Note to tutor: Most of the material required to do these examples is in the lecture notes. The lecture notes are available in html and pdf format on the homepage

http://brandes.phy.umist.ac.uk/QM/.

Students shoudl be encouraged to work though the lecture notes before doing the examples.

1.1 The Radiation Laws and the Birth of Quantum Mechanics

1.1.1 Kirchhoff (5 min)

What did Kirchhoff postulate for the spectral energy density u of black body radiation?

SOLUTION: The radiation energy u per volume and per frequency interval is only a function of the frequency ν and the temperature T of the walls, and does not depend, e.g., on the shape of the container:

$$u = u(\nu, T) \tag{1.1}$$

1.1.2 Rayleigh–Jeans law (5 min)

Why can the Rayleigh–Jeans law not be correct for all frequencies?

SOLUTION: The (**Rayleigh–Jeans–law**) is

$$u(\nu, T) = \rho(\nu)\bar{E}(\nu) = \frac{8\pi\nu^2}{c^3} k_B T, \tag{1.2}$$

where k_B is the Boltzmann constant. Rayleigh's law followed from the **density of states** $\rho(\nu) = 8\pi\nu^2/c^3$ (density of electromagnetic eigenmodes per volume, polarization direction and frequency) of the electromagnetic field in a cavity, and the theorem of thermodynamics that gives each degree of freedom of an oscillation in thermal equilibrium an average energy $\bar{E}(\nu) = k_B T$ ($1/2 k_B T$ for kinetic and potential energy each), independent of the frequency ν. It cannot hold for very large frequencies where the energy density would become infinite which clearly is unphysical.

1.1.3 * Planck's law (10 min)

Show that from Planck's law, the Wien law and the Rayleigh–Jeans law follow as limiting cases.

SOLUTION: Planck's law is

$$u(\nu, T) = \frac{8\pi\nu^2}{c^3} \frac{h\nu}{\exp\left(\frac{h\nu}{k_B T}\right) - 1}. \tag{1.3}$$

For small x, approximate $1/(\exp(x) - 1) \approx 1/x$ which gives the Rayleigh–Jeans–law as limiting case for $h\nu/k_B T$ small, i.e. small frequencies or large wave lengths. On the other hand, for large x, approximate $1/(\exp(x) - 1) \approx \exp(-x)$ which yields (**Wien's law**),

$$u(\nu, T) = \frac{4\nu^3}{c^3} b \exp\left(-\frac{a\nu}{T}\right), \quad a, b = const. \tag{1.4}$$

1.1.4 ** Stefan–Boltzmann constant (20-60 min)

Calculate the numerical value of the Stefan–Boltzmann constant

$$\sigma = (k_B T/h)^4 8\pi^5/15c^3$$

using the Planck radiation law for $u(\nu, T)$. In the calculation, you need the integral $\int_0^\infty dx x^3/(e^x - 1) = \pi^4/15$ which you should try to prove.

SOLUTION:

$$U(T) := \int_0^\infty d\nu u(\nu, T) = \int_0^\infty d\nu \frac{8\pi\nu^2}{c^3} \frac{h\nu}{\exp\left(\frac{h\nu}{k_B T}\right) - 1}$$
$$= \frac{8\pi (k_B T)^4}{h^4 c^3} \int_0^\infty dx \frac{x^3}{\exp(x) - 1} = \frac{8\pi^5 (k_B T)^4}{15 h^4 c^3}. \quad (1.5)$$

Furthermore,

$$\int_0^\infty dx \frac{x^3}{\exp(x) - 1} = \int_0^\infty dx \frac{x^3 e^{-x}}{1 - e^{-x}} = \sum_{n=0}^\infty \int_0^\infty dx x^3 e^{-x} e^{nx}$$
$$= \sum_{n=0}^\infty \frac{1}{(n+1)^4} \int_0^\infty dy y^3 e^{-y} = \zeta(4)\Gamma(4) = \frac{\pi^4}{90} 3! = \frac{\pi^4}{15}. \quad (1.6)$$

The value of the Zeta function $\zeta(4) = \sum_{n=0}^\infty 1/n^4$ can be obtained from a Fourier series.

1.2 Waves, particles, and wave packets

1.2.1 Macroscopic Object (5 min)

Is the de Broglie wave length of large, macroscopic objects very small or very large? Calculate the de Broglie wave length of a 70 kg mass point moving at a constant speed of 5 km/h. Compare it to typical 'macroscopic' sizes of cars, chairs etc.

SOLUTION: de Broglie wave lengths of large, macroscopic objects are very small:

$$p = h/\lambda \rightsquigarrow \lambda = \frac{6.626 \cdot 10^{-34} Js}{70kg(6000/3600)m/s} = 5.7 \cdot 10^{-36} m. \quad (1.7)$$

1.2.2 * Geometrical Optic (2 min)

For which limit of wave lengths is geometrical optics a limiting case of the wave theory of light?

SOLUTION: In the limit of very small wave lengths, geometrical optics is a limiting case of the wave theory of light.

1.3 Interpretation of the Wave Function

1.3.1 Schrödinger Equation (5 min)

a) Write down the Schrödinger Equation for the wave function $\Psi(x, t)$ for a particle with mass m moving in a potential $V(x)$ in one dimension.

b) Write down the Schrödinger Equation for the wave function $\Psi(\mathbf{x}, t)$ for a particle with mass m moving in a potential $V(\mathbf{x})$.

SOLUTION: a)

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \left[-\frac{\hbar^2 \partial_x^2}{2m} + V(x)\right] \Psi(x, t) \quad (1.8)$$

b)

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}, t) = \left[-\frac{\hbar^2 \Delta}{2m} + V(\mathbf{x})\right] \Psi(\mathbf{x}, t). \quad (1.9)$$

1.3.2 Interpretation of the Wave Function (2 min)

What is the physical meaning of the wave function ?

SOLUTION: $|\Psi(\mathbf{x}, t)|^2 d^3x$ is the probability for the particle to be in the (infinitesimal small) volume d^3x around $\mathbf{x}$ at time t.

1.3.3 Probability (2 min)

What is the probability $P(\Omega)$ for a particle with wave function $\Psi(\mathbf{x}, t)$ to be in a finite volume Ω of space?

SOLUTION: The probability $P(\Omega)$ for the particle to be in a finite volume Ω of space is given by the integral over this volume:

$$P(\Omega) = \int_\Omega d^3x |\Psi(\mathbf{x}, t)|^2. \tag{1.10}$$

1.3.4 Probability and current density of a particle (15 min)

Assume that a particle in an interval $[-L/2, L/2]$ is described by a wave function

$$\Psi(x, t) = \frac{1}{\sqrt{L}} e^{i(kx - \omega t)}.$$

What are the probability density $\rho(x, t)$ and the current density $j(x, t)$ for this wave function ? How can one express the current density by the probability density and the velocity? What is the probability to find the particle a) anywhere in the interval $[-L/2, L/2]$; b) in the interval $[-L/2, 0]$; c) in the interval $[0, L/4]$?

SOLUTION:

$$\begin{aligned}
\rho(x, t) &:= \Psi(x, t)\Psi^*(x, t) = \frac{1}{L} \\
j(x, t) &:= -\frac{i\hbar}{2m} \left[\Psi(x, t)^* \partial_x \Psi(x, t) - \Psi(x, t)\partial_x \Psi^*(x, t)\right] = \frac{\hbar k}{mL} = \frac{p}{m}\rho = v\rho,
\end{aligned}$$

where v is the particle velocity and $p = \hbar k$ (de Broglie) was used.

The probabilities are a) 1; b) 1/2; c) 1/4.

1.4 Fourier Transforms and the Solution of the Schrödinger Equation

1.4.1 Definition of the Fourier Integral (2 min)

Write down the decomposition into plane waves of a function $f(x)$ of one variable x by its **Fourier transform** $\tilde{f}(k)$.

SOLUTION: We define the decomposition into plane waves of a function $f(x)$ of one variable x by its **Fourier transform** $\tilde{f}(k)$,

$$\tilde{f}(k) := \int_{-\infty}^{\infty} dx f(x) e^{-ikx}, \quad f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \tilde{f}(k) e^{ikx}. \tag{1.11}$$

Remarks:
1. In this lecture, we define the Fourier transform with the factor $1/2\pi$ in front of $f(x)$. Some people define it symmetrically, i.e. $1/\sqrt{2\pi}$ in front of $f(x)$ and $\tilde{f}(k)$.
2. Remember the Minus signs in the exp functions.

1.4.2 ** Math: Gauß (20 min)

Look up who Gauß was, where he lived etc. Write down the definition of the Gauss function. Look up examples for areas of mathematics and physics where the Gauss function is used.

SOLUTION: The Gauss function is

$$g(x) := \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}}. \tag{1.12}$$

1.4.3 * Math: Gauß Integral 1 (10 min)

Use polar coordinates to calculate $\int_{-\infty}^{\infty} dxdy e^{-x^2-y^2}$ in order to prove the above $\int_{-\infty}^{\infty} dx e^{-x^2} = \sqrt{\pi}$.

SOLUTION:

$$\begin{aligned} \left(\int_{-\infty}^{\infty} dx e^{-x^2}\right)^2 &= \int_{-\infty}^{\infty} dxdy e^{-x^2-y^2} = 2\pi \int_0^{\infty} dr r e^{-r^2} \\ &= [x = r^2, dx = 2rdr] = \pi \int_0^{\infty} dx x e^{-x} = \pi. \end{aligned} \tag{1.13}$$

1.4.4 Math: Gauß Integral 2 (10 min)

Use $\int_{-\infty}^{\infty} dx e^{-x^2} = \sqrt{\pi}$ to prove the formula for the Gauß integral

$$\int_{-\infty}^{\infty} dx e^{-ax^2+bx} = \sqrt{\frac{\pi}{a}} e^{b^2/4a}, \quad a > 0. \tag{1.14}$$

SOLUTION:

$$\begin{aligned} \int_{-\infty}^{\infty} dx e^{-ax^2+bx} = \int_{-\infty}^{\infty} dx e^{-a(x-b/2a)^2+b^2/4a} = \\ = [y = \sqrt{a}(x - b/2a)] = \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} dy e^{-y^2+b^2/4a} = \sqrt{\frac{\pi}{a}} e^{b^2/4a}. \end{aligned} \tag{1.15}$$

1.4.5 Math: Fourier Transform of Gauss Function (20 min)

The Gauss function

$$f(x) := \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}} \tag{1.16}$$

is a convenient example to discuss properties of the Fourier transform. Show that it can be decomposed into plane waves by

$$\tilde{f}(k) = \int_{-\infty}^{\infty} dx f(x) e^{-ikx} = e^{-\frac{1}{2}\sigma^2 k^2}, \quad f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-\frac{1}{2}\sigma^2 k^2} e^{ikx}. \tag{1.17}$$

Draw $f(x)$ and $\tilde{f}(k)$ for different values of σ and discuss their relation.

SOLUTION: In principle, one first has to show that the formula 1.14 for the Gauss integral also holds for complex b. This can be proven by complex integration, but we will not do it here. Then, simple application of 1.14 with $b = -ik$ yields the result for $\tilde{f}(k)$. The equation for $f(x)$ then is simply the Fourier back–transformation (definition), but you can explicitely verify it again by calculating the Gauss integral.

Small σ: corresponds to a narrow Gauss function $f(x)$ in x–space and a broad distribution $\tilde{f}(k)$ of Fourier components in k–space.

Large σ: corresponds to a broad Gauss function $f(x)$ in x–space and a narrow distribution $\tilde{f}(k)$ of Fourier components in k–space.

1.4.6 * Wave packet (20 min)

We assume that a particle with energy $E = p^2/2m$ can be described by a function that is a superposition of plane waves,

$$\Psi(x,t) = \int_{-\infty}^{\infty} dk a(k) e^{i(kx-\omega(k)t)}, \quad \hbar\omega(k) = E = \hbar^2 k^2/(2m). \tag{1.18}$$

Use

$$a(k) = C\sqrt{\sigma^2/(2\pi)}e^{-k^2\sigma^2/2}$$

to calculate the wave packet $\Psi(x,t)$. Here, C is a constant. Show that

$$\Psi(x,t) = \frac{C}{\sqrt{1+i(\hbar t/m\sigma^2)}}\exp\left(-\frac{x^2}{2\sigma^2[1+i(\hbar t/m\sigma^2)]}\right).$$

To simplify your calculation, you can set $\hbar = 2m = 1$ during your calculation and re-install it in the result. Why does this 'trick' work? Discuss $\Psi(x,t)$ as a function of time.

SOLUTION: The solution of this problem is discussed in many text books. Basically, one has to calculate a Gauss integral of the type 1.14. As a function of time, $\Psi(x,t)$ becomes broader. Actually, the physical interesting quantity is the square $|\Psi(x,t)|^2$ which is the probability density to find the particle in the interval $[x, x+dx]$ at time t. We see from this calculation that this probability density becomes broader with increasing time: If the particle was initially localized near the origin $x = 0$, it 'spreads' out. However, this does not mean that the particle disintegrates into smaller pieces or even into a continuous mass distribution. $|\Psi(x,t)|^2$ is not a mass density but a probability density: if we 'look' at time t if the particle is in the interval $[x, x+dx]$, it is either there (with probability $|\Psi(x,t)|^2 dx$) or not.

1.5 Position and Momentum in Quantum Mechanics

1.5.1 Normalization (2min)

Write down the normalization condition for the wave function $\Psi(x,t)$ of a particle that is necessary to interpret $|\Psi(x,t)|^2$ as a probability density.

SOLUTION: The probability to find the particle *somewhere* in space must be one and hence

$$\int_{R^3} d^3x|\Psi(\mathbf{x},t)|^2 = 1. \tag{1.19}$$

1.5.2 Expectation values in quantum mechanics (5min)

Write down the expectation value of the position x and the momentum p of a particle with a normalized wave function $\Psi(x,t)$.

SOLUTION:

$$\langle x\rangle_t = \int dx\Psi^*(x,t)x\Psi(x,t), \quad \langle p\rangle_t = \int dx\Psi^*(x,t)\frac{\hbar\partial_x}{i}\Psi(x,t) \tag{1.20}$$

We recognize that the position x corresponds to the **operator** 'multiplication with x'. On the other hand, the momentum corresponds to the operator $-i\hbar\partial_x$.

1.5.3 Wave packet (10-30 min)

We consider the wave function (wave packet)

$$\Psi(x) = \frac{1}{\sqrt{\sqrt{\pi a^2}}} \exp\left(-\frac{x^2}{2a^2}\right). \tag{1.21}$$

1. Show that this wave function is normalized (remember what normalization means!)
2. Using this wave function, calculate the expectation values $\langle x^2 \rangle$, $\langle p^2 \rangle$, and their product $\langle x^2 \rangle \cdot \langle p^2 \rangle$. You have to use the integral $\int_{-\infty}^{\infty} dy y^2 e^{-a^2 y^2} = \sqrt{\pi}/(2a^3)$.

SOLUTION:

$$\begin{aligned}
\langle p^2 \rangle &= \int\limits_{-\infty}^{\infty} \psi(x)\,(-\hbar^2)\,\frac{\partial^2}{\partial x^2}\psi(x)\,dx = -\frac{\hbar^2}{a\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \mathrm{e}^{-x^2/(2a^2)}\,\frac{\partial^2}{\partial x^2}\,\mathrm{e}^{-x^2/(2a^2)}\,dx \\
&= -\frac{\hbar^2}{a\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \mathrm{e}^{-x^2/(2a^2)}\,\frac{\partial}{\partial x}\Big(-\frac{x}{a^2}\,\mathrm{e}^{-x^2/(2a^2)}\Big)\,dx \\
&= -\frac{\hbar^2}{a\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \Big(-\frac{1}{a^2} + \frac{x^2}{a^4}\Big)\,\mathrm{e}^{-x^2/(a^2)}\,dx \\
&= -\frac{\hbar^2}{a\sqrt{\pi}}\Big(-\frac{\sqrt{\pi}}{a} + \frac{\sqrt{\pi}}{2a}\Big) = -\frac{\hbar^2}{a\sqrt{\pi}}\Big(-\frac{\sqrt{\pi}}{2a}\Big) = \frac{\hbar^2}{2a^2} \\
\langle x^2 \rangle &= \int\limits_{-\infty}^{\infty} \psi(x)\,x^2\,\psi(x)\,dx = \frac{1}{a\sqrt{\pi}} \int\limits_{-\infty}^{\infty} x^2\,\mathrm{e}^{-x^2/(a^2)}\,dx \\
&= \frac{a^3}{a\sqrt{\pi}} \int\limits_{-\infty}^{\infty} u^2\,\mathrm{e}^{-u^2}\,du = \frac{a^2}{\sqrt{\pi}}\frac{\sqrt{\pi}}{2} = \frac{a^2}{2}.
\end{aligned} \tag{1.22}$$

1.5.4 * Hamilton function (10min)

Write down the Hamilton function of a classical particle moving in a one dimensional potential $V(x)$. Write down the corresponding quantum mechanical Hamilton operator ('Hamiltonian'). Write down the Schrödinger equation in 'abstract form', using the Hamilton operator.

SOLUTION: The total energy in classical mechanics for a conservative system of a particle of mass m in a potential $V(\mathbf{x})$ (energy is conserved) is given by a **Hamilton function**

$$H(\mathbf{p}, \mathbf{x}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}). \tag{1.23}$$

The **correspondence principle** from axiom 2 tells us that this Hamilton function in quantum mechanics has to be replaced by a **Hamilton operator** (**Hamiltonian**) $\hat{H}$

$$\hat{H} = -\frac{\hbar^2 \Delta}{2m} + V(\hat{\mathbf{x}}). \tag{1.24}$$

Here, we have used the definition of the Laplace operator $\Delta = \nabla \cdot \nabla$. In Cartesian coordinates, it is $\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2$. The Hamilton operator represents the total energy of the particle with mass m in the potential $V(\mathbf{x})$. We have introduced the hat as a notation for operators, but often the hat is omitted for simplicity. We make the important observation that $\hat{H}$ is exactly the expression that appears on the right hand side of the Schrödinger equation. This means we can write the Schrödinger equation as

$$i\hbar \frac{\partial}{\partial t}\Psi(\mathbf{x}, t) = \hat{H}\Psi(\mathbf{x}, t). \tag{1.25}$$

1.5.5 * Commutator 1 (10 min)

Prove the commutator relation in one dimension, $[\hat{x}, \hat{p}] := i\hbar$, where $[A, B] := AB - BA$.

SOLUTION: Position x and momentum p are operators in quantum mechanics. Acting on wave functions, the operator product xp has the property

$$\begin{aligned} \hat{x}\hat{p}\Psi(x) &= \frac{\hbar}{i} x \frac{\partial}{\partial x}\Psi(x) = \frac{\hbar}{i} x\Psi'(x) \\ \hat{p}\hat{x}\Psi(x) &= \frac{\hbar}{i}\frac{\partial}{\partial x} x\Psi(x) = \frac{\hbar}{i}\left(\Psi(x) + x\Psi'(x)\right) \end{aligned} \tag{1.26}$$

The result depends on the order of $\hat{x}$ and $\hat{p}$: both operators do not commute. One has

$$(\hat{x}\hat{p} - \hat{p}\hat{x})\Psi(x) = i\hbar\Psi(x) \tag{1.27}$$

Comparing both sides, we have the **commutation relation**

$$[\hat{x}, \hat{p}] := \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar. \tag{1.28}$$

2.6 The stationary Schrödinger Equation

2.6.1 Definitions (2min)

Write down the stationary Schrödinger equation in one and three dimensions for a particle of mass m in a potential $V(x)$.

SOLUTION: The **stationary Schrödinger equation** is

$$\hat{H}\psi(\mathbf{x}) = E\psi(\mathbf{x}) \longleftrightarrow \left[-\frac{\hbar^2\Delta}{2m} + V(\mathbf{x})\right]\psi(\mathbf{x}) = E\psi(\mathbf{x}) \tag{2.29}$$

in three dimensions, in one dimensions x instead of $\mathbf{x}$ and ∂_x^2 instead of Δ. Mathematically, the equation $\hat{H}\psi = E\psi$ with the operator $\hat{H}$ is an **eigen value equation**. We know eigenvalue equations from linear algebra where $\hat{H}$ is a matrix and ψ is a vector. The wave function has been separated according to (see lecture notes)

$$\Psi(\mathbf{x}, t) = \psi(\mathbf{x})e^{-iEt/\hbar}. \tag{2.30}$$

2.6.2 Piecewise constant potentials in one dimension (5min)

Write down the general solution of

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right]\psi(x) = E\psi(x), \quad x \in [x_1, x_2] \tag{2.31}$$

for $E < V$ and $E > V$. What is the difference between these two cases?

SOLUTION: This is a second order ordinary differential equation with constant coefficients. There are **two independent solutions**

$$\psi_+(x) = e^{ikx}, \quad \psi_-(x) = e^{-ikx}, \quad k := \sqrt{\frac{2m}{\hbar^2}(E - V)}. \tag{2.32}$$

1. If $E > V$, the **wave vector** k is a real quantity and the two solutions $\psi_\pm(x)$ are plane waves running in the positive and the negative x–direction. Such solutions are called oscillatory solutions.

2. If $E < V$, k becomes imaginary and we write

$$k = i\kappa := i\sqrt{\frac{2m}{\hbar^2}(V - E)} \tag{2.33}$$

with the real quantity κ. The two independent solutions then become exponential functions $e^{\pm\kappa x}$. Such solutions are called exponential solutions.

For fixed energy E, the general solution $\psi(x)$ will be a **superposition**, that is a linear combination

$$\psi(x) = ae^{ikx} + be^{-ikx} \tag{2.34}$$

with k either real or imaginary, $k = i\kappa$. Since the wave function in general is a complex function, the coefficients a, b can be complex numbers. Note that we can not have linear combinations with one real and one imaginary term in the exponential like $ae^{ikx} + be^{-\kappa x}, a, b \neq 0$.

2.7 The Infinite Potential Well

2.7.1 Energies and Eigenstates I (10-20 min)

Consider the motion of a particle of mass m within the interval $[x_1, x_2] = [0, L], L > 0$ between the infinitely high walls of the potential

$$V(x) = \begin{cases} \infty, & -\infty < x \leq 0 \\ 0, & 0 < x \leq L \\ \infty & L < x < \infty \end{cases} \tag{2.35}$$

Show that the normalized energy eigenstate wave functions and energies are

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad E = E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}, \quad n = 1, 2, 3, ... \tag{2.36}$$

SOLUTION: (see lecture notes) Outside the interval $[0, L]$ the particle can not exist and its wave function must be zero, i.e.

$$\psi(x) = \begin{cases} 0, & -\infty < x \leq 0 \\ ae^{ikx} + be^{-ikx}, & 0 < x \leq L \\ 0, & L < x < \infty \end{cases} \tag{2.37}$$

We demand that the wave function vanishes at $x = 0$ and $x = L$ so that it is continuous a these points. Clearly, this makes physically sense because at $x = 0, L$ the potential is infinitely high and the probability density $|\psi(x)|^2$ to find the particle there should be zero. We obtain

$$\begin{aligned} \psi(0) &= 0 \rightsquigarrow 0 = a + b \rightsquigarrow \psi(x) = c\sin(kx), \quad 0 \leq x \leq L, \quad c = const. \\ \psi(L) &= 0 \rightsquigarrow \sin(kL) = 0. \end{aligned} \tag{2.38}$$

The first condition tells us that the wave function must be a sine–function. The second condition is more interesting: it sets a condition for the possible values k_n that k can have,

$$kL = n\pi \rightsquigarrow k \equiv k_n = \frac{n\pi}{L}, \quad n = 1, 2, 3, ... \tag{2.39}$$

The second **boundary condition** at $x = L$ restricts the possible values of the energy E, because $k := \sqrt{(2m/\hbar^2)(E - V)} = \sqrt{(2m/\hbar^2)E}$. Therefore, the energy can only acquire values

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\hbar^2\pi^2}{2mL^2}, \quad n = 1, 2, 3, ... \tag{2.40}$$

In order to interpret the absolute square wave of the wave functions $\phi_n(x) = c\sin(k_n x)$ as a probability density, we have to demand

$$
\begin{aligned}
1 &= \int_0^L dx|\psi_n(x)|^2 = \int_0^L dx|c|^2 \sin^2(n\pi x/L) \\
&= \frac{1}{2}\int_0^L dx|c|^2[1-\cos(n2\pi x/L)] = \frac{|c|^2 L}{2} \\
|x|^2 &= \frac{2}{L} \rightsquigarrow c = \sqrt{\frac{2}{L}}e^{i\phi} \rightsquigarrow \psi_n(x) = \sqrt{\frac{2}{L}}\sin(n\pi x/L)e^{i\varphi}, \qquad (2.41)
\end{aligned}
$$

where $\varphi \in R$ is a (real) phase factor. This **normalization condition** determines the wave functions $\psi_n(x)$ uniquely only up to a **phase factor**.

2.7.2 Energies and Eigenstates II (10-20 min)

Consider the motion of a particle of mass m within the infinitely high potential well

$$
V(x) = \begin{cases} \infty, & -\infty < x \le -L/2 \\ 0, & -L/2 < x \le L/2 \\ \infty & L/2 < x < \infty \end{cases} \qquad (2.42)
$$

Determine the eigenfunctions $\psi_n(x)$ and energy eigenvalues E_n explicitly. What are the symmetry properties of the eigenfunctions? Can you recover them from the solutions of the infinite well on the interval $[0, L]$ (see above and lecture notes)?

SOLUTION: We write the general wave function as

$$
\psi(x) = \begin{cases} 0, & -\infty < x \le -L/2 \\ a'e^{ikx} + b'e^{-ikx}, & -L/2 < x \le L/2 \\ 0, & L/2 < x < \infty \end{cases} \qquad (2.43)
$$

To make our life easier, we write this by re–defining the coefficients a' and b' as

$$
\psi(x) = ae^{ik(x-L/2)} + be^{-ik(x-L/2)}, \quad -L/2 < x \le L/2. \qquad (2.44)
$$

From $\psi(L/2) = 0$ we immediately obtain $a + b = 0$ which is fine because it tells us $\psi(x) \propto \sin k(x - L/2)$. From $\psi(-L/2) = 0$ we immediately obtain $\sin kL = 0$ whence $kL = n\pi$, $n = 1, 2, 3, 4, ...$ ($n = 0$ is the zero solution, $n = -1, -2, ..$ give nothing new. The possible energies therefore are

$$
E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\hbar^2\pi^2}{2mL^2}, \quad n = 1, 2, 3, ... \qquad (2.45)
$$

We thus have (within the well)

$$
\psi(x) \propto \sin(kx - n\pi/2) \propto \begin{cases} \sin kx, & n = 2, 4, 6, ... \quad \text{even} \\ \cos kx, & n = 1, 3, 5, ... \quad \text{odd} \end{cases} \qquad (2.46)
$$

Writing $\propto$ is a convenient way to avoid too much notation until the point were we eventually have to become clear about the normalization: Within the well,

$$
\psi(x) = \begin{cases} \sqrt{\frac{2}{L}}\sin kx, & n = 2, 4, 6, ... \quad \text{odd function} \\ \sqrt{\frac{2}{L}}\cos kx, & n = 1, 3, 5, ... \quad \text{even function} \end{cases} \qquad (2.47)
$$

2.7.3 * Orthonormality (10 min)

Consider the Hilbert space $\mathcal{H}$ of wave functions $\psi(x)$ of the infinite potential well on the interval $[0, L]$ with $\psi(0) = \psi(L) = 0$. Show that the basis vectors

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

form an orthonormal system.

SOLUTION: We have to show that the $\psi_n(x)$ form an orthonormal basis:

$$\int_0^L dx \psi_n^*(x)\psi_m(x) = \delta_{nm}. \tag{2.48}$$

We therefore have to calculate the integral

$$\int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{m\pi x}{L}\right). \tag{2.49}$$

For $n = m$ we have already calculated this integral above when we obtained the normalization of the wave functions. For $n \neq m$ we have to show that 2.49 is zero: Do this by expanding the sin into exponentials and calculating the integrals, or use a theorem for trigonometric functions, or look it up in a table.

2.7.4 Time Evolution (2 min)

Consider a wave function $\psi(x)$ of the infinite potential well on the interval $[0, L]$. Consider the case when the wave function at time $t = 0$ is one of the eigenstates of energy E_n, i.e. $\Psi(x, t = 0) = \psi_n(x)$ and check that the time evolution of a wave function that is an energy eigenstate is just given by multiplication with the time–dependent phase factor $e^{-iE_n t/\hbar}$, that is

$$\Psi(x, t = 0) = \psi_n(x) \rightsquigarrow \Psi(x, t) = \psi_n(x)e^{-iE_n t/\hbar}. \tag{2.50}$$

SOLUTION: In principle, this is in general already clear from the definition of the stationary states (see lecture notes): To solve

$$i\hbar\frac{\partial}{\partial t}\Psi(x, t) = \hat{H}\Psi(x, t), \tag{2.51}$$

we had made a separation ansatz

$$\Psi(x, t) = \psi(x)f(t). \tag{2.52}$$

Inserting into the Schrödinger equation, we have

$$\frac{i\hbar\partial_t f(t)}{f(t)} = \frac{\hat{H}\psi(x)}{\psi(x)} = E, \tag{2.53}$$

where we have separated the t– and the x–dependence. Both sides of depend on t resp. x independently and therefore must be constant $= E$. Solving the equation for $f(t)$ yields $f(t) = \exp -iEt/\hbar$ and therefore

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar}. \tag{2.54}$$

We recognize: the time evolution of the wave function $\Psi(x, t)$ is solely determined by the factor $\exp -iEt/\hbar$. Furthermore, the constant E must be an energy (dimension!).

We can also check directly that $\Psi(x, t)$ fulfills the time–dependent Schrödinger equation:

$$\begin{aligned}\hat{H}\psi_n(x) = E_n\psi_n(x) \rightsquigarrow i\hbar\frac{\partial}{\partial t}\Psi(x, t) &= i\hbar\frac{\partial}{\partial t}\psi_n(x)e^{-iE_n t/\hbar} = E_n\psi_n(x)e^{-iE_n t/\hbar} \\ &= \hat{H}\psi_n(x)e^{-iE_n t/\hbar} = \hat{H}\Psi(x, t).\end{aligned} \tag{2.55}$$

2.7.5 Expectation values (15 min)

Calculate the expectation value of a) the momentum square p^2 and b) the kinetic energy of a particle in the one–dimensional infinite well on the interval $[0, L]$ with wave function $\Psi(x,t) = \psi_n(x)e^{-iE_nt/\hbar}$.

SOLUTION: Use $\partial_x^2\psi_n(x) = -(n^2\hbar^2/L^2)\psi_n(x)$:

$$
\begin{aligned}
\langle p^2\rangle_t &= \int_0^L dx\psi_n(x)\frac{\hbar^2\partial_x^2}{i^2}\psi_n(x) = -\hbar^2\int_0^L dx\psi_n(x)\left(-\frac{n^2\pi^2}{L^2}\right)\psi_n(x) \\
&= \frac{n^2\hbar^2\pi^2}{L^2} \rightsquigarrow \langle\frac{p^2}{2m}\rangle_t = \frac{n^2\hbar^2\pi^2}{2L^2m^2} = E_n. \qquad (2.56)
\end{aligned}
$$

This is a very obvious result: since the energy of the wave function $\psi_n(x)$ is E_n, the expectation value of the kinetic energy $E = p^2/2m$ (= the total energy), i.e. the value one obtains on averaging the results from many measurements on the same system with the same wave function, must be E_n. We can obtain this result even easier by calculating the **expectation value of the energy**

$$
\langle\hat{H}\rangle_t = \int_0^L dx\psi_n(x)H\psi_n(x) = \int_0^L dx\psi_n(x)E_n\psi_n(x) = E_n, \qquad (2.57)
$$

where we have used the Schrödinger equation $\hat{H}\psi_n = E_n\psi_n$ and the orthonormality of the ψ_n.

2.7.6 * Time evolution of superposition (10 min)

a) What is the time evolution of an arbitrary wave function $\Psi(x, t = 0)$,

$$
\Psi(x,t=0) = \sum_{n=0}^{\infty} c_n\psi_n(x), \quad c_n = \int_0^L dx\psi_n^*(x)\Psi(x)? \qquad (2.58)
$$

b) Consider the wave function

$$
\Psi(x,t=0) = \frac{1}{\sqrt{2}}\left(\psi_1(x)+\psi_2(x)\right). \qquad (2.59)
$$

What is the probability density to find the particle at x at time t?

SOLUTION:

a) The Schrödinger equation is a linear partial differential equation, so the answer is simple: it is just given by the superposition

$$
\begin{aligned}
\Psi(x,t) &= \sum_{n=0}^{\infty} c_n\psi_n(x)e^{-iE_nt/\hbar} \qquad (2.60) \\
&\rightsquigarrow i\hbar\partial_t\Psi(x,t) = \sum_{n=0}^{\infty} c_nE_n\psi_n(x)e^{-iE_nt/\hbar} \\
&= \sum_{n=0}^{\infty} c_n\hat{H}\psi_n(x)e^{-iE_nt/\hbar} = \hat{H}\sum_{n=0}^{\infty} c_n\psi_n(x)e^{-iE_nt/\hbar} = \hat{H}\Psi(x,t),
\end{aligned}
$$

where we used the fact that $\hat{H}$ is a linear operator.

b) The time evolution is obtained as

$$
\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_1(x)e^{-iE_1t/\hbar} + \psi_2(x)e^{-iE_2t/\hbar}\right). \qquad (2.61)
$$

From this we obtain the probability density

$$
|\Psi(x,t)|^2 = \frac{1}{2}\left(\psi_1^2(x) + \psi_2^2(x) + 2\psi_1(x)\psi_2(x)\cos[(E_1-E_2)t/\hbar]\right), \qquad (2.62)
$$

which is no longer constant as a function of time.

2.8 The Finite Potential Well

2.8.1 Parity (10 min)

Show that the solutions of the stationary Schrödinger equation with the one–dimensional potential

$$V(x) = \begin{cases} 0, & -\infty < x \leq -a \\ -V < 0, & -a < x \leq a \\ 0 & a < x < \infty \end{cases} \tag{2.63}$$

can be chosen as even and odd solutions.

SOLUTION: (see lecture notes) For **symmetric potentials** $V(x) = V(-x)$, the Schrödinger equation has an important property: If $\psi(x)$ is a solution of $\hat{H}\psi(x) = E\psi(x)$, then also $\psi(-x)$ is a solution with the same E, i.e. $\hat{H}\psi(-x) = E\psi(-x)$ (replace $-x \to x$ and note that $\partial_x^2 = \partial_{-x}^2$. Since $\hat{H}$ is linear, also linear combinations of solutions with the same eigenvalue E are solutions with eigenvalue E, in particular the symmetric (even) and anti symmetric (odd) linear combinations

$$\psi_e(x) := \frac{1}{\sqrt{2}}[\psi(x) + \psi(-x)], \quad \psi_o(x) := \frac{1}{\sqrt{2}}[\psi(x) - \psi(-x)]. \tag{2.64}$$

These are the solutions with even (e) and odd (o) parity, respectively.

2.8.2 Wave functions (5 min)

Draw the wave functions for energy $E < 0$ corresponding to the potential $V(x)$, (2.63). What about energies $E < -V$?

SOLUTION: There are no solutions for $E < -V$.

2.9 Scattering states in one dimension

2.9.1 Plane Waves (5 min)

Show that plane waves solve the one–dimensional stationary Schrödinger equation for zero potential. Derive the dispersion relation $E = E(k)$, where E is the energy and k the wave vector. Show that plane waves can not be normalized over the whole x–axis.

SOLUTION: We check this by inserting into the Schrödinger equation:

$$\begin{aligned} -\frac{\hbar^2\partial_x^2}{2m}\psi_k(x) &= E\psi_k(x), \quad \psi_k(x) = e^{ikx} \\ \rightsquigarrow E = E(k) &= \frac{\hbar^2 k^2}{2m}. \end{aligned} \tag{2.65}$$

A problem arises, because $\psi_k(x)$ can not be normalized over the whole x–axis according to

$$\int_{-\infty}^{\infty} dx |\psi_k(x)|^2 = 1, \tag{2.66}$$

because this integral is infinite. A practical solution is to consider a large, but finite interval $[-L/2, L/2]$ instead of the total x–axis, and to normalize the wave functions according to

$$\psi_k = \frac{1}{\sqrt{L}} e^{ikx}, \quad \int_{-L/2}^{L/2} dx |\psi_k(x)|^2 = 1. \tag{2.67}$$

See lecture notes for a further discussion.

2.9.2 Piecewise constant potential (25 min)

We consider a 1d piecewise constant potential and a stationary wave function at energy E.

$$V(x) = \begin{cases} V_1, & \\ V_2, & \\ V_3, & \\ ... & ... \\ V_N & \\ V_{N+1} & \end{cases} \quad \psi(x) = \begin{cases} a_1 e^{ik_1x} + b_1 e^{-ik_1x}, & -\infty < x \le x_1 \\ a_2 e^{ik_2x} + b_2 e^{-ik_2x}, & x_1 < x \le x_2 \\ a_3 e^{ik_3x} + b_3 e^{-ik_3x}, & x_2 < x \le x_3 \\ ... & ... \\ a_N e^{ik_Nx} + b_N e^{-ik_Nx}, & x_{N-1} < x \le x_N \\ a_{N+1} e^{ik_{N+1}x} + b_{N+1} e^{-ik_{N+1}x}, & x_N < x < \infty \end{cases} \tag{2.68}$$

a) Show that $k_j = \sqrt{(2m/\hbar^2)\,(E - V_j)}$. Discuss the behaviour of the wave functions in regions with $V_j < E$ and $V_j > E$.
b) We consider the case $E > V_1, V_{N+1}$ such that k_1 and k_{N+1} are real wave vectors and $\psi(x)$ describes running waves outside the 'scattering region' $[x_1, x_N]$. Prove the matrix equation

$$\mathbf{u}_1 = T_1 \mathbf{u}_2, \quad \mathbf{u}_i = \begin{pmatrix} a_i \\ b_i \end{pmatrix}, \quad i = 1, 2, \tag{2.69}$$

with

$$T_1 = \frac{1}{2k_1} \begin{pmatrix} (k_1 + k_2)e^{i(k_2-k_1)x_1} & (k_1 - k_2)e^{-i(k_1+k_2)x_1} \\ (k_1 - k_2)e^{i(k_2+k_1)x_1} & (k_1 + k_2)e^{-i(k_2-k_1)x_1} \end{pmatrix}. \tag{2.70}$$

SOLUTION: This problem looks complicated but it isn't. Most of it is described in detail in the lecture notes: We demand that $\psi(x)$ and its derivative $\psi'(x)$ are continuous at $x = x_1$. This gives two equations

$$\begin{aligned} a_1 e^{ik_1x_1} + b_1 e^{-ik_1x_1} &= a_2 e^{ik_2x_1} + b_2 e^{-ik_2x_1} \\ a_1 e^{ik_1x_1} - b_1 e^{-ik_1x_1} &= (k_2/k_1)(a_2 e^{ik_2x_1} - b_2 e^{-ik_2x_1}) \end{aligned} \tag{2.71}$$

or

$$\begin{aligned} a_1 &= \frac{1}{2}\left(\frac{k_2}{k_1} + 1\right) e^{i(k_2-k_1)x_1} a_2 + \frac{1}{2}\left(1 - \frac{k_2}{k_1}\right) e^{-i(k_2+k_1)x_1} b_2 \\ b_1 &= \frac{1}{2}\left(1 - \frac{k_2}{k_1}\right) e^{i(k_2+k_1)x_1} a_2 + \frac{1}{2}\left(1 + \frac{k_2}{k_1}\right) e^{-i(k_2-k_1)x_1} b_2 \end{aligned} \tag{2.72}$$

which can be written in the above **matrix form**.

2.9.3 Transfer matrix (5 min)

How is the definition of the transfer matrix M, defined by

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} a_{N+1} \\ b_{N+1} \end{pmatrix}? \tag{2.73}$$

Express M as a product of matrices of the type (2.70).

SOLUTION: (again see lecture notes) In completely the same manner as in the above problem, we obtain the **transfer matrix** T_2 at the 'slice' $x = x_2$ and

$$\mathbf{u}_2 = T_2 \mathbf{u}_3 \rightsquigarrow \mathbf{u}_1 = T_1 \mathbf{u}_2 = T_1 T_2 \mathbf{u}_3. \tag{2.74}$$

Doing this for all the slices $x_1, ..., x_N$, we obtain the complete transfer matrix M that connects the wave function on the left side of the potential with the one on the right side,

$$\mathbf{u}_1 = M \mathbf{u}_{N+1}, \quad M = T_1 T_2 ... T_N. \tag{2.75}$$

2.9.4 Transmission, * Reflection (10min)

We define the transmission coefficient T and the reflection coefficient R as

$$T := \frac{k_{N+1}}{k_1}\left|\frac{a_{N+1}}{a_1}\right|^2, \quad R := \left|\frac{b_1}{a_1}\right|^2, \tag{2.76}$$

where the scattering condition $b_{N+1} = 0$ is assumed. Formulate this scattering condition in words. Show

$$T = \frac{k_{N+1}}{k_1}\frac{1}{|M_{11}|^2}, \quad R = \left|\frac{M_{21}}{M_{11}}\right|^2, \tag{2.77}$$

where M_{ij} are the matrix elements of the transfer matrix.

SOLUTION: From

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} a_{N+1} \\ b_{N+1} \end{pmatrix} \tag{2.78}$$

and the scattering condition $b_{N+1} = 0$ it follows

$$\begin{aligned} a_1 &= M_{11}a_{N+1} + M_{12}b_{N+1} = M_{11}a_{N+1} \\ b_1 &= M_{21}a_{N+1} + M_{22}b_{N+1} = M_{21}a_{N+1} = M_{21}a_1/M_{11} \\ \rightsquigarrow T &= \frac{k_{N+1}}{k_1}\frac{1}{|M_{11}|^2}, \quad R = \left|\frac{M_{21}}{M_{11}}\right|^2. \end{aligned} \tag{2.79}$$

To calculate the transmission and reflection coefficient through a piecewise constant one–dimensional potential, it is therefore sufficient to know the **total transfer matrix** M. The fact that $M = T_1T_2...T_N$ is just the product of the individual two–by two transfer matrices makes it a very convenient tool for computations. The scattering condition $b_{N+1} = 0$ means that we are only looking for solutions where no waves are coming in from the far right of the barrier.

2.10 The Tunnel Effect and Scattering Resonances

2.10.1 M–matrix for tunnel barrier (15 min)

Calculate the elements M_{11} and M_{12} of the transfer matrix $M = T_1T_2$ for a rectangular barrier. In (2.68), set $N = 2$, $x_2 = -x_1 = a$, $V_1 = V_3 = 0$, and $V_2 = V > 0$.

SOLUTION: By matrix multiplication:

$$\begin{aligned}
M &= \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \\
&= \frac{1}{4k_1k_2}\begin{pmatrix} (k_1+k_2)e^{i(k_2-k_1)x_1} & (k_1-k_2)e^{-i(k_1+k_2)x_1} \\ (k_1-k_2)e^{i(k_2+k_1)x_1} & (k_1+k_2)e^{-i(k_2-k_1)x_1} \end{pmatrix}. \\
&\times \begin{pmatrix} (k_2+k_1)e^{i(k_1-k_2)x_2} & (k_2-k_1)e^{-i(k_2+k_1)x_2} \\ (k_2-k_1)e^{i(k_1+k_2)x_2} & (k_2+k_1)e^{-i(k_1-k_2)x_2} \end{pmatrix} \\
\rightsquigarrow M_{12} &= \frac{1}{4k_1k_2}\Big[(k_1+k_2)(k_2-k_1)e^{i(k_1-k_2)a-i(k_2+k_1)a} \\
&+ (k_1-k_2)(k_2+k_1)e^{i(k_1+k_2)a-i(k_1-k_2)a}\Big] \\
&= \frac{k_2^2-k_1^2}{4k_1k_2}\left[e^{-2ik_2a}-e^{2ik_2a}\right] = \frac{k_1^2-k_2^2}{4k_1k_2}2i\sin(2k_2a) \\
\rightsquigarrow M_{11} &= \frac{1}{4k_1k_2}\Big[(k_1+k_2)(k_2+k_1)e^{i(k_1-k_2)a-i(k_2-k_1)a} \\
&+ (k_1-k_2)(k_2-k_1)e^{i(k_1+k_2)a+i(k_2+k_1)a}\Big] \\
&= \frac{e^{2ik_1a}}{4k_1k_2}\left[(k_1+k_2)^2e^{-2ik_2a}-(k_1-k_2)^2e^{2ik_2a}\right] \\
&= e^{2ik_1a}\left[\frac{k_1^2+k_2^2}{2k_1k_2}i\sin(-2k_2a)+\cos(2k_2a)\right].
\end{aligned} \tag{2.80}$$

Correspondingly for M_{21} and M_{22}.

2.10.2 * Transmission coefficient (15 min)

Verify the expressions for the transmission coefficients of the tunnel barrier, given in the lecture notes.

2.10.3 Transmission coefficient (10 min)

a) Draw the transmission coefficient of a tunnel barrier (roughly) as a function of energy E. What are transmission resonances?
b) Draw the transmission coefficient of a potential step (roughly) as a function of energy E.

2.10.4 ** Determinant of M (10 min)

Consider the case $k_1 = k_{N+1}$ in (2.68). Use the definitions for T_1 (T_n correspondingly) and M

$$T_1 = \frac{1}{2k_1}\begin{pmatrix} (k_1+k_2)e^{i(k_2-k_1)x_1} & (k_1-k_2)e^{-i(k_1+k_2)x_1} \\ (k_1-k_2)e^{i(k_2+k_1)x_1} & (k_1+k_2)e^{-i(k_2-k_1)x_1} \end{pmatrix}, \quad M = T_1T_2...T_N, \tag{2.81}$$

to show that the determinant of the transfer matrix $\det(M) = 1$.

SOLUTION: The determinant of a matrix product is the product of the determinants,

$$\det(M) = \det T_1 ... \det T_n. \tag{2.82}$$

Furthermore,

$$\begin{aligned}
\det T_1 &= \frac{1}{4k_1^2}\left[(k_1+k_2)^2-(k_1-k_2)^2\right] = \frac{k_2}{k_1} \\
\det T_1 ... \det T_n &= \frac{k_2}{k_1}\frac{k_3}{k_2}...\frac{k_{N+1}}{k_N} = \frac{k_{N+1}}{k_1} = 1.
\end{aligned} \tag{2.83}$$

2.10.5 ** A more general definition of the transfer matrix M (>30 min)

We consider a one–dimensional potential of the form

$$V(x) = \left\{ \begin{array}{c} 0, \\ v(x), \\ 0 \end{array} \right. \qquad \psi(x) = \left\{ \begin{array}{cc} ae^{ikx} + be^{-ikx}, & -\infty < x \leq x_1 \\ \phi(x), & x_1 < x \leq x_2 \\ ce^{ikx} + de^{-ikx}, & x_2 < x < \infty \end{array} \right. \tag{2.84}$$

Here, $v(x)$ is an arbitrary real potential. The central part $\phi(x)$ of the wave function $\psi(x)$ therefore in general is very difficult to calculate. We can, however, relate the coefficients a, b (left side) with the coefficients c, d (right side): if some fixed values for c and d are chosen, this determines the solution $\psi(x)$ everywhere on the x–axis and therefore in particular a and b. We write this relation as

$$\left(\begin{array}{c} a \\ b \end{array} \right) = \left(\begin{array}{cc} M_{11} & M_{12} \\ M_{21} & M_{22} \end{array} \right) \left(\begin{array}{c} c \\ d \end{array} \right). \tag{2.85}$$

a) With $\psi(x)$ also the conjugate complex $\psi^*(x)$ must be a solution of the stationary Schrödinger equation $\hat{H}\psi(x) = E\psi(x)$. Why ?
b) Take the conjugate complex $\psi^*(x)$ in (2.84) and show that this leads to the exchange $a \leftrightarrow b^*$ and $c \leftrightarrow d^*$ in (2.85).
c) Take the conjugate complex of the whole equation (2.85) and compare with the equation you obtain from part b). Show that

$$M_{11}^* = M_{22}, \quad M_{12}^* = M_{21}. \tag{2.86}$$

d) Consider the current density and show that

$$|a|^2 - |b|^2 = |c|^2 - |d|^2. \tag{2.87}$$

Write this equation as a scalar product of vectors in the form

$$(a^* b^*) \left(\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right) \left(\begin{array}{c} a \\ b \end{array} \right) = (c^* d^*) \left(\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right) \left(\begin{array}{c} c \\ d \end{array} \right). \tag{2.88}$$

Use the matrix M to derive from this

$$\det(M) = 1. \tag{2.89}$$

3.11 Axioms of Quantum Mechanics and the Hilbert Space

3.11.1 Definition (2min)

What is a Hilbert space?

Def.: A **Hilbert space** *is a complete unitary space.*

3.11.2 Orthonormality (5 min)

Consider the Hilbert space $\mathcal{H}$ of wave functions $\psi(x)$ of the infinite potential well on the interval $[0, L]$ with $\psi(0) = \psi(L) = 0$. Show that the basis vectors

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

form an orthonormal system.

3.11.3 * Expansion into eigenmodes (40 min)

Consider the vector $f \in \mathcal{H}$, $f(x) = cx(L-x)$.
a) Calculate the constant c such that f is normalized, i.e. $\|f\| = 1$. Show that $c = \sqrt{30/L}/L^2$.

$$\begin{aligned} 1 &= \|f\|^2 = \int_0^L dx f^*(x) f(x) = c^2 \int_0^L x^2(L-x)^2 = \\ &= c^2 \int_0^L dx[x^4 - 2Lx^3 + L^2x^2] = c^2 L^5 \left[\frac{1}{5} - \frac{2}{4} + \frac{1}{3}\right] \rightsquigarrow c = \sqrt{\frac{30}{L}} \frac{1}{L^2}. \end{aligned}$$

b) Show that f can be expanded in the basis ψ_n as

$$f = \sum_{n=1}^{\infty} c_n \psi_n, \quad c_n = 2\sqrt{60} \frac{1-(-1)^n}{n^3\pi^3} \tag{3.90}$$

$$\begin{aligned} c_n &= \langle \psi_n | f \rangle = c\sqrt{\frac{2}{L}} \int_0^L dx x(L-x) \sin\left(\frac{n\pi x}{L}\right) = [y = x/L) = \\ &= \sqrt{60} \int_0^1 dy (y - y^2) \sin(n\pi y). \end{aligned}$$

We have

$$\begin{aligned} \int_0^1 dy y \sin(n\pi y) &= -\frac{\cos(n\pi)}{n\pi} \\ \int_0^1 dy y^2 \sin(n\pi y) &= -\frac{2}{n^3\pi^3} + \frac{2 - n^2\pi^2}{n^3\pi^3} \cos(n\pi) \\ &\rightsquigarrow \int_0^1 dy (y - y^2) \sin(n\pi y) = 2\frac{1-(-1)^n}{n^3\pi^3} \end{aligned}$$

c) Use b) to prove the formula

$$\frac{\pi^3}{32} = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^3}.$$

We have

$$\begin{aligned} \sqrt{\frac{30}{L}} \frac{1}{L^2} x(L-x) &= \sqrt{60} \sum_{n=1}^{\infty} 2\frac{1-(-1)^n}{n^3\pi^3} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad \text{set} x = L/2 \\ (1/2)(1/4) &= \sum_{n=1}^{\infty} 2\frac{1-(-1)^n}{n^3\pi^3} \sin\left(\frac{n\pi}{2}\right) = [n = 2k+1] = \sum_{k=0}^{\infty} \frac{4(-1)^k}{\pi^3(2k+1)^3} \\ \rightsquigarrow \frac{\pi^3}{32} &= \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^3}. \end{aligned}$$

3.11.4 * Scalar product (20 min)

a) Use the bra and ket notation to show that for an orthonormal basis $\{|\psi_n\rangle\}$ and two Hilbert space vectors $|\psi\rangle$ and $|\chi\rangle$, one has

$$\langle \psi | \chi \rangle = \sum_{n=0}^{\infty} \langle \psi | \psi_n \rangle \langle \psi_n | \chi \rangle. \tag{3.91}$$

b) Show that in the case of vectors $\mathbf{x}$, $\mathbf{y} \in R^d$, this reduces to the standard formula for the scalar product in R^d,

$$\langle \mathbf{x}|\mathbf{y}\rangle = \sum_{i=1}^{d} x_i^* y_i.$$

c) Use Eq.(3.91) and Eq.(3.90) to prove

$$\frac{\pi^6}{960} = \sum_{k=0}^{\infty} \frac{1}{(2k+1)^6}$$

3.12 Operators and Measurements in Quantum Mechanics

3.12.1 Definitions (2 min)

Show that the momentum operator $\hat{\mathbf{p}} = -i\hbar\nabla$ is a linear operator.

Apply $-i\hbar\nabla$ to a linear combination of two wave functions.

3.12.2 Adjoint operator (10 min)

Consider the complex two–dimensional Hilbert space with basis vectors $(1,0)$ and $(0,1)$. Use the definition of the adjoint operator to prove the following for the adjoint $A^\dagger$ of the operator A: If A is given as a complex two–by– two matrix,

$$A = \left(\begin{array}{cc} a & b \\ c & d \end{array}\right) \rightsquigarrow A^\dagger = \left(\begin{array}{cc} a^* & c^* \\ b^* & d^* \end{array}\right).$$

Def.: The adjoint operator $A^\dagger$ of a linear operator A acting on a Hilbert space $\mathcal{H}$ is defined by

$$\langle \psi|A\phi\rangle = \langle A^\dagger\psi|\phi\rangle, \quad \forall \phi, \psi \in \mathcal{H}. \tag{3.92}$$

We calculate the scalar products with the basis vectors $\mathbf{e}_1, \mathbf{e}_2$:

$$A_{11} = (\mathbf{e}_1, A\mathbf{e}_1) = a = (A^\dagger\mathbf{e}_1, \mathbf{e}_1) = (A^\dagger_{11}\mathbf{e}_1, \mathbf{e}_1) = \left(A^\dagger_{11}\right)^*. \tag{3.93}$$

By this we have the element $A^\dagger_{11}$ of the adjoint matrix of A. Here, we used the fact that a scalar c in the first argument of the scalar product appears as its conjugate complex when pulled out, $(c\psi, \phi) = c^*(\psi, \phi)$. In completely the same manner we prove it for the other matrix elements.

3.12.3 Observables (5 min)

Which of the following matrices could describe physical observables in a Hilbert space of two states ?

$$A = \left(\begin{array}{cc} 1 & 1 \\ 0 & 2 \end{array}\right), \quad B = \left(\begin{array}{cc} -1 & 0 \\ 0 & 0 \end{array}\right), \quad C = \left(\begin{array}{cc} -100 & i+1 \\ i+1 & 2 \end{array}\right), \quad D = \left(\begin{array}{cc} 0 & -i \\ i & 0 \end{array}\right).$$

Physical observabes are represented hermitian operators. *Def.:* A linear operator A on the Hilbert space $\mathcal{H}$ is called **hermitian**, if the following relation holds:

$$\langle A\psi|\phi\rangle = \langle \psi|A\phi\rangle, \quad \forall \phi, \psi \in \mathcal{H}. \tag{3.94}$$

Therefore, only B and D describe physical observables. For example, B could describe a two level atom in the basis of its two eigenstates with energy -1 and 0 (in some energy unit). D is the Pauli matrix σ_y and could describe the Zeeman energy of a spin 1/2 in a magnetic field in y direction in the basis of spin states for magnetic field in the z direction. Alternatively, it could be an operator that simply performs a flip of a spin 1/2, or an operator that describes the tunneling of a particle from one side of a well to another.

3.12.4 Eigenvalues (5min)

Show that the eigenvalues of a hermitian operator are real numbers.

Theorem: The eigenvalues of hermitian operators A are real. This is because

$$A|\psi\rangle = \lambda|\psi\rangle \rightsquigarrow \lambda = \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle} \in R. \tag{3.95}$$

Furthermore,

$$\langle\psi|A\psi\rangle = \langle A^\dagger\psi|\psi\rangle = \langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle^*. \tag{3.96}$$

3.13 The Two–Level System I

3.13.1 Model (20 min)

Repeat the steps that lead to the form

$$\hat{H} = \begin{pmatrix} \varepsilon_L & T \\ T* & \varepsilon_R \end{pmatrix} \tag{3.97}$$

of the Hamiltonian of the two–level system, see Fig. 3.1. Explain the terms appearing in the

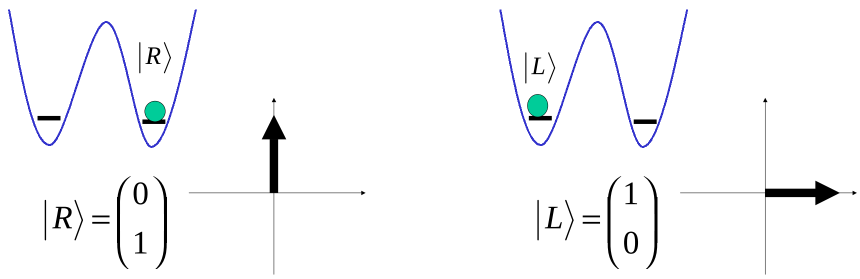

Fig. 3.1: Vector representation of left and right lowest states of double well potential.

two–by–two matrix $\hat{H}$.

3.13.2 Eigenvalues of the energy, eigenvectors (50 min)

Calculate the two eigenvectors $|i\rangle$ and eigenvalues ε_i of $\hat{H}$, eq. (3.97), that is the solutions of

$$\hat{H}|i\rangle = \varepsilon_i|i\rangle, \quad i = 1, 2. \tag{3.98}$$

Show that

$$\begin{aligned}
|1\rangle &= \frac{1}{N_1}\left[-2T|L\rangle + (\Delta+\varepsilon)|R\rangle\right], \quad \varepsilon_1 = \frac{1}{2}\left(\varepsilon_L+\varepsilon_R-\Delta\right)\\
|2\rangle &= \frac{1}{N_2}\left[\ \ 2T|L\rangle + (\Delta-\varepsilon)|R\rangle\right], \quad \varepsilon_2 = \frac{1}{2}\left(\varepsilon_L+\varepsilon_R+\Delta\right)\\
\varepsilon &:= \varepsilon_L-\varepsilon_R, \quad \Delta := \varepsilon_2-\varepsilon_1 = \sqrt{\varepsilon^2+4|T|^2}\\
N_{1,2} &:= \sqrt{4|T|^2+(\Delta\pm\varepsilon)^2}.
\end{aligned} \tag{3.99}$$

3.13.3 Absorption Experiment (5 min)

In an experiment, microwaves are irradiated upon a double quantum well. An absorption peak is observed when electrons absorb a photon $h\nu$ that matches the energy difference between the lowest state 1 and the first excited state 2 of the system. Plot the absorption peak photon energy as a function of the tunnel coupling T between both wells, when the energies in both wells are kept fixed.

The absorption energy $h\nu$ has to match the energy difference

$$\Delta := \varepsilon_2-\varepsilon_1 = \sqrt{\varepsilon^2+4|T|^2}$$

between the ground and the excited state. We thus have to plot $\Delta(T)$!

3.13.4 * Vector Representation (10 min)

Represent the eigenvectors of the two–level system for arbitrary real, negative $T=-|T|$ and arbitrary ε as vectors in the two–dimensional plane.

3.14 The Two–Level System: Measurements and Probabilities

3.14.1 Qubit 1 (5 min)

A Qubit is a state in a two–dimensional complex Hilbert space. If $|0\rangle$ and $|1\rangle$ are denoted as basis vectors of this space, what is the general form of a qubit?

A general superposition is

$$c_0|0\rangle + c_1|1\rangle, \quad |c_1|^2+|c_2|^2=1,$$

with complex coefficients c_1 and c_2.

3.14.2 Qubit 2 (5 min)

We assume that the above qubit is realized as a particle that can tunnel between two regions of space 0 and 1. What is the probability to find it in region 0 (state $|0\rangle$) if the qubit is in the quantum state

$$\frac{1}{\sqrt{2}}\left(i|0\rangle - 1|1\rangle\right), \quad i=\sqrt{-1}?$$

$$P(0) = \left|\frac{1}{\sqrt{2}}i\right|^2 = \frac{1}{2}.$$

3.14.3 Qubit 3: NOT-Gate (5 min)

Construct the quantum mechanical operator 'NOT' that flips the qubit

$$|0\rangle \to |1\rangle, \quad |1\rangle \to |0\rangle.$$

Write 'NOT' as a two–by–two matrix in the basis $\{|0\rangle = (1,0)^T, |1\rangle = (0,1)^T\}$. How does 'NOT' operate on a general qubit?

$$NOT = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{3.100}$$

3.14.4 * Qubit 4: HADAMARD–Gate (10 min)

Construct a gate (2 by 2 matrix) $\hat{H}$ that shifts the basis vectors into superpositions

$$|0\rangle \to \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right), \quad |1\rangle \to \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right). \tag{3.101}$$

Write down the explicit form of $\hat{H}$.

$$\hat{H} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{3.102}$$

4.15 The Harmonic Oscillator I

4.15.1 Model (2 min)

Write down the Hamiltonian of the one–dimensional harmonic oscillator of mass m and frequency ω.

SOLUTION:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{4.103}$$

4.15.2 Energies (2 min)

Write down the energy eigenvalues of the one–dimensional harmonic oscillator of mass m and frequency ω.

SOLUTION:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, 3, ... \tag{4.104}$$

4.15.3 Linear combination (10-20 min)

We introduce our 'vector notation' (Dirac notation) from section 3, where the normalized wave functions $\psi_n(x)$ are denoted as $|n\rangle$, because they are vectors in a Hilbert space. In this problem, the $|n\rangle$ shall correspond to the normalized wave functions of the one–dimensional harmonic oscillator of frequency ω. The $|n\rangle$ form an orthogonal system; we write the scalar product as

$$\langle n|m\rangle \equiv \int_{-\infty}^{\infty} dx \psi_n^*(x)\psi_m(x) = \delta_{n,m}. \tag{4.105}$$

1. Consider the state

$$|\phi\rangle = a|1\rangle + b|3\rangle, \quad a, b, \in C. \tag{4.106}$$

Which condition must the coefficients a,b fulfill in order that $|\phi\rangle$ is normalized? Write the normalization condition in the 'abstract, elegant form', using

$$\langle\phi| = a^*\langle 1| + b^*\langle 3|, \tag{4.107}$$

as $1 = \langle\phi|\phi\rangle = ...$
2. What is the probability to find the energy values E_1 and E_3 in an energy measurement of a system in the state $|\psi\rangle$?
3. Calculate the expectation value of the energy in the state $|\phi\rangle$ for general a and b and for $a = b = 1/\sqrt{2}$.

SOLUTION:
1.

$$|a|^2 + |b|^2 = 1. \tag{4.108}$$

2.

$$prob(E_1) = |a|^2, \quad prob(E_3) = |b|^2. \tag{4.109}$$

3.

$$\begin{aligned}
\langle\phi|\hat{H}|\phi\rangle &= a\langle\phi|\hat{H}|1\rangle + b\langle\phi|\hat{H}|3\rangle = aE_1\langle\phi|1\rangle + bE_3\langle\phi|3\rangle \\
&= aE_1(a^*\langle 1|1\rangle + b^*\langle 3|1\rangle) + bE_3(a^*\langle 1|3\rangle + b^*\langle 3|3\rangle \\
&= |a|^2E_1 + |b|^2E_3 \\
&= \hbar\omega\left(|a|^2\frac{3}{2} + |b|^2\frac{5}{2}\right) \\
a = b = \frac{1}{\sqrt{2}} \leadsto \langle\phi|\hat{H}|\phi\rangle &= \hbar\omega\left(\frac{3}{4} + \frac{5}{4}\right) = 2\hbar\omega.
\end{aligned} \tag{4.110}$$

4.16 The Harmonic Oscillator II

4.16.1 ** Generating Function (5-30 min)

We define the generating function of the Hermite polynomials as

$$e^{2tx-t^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!}t^n, \quad -\infty < x, t < \infty....... \tag{4.111}$$

Prove the formula of Rodrigues,

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}(e^{-x^2}).$$

Hint: Differentiate with respect to t.
SOLUTION:

$$\begin{aligned} H_n(x) &= \frac{\partial^n}{\partial t^n} e^{2tx-t^2}\Big|_{t=0} = \frac{\partial^n}{\partial t^n} e^{x^2-(t-x)^2}\Big|_{t=0} \\ &= e^{x^2} \frac{\partial^n}{\partial t^n} e^{-(t-x)^2}\Big|_{t=0} = e^{x^2} \frac{\partial^n}{\partial (-x)^n} e^{-(t-x)^2}\Big|_{t=0} = (-1)^n e^{x^2} \frac{\partial^n}{\partial x^n} e^{-x^2} \end{aligned}$$

4.17 Ladder Operators and Phonons

4.17.1 Commutator (5 min)

Define

$$a := \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}, \quad a^+ := \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}. \tag{4.112}$$

and show that

$$[a, a^+] = 1. \tag{4.113}$$

SOLUTION:
Use the commutator $[x, p]$.

4.17.2 Hamiltonian (10 min)

Prove that the Hamiltonian of the one–dimensional harmonic oscillator can be rewritten with the help of ladder operators as

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \hbar\omega\left(a^+a + \frac{1}{2}\right), \tag{4.114}$$

SOLUTION:
Use the commutator $[a, a^+]$.

4.17.3 Ladder Operator (5 min)

Prove the equation

$$\hat{N}a^+ = a^+(\hat{N} + 1), \quad \hat{N} := a^+a. \tag{4.115}$$

Hint: Use the commutator $[a, a^+]$.

4.17.4 Ladder Operator (15 min)

Use the above equation to show that $a^+|n\rangle$ is an eigenstate of the number operator $\hat{N}$. Show that

$$a^+|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{4.116}$$

(The $|n\rangle$ are normalized).

4.17.5 Ground state (20 min)

Use the operator a to calculate the ground state wave function $\psi_0(x)$ explicitely. Start from the operation

$$a|0\rangle = 0 \rightsquigarrow a\psi_0(x) = 0, \tag{4.117}$$

and use the definition of a to derive an ordinary differential equation for $\psi_0(x)$ that you can solve.

SOLUTION:

Write a in terms of x and p and solve the resulting differential equation:

$$\begin{aligned} \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{\hbar}{\sqrt{2m\hbar\omega}}\psi_0'(x) &= 0 \\ \frac{m\omega}{\hbar}x + \psi_0'(x) &= 0 \rightsquigarrow \psi_0(x) \propto \exp\left(-m\omega x^2/2\hbar\right). \end{aligned} \tag{4.118}$$

4.18 Central Potentials in Three Dimensions

4.18.1 Separations of Variables (20 min)

Show by using the definition of the Laplace operator in polar coordinates and the definition of the angular momentum square,

$$\hat{\mathbf{L}}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \tag{4.119}$$

that the stationary Schrödinger equation for energy E for the motion of a particle with mass m in a central potential $U(r)$ can be separated with the Ansatz for the wave function

$$\Psi(r,\theta,\phi) = R(r)Y_{lm}(\theta,\phi). \tag{4.120}$$

In order to do so, define the radial function $\chi(r) := rR(r)$ and show

$$\frac{d^2\chi(r)}{dr^2} + \left[\frac{2m}{\hbar^2}(E - U(r)) - \frac{l(l+1)}{r^2}\right]\chi(r) = 0. \tag{4.121}$$

Which values are possible for l (without proof)?

SOLUTION: See lecture notes chapter 4.4 and 4.5.

4.18.2 * Behavior for $r \to 0$ und $r \to \infty$ (10-20 min)

Verify that functions $\chi(r)$ with the following properties

$$\lim_{r\to 0} \quad \chi(r) \propto r^{l+1}, \quad \lim_{r\to\infty}\chi(r) \propto e^{-r\sqrt{-2mE/\hbar^2}}, \quad E < 0 \tag{4.122}$$

fulfill the radial part of the Schrödinger equation for ‘reasonable’ potentials $U(r)$.