Quantum Mechanics I (Example Sheets)

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

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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?

1.1.2 Rayleigh–Jeans law (5 min)

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

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.

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.

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.

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?

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 $V(\mathbf{x})$.

1.3.2 Interpretation of the Wave Function (2 min)

What is the physical meaning of the wave function ?

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?

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 $[0, L/4]$?

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** $\tilde{f}(k)$.

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.

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 $\int_{-\infty}^{\infty} dx e^{-x^2} = \sqrt{\pi}$.

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

$$\int_{-\infty}^{\infty} dx e^{-ax^2+bx} = \sqrt{\frac{\pi}{a}} e^{b^2/4a}, \quad a > 0. \tag{1.1}$$

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

The Gauss function

$$f(x) := \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}} \tag{1.2}$$

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

$$\tilde{f}(k) = \int_{-\infty}^{\infty} dx f(x) e^{-ikx} = e^{-\frac{1}{2}\sigma^2 k^2}, \quad f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-\frac{1}{2}\sigma^2 k^2} e^{ikx}. \tag{1.3}$$

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

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,

$$\Psi(x,t) = \int_{-\infty}^{\infty} dk a(k) e^{i(kx-\omega(k)t)}, \quad \hbar\omega(k) = E = \hbar^2 k^2/(2m). \tag{1.4}$$

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.

1.5 Position and Momentum in Quantum Mechanics

1.5.1 Normalization (2min)

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

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 $\Psi(x,t)$.

1.5.3 Wave packet (10-30 min)

We consider the wave function (wave packet)

$$\Psi(x) = \frac{1}{\sqrt{\sqrt{\pi a^2}}} \exp\left(-\frac{x^2}{2a^2}\right). \tag{1.5}$$

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 $\int_{-\infty}^{\infty} dy y^2 e^{-a^2y^2} = \sqrt{\pi}/(2a^3)$.

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.

1.5.5 * Commutator 1 (10 min)

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

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 $V(x)$.

2.6.2 Piecewise constant potentials in one dimension (5min)

Write down the general solution of

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V\right]\psi(x) = E\psi(x), \quad x\in[x_1,x_2] \tag{2.6}$$

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

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

$$V(x)=\begin{cases}\infty, & -\infty<x\le 0\\ 0, & 0<x\le L\\ \infty & L<x<\infty\end{cases} \tag{2.7}$$

Show that the normalized energy eigenstate wave functions and energies are

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad E=E_n=\frac{n^2\hbar^2\pi^2}{2mL^2}, \quad n=1,2,3,... \tag{2.8}$$

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

$$V(x)=\begin{cases}\infty, & -\infty<x\le -L/2\\ 0, & -L/2<x\le L/2\\ \infty & L/2<x<\infty\end{cases} \tag{2.9}$$

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)?

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.

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

$$\Psi(x, t = 0) = \psi_n(x) \rightsquigarrow \Psi(x, t) = \psi_n(x)e^{-iE_n t/\hbar}. \tag{2.10}$$

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

2.7.6 * Time evolution of superposition (10 min)

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

$$\Psi(x, t = 0) = \sum_{n=0}^{\infty} c_n \psi_n(x), \quad c_n = \int_0^L dx \psi_n^*(x)\Psi(x)? \tag{2.11}$$

b) Consider the wave function

$$\Psi(x, t = 0) = \frac{1}{\sqrt{2}} (\psi_1(x) + \psi_2(x)). \tag{2.12}$$

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

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

$$V(x) = \begin{cases} 0, & -\infty < x \leq -a \\ -V < 0, & -a < x \leq a \\ 0 & a < x < \infty \end{cases} \tag{2.13}$$

can be chosen as even and odd solutions.

2.8.2 Wave functions (5 min)

Draw the wave functions for energy $E < 0$ corresponding to the potential $V(x)$, (2.13). What about energies $E < -V$?

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.

2.9.2 Piecewise constant potential (25 min)

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

$$V(x) = \begin{cases} V_1, \\ V_2, \\ V_3, \\ \ldots \quad \ldots \\ V_N \\ V_{N+1} \end{cases} \qquad \psi(x) = \begin{cases} a_1 e^{ik_1 x} + b_1 e^{-ik_1 x}, & -\infty < x \leq x_1 \\ a_2 e^{ik_2 x} + b_2 e^{-ik_2 x}, & x_1 < x \leq x_2 \\ a_3 e^{ik_3 x} + b_3 e^{-ik_3 x}, & x_2 < x \leq x_3 \\ \ldots & \ldots \\ a_N e^{ik_N x} + b_N e^{-ik_N x}, & x_{N-1} < x \leq x_N \\ a_{N+1} e^{ik_{N+1} x} + b_{N+1} e^{-ik_{N+1} x}, & x_N < x < \infty \end{cases} \tag{2.14}$$

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

$$\mathbf{u}_1 = T^1 \mathbf{u}_2, \quad \mathbf{u}_i = \begin{pmatrix} a_i \\ b_i \end{pmatrix}, \quad i = 1, 2, \tag{2.15}$$

with

$$T^1 = \frac{1}{2k_1} \begin{pmatrix} (k_1 + k_2) e^{i(k_2 - k_1)x_1} & (k_1 - k_2) e^{-i(k_1 + k_2)x_1} \\ (k_1 - k_2) e^{i(k_2 + k_1)x_1} & (k_1 + k_2) e^{-i(k_2 - k_1)x_1} \end{pmatrix}. \tag{2.16}$$

2.9.3 Transfer matrix (5 min)

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

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} a_{N+1} \\ b_{N+1} \end{pmatrix}? \tag{2.17}$$

Express M as a product of matrices of the type (2.16).

2.9.4 Transmission, * Reflection (10min)

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

$$T := \frac{k_{N+1}}{k_1} \left| \frac{a_{N+1}}{a_1} \right|^2, \quad R := \left| \frac{b_1}{a_1} \right|^2, \tag{2.18}$$

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

$$T = \frac{k_{N+1}}{k_1} \frac{1}{|M_{11}|^2}, \quad R = \left| \frac{M_{21}}{M_{11}} \right|^2, \tag{2.19}$$

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

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 $M = T^1 T^2$ for a rectangular barrier. In (2.14), set $N = 2$, $x_2 = -x_1 = a$, $V_1 = V_3 = 0$, and $V_2 = V > 0$.

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 (2.14). Use the definitions for T^1 (T^n correspondingly) and M

$$T^1 = \frac{1}{2k_1}\begin{pmatrix} (k_1+k_2)e^{i(k_2-k_1)x_1} & (k_1-k_2)e^{-i(k_1+k_2)x_1} \\ (k_1-k_2)e^{i(k_2+k_1)x_1} & (k_1+k_2)e^{-i(k_2-k_1)x_1} \end{pmatrix}, \quad M = T^1T^2...T^N, \tag{2.20}$$

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

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

We consider a one–dimensional potential of the form

$$V(x) = \begin{cases} 0, \\ v(x), \\ 0 \end{cases} \qquad \psi(x) = \begin{cases} ae^{ikx} + be^{-ikx}, & -\infty < x \le x_1 \\ \phi(x), & x_1 < x \le x_2 \\ ce^{ikx} + de^{-ikx}, & x_2 < x < \infty \end{cases} \tag{2.21}$$

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

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} c \\ d \end{pmatrix}. \tag{2.22}$$

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 (2.21) and show that this leads to the exchange $a \leftrightarrow b^*$ and $c \leftrightarrow d^*$ in (2.22).
c) Take the conjugate complex of the whole equation (2.22) and compare with the equation you obtain from part b). Show that

$$M_{11}^* = M_{22}, \quad M_{12}^* = M_{21}. \tag{2.23}$$

d) Consider the current density and show that

$$|a|^2 - |b|^2 = |c|^2 - |d|^2. \tag{2.24}$$

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

$$(a^*b^*)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = (c^*d^*)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} c \\ d \end{pmatrix}. \tag{2.25}$$

Use the matrix M to derive from this

$$\det(M) = 1. \tag{2.26}$$

3.11 Axioms of Quantum Mechanics and the Hilbert Space

3.11.1 Definition (2min)

What is a Hilbert 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 $c = \sqrt{30/L}/L^2$.
b) Show that f can be expanded in the basis ψ_n as

$$f = \sum_{n=1}^{\infty} c_n \psi_n, \quad c_n = 2\sqrt{60}\frac{1 - (-1)^n}{n^3\pi^3} \tag{3.27}$$

c) Use b) to prove the formula

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

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

$$\langle\psi|\chi\rangle = \sum_{n=0}^{\infty} \langle\psi|\psi_n\rangle\langle\psi_n|\chi\rangle. \tag{3.28}$$

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.(3.28) and Eq.(3.27) 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.

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,

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \rightsquigarrow A^\dagger = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}.$$

3.12.3 Observables (5 min)

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

$$A = \begin{pmatrix} 1 & 1 \\ 0 & 2 \end{pmatrix}, \quad B = \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}, \quad C = \begin{pmatrix} -100 & i+1 \\ i+1 & 2 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

3.12.4 Eigenvalues (5min)

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

3.13 The Two–Level System I

3.13.1 Model (20 min)

Repeat the steps that lead to the form

$$\hat{H} = \begin{pmatrix} \varepsilon_L & T \\ T* & \varepsilon_R \end{pmatrix} \tag{3.29}$$

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

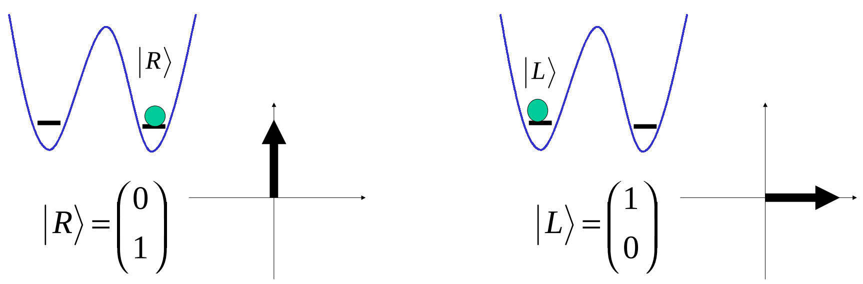

Fig. 3.1: Vector representation of left and right lowest states of double well potential.

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. (3.29), that is the solutions of

$$\hat{H}|i\rangle = \varepsilon_i |i\rangle, \quad i = 1, 2. \tag{3.30}$$

Show that

$$
\begin{aligned}
|1\rangle &= \frac{1}{N_1}\left[-2T|L\rangle + (\Delta+\varepsilon)|R\rangle\right], \quad \varepsilon_1 = \frac{1}{2}\left(\varepsilon_L + \varepsilon_R - \Delta\right)\\
|2\rangle &= \frac{1}{N_2}\left[\ \ 2T|L\rangle + (\Delta-\varepsilon)|R\rangle\right], \quad \varepsilon_2 = \frac{1}{2}\left(\varepsilon_L + \varepsilon_R + \Delta\right)\\
\varepsilon &:= \varepsilon_L - \varepsilon_R, \quad \Delta := \varepsilon_2 - \varepsilon_1 = \sqrt{\varepsilon^2 + 4|T|^2}\\
N_{1,2} &:= \sqrt{4|T|^2 + (\Delta \pm \varepsilon)^2}.
\end{aligned} \tag{3.31}
$$

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.

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?

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

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

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?

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

$$|0\rangle \to \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right), \quad |1\rangle \to \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right). \tag{3.32}$$

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

4.15 The Harmonic Oscillator

4.15.1 Model (2 min)

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

4.15.2 Energies (2 min)

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

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

$$\langle n|m\rangle \equiv \int_{-\infty}^{\infty} dx \psi_n^*(x)\psi_m(x) = \delta_{n,m}. \tag{4.33}$$

1. Consider the state

$$|\phi\rangle = a|1\rangle + b|3\rangle, \quad a, b, \in C. \tag{4.34}$$

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

$$\langle\phi| = a^*\langle 1| + b^*\langle 3|, \tag{4.35}$$

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 $a = b = 1/\sqrt{2}$.

4.15.4 ** Generating Function (5-30 min)

We define the generating function of the Hermite polynomials as

$$e^{2tx-t^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n, \quad -\infty < x, t < \infty....... \tag{4.36}$$

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.

4.16 Ladder Operators and Phonons

4.16.1 Commutator (5 min)

Define

$$a := \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}, \quad a^+ := \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}. \tag{4.37}$$

and show that

$$[a, a^+] = 1. \tag{4.38}$$

4.16.2 Hamiltonian (10 min)

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

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \hbar\omega\left(a^+a + \frac{1}{2}\right), \tag{4.39}$$

4.16.3 Ladder Operator (5 min)

Prove the equation

$$\hat{N}a^+ = a^+(\hat{N}+1), \quad \hat{N} := a^+a. \tag{4.40}$$

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

4.16.4 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

$$a^+|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{4.41}$$

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

4.16.5 Ground state (20 min)

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

$$a|0\rangle = 0 \rightsquigarrow a\psi_0(x) = 0, \tag{4.42}$$

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

4.17 Central Potentials in Three Dimensions

4.17.1 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,

$$\hat{\mathbf{L}}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right] \tag{4.43}$$

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

$$\Psi(r, \theta, \phi) = R(r) Y_{lm}(\theta, \phi). \tag{4.44}$$

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

$$\frac{d^2\chi(r)}{dr^2} + \left[\frac{2m}{\hbar^2}(E - U(r)) - \frac{l(l+1)}{r^2} \right] \chi(r) = 0. \tag{4.45}$$

Which values are possible for l (without proof)?

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

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

$$\lim_{r\to 0} \quad \chi(r) \propto r^{l+1}, \quad \lim_{r\to\infty} \chi(r) \propto e^{-r\sqrt{-2mE/\hbar^2}}, \quad E < 0. \tag{4.46}$$

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