

Quantum Physics

Collection of problems

This is a collection of problems in quantum mechanics for undergraduate physics students, put together by Prof. Dr. Ana-Sunčana Smith and her group at FAU Erlangen–Nürnberg.

Many of these exercises were collected from materials presented over the years at Friedrich-Alexander-University Erlangen-Nürnberg, Germany and University of Zagreb, Croatia. Some of the exercises were conceived by Prof. Dr. T. Franosch (University of Innsbruck, Austria), Prof. Dr. T. Nikšić (University of Zagreb, Croatia) and the authors of the script.

All users of this collection are requested to kindly report any errors and omissions to Smith Group at FAU Erlangen-Nürnberg, in particular to [Mislav Cvitković](#) or [Robert Blackwell](#).

1 Introduction and Analogies

Problem 1.1 *Delta function*

a) The δ -function can be represented as the limit, as $N \rightarrow \infty$, of the sum

$$\sum_{k=-N}^N e^{2\pi i k x} .$$

Show the above sum is equal to

$$f(x) = \frac{\sin[2\pi(N + \frac{1}{2})x]}{\sin(\pi x)} \quad (1.1)$$

for $x \neq 0$. Hint: Use Euler's formula and the identity

$$\sum_{k=0}^{2N} z^k = \frac{z^{2N+1} - 1}{z - 1} .$$

The 3-dimensional δ -function can be analogously represented as

$$\lim_{N \rightarrow \infty} \sum_{h=-N}^N \sum_{k=-N}^N \sum_{l=-N}^N e^{2\pi i (hx+ky+lz)} .$$

Show for $x, y, z \neq 0$, the above sum is equal to $f(x)f(y)f(z)$ where $f(x)$ is as defined in (1.1).

b) Evaluate the following integrals:

(i)

$$\int_0^3 x^3 \delta(x+1) dx$$

(ii)

$$\int_{-1}^1 9x^2 \delta(3x+1) dx$$

(iii)

$$\int_{V'} (r^2 + 2) \nabla \cdot \left(\frac{\mathbf{e}_r}{r^2} \right) dV,$$

where V' is a sphere of radius R centred at the origin, and \mathbf{e}_r is the unit vector in the radial direction. Hint: Use the fact that $\nabla \cdot \left(\frac{\mathbf{e}_r}{r^2} \right) = 4\pi\delta^3(\mathbf{r})$.

(iv)

$$\int_{V'} |\mathbf{r} - \mathbf{b}|^2 \delta^3(5\mathbf{r}) dV,$$

where V' is a cube of side 2, centred on the origin, and $\mathbf{b} = 4\mathbf{e}_y + 3\mathbf{e}_z$.

Problem 1.2 *Spherical harmonics*

a) The ‘associated’ Legendre polynomials P_l^m

$$P_l^m(x) = \frac{(-1)^m}{2^l l!} (1-x^2)^{m/2} \frac{\partial^{l+m}}{\partial x^{l+m}} (x^2-1)^l$$

can be calculated for $-l \leq m \leq l$. Verify that for $l = 0, \dots, 3$ they fulfil the differential equation

$$\frac{\partial}{\partial x} \left[(1-x^2) \frac{\partial P_l^m(x)}{\partial x} \right] + \left[l(l+1) - \frac{m^2}{1-x^2} \right] P_l^m(x) = 0.$$

b) The spherical harmonics $Y_{lm}(\vartheta, \varphi)$ are defined by

$$Y_{lm}(\vartheta, \varphi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos \vartheta) e^{im\varphi}.$$

Verify for $l, l' \leq 2$ the orthonormality condition

$$\int_0^{2\pi} d\varphi \int_0^\pi \sin \vartheta d\vartheta Y_{l'm'}^*(\vartheta, \varphi) Y_{lm}(\vartheta, \varphi) = \delta_{ll'} \delta_{mm'}.$$

Problem 1.3 *Eikonal Equation and Fermat’s Principle*

The refractive index in the atmosphere varies weakly in space and may be approximated by a linear change with respect to the z -axis

$$n(z) = n(0) - z n'(0), \quad n(0) > 0, \quad n'(0) > 0,$$

where $n(0)$ corresponds to the refractive index at ground level. The problem is to be discussed in the limit of geometrical optics, where for the wavelength of the ray $\lambda n'(z) \ll 1$ is valid.

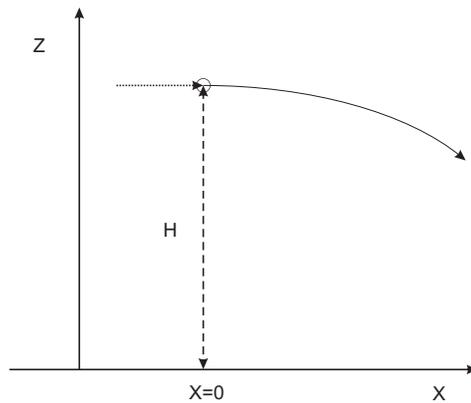


Fig. 1: Scheme of the light trajectory.

a) Calculate the trajectory of a light ray in the atmosphere (see fig. 1). Use the equations of the method of characteristics (ray equations) for the eikonal equation to determine $x(\ell), z(\ell)$ as a function of the flow parameter ℓ . Eliminate ℓ in favor of x to obtain a description for the trajectory $z(x)$.

b) In addition determine $z(x)$ relying on Fermat's principle by minimizing the optical path

$$S = \int n ds.$$

Use the methods of Euler-Lagrange to obtain a description for $z(x)$.

Problem 1.4 *Electromagnetic Wave as Analogy to Quantum Matter Waves*

Consider an electromagnetic monochromatic plane wave propagating in vacuum $\varepsilon = 1$ and $\mu = 1$ with a wave vector $\mathbf{k} = (0, 0, k)$. The electric field vector should oscillate in time and space with $\mathbf{E}(\mathbf{r}, t) = (0, 0, E_z(x, t))$ where $E_z(x, t) = \exp[i(kx - \omega t)]$ for a given frequency ω . At position $x = 0$ a dielectric medium fills the half space $x > 0$, which is characterized by $\varepsilon \geq 1$ and $\mu = 1$. The medium is assumed to be transparent, so ε is real. A part of the wave is transmitted through the dielectric medium.

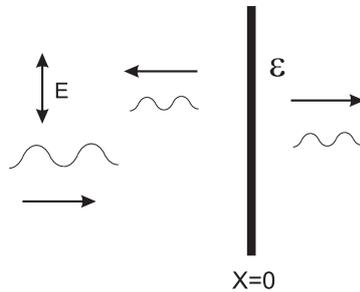


Fig. 2: Scheme of reflection.

- What can be inferred on the the frequencies ω' for the transmitted wave?
- The stationary electric field has to fulfill the wave equation,

$$\left[\varepsilon(x) \frac{\omega^2}{c^2} + \frac{d^2}{dx^2} \right] E_z(x) = 0,$$

which is a one dimensional problem only. Discuss the following ansatz for the solutions

$$E_z(x) = \begin{cases} e^{ikx} + r e^{-ikx} & \text{for } x < 0, \\ t e^{ik'x} & \text{for } x > 0 \end{cases}$$

- Write down the dispersion relations for $x < 0$ and $x > 0$.
- Use the continuity conditions for the fields at the interface to express the amplitudes in terms of ε .
- Calculate the transmission coefficient T and the reflection coefficient R . Show, that $T + R = 1$.

Problem 1.5 *Tunnel Effect*

Consider a thin film of thickness $2a$ characterized by a dielectric constant ε_m dividing the three-dimensional space (dielectric constant ε); see fig. 1.5. A monochromatic electromagnetic plane wave is incident on the film. Choose a coordinate system such that the incident wave vector reads $\mathbf{k}_i = (k, k_{\parallel}, 0)$. Discuss the case of a polarization of the incident electric field parallel to the interfaces, $\mathbf{E}_i = (0, 0, E_i)$.

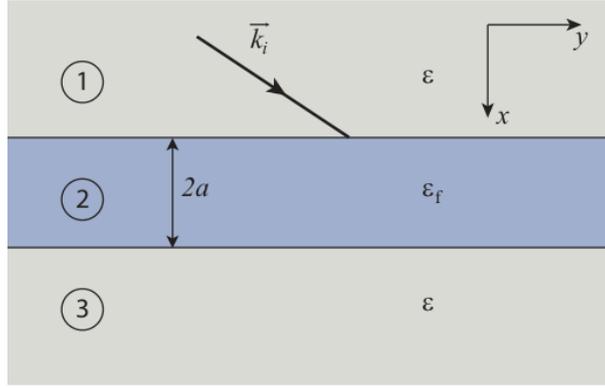


Fig. 3: Scheme of the Problem 1.5.

- Determine the dispersion relation $\omega = \omega(\mathbf{k})$ separately in each region.
- Argue that the polarization of the electric field is parallel to the interface in all three regions.
- Since the tangential component of the electric field is continuous at the interfaces, the spatio-temporal modulation at the interface are identical. Justify the following ansatz for the electric field

$$E_z(\mathbf{x}, t) = e^{i k_{\parallel} y - i \omega t} \begin{cases} E_i e^{i k x} + E_r e^{-i k x} & \text{for } x < -a, \\ E_+ e^{i q x} + E_- e^{-i q x} & \text{for } -a < x < a, \\ E_t e^{i k x} & \text{for } x > a, \end{cases}$$

and interpret the individual terms. Show that q becomes purely imaginary for $k_{\parallel}^2 > \epsilon_m \omega^2 / c^2$.

- Establish the conditions of continuity for the tangential components of \mathbf{H} ($= \mathbf{B}$ here) and calculate the effective transmission amplitude $t = E_t / E_i$ and the effective reflection amplitude $r = E_r / E_i$.

Problem 1.6 Paraxial Beams

Consider a monochromatic electromagnetic beam of angular frequency $\omega = ck$ propagating essentially along the positive z -direction.

- Argue that the components of the electric field allow for a representation as

$$E(\mathbf{x}_{\perp}, z; t) = e^{-i \omega t} \int \frac{d^2 \mathbf{k}_{\perp}}{(2\pi)^2} a(\mathbf{k}_{\perp}) \exp(i \mathbf{k}_{\perp} \mathbf{x}_{\perp} + i k_{\parallel} z),$$

where $k_{\parallel} = (k^2 - \mathbf{k}_{\perp}^2)^{1/2}$ is to be eliminated in favor of \mathbf{k}_{\perp} .

- The complex amplitudes $a(\mathbf{k}_{\perp})$ are assumed to contribute only for $|\mathbf{k}_{\perp}| \ll k$. Expanding the square root, $k_{\parallel} \simeq k - \mathbf{k}_{\perp}^2 / 2k$ to leading order in k_{\perp} / k , show that the field assumes the following form

$$E(\mathbf{x}_{\perp}, z; t) = e^{i k z - i \omega t} \mathcal{E}(\mathbf{x}_{\perp}, z),$$

where the *envelope function* \mathcal{E} is slowly varying along z on the scale of a wavelength, $\partial_z \mathcal{E} \ll k \mathcal{E}$. Relate the envelope to the amplitudes $a(\mathbf{k}_{\perp})$. Show that the envelope satisfies a field equation of the Schrödinger type,

$$i \partial_z \mathcal{E}(\mathbf{x}_{\perp}, z) = -\frac{1}{2k} \nabla_{\perp}^2 \mathcal{E}(\mathbf{x}_{\perp}, z).$$

In particular, the field equation is first order in the z -direction.

c) Evaluate the electric field $E(\mathbf{x}_\perp, z; t)$ for a Gaussian amplitude function

$$a(\mathbf{k}_\perp) \propto \exp\left(-\frac{1}{4}w_0^2\mathbf{k}_\perp^2\right), \quad w_0 > 0,$$

and show that the intensity $I \propto |E|^2$ exhibits a Gaussian profile in the perpendicular direction \mathbf{x}_\perp and a width that depends on z . Where is the width minimal?

Problem 1.7 *Angular Momentum Conservation Law*

The angular momentum density of the electromagnetic field is defined by the antisymmetric tensor field

$$L_{ij}(\mathbf{x}, t) = \frac{1}{c^2}(x_i S_j - x_j S_i),$$

where \mathbf{S} denotes the Poynting vector.

a) Employ the momentum balance law to construct a local balance law for the angular momentum density of the form

$$\partial_t L_{ij} + \nabla_k M_{ijk} = -D_{ij}.$$

Determine the angular momentum current tensor M_{ijk} as well as the mechanical torque tensor D_{ij} . Rewrite the balance law in terms of the pseudo-vector field

$$L_i(\mathbf{x}, t) = \frac{1}{2}\varepsilon_{ijk}L_{jk},$$

and suitable M_{ik} and D_i .

b) Formulate the angular momentum conservation law in integral form, for $\mathcal{L}_i = \int_V L_i dV$.
c) Demonstrate that in the gauge $\varphi = 0$, the angular momentum of the field can be decomposed, $\mathcal{L} = \mathcal{L}_S + \mathcal{L}_B$, in a ‘spin’ part

$$\mathcal{L}_S = \frac{1}{4\pi c^2} \int_V \mathbf{A} \times \dot{\mathbf{A}} dV,$$

and an ‘orbital’ part \mathcal{L}_B that depends explicitly on the point of reference of the coordinate system.

Problem 1.8 *Radiation Loss of a Harmonically Oscillating Charge*

a) A positive charge is attached to a spring (Fig. 6) in such a way that a radiating harmonic oscillator results. Show that small radiation losses with a minor reaction on a motion of the oscillator may be described by introducing a frictional force proportional to the third derivative of the elongation.

b) Consider an isolated system which emits dipole radiation mainly with the frequency ω_0 . Due to the radiation, the energy of the system is diminished permanently. This implies that the frequencies $\omega = \omega_0 + \Delta\omega$ adjacent to ω_0 are emitted by the system. $\Delta\omega$ is called the natural width of the emission line. Show that for a radiating harmonic oscillator of mass m and charge e , in case of weak damping, the natural line width is given by $\Delta\omega = \frac{2}{3} \frac{e^2 \omega_0^2}{mc^3}$.

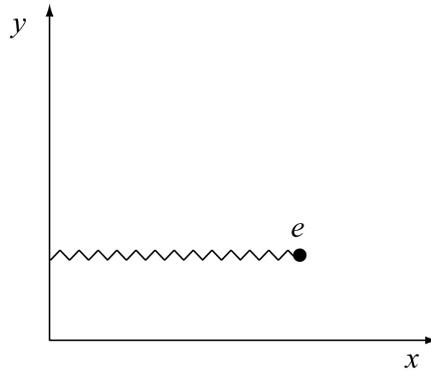


Fig. 6: A charge attached to a spring.

Problem 1.9 *Linear Response to the Field — Lorentz–Drude Model*

Consider the constitutive equation of the Lorentz–Drude model,

$$\partial_t^2 \mathbf{P}(\mathbf{x}, t) + \frac{1}{\tau} \partial_t \mathbf{P}(\mathbf{x}, t) + \omega_0^2 \mathbf{P}(\mathbf{x}, t) = \frac{\omega_p^2}{4\pi} \mathbf{E}(\mathbf{x}, t),$$

with the relaxation time τ , characteristic frequency ω_0 and the plasma frequency ω_p .

- a) Perform a spatio-temporal Fourier transform and determine the complex susceptibility $\chi(\omega)$, with $\mathbf{P}(\mathbf{k}, \omega) = \chi(\omega) \mathbf{E}(\mathbf{k}, \omega)$, as well as the dielectric function $\varepsilon(\omega) = 1 + 4\pi\chi(\omega)$.
- b) Argue that the longitudinal modes follow from the zero of the dielectric function, $\varepsilon(\omega_*) = 0$, and determine the complex frequency ω_* in the case of weak damping.
- c) Ignoring the damping (i.e. $\tau \rightarrow \infty$) determine the dispersion relation of the transverse modes.
- d) Explain without calculation, in what frequency regime the damping is most important.

Problem 1.10 *Classical Hydrogen Atom, s-orbitals*

Quantum mechanics reveals that the electron in a hydrogen atom should be described in terms of a wave function $\psi(\mathbf{r})$ (probability amplitude) giving rise to a smeared electron cloud corresponding to a charge density, $\rho_e(\mathbf{r}) = -e|\psi(\mathbf{r})|^2$. At the center of the atom, the proton is localized at a much smaller length scale, and the contribution to the charge density may be modelled as a point charge, $e\delta(\mathbf{r})$. Determine the (total) electrostatic potential φ

- a) for the (1s-orbital, K-shell) ground state of the hydrogen atom. Here the wave function is spherically symmetric

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

where $a = \hbar^2/2me^2 = 0.529 \times 10^{-8} \text{cm}$ denotes the Bohr radius.

- b) for the spherically symmetric first excited state (2s-orbital, L-shell)

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{8\pi a^3}} \left(1 - \frac{r}{2a}\right) e^{-r/2a}.$$

Problem 1.11 *Classical Hydrogen Atom, p-orbitals*

The electronic charge distribution of a hydrogen atom in a p -orbital has the following form in spherical coordinates

$$\rho(\mathbf{r}) = -\frac{e}{64\pi a^3} \left(\frac{r}{a}\right)^2 e^{-r/a} \sin^2 \vartheta$$

where a is the Bohr radius and e is the elementary charge.

a) Calculate the multipole moment

$$q_{lm} = \int_{\mathbb{R}^3} Y_{lm}^*(\vartheta', \varphi') r'^l \rho(\mathbf{r}) dV'$$

and the multipole expansion

$$\bar{\Phi}(\mathbf{r}) := \sum_{l,m} \frac{4\pi}{2l+1} \frac{q_{lm}}{r^{l+1}} Y_{lm}(\vartheta, \varphi).$$

Hint: $\sin^2 \vartheta$ can be expressed as a linear combination of spherical harmonics.

b) How and why is $\bar{\Phi}$ different from the exact potential

$$\Phi(\mathbf{r}) = \int_{\mathbb{R}^3} \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV' ?$$

Hint: You may use the following relation

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{4\pi}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_{lm}(\vartheta, \varphi) Y_{lm}^*(\vartheta', \varphi'),$$

where $r_{>}$ ($r_{<}$) denotes absolute value of the larger (smaller) of the two radius vectors \mathbf{r} and \mathbf{r}' .

c) What is the behaviour of $\Phi(\mathbf{r})$ for $r \ll a$?

Problem 1.12 *Gaussian Wave Packet — Heisenberg's Uncertainty Relation*

Consider a particle that is described by the wave function

$$\psi(x) = A e^{-\frac{x^2}{4a^2}}$$

where a is real and positive.

a) Normalize the wave function.

b) Calculate $\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$, $\langle p^2 \rangle$.

c) Evaluate the product of the standard deviations $\sigma_x \sigma_p$. Compare it to Heisenberg's uncertainty relation $\sigma_x \sigma_p \geq \hbar/2$.

2 Algebra, Operators, Representations

Problem 2.1 Hilbert Space

- For what range of ν is the function $f(x) = x^\nu$ in Hilbert space, on the interval $(0, 1)$? Assume ν is real, but not necessarily positive.
- For the specific case $\nu = 1/2$, is $f(x)$ in Hilbert space? What about $xf(x)$? How about $(d/dx)f(x)$?

Problem 2.2 Commutator Rules

Show the following relations for the commutator $[A, B]$ of the two linear operators A, B :

- $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$ (Jacobi rule).
- $[AB, C] = A[B, C] + [A, C]B$ (Leibnitz rule).
- $[A, [A, B]] = 0 \Rightarrow [A^n, B] = nA^{n-1}[A, B], \forall n \in \mathbb{N}$.
- $f(x) = \sum_{n=0}^{\infty} a_n x^n$ and $[A, [A, B]] = 0 \Rightarrow [f(A), B] = f'(A)[A, B]$.

Problem 2.3 Dirac Notation

Consider the three-dimensional Hilbert space spanned by the orthonormal basis $\{|1\rangle, |2\rangle, |3\rangle\}$. Two kets are given: $|\alpha\rangle = i|1\rangle - 4|2\rangle - 2i|3\rangle$, $|\beta\rangle = 2i|1\rangle + 2|3\rangle$.

- Write down $\langle\alpha|$ and $\langle\beta|$. Calculate $\langle\alpha|\alpha\rangle$, $\langle\beta|\beta\rangle$, $\langle\beta|\alpha\rangle$ and $\langle\alpha|\beta\rangle$. Verify $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$.
- What are the matrix elements of the operator $A = |\alpha\rangle\langle\beta|$ in the basis $\{|1\rangle, |2\rangle, |3\rangle\}$.
- Find the energy eigenvalues and the corresponding eigenkets for a system characterized by the Hamiltonian $H = a(|2\rangle\langle 1| + |1\rangle\langle 2| + 2|3\rangle\langle 3|)$. Don't forget to normalize your result.

Problem 2.4 Bra-Ket Trainer

Let $\{|a_i\rangle : i = 1, \dots, N \in \mathbb{N}\}$ and $\{|b_i\rangle : i = 1, \dots, N \in \mathbb{N}\}$ be two different complete sets of orthonormal vectors, which span the N -dimensional complex Hilbert space \mathcal{H} .

$$|a_j\rangle = \sum_{i=1}^N U_{ij}|b_i\rangle, \text{ where } U_{ij} = \langle b_i | a_j \rangle.$$

Use the bra-ket notation to solve the following exercises:

- Show that the operator

$$U := \sum_{i,k} |a_i\rangle\langle b_i | a_k \rangle \langle a_k | = \sum_{i,k} |a_i\rangle U_{ik} \langle a_k |$$

fulfills $|a_i\rangle = U|b_i\rangle \forall i = 1, \dots, N$. Show that U is unitary, meaning $U^\dagger U = 1$.

- For any linear operator A show that $\text{tr}(A) := \sum_i \langle a_i | A | a_i \rangle$ does not depend on the choice of the basis, i.e. show $\text{tr}(A) = \sum_i \langle b_i | A | b_i \rangle$.

Problem 2.5 *Adjoint and Hermitian Operators*

The scalar product with some operator A is defined as

$$(\varphi, A\psi) = \int \varphi^*(\mathbf{r})A\psi(\mathbf{r}) \, d\mathbf{r}.$$

The adjoint operator is called A^\dagger , if

$$(\varphi, A\psi) = (A^\dagger\varphi, \psi)$$

or equivalently

$$\int \varphi^*(\mathbf{r})A\psi(\mathbf{r}) \, d\mathbf{r} = \int (A^\dagger\varphi(\mathbf{r}))^* \psi(\mathbf{r}) \, d\mathbf{r}.$$

- Determine the adjoint operator of the operator αA , $\alpha \in \mathbb{C}$.
- Show, that for two Hermitian operators $\alpha A + \beta B$ is Hermitian, if $\alpha, \beta \in \mathbb{R}$.
- Prove, that the momentum operator $\mathbf{P} = \frac{\hbar}{i}\nabla$ is Hermitian.
- What is the adjoint operator to the product operator $C = AB$, which is defined as

$$C\psi(\mathbf{r}) = (AB)\psi(\mathbf{r}) = A(B\psi(\mathbf{r})).$$

If A and B are Hermitian, when is AB Hermitian?

- Show, that $H = -\frac{\hbar^2}{2m}\Delta + V(\mathbf{Q})$ and $\mathbf{L} = \mathbf{Q} \times \frac{\hbar}{i}\nabla$ (only one component) are Hermitian.

Problem 2.6 *Properties of the Hermitian Operators*

- Show that the sum of two Hermitian operators is Hermitian.
- Suppose \hat{Q} is Hermitian, and α is a complex number. Under what condition on α is $\alpha\hat{Q}$ Hermitian?
- When is the product of two Hermitian operators Hermitian?
- Show that the position operator ($\hat{x} = x$) and the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

are Hermitian.

- Show that the eigenvalues of Hermitian operator are real.
- Show that if $\langle h|\hat{Q}h\rangle = \langle \hat{Q}h|h\rangle$ for all functions h (in Hilbert space), then $\langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle$ for all f and g .

Problem 2.7 *Probability Current*

Max Born first suggested that the mod-square of a particle's wave function

$$\rho(\mathbf{x}, t) \equiv |\Psi(\mathbf{x}, t)|^2$$

is the probability density of finding the particle near \mathbf{x} at time t . Since the particle is certain to be found *somewhere* at each instant of time t , for this interpretation to make sense we must have

$$\int |\Psi(\mathbf{x}, t)|^2 \, d^3\mathbf{x} = 1. \quad (2.3)$$

a) Defining the *probability current* \mathbf{J} as

$$\mathbf{J}(\mathbf{x}) = \frac{i\hbar}{2m} (\Psi \nabla \Psi^* - \Psi^* \nabla \Psi)$$

show that the following *continuity equation* is satisfied:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}.$$

b) With the help of the continuity equation, show that

$$\frac{d}{dt} \int_{\text{all space}} \rho d^3\mathbf{x} = 0$$

showing that eq. (2.3) is indeed satisfied.

c) Writing Ψ as

$$\Psi(\mathbf{x}) = S(\mathbf{x})e^{i\varphi(\mathbf{x})}$$

with S and φ real, show that the velocity \mathbf{v} of the probability current, defined as $\mathbf{J} = \rho\mathbf{v}$, is

$$\mathbf{v} = \frac{\hbar \nabla \varphi}{m}.$$

Problem 2.8 Ladder Operators

a) Let $B = cA + sA^\dagger$, where $c \equiv \cosh \vartheta$, $s \equiv \sinh \vartheta$ with ϑ a real constant and A, A^\dagger are the usual ladder operators. Show that $[B, B^\dagger] = 1$.

b) Consider the Hamiltonian

$$H = \varepsilon A^\dagger A + \frac{1}{2}\lambda(A^\dagger A^\dagger + AA)$$

where ε and λ are real and such that $\varepsilon > \lambda > 0$. Show that when

$$\varepsilon c - \lambda s = Ec \quad ; \quad \lambda c - \varepsilon s = Es$$

with E a constant, $[B, H] = EB$. Hence determine the spectrum of H in terms of ε and λ .

Problem 2.9 Fermi Oscillator

A *Fermi oscillator* has the Hamiltonian $H = f^\dagger f$, where f is an operator that satisfies

$$f^2 = 0; \quad f f^\dagger + f^\dagger f = 1.$$

Show that $H^2 = H$, and thus find the eigenvalues of H . If the ket $|0\rangle$ satisfies $H|0\rangle = 0$ with $\langle 0|0\rangle = 1$, what are the kets $|a\rangle \equiv f|0\rangle$, and $|b\rangle \equiv f^\dagger|0\rangle$?

In quantum field theory the vacuum is pictured as an assembly of oscillators, one for each possible value of the momentum of each particle type. A boson is an excitation of a harmonic oscillator, while a fermion is an excitation of a Fermi oscillator. Explain the connection between the spectrum of $f^\dagger f$ and the Pauli principle.

Problem 2.10 *Baker-Hausdorff Identity*

Prove that for two operators A, B and a complex parameter y , the so-called Baker-Hausdorff identity

$$e^{yA} B e^{-yA} = B + y[A, B] + \frac{y^2}{2!} [A, [A, B]] + \dots + \frac{y^n}{n!} [A, [A, \dots [A, B] \dots]]_n + \dots$$

holds. *Hint:* Define $F(y) = e^{yA} B e^{-yA}$ and consider $\frac{dF}{dy}$.

Problem 2.11 *Translation Operator*

a) In this problem you derive the wavefunction

$$\langle \mathbf{x} | \mathbf{p} \rangle = e^{i\mathbf{p} \cdot \mathbf{x} / \hbar} \quad (2.6)$$

of a state of well defined momentum for the properties of the translation operator $U(\mathbf{a})$. The state $|\mathbf{k}\rangle$ is one of well-defined momentum $\hbar\mathbf{k}$. How would you characterise the state $|\mathbf{k}'\rangle \equiv U(\mathbf{a})|\mathbf{k}\rangle$? Show that the wavefunctions of these states are related by $u_{\mathbf{k}'}(\mathbf{x}) = e^{-i\mathbf{a} \cdot \mathbf{k}} u_{\mathbf{k}}(\mathbf{x})$ and $u_{\mathbf{k}'}(\mathbf{x}) = u_{\mathbf{k}}(\mathbf{x} - \mathbf{a})$. Hence obtain equation (2.6).

b) The relation $[v_i, J_j] = i \sum_k \varepsilon_{ijk} v_k$ holds for any operator whose components v_i form a vector. The expectation value of this operator relation in any state $|\psi\rangle$ is then

$$\langle \psi | [v_i, J_j] | \psi \rangle = i \sum_k \varepsilon_{ijk} \langle \psi | v_k | \psi \rangle.$$

Check that with $U(\boldsymbol{\alpha}) = e^{-i\boldsymbol{\alpha} \cdot \mathbf{J}}$ this relation is consistent under a further rotation $|\psi\rangle \rightarrow |\psi'\rangle = U(\boldsymbol{\alpha})|\psi\rangle$ by evaluating both sides separately.

Problem 2.12 *Rotation Operator*

a) Show that the vector product $\mathbf{a} \times \mathbf{b}$ of two classical vectors transforms like a vector under rotations. Hint: A rotation matrix \mathbf{R} satisfies the relations $\mathbf{R} \cdot \mathbf{R}^T = \mathbf{I}$ and $\det(\mathbf{R}) = 1$, which in tensor notation read $\sum_p R_{ip} R_{tp} = \delta_{it}$ and $\sum_{ijk} \varepsilon_{ijk} R_{ir} R_{js} R_{kt} = \varepsilon_{rst}$.

(i) Let the matrices J_x, J_y and J_z be such that $\exp(-i\boldsymbol{\alpha} \cdot \mathbf{J}) \equiv \mathbf{R}(\boldsymbol{\alpha})$, where the exponential of a matrix is defined in terms of the power series for e^x . Here $\boldsymbol{\alpha}$ is a vector that specifies a rotation through an angle $|\boldsymbol{\alpha}|$ around the direction of the unit vector $\hat{\boldsymbol{\alpha}}$. Show that J_i are Hermitian matrices.

(ii) Show that for any two vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ the product $\mathbf{R}^T(\boldsymbol{\alpha})\mathbf{R}(\boldsymbol{\beta})\mathbf{R}(\boldsymbol{\alpha})$ is an orthogonal matrix with determinant +1, so it is a rotation matrix.

(iii) Make a Taylor expansion of $\exp(-i\boldsymbol{\alpha} \cdot \mathbf{J}) \equiv \mathbf{R}(\boldsymbol{\alpha})$ for small $|\boldsymbol{\alpha}|$ and $|\boldsymbol{\beta}|$ and show $[J_i, J_j] = i \sum_k \varepsilon_{ijk} J_k$.

b) Show that if $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are non-parallel vectors, $\boldsymbol{\alpha}$ is not invariant under the combined rotation $\mathbf{R}(\boldsymbol{\alpha})\mathbf{R}(\boldsymbol{\beta})$. Hence show that $\mathbf{R}^T(\boldsymbol{\beta})\mathbf{R}^T(\boldsymbol{\alpha})\mathbf{R}(\boldsymbol{\beta})\mathbf{R}(\boldsymbol{\alpha})$ is not the identity operation. Explain the physical significance of this result.

c) The matrix for rotating an ordinary vector by φ around the z axis is

$$\mathbf{R}(\varphi) \equiv \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

By considering the form taken by \mathbf{R} for infinitesimal φ calculate from \mathbf{R} the matrix \mathbf{J}_z that appears in $\mathbf{R}(\varphi) = \exp(-i\mathbf{J}_z\varphi)$. Introduce new coordinates $u_1 \equiv (-x + iy)/\sqrt{2}$, $u_2 = z$

and $u_3 \equiv (x + iy)/\sqrt{2}$. Write down the matrix \mathbf{M} that appears in $\mathbf{u} = \mathbf{M} \cdot \mathbf{x}$ [where $x \equiv (x, y, z)$] and show that it is unitary. Then show that

$$\mathbf{J}'_z \equiv \mathbf{M} \cdot \mathbf{J}_z \cdot \mathbf{M}^\dagger \quad (2.7)$$

is identical with S_z in the set of spin-one Pauli analogues

$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (2.8)$$

Write down the matrix \mathbf{J}_z whose exponential generates rotations around the x axis, calculate \mathbf{J}'_x by analogy with equation (2.7) and check that your result agrees with S_x in the set (2.8). Explain as fully as you can the meaning of these calculations.

Problem 2.13 *Shift Operator and Heisenberg Algebra*

Let $\Psi : \mathbb{R} \rightarrow \mathbb{C}$ be an arbitrary wavefunction. The shift operator T_a , $a \in \mathbb{R}$, is defined through

$$(T_a \Psi)(x) = \Psi(x + a).$$

Let $\Psi : \mathbb{R}^3 \rightarrow \mathbb{C}$ be an arbitrary wavefunction. The momentum and position operators P_i, Q_i ($i = 1, 2, 3$) are defined as following:

$$(Q_i \Psi)(\mathbf{r}) = r_i \Psi(\mathbf{r}),$$

$$(P_i \Psi)(\mathbf{r}) = \frac{\hbar}{i} \frac{\partial}{\partial r_i} \Psi(\mathbf{r}),$$

- Express T_a in terms of the momentum operator $P = \frac{\hbar}{i} \frac{\partial}{\partial x}$.
- Calculate all commutators $[Q_i, Q_j], [P_i, P_j], [Q_i, P_j]$, $i, j = 1, 2, 3$.
- Calculate $[Q, P], [Q, H], [P, H]$ for the Hamiltonian of the harmonic oscillator:

$$H = \frac{1}{2m} P^2 + \frac{m\omega^2}{2} Q^2.$$

3 Dynamics, Time Evolution

Problem 3.1 *Localized Particle*

Consider a free particle that is localized in the range $-a < x < a$ at time $t = 0$:

$$\psi(x, 0) = \begin{cases} A, & \text{if } -a < x < a; \\ 0, & \text{otherwise.} \end{cases}$$

- Normalize the given wave function and calculate its representation in momentum space $\hat{\psi}(k, 0)$.
- Discuss and compare $\psi(x, 0)$ versus $\hat{\psi}(k, 0)$ for the two limiting cases of very small and very large a . Interpret your result in terms of Heisenberg uncertainty principle.
- Derive an expression to calculate the wave function $\psi(x, t)$ for later times t in terms of $\hat{\psi}(k, 0)$.

Problem 3.2 *Time Evolution of Superposition States*

At time $t = 0$ a particle is assumed to be in a superposition of two stationary states ψ_0, ψ_1 with energies E_0, E_1 , respectively:

$$\psi(x, 0) = c_0\psi_0(x) + c_1\psi_1(x).$$

- What is the wave function $\psi(x, t)$ at later times? Calculate the probability density $|\psi(x, t)|^2$. For simplicity assume that the coefficients c_0, c_1 as well as the wave functions ψ_0, ψ_1 are real.
- What is the consequence of the interference between ψ_0 and ψ_1 ? Describe the motion of $|\psi(x, t)|^2$. Compare this to the case $c_1 = 0$.
- Evaluate $|\psi(x, t)|^2$ for the case of ψ_0, ψ_1 being the ground and first excited state of a particle confined in an infinitely deep square well potential of width L and $c_0 = c_1 = 1/\sqrt{2}$.

Problem 3.3 *Evolution of Gaussian Wave Package*

Consider a free particle described by a Gaussian wave package at time $t = 0$:

$$\psi(x, 0) = \frac{1}{(2\pi a^2)^{1/4}} e^{-\frac{x^2}{4a^2}}.$$

- Find $\psi(x, t)$ for later times t .
- Calculate the probability density and sketch $|\psi|^2$ for $t = 0$. How does it evolve? How does it look like for very large times?

Problem 3.4 *Time Evolution, Conserved Observables*

Consider an arbitrary time-dependent normalized wave function:

$$\Psi(t) : \begin{cases} \mathbb{R}^3 \rightarrow \mathbb{C}, \\ \mathbf{r} \mapsto \Psi(\mathbf{r}, t), \end{cases}$$

$$\int d^3r |\Psi(\mathbf{r}, t)|^2 = 1, \quad \forall t.$$

Let A be a *time-independent* linear operator (e.g. an operator corresponding to a physical observable) with $[A, H] = 0$.

- Verify $[A^n, H] = 0$.
- Calculate $\frac{d}{dt}\langle A^n \rangle(t)$, where $\langle A^n \rangle(t)$ is the expectation value of the operator A^n in the state $\Psi(t)$.

Problem 3.5 *Ehrenfest Theorem and Quantum-Classical Correspondence*

- Show that $[Q, F(P)] = i\hbar\frac{\partial F}{\partial P}$ and $[P, G(Q)] = -i\hbar\frac{\partial G}{\partial Q}$ for any differentiable functions $F(P)$ and $G(Q)$.

b) Derive the Ehrenfest theorem,

$$m \frac{d^2}{dt^2} \langle Q \rangle = \frac{d}{dt} \langle P \rangle = -\langle \nabla V(Q) \rangle \quad (3.1)$$

for any $H = \frac{1}{2m} P^2 + V(Q)$. Interpret it and relate it to Newton's second law.

c) The Poisson brackets for classical quantities $f(p, q)$ and $g(p, q)$ are defined as

$$\{f, g\} = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q}.$$

Show that

$$\frac{d}{dt} f(p, q) = \{f, H(p, q)\}, \quad (3.2)$$

where $H(p, q)$ is the Hamiltonian of the classical system. What is the condition for $f(p, q)$ to be a constant of motion?

d) Show that $\frac{1}{i\hbar} [Q^2, P^2]$ corresponds to $\{q^2, p^2\}$.

Problem 3.6 Virial Theorem

a) Prove that for any two differentiable functions of operators F and G (which are operators, too) and linear operators A and B which satisfy conditions: (i) $[A, [A, B]] = 0$, (ii) $[B, [B, A]] = 0$ and (iii) $[[A, B], B^n] = 0 \forall n \in \mathbb{N}$ the following relation is valid:

$$[F(A, B), G(A, B)] = \frac{\partial F}{\partial A} \frac{\partial G}{\partial B} [A, B] + \frac{\partial F}{\partial B} \frac{\partial G}{\partial A} [B, A],$$

which is generalisation of the Problem 2.2 d).

b) Using a), show that the time derivative of function $F(\mathbf{p}, \mathbf{r})$, where \mathbf{p} and \mathbf{r} are momentum and position operators, respectively, is given by commutator with Hamiltonian:

$$\frac{dF(\mathbf{p}, \mathbf{r})}{dt} = \frac{1}{i\hbar} [F(\mathbf{p}, \mathbf{r}), H]$$

which is a quantum analogue to classical relation $df/dt = \{f, H\}$.

c) Prove the *virial theorem* that formulates a general relation between the mean value of the kinetic energy and the potential $V(\mathbf{r})$:

$$2\langle E_{\text{kin}} \rangle = \langle \mathbf{r} \cdot \nabla V(\mathbf{r}) \rangle$$

and has the same form in classical and quantum physics.

d) Show that for a spherically symmetric potential $V(\mathbf{r}) = Cr^\alpha$ the mean kinetic energy is directly given by mean potential energy:

$$2\langle E_{\text{kin}} \rangle = \alpha \langle V(\mathbf{r}) \rangle.$$

Problem 3.7 *Parity Operator and Quantum Zeno Effect*

A quantum system is described by two energy eigenstates $|1\rangle$ and $|2\rangle$ with the corresponding energies E_1 and E_2 . Consider the parity operator \mathcal{P} , which is acting on the eigenstates in the following:

$$\mathcal{P}|1\rangle = |2\rangle, \quad \mathcal{P}|2\rangle = |1\rangle.$$

- Find the eigenstates of the parity operator and calculate the time evolution for the case of being initially in the positive parity eigenstate $|+\rangle$.
- At time t a parity measurement is made on the system. What is the probability to measure positive parity?
- Imagine you make a series of parity measurements at the times $\Delta t, 2\Delta t, \dots, N\Delta t = T$, where $\Delta t \ll \frac{1}{\omega}$ and $\omega = \frac{E_2 - E_1}{2\hbar}$. What is the probability that the *initially prepared* positive parity state survives at time T within that series of measurements? Investigate then the case of $N \gg 1$ and finally the limit $N \rightarrow \infty$ at constant T .

Problem 3.8 *1D Quantum Well — Time Evolution*

A particle (mass m) is confined in the infinite quantum well of the length L :

$$V(x) = \begin{cases} 0, & 0 < x < L, \\ \infty, & \text{else.} \end{cases}$$

The wave function at the time $t = 0$ reads

$$\Psi(x, 0) = \begin{cases} 2b\frac{x}{L}, & 0 < x \leq \frac{L}{2}, \\ 2b\left(1 - \frac{x}{L}\right), & \frac{L}{2} < x < L. \end{cases}$$

- Normalize the wavefunction (calculate b). Plot the probability density $|\Psi(x, 0)|^2$
- Using Schrödinger equation, calculate the wavefunction $\Psi(x, t)$ at later times $t > 0$. Hint: Expand $\Psi(x, 0)$ in the eigenbasis of the infinite quantum well. Use the orthonormality of the eigenstates φ_n :

$$\langle u_n | u_l \rangle = \int_0^L dx \langle u_n | x \rangle \langle x | u_l \rangle = \int_0^L dx u_n^*(x) u_l(x) = \delta_{n,l}.$$

- Calculate the time-dependent expectation value of the energy, i.e. $\langle H \rangle(t)$, in the state $\Psi(t)$. You can use without proof

$$\sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} = \frac{\pi^2}{8}.$$

Problem 3.9 *Harmonic Oscillator — Galilei Invariance*

Consider a particle in a quadratic potential that moves along the x-axis at constant speed:

$$H = \frac{1}{2m}P^2 + \frac{k}{2}(Q - vt)^2.$$

- a) Transform into the reference frame moving with the potential by introducing the new variables $\tilde{x} = x - vt$ and $\tilde{t} = t$. Show that the Schrödinger equation can be rewritten as

$$i\hbar\left(\frac{\partial}{\partial\tilde{t}} - v\frac{\partial}{\partial\tilde{x}}\right)\tilde{\Psi}(\tilde{x},\tilde{t}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\tilde{x}^2}\tilde{\Psi}(\tilde{x},\tilde{t}) + \frac{k}{2}\tilde{x}^2\tilde{\Psi}(\tilde{x},\tilde{t}). \quad (3.10)$$

- b) Eliminate the term $\frac{\partial}{\partial\tilde{x}}$ on the left hand side of (3.10) by introducing $\Psi(\tilde{x},\tilde{t}) = e^{-i\alpha(\tilde{x},\tilde{t})}\tilde{\Psi}(\tilde{x},\tilde{t})$. What are the solutions of the Schrödinger equation in the comoving frame and in the laboratory frame?
- c) Generalize the result of b): Assume you know the energy eigenstates $\Psi_n(x)$ for a given Hamiltonian $H = P^2/2m + V(Q)$. Prove that

$$\Phi(x, t) = e^{-i(E + \frac{mv^2}{2})t/\hbar} e^{imvx/\hbar} \Psi(x - vt) \quad (3.11)$$

is a solution of the Schrödinger equation for a particle subject to a moving potential $V(Q - vt)$.

Problem 3.10 Möbbauer Effect

We want to calculate the quantum-mechanical effects of a momentum transfer δp (e.g. from emission, absorption, scattering, etc.) on a bound system. Consider a nucleus bound via the potential $V(Q)$. Before the absorption the nucleus is in the initial state $|\Psi_{\text{in}}\rangle$, which is an (arbitrary) eigenstate of the Hamiltonian. Now the nucleus absorbs a photon with the wavenumber δk (i.e. momentum $\delta p = \hbar\delta k$). The new state $|\Psi_{\text{new}}\rangle$ of the nucleus can be expressed as

$$|\Psi_{\text{new}}\rangle = N \exp\left(i\frac{\delta p}{\hbar}Q\right)|\Psi_{\text{in}}\rangle,$$

where Q is the position operator and N a normalization constant.

- a) Calculate the normalization constant N .
- b) Convince yourself that $|\Psi_{\text{new}}\rangle$ is an appropriate state to describe the momentum transfer: Calculate the change of the expectation value of P and verify

$$\delta p = \langle\Psi_{\text{new}}|P|\Psi_{\text{new}}\rangle - \langle\Psi_{\text{in}}|P|\Psi_{\text{in}}\rangle.$$

Hint: The action of Q in momentum space is $Q\tilde{\Psi}(k) = i\partial_k\tilde{\Psi}(k)$. Recall the shift operator T_a in coordinate space. What is its analogue in momentum space?

- c) Calculate the change of the expectation value of the energy δE and compare it with the classical expectation.

$$\delta E := \langle\Psi_{\text{new}}|H|\Psi_{\text{new}}\rangle - \langle\Psi_{\text{in}}|H|\Psi_{\text{in}}\rangle.$$

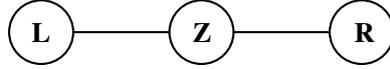
- d) Up to here we considered arbitrary potentials $V(Q)$. Now we specialize to the case of the harmonic oscillator: $V(Q) = m\omega^2 Q^2/2$. This can be regarded as a model for a nucleus bound on a lattice site of a crystal. The initial state $|\Psi_{\text{in}}\rangle$ is the ground state of the harmonic oscillator, i.e. $|\Psi_{\text{in}}\rangle = |0\rangle$. Calculate the probability $P_n := |\langle n|\Psi_{\text{new}}\rangle|^2$ for the nucleus to be in the n -th eigenstate of the harmonic oscillator after the absorption. Hint: You can use without proof the Baker-Campbell-Hausdorff identity:

$$[A, [A, B]] = [B, [A, B]] = 0 \Rightarrow \exp(A + B) = \exp(A)\exp(B)\exp\left(-\frac{1}{2}[A, B]\right).$$

What is the probability to stay in the ground state? What does it look like for small δp ?

Problem 3.11 *Linear Molecule*

Consider an electron in a linear molecule consisting of three atoms, where the central atom Z is located between the left and the right atoms L and R like in figure below.



$|L\rangle$, $|Z\rangle$ and $|R\rangle$ denote three orthonormal vectors that correspond to the electron localized at the atoms L , Z and R respectively and span a three-dimensional Hilbert space. With respect to the basis $\{|L\rangle, |Z\rangle, |R\rangle\}$ the Hamiltonian of the electron has the matrix form

$$H = \begin{pmatrix} b & -a & 0 \\ -a & b & -a \\ 0 & -a & b \end{pmatrix}, \quad a > 0.$$

a) Verify that the three states $|0\rangle$, $|\pm\rangle$,

$$|0\rangle := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|L\rangle - |R\rangle),$$

$$|\pm\rangle := \frac{1}{2} \begin{pmatrix} 1 \\ \mp\sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2} (|L\rangle \mp \sqrt{2}|Z\rangle + |R\rangle),$$

are eigenstates of H and calculate the corresponding eigenenergies.

b) Let the electron be in the state $|-\rangle$. Calculate the probability $P_\alpha := |\langle\alpha|-\rangle|^2$ to find the electron in the state $|\alpha\rangle$ for every $\alpha \in \{L, Z, R\}$.

c) Calculate the expectation value $\langle H \rangle$ and the variance $\langle H^2 \rangle - \langle H \rangle^2$ of the Hamiltonian in the state $|L\rangle$.

d) At $t = 0$ the electron is localized at the atom Z , i.e. it is in the state $|\Psi(0)\rangle = |Z\rangle$. Calculate the time evolution $|\Psi(t)\rangle$ and the probability $P(t) := |\langle Z|\Psi(t)\rangle|^2$ to find the electron in the state $|Z\rangle$ for $t \neq 0$.

4 Barriers, Traps and Potentials

Problem 4.1 *Quantum Scattering and Resonances*

Given the potential barrier

$$V(x) = \begin{cases} 0 & \text{for } |x| < \frac{L}{2}, \\ V_0 & \text{otherwise} \end{cases}$$

consider the unbound solutions with $E > V_0$ (*scattering states*). The most general ansatz to solve the stationary Schrödinger equation is

$$\psi(x) = \begin{cases} \alpha_+ e^{ik_0 x} + \alpha_- e^{-ik_0 x} & \text{for } x < -\frac{L}{2}, \\ \beta_+ e^{ikx} + \beta_- e^{-ikx} & \text{for } -\frac{L}{2} \leq x \leq \frac{L}{2}, \\ \gamma_+ e^{ik_0 x} + \gamma_- e^{-ik_0 x} & \text{for } x > \frac{L}{2}. \end{cases}$$

- a) Relate the wave numbers in each region to the energy E .
 b) Formulate the continuity conditions for the above mentioned most general case and write them as a matrix equations

$$\begin{pmatrix} \alpha_+ \\ \alpha_- \end{pmatrix} = \mathcal{M}\left(k_0, k, -\frac{L}{2}\right) \begin{pmatrix} \beta_+ \\ \beta_- \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \beta_+ \\ \beta_- \end{pmatrix} = \mathcal{M}\left(k, k_0, \frac{L}{2}\right) \begin{pmatrix} \gamma_+ \\ \gamma_- \end{pmatrix}$$

where $\mathcal{M}(k_0, k, -\frac{L}{2}) \in \mathbb{K}_{2 \times 2}$ and $\mathcal{M}(k, k_0, \frac{L}{2}) \in \mathbb{K}_{2 \times 2}$ are to be determined.

- c) Express only the coefficients of $|x| > \frac{L}{2}$ by each other, introduce new variables

$$\varepsilon_+ = \frac{k}{k_0} + \frac{k_0}{k} \quad \text{and} \quad \varepsilon_- = \frac{k}{k_0} - \frac{k_0}{k}$$

and adapt the conditions $\gamma_- = 0$, $\gamma_+ = S$ and $\alpha_+ = 1$, which describe the physical situation of an incoming quantum particle from $x = -\infty$ which is scattered at the potential. Determine S as a function of $k, k_0, \varepsilon_-, \varepsilon_+$ and L .

- d) Calculate the currents for the incident, reflected and transmitted wave: j_I, j_R, j_T .
 e) Determine explicitly the transmission coefficient T . Find out the energies, for which transmission is optimized. What is different between quantum and classical scattering in this scenario?

Problem 4.2 Potential Barrier — Quantum Tunnelling

Consider again the one-dimensional motion of a particle that is incident on a potential barrier, $V_0 > 0$,

$$V(x) = \begin{cases} V_0 & \text{for } 0 \leq x \leq d \\ 0 & \text{else} \end{cases}$$

- a) Discuss the limit of thin and high barriers $V_0 \rightarrow \infty, d \rightarrow 0$ such that the area $V_0 d := \hbar^2/2m\ell$ under the potential remains finite. Thus the potential barrier degenerates to

$$V(x) = \frac{\hbar^2}{2m\ell} \delta(x)$$

where $\delta(\cdot)$ denotes the Dirac δ -distribution. The wavefunction remains continuous at $x = 0$ in this limit. Yet in the same limit, the derivatives exhibit a jump,

$$\lim_{x \downarrow 0} \psi'(x) - \lim_{x \uparrow 0} \psi'(x) = \frac{1}{\ell} \psi(0)$$

Show that the conditions can be obtained by inspecting the Schrödinger equation upon integrating over a small interval containing the singularity. Discuss the transmission coefficient for the δ -potential.

Problem 4.3 Double Step Potential

A particle is incident from the left on the double potential step

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } 0 \leq x \leq d \\ V_1 & \text{for } x > d \end{cases}$$

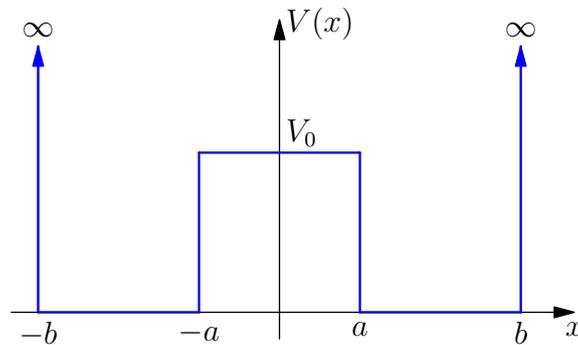
with $0 < V_0 < V_1 < E$, where E denotes the energy of the particle. Calculate the reflection and transmission amplitude. For what value of V_0 and width d does the reflection vanish?

Problem 4.4 *Double Well Oscillations*

A particle of mass m and energy $E < V_0$ moves in a one-dimensional potential box

$$V(x) = \begin{cases} \infty & \text{for } |x| > b, \\ V_0 & \text{for } |x| < a, \\ 0 & \text{for } a < |x| < b. \end{cases}$$

as shown in the figure below:



- Solve the Schrödinger eq. and find the eigenvalues and an algebraic equation for eigen energies of the system.
- How does the potential define the number of states with $E < V_0$?
- From the symmetry it is clear that system has well defined parity. Is the ground state odd or even? Construct and sketch the wave functions of the first two states and their superposition.
- Calculate the time evolution for the case of being initially in the right well. There is some probability to penetrate through the finite barrier. Can we ever be sure that we'll find the particle in the left well? If no, why? If yes, what time do we have to wait to have particle on the left?

Problem 4.5 *Attractive δ -potential – Scattering and Bound States*

Consider the one-dimensional stationary Schrödinger equation with the attractive delta potential

$$V(x) = -\frac{\hbar^2}{2m\ell} \delta(x),$$

where m denotes the mass of the particle and $\ell > 0$.

- Consider the scattering problem: A particle with energy $E > 0$ is incident from the left on the potential. Use the ansatz

$$\psi(x) = \begin{cases} e^{ikx} + r e^{-ikx} & \text{for } x < 0, \\ t e^{ikx} & \text{for } x > 0, \end{cases}$$

and determine the wave number k , the coefficients r , t and the transmission amplitude $T = |t|^2$. Compare the results with those for the repulsive delta peak.

- Solve the stationary Schrödinger equation for possible bound (localized) states, i.e. states with energy $E < 0$.

Problem 4.6 *Double δ -function Potential*

Consider the double delta-function potential

$$V(x) = -\alpha(\delta(x+a) + \delta(x-a)),$$

where α and a are positive constants.

- a) Sketch this potential.
- b) How many bound states does it possess? Find the allowed energies for $\alpha = \hbar^2/ma$ and for $\alpha = \hbar^2/4ma$ and sketch the wave functions.

Problem 4.7 *Floquet's Theorem*

Solve the Schrödinger equation and find the allowed energies for a potential of the form

$$V(x) = \frac{\hbar^2}{m} \Omega \sum_{n=-\infty}^{+\infty} \delta(x+na).$$

Hint: First we have to prove the validity of the Floquet's theorem, which says that if the potential is periodic ($V(x+a) = V(x)$), then $\psi(x+a) = e^{ika}\psi(x)$.

Problem 4.8 *Periodic δ -comb — Energy Bands*

Calculate possible eigenenergies of the one-dimensional Hamiltonian with the external potential V corresponding to a periodic delta-comb:

$$V(x) = -\frac{\hbar^2}{2m\ell} \sum_{n=-\infty}^{\infty} \delta(x-na)$$

Note: This problem can be interpreted as a simple model for a one-dimensional crystal with ions fixed on positions na , $n \in \mathbb{Z}$, and the single-ion potential $-\frac{\hbar^2}{2m\ell}\delta(x)$.

Let Ψ be a solution of the corresponding Schrödinger equation. By symmetry one argues that the electron density is periodic: $|\Psi(x)|^2 = |\Psi(x+a)|^2$, meaning that the wavefunction itself is only allowed to accumulate an arbitrary phase (Bloch theorem):

$$\Psi(x+na) = e^{inKa}\Psi(x), \quad Ka \in [-\pi, \pi) \text{ arbitrary}, \quad n \in \mathbb{Z}. \quad (4.10)$$

Consider a plane-wave ansatz for $x \in (0, a)$:

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}, \quad x \in (0, a).$$

- a) Continue this ansatz to all regions $((n-1)a, na)$, $n \in \mathbb{Z}$, such that the Bloch condition (4.10) is fulfilled. You should obtain

$$\begin{aligned} \Psi(x) &= e^{i(n-1)Ka} u[x - (n-1)a], \quad \text{for } x \in ((n-1)a, na), \quad n \in \mathbb{Z}, \\ u(x) &= Ae^{ikx} + Be^{-ikx}. \end{aligned}$$

- b) Write down the matching conditions for Ψ at $x = a$. What do the matching conditions at other points $x = na$ look like? Rewrite the matching conditions in the form

$$M \begin{pmatrix} A \\ B \end{pmatrix} = 0,$$

with a 2×2 matrix M .

- c) Derive the condition for the matrix M in order for this linear equation to have nontrivial solutions $(A, B) \neq (0, 0)$. Check:

$$\cos(Ka) = \cos(ka) - \frac{a}{2\ell} \frac{\sin(ka)}{ka}. \quad (4.11)$$

- d) Here we consider only solutions with positive energies, i.e. $k \in \mathbb{R}$. Convince yourself — graphically — that Eq. (4.11) allows only for energies E (or wavevectors k) from certain intervals — these intervals are known as the energy bands of the crystal.
- e) What are the allowed energies for $a/\ell \rightarrow \infty$ and $a/\ell \rightarrow 0$? At constant a/ℓ , how does the width of the energy bands behave for increasing ak ?

Problem 4.9 Bloch Bands

A simple model for a one-dimensional crystal with ions fixed on positions na , $n \in \mathbb{Z}$, is the comb of the single-ion potentials $\frac{\hbar^2\Omega}{m}\delta(x)$:

$$V(x) = \frac{\hbar^2\Omega}{m} \sum_{n=-\infty}^{\infty} \delta(x + na).$$

Using *Bloch's theorem*

$$\Psi(x + na) = e^{inKa} \Psi(x), \quad Ka \in [-\pi, \pi) \text{ arbitrary, } n \in \mathbb{Z},$$

and plane-wave ansatz we have obtained in Problem 4.7 the condition (4.9) for energies:

$$\cos(Ka) = \cos(ka) + a\Omega \frac{\sin(ka)}{ka}. \quad (4.15)$$

- a) Show (graphically) that (4.15) allows only for energies E (or wave vectors k) from certain intervals. These intervals are known as the *energy bands* of the crystal.
- b) Plot the energy as a function of Ka . How does the width of the energy bands behave for increasing k ?
- c) What are the allowed energies for $a\Omega \rightarrow \infty$ and $a\Omega \rightarrow 0$?

Problem 4.10 Separation of Variables in Axial Symmetry

Make a separation of variables for the Schrödinger equation in a potential that depends only on the distance from the z -axis.

Problem 4.11 Particle Between Two Parallel Cylinders

The particle of mass m is in the space between two infinitely long concentric cylinders with radii $r = a$ and $r = b$. The edge of every cylinder is an infinitely repulsive potential for the particle. Determine the energy and wave function of the particle in the ground, $n_p = 0$ state.

Problem 4.12 *Finite Spherical Potential Well*

A particle is in a spherical finite potential well of the form

$$V(r) = \begin{cases} -V_0, & r < a; \\ 0, & r \geq a. \end{cases}$$

Find the bound energy states for $l = 0$ and $l = 1$.

Problem 4.13 *Spherical Shell*

A particle of mass m moves in the space bounded by two concentric spheres with radii $r_< = a$ and $r_> = b$. The sides of the spheres represent an infinite repelling potential for the particle. Calculate the energy and the wave function in the ground state ($l = 0$).

Problem 4.14 *Landau levels*

For a particle of mass m and charge Q in a magnetic field \mathbf{B} , the Hamiltonian proves, from relativistic reasons, to be

$$H = \frac{1}{2m} (\mathbf{p} - Q\mathbf{A})^2$$

where \mathbf{A} is the magnetic vector potential. For a particular case, let $\mathbf{B} = B\hat{z}$, and choose $\mathbf{A} = \frac{1}{2}B(-y, x, 0)^T$.

a) Express H in terms of p_z and the dimensionless operators

$$\pi_x \equiv \frac{p_x + \frac{1}{2}m\omega y}{\sqrt{m\omega\hbar}}; \quad \pi_y \equiv \frac{p_y - \frac{1}{2}m\omega x}{\sqrt{m\omega\hbar}}$$

where $\omega = QB/m$ is the *Larmor frequency*. Show that H can be seen as the sum of that of a free particle in one dimension and of that of a harmonic oscillator. Find the ladder operators corresponding to the harmonic oscillator part of the Hamiltonian, and also the corresponding energy levels (called **Landau levels**).

b) To find the wavefunction of a given Landau level, write down the ground state's defining equation, $A|0\rangle = 0$ (where A is the lowering ladder operator), in the position representation. Solve it to find $\langle \mathbf{x}|0\rangle$ and subsequently $\langle \mathbf{x}|n\rangle$.

c) In classical physics, a particle is not affected by an electromagnetic field that is restricted to a region where the particle does not pass through. This is not so in quantum mechanics.

Consider an infinitely long and infinitely thin solenoid placed along the z -axis. There is a strong magnetic field \mathbf{B} inside the solenoid, and, due to its infinite length, none outside it. Suppose a screen is placed along the plane $y = 0$, with two slits along the lines $x = \pm s$. The screen is bombarded from the side $y < 0$ with particles that have well-defined momenta $\mathbf{p} = p\hat{y}$, and their arrival is detected on a screen P placed along the plane $y = L$. Show that the particles, which never enter the region of non-zero \mathbf{B} , are still affected by \mathbf{B} .

Problem 4.15 *Decomposition of Arbitrary Potential and α -decay*

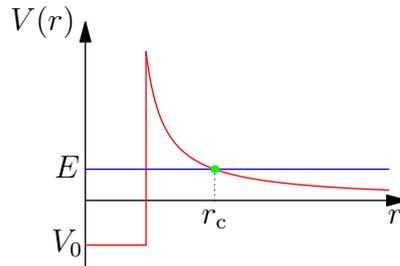
In the Problem 4.1 the transmission probability for a quantum particle at a finite potential barrier V_0 of thickness L was determined.

- Use the result and derive the transmission coefficient for the case $E < V_0$, which is the tunnel effect through a constant barrier. Express all terms in favor of E and V_0 .
- Find a convenient approximation for the case of a high and thick potential barrier, which means $\kappa L \gg 1$. As a result one gets

$$T \approx \frac{16E(V_0 - E)}{V_0^2} \exp\left(-\frac{2}{\hbar}\sqrt{2m(V_0 - E)L}\right).$$

In the limit of high potentials the tunnel probability is dominated by the exponential. Therefore the prefactor is neglected in the following.

- To describe the transmission through a continuously varying potential, decompose the potential within the classical forbidden area into N rectangular barrier segments of length Δx of the above described barrier type. Determine the transmission probability for each segment i and then for the whole approximated potential. Assume as a further approximation that no inner reflections occur. Finally apply the limit $\Delta x \rightarrow 0$. Within this procedure, determine the *Gamow factor* G , defined as $T \approx \exp(-G)$.
- One of the most prominent applications of this formula is the α -decay. Consider a formed α -particle $E > 0$ moving within the center of a nucleus. Inside the alpha-particle feels a constant negative potential coming from the nuclear interaction with the other nucleons. Beyond the average radius R of the nucleus the Coulomb potential $V_C(r) = \frac{\gamma}{r}$ forms a finite potential barrier, which is classically impenetrable.



Here $\gamma = 2Ze^2/4\pi\epsilon_0$ and Z is the number of protons in the nucleus. Determine the classical forbidden interval $[R, r_c]$. Calculate the Gamow-factor and expand it in lowest order for R/r_c . Use the integral

$$\int_R^{r_c} dr \sqrt{\frac{1}{r} - \frac{1}{r_c}} = \sqrt{r_c} \left(\frac{\pi}{2} - \arcsin \sqrt{\frac{R}{r_c}} - \sqrt{\frac{R}{r_c}} \left(1 - \frac{R}{r_c}\right) \right).$$

Introduce *fine-structure constant* $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$ and the common nuclear radius estimate $R \approx r_0 A^{\frac{1}{3}}$ (with $r_0 = 1.2$ fm and A being mass number). Express G in terms of Z , E , A and α .

- The average life time of the state can be approximated with $\tau \approx \frac{t_{\text{nuc}}}{T}$, where $t_{\text{nuc}} = \frac{2R}{v}$ is the time to move through the nucleus. Derive the so called *Geiger-Nutall rule*

$$\ln \tau \approx c_0 + c_1 \frac{Z}{\sqrt{E}} + c_2 \sqrt{ZA^{\frac{1}{3}}}$$

The explanation of the α -decay and the qualitative correct predictions of the average life times could be seen as a big success of quantum mechanics.

Problem 4.16 *Thomas–Reiche–Kuhn Sum Rules*

Prove the so-called *Thomas–Reiche–Kuhn sum rules* for particle of mass m moving in a potential V :

$$\sum_j |x_{ij}|^2 (E_j - E_i) = \frac{\hbar^2}{2m} \quad \text{and} \quad \sum_j |p_{ij}|^2 (E_j - E_i) = \frac{\hbar^2}{2} \left\langle \frac{\partial^2 V}{\partial x^2} \right\rangle,$$

where E_i is the energy of state $|i\rangle$, $x_{ij} \equiv \langle i|x|j\rangle$ and $p_{ij} \equiv \langle i|p|j\rangle$.

4.1 Harmonic Oscillator**Problem 4.17** *Harmonic Oscillator — Virial Theorem, Ground State, Uncertainty*

- a) Prove the quantum analogue of the virial theorem for a system with Hamiltonian $H = \frac{1}{2m}P^2 + V(Q)$

$$\frac{d}{dt} \langle QP \rangle = \frac{1}{m} \langle P^2 \rangle - \langle Q \nabla V(Q) \rangle. \quad (4.26)$$

- b) Now consider the special case of a harmonic oscillator, $H = \frac{1}{2m}P^2 + \frac{k}{2}Q^2$. What does the virial theorem state? Show that, if the system is in an energy eigenstate ($\langle a^\dagger a \rangle = n$),

$$\frac{1}{2m} \langle P^2 \rangle = \frac{k}{2} \langle Q^2 \rangle = \frac{1}{2} \langle H \rangle = \frac{\hbar\omega}{2} \left(n + \frac{1}{2} \right), \quad (4.27)$$

where $\omega = \sqrt{k/m}$.

- c) Using the previous results, calculate the position-momentum uncertainty of a harmonic oscillator in the n th energy eigenstate.

Problem 4.18 *Harmonic Potential*

A particle is in the potential of a harmonic oscillator. For the first three eigenstates of the Hamiltonian calculate the probability that the particle is in the classically forbidden region.

Problem 4.19 *Harmonic Oscillator — Coherent States*

The coherent state of the harmonic oscillator can be defined as the eigenstate of the annihilation operator $a\varphi_\alpha(\xi) = \alpha\varphi_\alpha(\xi)$. The operator $a = \frac{1}{\sqrt{2}}(\xi + \frac{d}{d\xi})$ is rescaled with respect to the oscillator length $x_0 = \sqrt{\frac{\hbar}{\omega m}}$ with $\xi = \frac{x}{x_0}$. The eigenvalue α of the annihilation operator a is complex, so $\alpha = \Re\{\alpha\} + i\Im\{\alpha\} = |\alpha| \exp(i\delta)$.

- In opposite to the algebraic solution shown in the lecture directly determine $\varphi_\alpha(x) \equiv \varphi_\alpha(\frac{x}{x_0})$ via solving the differential equation.
- Determine the dynamics $\varphi_\alpha(x, t)$ by assuming $\alpha \rightarrow \alpha(t)$ and a time dependent prefactor $N \rightarrow N(t)$ concerning the above derived solution. Insert the ansatz into the time dependent Schrödinger equation and evaluate $N(t)$ and $\alpha(t)$.
- Normalize the wavefunction for $t = 0$ and calculate then $|\varphi_\alpha(x, t)|^2$. Which shape does it have?
- Calculate the expectation values $\langle Q \rangle_t, \langle P \rangle_t, \langle Q^2 \rangle_t, \langle P^2 \rangle_t$.
- Evaluate the product of the standard deviations $\sigma_Q \sigma_P$. Compare it to Heisenberg's uncertainty relation $\sigma_Q \sigma_P \geq \hbar/2$.

Problem 4.20 *Harmonic Oscillator — Energy Spectrum*

We want to obtain all possible energies E_n and wavefunctions Ψ_n which obey

$$H\Psi_n = E_n\Psi_n, \text{ where}$$

$$H = \frac{1}{2m}P^2 + \frac{m\omega^2}{2}Q^2.$$

First we define the operators a^\dagger, a and express the momentum and coordinate in terms of a, a^\dagger :

$$a^\dagger := \sqrt{\frac{\omega m}{2\hbar}}Q - i\sqrt{\frac{1}{2m\omega\hbar}}P, \quad a := \sqrt{\frac{\omega m}{2\hbar}}Q + i\sqrt{\frac{1}{2m\omega\hbar}}P,$$

$$\Rightarrow Q = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \quad P = i\sqrt{\frac{\hbar\omega m}{2}}(a^\dagger - a).$$

- a) Verify $[a, a^\dagger] = 1$ (this means $aa^\dagger = 1 + a^\dagger a$).
 b) Use the expression of Q, P in terms of a^\dagger, a to verify

$$H = \frac{\hbar\omega}{2}(aa^\dagger + a^\dagger a) = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right).$$

- c) Using a) and b), verify $Ha^\dagger = a^\dagger(H + \hbar\omega)$.
 d) Now assume that Ψ is a solution of the stationary Schrödinger equation with the energy E , i.e. $H\Psi = E\Psi$. Use c) to show that $a^\dagger\Psi$ is solution with the energy $E' = E + \hbar\omega$.
 e) Show that the Gaussian

$$\Psi_0(x) = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{1}{4}} \exp\left(-\frac{1}{4}\frac{x^2}{\sigma^2}\right)$$

is a solution and calculate σ and the corresponding energy. Why is it the ground state?

- f) Starting with the ground state Ψ_0 one can now obtain all Ψ_n using d): $\Psi_n = \frac{1}{\sqrt{n!}}(a^\dagger)^n \Psi_0$. Calculate Ψ_1 . (Note: since $E_0 = \frac{1}{2}\hbar\omega$, one gets with d) $E_n = \hbar\omega(n + 1/2)$. This is the energy spectrum of the quantum mechanical harmonic oscillator!)

Problem 4.21 *Eigenstates of Harmonic Oscillator — Analytic vs. Algebraic Approach*

Recall the eigenfunctions of the harmonic oscillator in terms of Hermite polynomials $H_n(z)$ that have been found by an analytic analysis of the stationary Schrödinger Equation

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi} x_0}} H_n\left(\frac{x}{x_0}\right) \exp\left(-\frac{x^2}{2x_0^2}\right).$$

Using the so called creation and annihilation operator,

$$a^\dagger := \sqrt{\frac{\omega m}{2\hbar}}Q - i\sqrt{\frac{1}{2m\omega\hbar}}P, \quad a := \sqrt{\frac{\omega m}{2\hbar}}Q + i\sqrt{\frac{1}{2m\omega\hbar}}P,$$

($\Rightarrow Q = \sqrt{\hbar/2m\omega}(a + a^\dagger)$ and $P = i\sqrt{\hbar\omega m/2}(a^\dagger - a)$), the Hamiltonian can be expressed as $H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$. We define the number operator $N = a^\dagger a$ and denote the eigenkets and eigenvalues of N according to $N|n\rangle = n|n\rangle$.

- a) Show $[a, a^\dagger] = 1$ and use the expression of Q and P in terms of a^\dagger and a to verify $H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right)$.
- b) Calculate $H|n\rangle = E_n|n\rangle$ and compare E_n to the result from the analytic calculation.
- c) Determine the commutators $[N, a]$, $[N, a^\dagger]$ and use this to find $Na^\dagger|n\rangle$, $Na|n\rangle$. Argue that $a|n\rangle = c|n-1\rangle$ where c is a multiplicative constant. Use the norm of $|n\rangle$ and $|n-1\rangle$ to show

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

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

Argue that n must be a nonnegative integer and comment on the names of a^\dagger and a . Starting from $|0\rangle$, how do you determine $|n\rangle$ with this algebraic approach?

- d) Use the representation of a in terms of position and momentum operator Q, P to express $\langle x|a|0\rangle$ in terms of $\langle x|0\rangle$. *Note:* $\langle x|Q\varphi\rangle = x\langle x|\varphi\rangle$ and $\langle x|P\varphi\rangle = -i\hbar\partial_x\langle x|\varphi\rangle$. Show that $a|0\rangle = 0$ leads to a differential equation that determines $\langle x|0\rangle$. Compare the solution to the ground state wave function $\psi_0(x)$.
- e) Use the recursion formula for Hermite polynomials $H_{n+1}(z) = 2zH_n(z) - H'_n(z)$ and $\langle x|1\rangle = \langle x|a^\dagger|0\rangle$, $\langle x|2\rangle = \langle x|(a^\dagger)^2|0\rangle/\sqrt{2}$, etc., to verify $\psi_n(x) = \langle x|n\rangle$.

Problem 4.22 Harmonic Oscillator — Heisenberg Representation

In the Heisenberg representation of quantum mechanics the states are time independent, but the observables have a time dependence which is given through a unitary operator $U(t)$ (Note: $U(0) = 1$). We denote an operator in Schrödinger representation (which is allowed to be explicitly time dependent) as $A_S(t)$. Then, the corresponding time dependent operator in Heisenberg representation $A_H(t)$ reads

$$A_H(t) = U^\dagger(t)A_S(t)U(t).$$

The central equation of motion is the Heisenberg equation:

$$\frac{d}{dt}A_H(t) = \frac{i}{\hbar}[H_H(t), A_H(t)] + \left(\frac{\partial}{\partial t}A_S(t) \right)_H.$$

In this exercise we want to obtain the time dependence of the momentum operator P and the coordinate operator Q in the Heisenberg representation for the harmonic oscillator. Our Hamiltonian in Schrödinger representation is time independent and reads

$$H_S = \frac{1}{2m}P_S^2 + \frac{m\omega^2}{2}Q_S^2.$$

- a) For two operators (in Schrödinger representation) A_S, B_S , show $[A_H, B_H] = [A_S, B_S]_H$
- b) Express Q_S, P_S in terms of a_S, a_S^\dagger and, using the Heisenberg equation, calculate $\frac{d}{dt}a_H(t)$ and $\frac{d}{dt}a_H^\dagger(t)$.
- c) Using the results from c), calculate $a_H(t), a_H^\dagger(t)$ and then, using a), calculate $Q_H(t), P_H(t)$.

Problem 4.23 *Harmonic Oscillator — Symmetry and Matrix Elements*

Let $|n\rangle$, $n \in \mathbb{N}_0$, be the n -th eigenstate of the one dimensional harmonic oscillator. As discussed in the lecture, the energy eigenstates $\Psi_n(x)$ of a quantum mechanical harmonic oscillator are given by

$$\Psi_n(x) = (2^n n!)^{-\frac{1}{2}} \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) H_n\left(\sqrt{m\omega/\hbar}x\right) \quad (4.28)$$

where the Hermite polynomials $H_n(x)$, $n \in \mathbb{N}$ are defined via the generating function

$$\varphi(x, t) = \exp(2xt - t^2) = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x). \quad (4.29)$$

It was also shown that for the creation and annihilation operator,

$$a^\dagger := \sqrt{\frac{\omega m}{2\hbar}} Q - i\sqrt{\frac{1}{2m\omega\hbar}} P, \quad a := \sqrt{\frac{\omega m}{2\hbar}} Q + i\sqrt{\frac{1}{2m\omega\hbar}} P, \quad (4.30)$$

following properties are valid

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \quad (4.31)$$

- Using the symmetry of $\varphi(x, t)$ for $t \rightarrow -t$ find the symmetry of the Hermite polynomials $H_n(x)$ for $x \rightarrow -x$.
- Calculate the matrix elements $\langle m|Q|n\rangle$, $\langle m|P|n\rangle$, $\langle m|Q^2|n\rangle$, $\langle m|P^2|n\rangle$ of the Q and P operators using algebraic properties of the harmonic oscillator. Hint: Express Q , P in terms of a , a^\dagger and use (4.31).
- Using the following recursion relation for the Hermite polynomials:

$$H_{n+1}(x) = 2x H_n(x) - 2n H_{n-1}(x) \quad (4.32)$$

and the coordinate representation of the eigenstates $|n\rangle$ (4.28), calculate the matrix elements $\langle m|Q|n\rangle$ of the position operator.

Note: The algebraic properties of a , a^\dagger and $|n\rangle$ fully correspond to the recursion relations of the Hermite polynomials.

- Now consider a particle of mass m subject to a potential of the form

$$V(x) = \begin{cases} \infty & \text{for } x < 0, \\ \frac{k}{2} x^2 & \text{for } x > 0. \end{cases} \quad (4.33)$$

What are the eigenstates $\Psi_n^>(x)$ and eigenenergies $E_n^>$ of the system?

- What are the expectation values $\langle Q^2 \rangle$, $\langle P^2 \rangle$ and $\langle H \rangle$ for the ground state of the harmonic oscillator and of this system (4.33)?
- Calculate the uncertainty product $\Delta Q \Delta P$ for the ground state of harmonic oscillator and of system (4.33) and check the Heisenberg uncertainty relation.
- Write the Schrödinger equation for an oscillator in the p representation and determine the probability distribution for different values of momentum.

Problem 4.24 *3D Harmonic Oscillator Degeneration*

A three dimensional isotropic harmonic oscillator has the energy eigenvalues $\hbar\omega(n + \frac{3}{2})$, where $n \in \{0, 1, 2, 3, \dots\}$. What is the degree of degeneracy d_n of the quantum state $|n\rangle$?

4.2 Hydrogen Atom

Problem 4.25 *Central Potential*

Assume a central potential of the form

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 c}{2m_e r^2}.$$

Note that the second term is a small correction to the Coulomb potential ($c \ll 1$).

- a) Evaluate the eigenenergies. (Hint: Introduce l' by the relation $l'(l' + 1) = l(l + 1) + c$.)
- b) Show that the additional term in the potential eliminates the (accidental) degeneration of the Coulomb potential with respect to the azimuthal quantum number l . (Hint: You can approximate $l' \approx l + c/(2l + 1)$. Why that?)

Problem 4.26 *Two Body Problem in Quantum Mechanics*

The Hamiltonian for a bound hydrogen-like atom with one electron and a nucleus consisting of a charge Ze reads

$$H = \frac{P_N^2}{2m_N} + \frac{P_e^2}{2m_e} + V(|\mathbf{r}_N - \mathbf{r}_e|),$$

with the Coulomb potential $V(|\mathbf{r}_N - \mathbf{r}_e|) = -\frac{Ze^2}{4\pi\epsilon_0|\mathbf{r}_N - \mathbf{r}_e|}$, where m_e is the electron mass and the nucleus mass $m_N < \infty$.

- a) Express the Schrödinger equation for $\psi(\mathbf{r}_N, \mathbf{r}_e)$ in terms of center of mass coordinates $\mathbf{R} = \frac{1}{M}(m_N\mathbf{r}_N + m_e\mathbf{r}_e)$ and relative coordinates $\mathbf{r} = \mathbf{r}_N - \mathbf{r}_e$. Finally introduce the total mass $M = m_e + m_N$ and the reduced mass $\mu = \frac{m_e m_N}{m_e + m_N}$.
- b) Formulate the Hamilton operator $\hat{H}(\mathbf{P}_R, \mathbf{P}_r, \mathbf{r}_R, \mathbf{r}_r)$ and show that the operator components of the central of mass momenta and coordinates as well as the operator components of the relative momenta and coordinates fulfil the commutator relations

$$[Q_{R,x}, P_{R,x}] = [Q_{r,x}, P_{r,x}] = i\hbar.$$

- c) Apply a separation ansatz (why?) $\hat{\psi}(\mathbf{R}, \mathbf{r}) = \chi(\mathbf{R})\varphi(\mathbf{r})$ and determine the energy E of the whole system by comparing with the Coulomb problem solved in the lectures. Where are the differences?

Problem 4.27 *Expectation Values for the Hydrogen Atom*

We want to prove the following recursion formula for the expectation values $\langle r^s \rangle$ for the eigenstates ψ_{nl} of the hydrogen atom ($s \geq 0$);

$$\frac{s+1}{n^2} \langle r^s \rangle - (2s+1)a_B \langle r^{s-1} \rangle + \frac{s}{4} [(2l+1)^2 - s^2] a_B^2 \langle r^{s-2} \rangle = 0, \quad (4.42)$$

where $a_B = \hbar^2/m_e e^2$. Using dimensionless parameters $\rho = kr$ and $y_{nl}(\rho) = k^{-1/2}u_{nl}(\rho)$ with $k = \sqrt{-2mE}/\hbar$, the Schrödinger equation for the radial part of the wave function $R_{nl}(r) = u_{nl}(r)/r$ can be expressed as

$$\left[\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{2n}{\rho} - 1 \right] y_{nl}(\rho) = 0 \quad (4.43)$$

a) Write down the recursion formula for $\langle r^s \rangle$ in terms of $\langle \rho^s \rangle$.

b) Prove the following identities:

$$1. \int d\rho \rho^s y_{nl}(\rho)^2 = \langle \rho^s \rangle$$

$$2. \int d\rho \rho^s y_{nl}(\rho) y'_{nl}(\rho) = -\frac{s}{2} \langle \rho^{s-1} \rangle$$

$$3. \int d\rho \rho^s y_{nl}(\rho) y''_{nl}(\rho) = -\int d\rho \rho^s y'_{nl}(\rho)^2 + \frac{s(s-1)}{2} \langle \rho^{s-2} \rangle$$

$$4. \int d\rho \rho^s y'_{nl}(\rho) y''_{nl}(\rho) = -\frac{s}{2} \int d\rho \rho^{s-1} y'_{nl}(\rho)^2.$$

(Hint: use integration by parts.)

c) Multiply Eq. (4.43) once with $\rho^s y_{nl}(\rho)$ and another time with $\rho^{s+1} y'_{nl}(\rho)$ and integrate over ρ . From these two expressions prove the recursion formula for $\langle \rho^s \rangle$.

d) The virial theorem states $\langle e^2/r \rangle = -2E_n$. Use this and (4.42) to calculate $\langle r \rangle$ and $\langle r^2 \rangle$.

5 Symmetries

Problem 5.1 Rotation Group $SO(3)$

The generators of rotations in three dimensions Ω_i , which correspond to “infinitesimal” rotations, are:

$$\Omega_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \Omega_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \Omega_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Let $\mathbf{n} = (n_1, n_2, n_3)$, $\mathbf{n}^2 = 1$ and $\varphi \in [0, 2\pi)$. The components $(D(\mathbf{n}, \varphi))_{ij}$, $i, j \in \{1, 2, 3\}$ of the rotation matrix $D(\mathbf{n}, \varphi)$ for the rotation around the axis \mathbf{n} with the rotation angle φ read

$$(D(\mathbf{n}, \varphi))_{ij} = (1 - \cos \varphi) n_i n_j + \cos \varphi \delta_{ij} + \sin \varphi \varepsilon_{ijk} n_k.$$

In this exercise we want to obtain this rotation matrix from the generators Ω_i of the rotation group, more precisely, we want to show

$$e^{\varphi \mathbf{n} \cdot \boldsymbol{\Omega}} = D(\mathbf{n}, \varphi).$$

a) Prove that $[\Omega_i, \Omega_j] = \varepsilon_{ijk} \Omega_k$.

b) We denote $\Omega(\mathbf{n}) := \mathbf{n} \cdot \boldsymbol{\Omega} := \sum_{i=1}^3 n_i \Omega_i$. Show that $(\Omega(\mathbf{n}))^2 = -(\mathbf{1}_3 - \mathbf{n} \otimes \mathbf{n})$, where $\mathbf{n} \otimes \mathbf{n}$ is defined through

$$(\mathbf{n} \otimes \mathbf{n})_{ij} := n_i n_j.$$

c) Show that $\mathbf{n} \otimes \mathbf{n}$ is a projector. Thus $(\mathbf{1}_3 - \mathbf{n} \otimes \mathbf{n})$ is also a projector.

d) Show that $\exp(\varphi \Omega_1)$ is the matrix for the rotation around the x -axis with the rotation angle φ . In general, calculate $\exp(\varphi \mathbf{n} \cdot \boldsymbol{\Omega})$ and show $\exp(\varphi \mathbf{n} \cdot \boldsymbol{\Omega}) = D(\mathbf{n}, \varphi)$.

Problem 5.2 *Expansion in Matrices*

Consider four Hermitian matrices I , σ_1 , σ_2 and σ_3 , where I is the unit matrix, and the others satisfy the relation $\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}$. Without using any specific representation of matrices:

- Prove that $\text{Tr}(\sigma_i) = 0$.
- Show that eigenvalues of σ_i are ± 1 and that $\det(\sigma_i) = -1$.
- Show that the four matrices are linearly independent.
- Because of (c), any 2×2 matrix can be expanded in terms of these four matrices:

$$M = m_0 I + \sum_{i=1}^3 m_i \sigma_i.$$

Derive m_i for $i = 1, 2, 3, 4$.

Problem 5.3 *Many Eigenvalues*

Three matrices M_x , M_y and M_z , each with 256 rows and columns, obey the commutation rules $[M_x, M_y] = i M_z$ with cyclic permutations of x , y and z . M_x has the following eigenvalues: ± 2 , each once; $\pm 3/2$, each 8 times; ± 1 , each 28 times; $\pm 1/2$, each 56 times; and 0, 70 times. State the 256 eigenvalues of the matrix $M^2 = M_x^2 + M_y^2 + M_z^2$.

Problem 5.4 *A Symmetry Argument*

A molecule in the form of an equilateral triangle can capture an extra electron. To a good approximation, this electron can go into one of three orthogonal states ψ_A , ψ_B and ψ_C localized near the corners of the triangle. To a better approximation, the energy eigenstates of the electron are linear combinations of ψ_A , ψ_B and ψ_C determined by an effective Hamiltonian which has equal expectation values for all the three states and equal matrix elements V_0 between each pair of the three states.

- What does the symmetry under rotation through $2\pi/3$ imply about the coefficients of ψ_A , ψ_B and ψ_C in the eigenstates of the effective Hamiltonian?
- There is also symmetry under interchange of B and C . What additional information does this give about the eigenvalues of the effective Hamiltonian?
- At time $t = 0$ electron is captured into the state ψ_A . Find the probability that it will be found in ψ_A at time t .

6 Angular Momentum

Problem 6.1 *Angular Momentum and Spherical Harmonics*

- Determine the Cartesian components of the angular momentum operator $\mathbf{L} = \mathbf{r} \times \frac{\hbar}{i} \nabla$ (position representation) given in spherical coordinates (r, ϑ, φ) . Note that ∇ is defined in spherical coordinates as

$$\nabla = \mathbf{u}_r \frac{\partial}{\partial r} + \mathbf{u}_\vartheta \frac{1}{r} \frac{\partial}{\partial \vartheta} + \mathbf{u}_\varphi \frac{1}{r \sin \vartheta} \frac{\partial}{\partial \varphi},$$

where \mathbf{u}_r , \mathbf{u}_φ and \mathbf{u}_ϑ are the local orthogonal unit vectors.

Check up: $L_x = i\hbar \left(\sin \varphi \frac{\partial}{\partial \vartheta} + \cot \vartheta \cos \varphi \frac{\partial}{\partial \varphi} \right)$

- b) Evaluate $L_x Y_1^m(\vartheta, \varphi)$ for $m \in \{-1, 0, 1\}$ and express the result in terms of spherical harmonics. An explicit form of the spherical harmonics $Y_l^m(\vartheta, \varphi)$ can be found, e. g. on http://en.wikipedia.org/wiki/Spherical_harmonics#Conventions.
- c) Solve the eigenvalue problem for the x -component of the angular momentum L_x in the subspace of wave functions with $l = 1$: $L_x X_{l=1}(\vartheta, \varphi) = \lambda X_{l=1}(\vartheta, \varphi)$. Use the fact that for fixed l the spherical harmonics $Y_l^m(\vartheta, \varphi)$ form a basis of the subspace of wave functions with this particular l . Express the orthonormal eigenfunctions $X_{l=1}(\vartheta, \varphi)$ in terms of the spherical harmonics with $l = 1$.

Problem 6.2 Visualization of the Spherical Harmonics

From the lecture you know that the spherical harmonics Y_l^m are eigenfunctions of the operators of angular momentum \mathbf{L}^2 , L_z . Furthermore they correspond to eigenfunctions (orbitals) of the hydrogen atom.

- a) Using an applet

<http://demonstrations.wolfram.com/SphericalHarmonics>

(you can either download Mathematica code or standalone .CDF application), visualize Y_l^m for $l \leq 5$ and all possible m s. This is actually parametric plot where radial distance r for some (ϑ, φ) is given the value of spherical harmonic at these coordinates: $r = Y_l^m(\vartheta, \varphi)$.

- b) Plot the values of $|Y_l^m(\vartheta, \varphi)|^2$ (i.e angular density of angular momentum) on the spherical surface, with colors indicating the functional value of spherical harmonics.

Problem 6.3 Angular Momentum

The quantum mechanical operator $\mathbf{L} = (L_1, L_2, L_3)$ which corresponds to angular momentum in three dimensions is defined as following:

$$\mathbf{L} = \mathbf{Q} \times \mathbf{P}, \text{ i.e.}$$

$$L_i = \varepsilon_{ijk} Q_j P_k, \quad i \in \{1, 2, 3\}.$$

Using the commutator $[Q_i, P_j]$ and general commutator relations solve the following exercises:

- a) Show $[L_i, L_j] = i\hbar \varepsilon_{ijk} L_k$. Hint: You can use $\sum_k \varepsilon_{ijk} \varepsilon_{klm} = \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}$.
- b) We define $\mathbf{L}^2 := \sum_i L_i^2$ and $L_\pm := L_1 \pm iL_2$. Calculate $[L^2, L_i]$, $[L^2, L_\pm]$ and $[L_+, L_-]$.
- c) Show $[L_3, L_\pm^k] = \pm \hbar k L_\pm^k$ for any $k \in \mathbb{N}$.
- d) Calculate $[L_i, Q_j]$, $[L_i, P_j]$ and $[L_i, \mathbf{P} \cdot \mathbf{Q}]$.

Note. The components L_i of the angular momentum obey the same commutator relations as the generators Ω_i of the rotation group $SO(3)$ from Problem 5.1. They are called a representation of the rotation group (more precisely: of the corresponding Lie-Algebra). The corresponding group elements $\exp(i\varphi \mathbf{n} \cdot \mathbf{L})$ “rotate” the wave function.

Problem 6.4 Angular Momentum Operator

The wave function of a particle subjected to a spherically symmetrical potential $V(r)$ is given by

$$\psi(\mathbf{x}) = (x + y + 3z)f(r).$$

- a) Is ψ an eigenfunction of \mathbf{L}^2 ? If so, what is the l -value? If not, what are the possible values of l we may obtain when \mathbf{L}^2 is measured?
- b) What are the probabilities for the particle to be found in various m_l states?
- c) Suppose it is known somehow that $\psi(\mathbf{x})$ is an eigenfunction with eigenvalue E . Indicate how we may find $V(r)$.

Problem 6.5 *Coupling of Angular Momentum*

Two interacting particles are moving in a central symmetric field (for example: helium atom). The Hamilton operator is given by

$$H = \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + V_1(Q_1) + V_2(Q_2) + V(|\mathbf{Q}_1 - \mathbf{Q}_2|).$$

Prove that the coupled angular momentum $L_z = L_z^1 + L_z^2$ of the two particles commutes with the Hamiltonian operator.

Problem 6.6 *Pauli Matrices for Spin 1*

Construct the spin matrices (S_x, S_y, S_z) for a particle of spin 1.

Problem 6.7 *System of Two Spin = 1 Particles*

Consider a system of two particles with spin 1.

- a) Express all the eigen-states $|j m\rangle$ in the base of total angular momentum using vectors from the bases of particles $|j_1 j_2; m_1 m_2\rangle$:

$$|j m\rangle = \sum_{m=m_1+m_2} \langle j_1 j_2; m_1 m_2 | j_1 j_2; j m\rangle |j_1 j_2; m_1 m_2\rangle$$

using ladder operators.

- b) Express all the eigen-states $|j m\rangle$ in the base of total angular momentum using vectors from the bases of particles $|j_1 j_2; m_1 m_2\rangle$ without usage of the ladder operators, but using the spin operators of the two particles.

7 Spin = $\frac{1}{2}$ Systems

Problem 7.1 *Spin Measurement*

Evaluate the eigenvalues and eigenstates of the operator $O = \alpha(S_x - S_y)$ with $\alpha \in \mathbb{R}$ for a particle with spin 1/2. What is the probability to observe the value $-\hbar/2$ when measuring S_z for a particle prepared in an eigenstate of O ?

Problem 7.2 *Pauli Matrices*

We consider quantum mechanics in a 2-dimensional complex Hilbert space, which is isomorphic to \mathbb{C}^2 with the standard scalar product. We choose two orthonormal vectors, $|+\rangle$ and $|-\rangle$, as a basis, i.e

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

We consider observables $\sigma_1, \sigma_2, \sigma_3$. With respect to our basis they have the following matrix representation:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- Calculate the eigenvalues and the corresponding eigenvectors of $\sigma_1, \sigma_2, \sigma_3$.
- Calculate σ_i^2 and $[\sigma_i, \sigma_j]$ for $i, j \in \{1, 2, 3\}$.
- Assume that the larger eigenvalue of σ_1 has been measured. What is the probability to measure the eigenvalues of σ_2 immediately after the first measurement?
- Consider the product of uncertainties $\langle(\Delta\sigma_1)^2\rangle\langle(\Delta\sigma_2)^2\rangle$ for the same state. In which states does this product take its maximal/minimal value? Hint: Use the general uncertainty principle for σ_1, σ_2 from the lecture.

Problem 7.3 *Pauli Matrices*

We consider quantum mechanics in the \mathbb{C} -Hilbert space \mathbb{C}^2 with the standard scalar product. We choose two orthonormal vectors, $|\uparrow\rangle$ and $|\downarrow\rangle$, as a basis and consider observables $\sigma_1, \sigma_2, \sigma_3$. With respect to our basis they have the following matrix representation:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Note: all σ_i are hermitian. Our main aim is to find a unitary operator $V(\mathbf{n}, \varphi)$, which, in analogy to the rotation matrix $D(\mathbf{n}, \varphi)$ in three dimensions, rotates the vector $\boldsymbol{\sigma} := (\sigma_1, \sigma_2, \sigma_3)$, i.e.:

$$V^\dagger(\mathbf{n}, \varphi) \sigma_i V(\mathbf{n}, \varphi) = \sum_{j=1}^3 D(\mathbf{n}, \varphi)_{ij} \sigma_j.$$

We recall: $D(\mathbf{n}, \varphi) = \exp(\varphi \mathbf{n} \cdot \boldsymbol{\Omega})$ and the generators Ω_i obey $[\Omega_i, \Omega_j] = \varepsilon_{ijk} \Omega_k$. The rotation axis \mathbf{n} is normalized, $\sum_i n_i^2 = 1$. Furthermore $(\mathbf{n} \cdot \boldsymbol{\Omega})_{ij} = -\varepsilon_{ijk} n_k$.

- Calculate σ_i^2 and verify $[\sigma_i, \sigma_j] = 2i \varepsilon_{ijk} \sigma_k$, for $i, j \in \{1, 2, 3\}$.
- Calculate the anti-commutator $\{\sigma_i, \sigma_j\} := \sigma_i \sigma_j + \sigma_j \sigma_i$ and verify $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$.
- To obtain exactly the same commutator relations as for the generators Ω_i of rotations in three dimensions, we define the operators $S_i := -(i/2)\sigma_i$. Convince yourself that $[S_i, S_j] = \varepsilon_{ijk} S_k$.
- In analogy to rotations in three dimensions we define $V(\mathbf{n}, \varphi) := \exp(\varphi \mathbf{n} \cdot \mathbf{S}) = \exp\left(-\frac{i}{2}\varphi \mathbf{n} \cdot \boldsymbol{\sigma}\right)$. For infinitesimally small rotations, i.e. up to $\mathcal{O}(\varphi)$, verify that $V^\dagger \boldsymbol{\sigma} V$ rotates $\boldsymbol{\sigma}$.
- Calculate $\exp\left(-\frac{i}{2}\varphi \mathbf{n} \cdot \boldsymbol{\sigma}\right)$. *Hint:* First calculate $(\mathbf{n} \cdot \boldsymbol{\sigma})^2$.
- Prove $A_i := V^\dagger \sigma_i V = \sum_j D_{ij} \sigma_j =: B_i$ by considering the derivative $\frac{d}{d\varphi} A_i$ and the corresponding differential equation.

Problem 7.4 Stern-Gerlach Experiment

In the *Stern-Gerlach experiment* we have a beam of silver atoms moving in vacuum, and passing through some filters. The filters, which are inhomogeneous magnetic fields pointing in some direction, split up the beam according to the magnetic dipole of the incoming particles, blocking a particular spin component of the beam. Consider a situation with three Stern-Gerlach filters, as shown on the figure below.

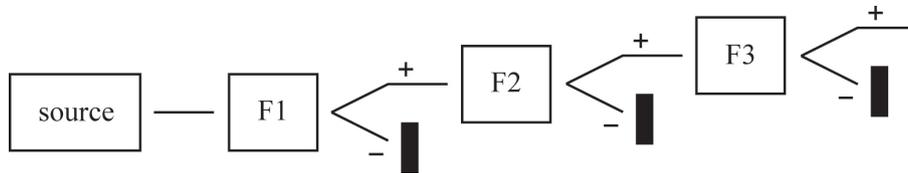


Fig. 29: Experiment with three Stern-Gerlach filters.

The first one has a magnetic field pointing in the z -direction, the second one in the $\mathbf{n}_1 = (0, \sin \vartheta, \cos \vartheta)$ direction, and the third one in the $\mathbf{n}_2 = (0, \sin \varphi, \cos \varphi)$ direction, where ϑ and φ are the angles between \mathbf{n} and the z -axis.

- Calculate the probability for particles with spin $1/2$ to pass through the second filter, and also the probability for them to pass through the third filter. Consider the special case of $\vartheta = \frac{\pi}{2}$ and $\varphi = \pi$. What will happen if the second filter is not there and $\varphi = \pi$?
- Calculate the corresponding probability for spin-one particles (the filter now blocks all the components of the beam except the one for $m = +1$).
- Comment about what would happen in the classical limit case (when the spin s becomes very large).

Problem 7.5 Spin Precession

As an example of spin dynamics we consider a particle of spin $\frac{1}{2}$ in a constant magnetic field. We assume that the particle is immobile to focus on the spin degrees of freedom. The Hamiltonian is given by $H = -\frac{e\hbar}{2m}\boldsymbol{\sigma} \cdot \mathbf{B}$, where the magnetic spin moment $\mathbf{m}_\sigma = \frac{e\hbar}{2m}\boldsymbol{\sigma}$ couples linearly to the magnetic field. We chose the magnetic field to be parallel to the z -direction, so $\mathbf{B} = (0, 0, B)$.

- Evaluate the motion of the spinor wave function

$$\psi(t) = \begin{pmatrix} \psi_+(t) \\ \psi_-(t) \end{pmatrix}$$

by introducing the Larmor frequency $\omega_L = \frac{eB}{2m}$.

- Calculate the expectation values of the spin components $\langle S_x \rangle$, $\langle S_y \rangle$ and $\langle S_z \rangle$ for the condition

$$\psi(0) = \begin{pmatrix} a \\ b \end{pmatrix}, \quad a, b \in \mathcal{R}$$

and interpret the results.

Problem 7.6 *Arbitrary Spin Direction and Spin Precession*

We consider again a spin measurements of a particle with spin $\frac{1}{2}$. The measurement occurs concerning an arbitrary space direction, which is defined as $\hat{\mathbf{e}} = \sin \vartheta \cos \varphi \hat{\mathbf{e}}_1 + \sin \vartheta \sin \varphi \hat{\mathbf{e}}_2 + \cos \vartheta \hat{\mathbf{e}}_3$.

- Calculate the eigenvalues and the eigenstates $|\hat{\mathbf{e}}_{\pm}\rangle$ of the spin projection $\mathbf{S} \cdot \hat{\mathbf{e}}$ and express them in terms of $\frac{\vartheta}{2}$ and φ .
- Consider now a magnetic field $\mathbf{B} = B\hat{\mathbf{e}}$, such that the Hamiltonian can be written as $H = -\hbar\omega_L \boldsymbol{\sigma} \cdot \hat{\mathbf{e}}$ with the well known Larmor frequency $\omega_L = \frac{eB}{2m}$. Calculate the time evolution, if at $t = 0$ the particle is in the eigenstate $|\psi(0)\rangle = a|+\rangle + b|-\rangle$.
- If $a = 1$ (i.e. at the beginning particle is in S_z eigenstate $|+\rangle$), find the probability to find the particle for $t > 0$ in the eigenstate $|+\rangle$. What do you get for $\hat{\mathbf{e}} = \hat{\mathbf{z}}$?
- Assume that $\hat{\mathbf{e}} = \hat{\mathbf{z}}$ (that is, \mathbf{B} has $\hat{\mathbf{z}}$ -direction) and calculate the expectation values of the spin components $\langle S_x \rangle$, $\langle S_y \rangle$ and $\langle S_z \rangle$ at time t . Interpret the results.

Problem 7.7 *Magnetic Spin Resonance*

We consider an electron which rests in the origin of the reference frame and apply a constant magnetic field $B_z \mathbf{e}_z$ as well as a rotating magnetic field $B_0 (\cos(\omega_0 t) \mathbf{e}_x + \sin(\omega_0 t) \mathbf{e}_y)$, where \mathbf{e}_i is the unit vector in the direction i . In the following we consider only the spin degrees of freedom of the electron. The Hamiltonian of the system reads $H = \gamma \mathbf{B} \cdot \boldsymbol{\sigma} =$ where $\gamma > 0$ is constant and σ_i are the Pauli matrices. Our aim is to solve the corresponding Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle.$$

The difficulty lies in the fact that our Hamiltonian is time dependent. To address the problem we first have to take care of some mathematical technicalities.

- In analogy to Problem 7.3, we define the unitary operator $V(\varphi) := \exp\left(-i\frac{\varphi}{2}\sigma_3\right)$. Verify the following identities:

$$V^\dagger \sigma_1 V = \cos(\varphi) \sigma_1 - \sin(\varphi) \sigma_2; \quad V^\dagger \sigma_2 V = \cos(\varphi) \sigma_2 + \sin(\varphi) \sigma_1; \quad V^\dagger \sigma_3 V = \sigma_3.$$

- We transform our system via the unitary transformation $V(\omega t)$ to a reference frame uniformly rotating around the z -axis. Derive the corresponding equation for $|\Phi(t)\rangle := V^\dagger(\omega t) |\Psi(t)\rangle$ and write it in the form

$$i\hbar \frac{\partial}{\partial t} |\Phi(t)\rangle = H_{\text{eff}}(t) |\Phi(t)\rangle,$$

where $H_{\text{eff}}(t)$ is the effective Hamiltonian of the system. Calculate H_{eff} .

- How do we have to choose ω in order for the effective Hamiltonian H_{eff} to be time independent?
- Since our effective Hamiltonian now is time-independent, we can directly solve the Schrödinger equation. Assume that, in the original reference frame, the electron is in the spin-up state $|+\rangle = (1, 0)^\top$ at $t = 0$. Calculate the probability $P(t)$ to measure the electron in the spin-down state $|-\rangle = (0, 1)^\top$ at $t > 0$.
- For which value of ω_0 is $P(t) = 1$ the maximal value of P ? (*Resonance condition*).

Problem 7.8 *Spin-half Atoms in a Crystal*

Consider two spin-half atoms in a crystal to be two magnetic dipoles $\boldsymbol{\mu}_1 = \mu \mathbf{S}^{(1)}$ and $\boldsymbol{\mu}_2 = \mu \mathbf{S}^{(2)}$ at distance a , where μ is constant, and $\mathbf{S}^{(1)}$ and $\mathbf{S}^{(2)}$ are respective spin operators.

a) Prove that the interaction between them is described by the Hamiltonian

$$H = K \left(\mathbf{S}^{(1)} \cdot \mathbf{S}^{(2)} - 3 \frac{(\mathbf{S}^{(1)} \cdot \mathbf{a})(\mathbf{S}^{(2)} \cdot \mathbf{a})}{a^2} \right),$$

where $K \equiv \frac{\mu_0 \mu^2}{4\pi a^3}$ is a constant with dimension of energy.

b) Show that $S_x^{(1)} S_x^{(2)} + S_y^{(1)} S_y^{(2)} = \frac{1}{2}(S_+^{(1)} S_-^{(2)} + S_-^{(1)} S_+^{(2)})$. Show that the mutual eigenkets of the total spin operators S^2 and S_z are also eigenstates of H and find the corresponding eigenvalues.

c) At time $t = 0$ particle 1 has its spin parallel to \mathbf{a} , while the other particle's spin is antiparallel to \mathbf{a} . Find the time required for both spins to reverse their orientations.

Problem 7.9 *Properties of Clebsch-Gordan Coefficients*

If we have two particles with angular momenta \mathbf{J}_1 and \mathbf{J}_2 , the total angular momentum operator is defined as $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$. The eigenkets of this operator $|jm\rangle$ are linear combinations of the composite states $|j_1 m_1\rangle |j_2 m_2\rangle$, and the connection is given by the *Clebsch-Gordan coefficients*. The general expression reads:

$$|j_1 j_2; jm\rangle = \sum_{m_1} \sum_{m_2} \langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle |j_1 j_2; m_1 m_2\rangle$$

where $\langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle \equiv C_{m_1 m_2 m}^{j_1 j_2 j}$ are the Clebsch-Gordan coefficients. Prove that:

- a) the coefficients will vanish unless $m = m_1 + m_2$.
- b) the coefficients will vanish unless $|j_1 - j_2| \leq j \leq j_1 + j_2$.

Problem 7.10 *Clebsch-Gordan Coefficients for $\frac{1}{2}$ and other spin*

Work out the Clebsch-Gordan coefficients for the case $s_1 = 1/2$, $s_2 = \text{anything}$. *Hint:* You are looking for the coefficients A and B in

$$|s m\rangle = A \left| \frac{1}{2} \frac{1}{2} \right\rangle |s_2(m - \frac{1}{2})\rangle + B \left| \frac{1}{2} (-\frac{1}{2}) \right\rangle |s_2(m + \frac{1}{2})\rangle,$$

such that $|s m\rangle$ is an eigenstate of \mathbf{S}^2 . Use this general result to construct the $(1/2) \times 1$ table of Clebsch-Gordan coefficients, and check it against the *Table of Clebsch-Gordan coefficients*. *Answer:*

$$A = \sqrt{\frac{s_2 \pm m + 1/2}{2s_2 + 1}}; \quad B = \pm \sqrt{\frac{s_2 \mp m + 1/2}{2s_2 + 1}},$$

where the signs are determined by $s = s_2 \pm 1/2$.

8 Perturbation Theory

8.1 Time independent

Problem 8.1 *Two-state System: Exact and Perturbation Solution*

The Hamiltonian matrix for a two-state system can be written as

$$H = \begin{pmatrix} E_1^0 & \lambda V \\ \lambda V & E_2^0 \end{pmatrix}$$

- Solve this problem exactly to find the energy eigenstates and the energy eigenvalues. Plot the eigenenergies as a function of $\Delta E = E_1^0 - E_2^0$. What is the separation of the energy levels for $\Delta E = 0$?
- Assuming that $\lambda|V| \ll |\Delta E|$, solve this problem using time-independent perturbation theory up to first and second order in the energy eigenvalues. Compare to the results obtained in a).
- Suppose the two unperturbed energies are "almost degenerate", i.e. $|\Delta E| \ll \lambda|V|$. Show that the exact results obtained in a) closely resemble what you would expect by applying degenerate perturbation theory to this problem with E_1^0 set exactly equal to E_2^0 .

Problem 8.2 *Harmonic oscillator — Perturbation theory*

Consider a harmonic oscillator in one dimension subjected to a perturbation:

$$H = \frac{P^2}{2m} + \frac{k}{2}Q^2 + V(Q). \quad (8.1)$$

- For $V = \frac{1}{2}\varepsilon m\omega^2 Q^2$ calculate exactly the eigenenergies. Calculate the energy of the ground state to second order (and the perturbed eigenket to first order) by applying perturbation theory. Compare the energies to those that you get from an exact treatment of a problem.
- For $V = bQ$ solve the problem exactly and calculate the energy shift of the ground state to lowest non-vanishing order. Compare your results.
- Calculate in first order perturbation theory the corrected ground state $|0'\rangle$ and its energy for a particle challenged by a sinusoidal force described by the perturbation $V = \lambda \sin(\kappa Q)$.
- Determine the expectation value of the position operator $\langle 0'|Q|0'\rangle$ in the lowest nontrivial order of λ for perturbation from c).

Problem 8.3 *Anharmonic Oscillator*

Consider an anharmonic oscillator with the following Hamiltonian:

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + \alpha x^3$$

where α is small, and we can use perturbation theory. Calculate the first and second order corrections to the energy. Compare the energy levels of the anharmonic oscillator to the ones of the harmonic oscillator.

Problem 8.4 *Quantum Pendulum*

A mass m is attached by a massless rod of length l to a pivot P and swings in a vertical plane under the influence of gravity.

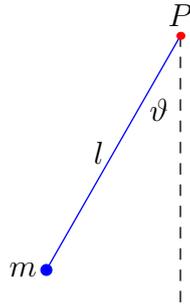


Fig. 31: Scheme of the system.

Find the energy levels in the small angle approximation as well as the first and second order correction to ground state energy resulting from inaccuracy of the small angle approximation.

Problem 8.5 *Van der Waals Interaction*

Consider two atoms at distance R apart. Because they are electrically neutral you might suppose there would be no force between them, but if they are polarizable there is in fact a weak attraction. To model this system, picture each atom as an electron (mass m , charge $-e$) attached by a spring (spring constant k) to the nucleus (charge $+e$), as in figure below.



Fig. 32: Two nearby polarizable atoms.

We'll assume the nuclei are heavy, and essentially motionless. The Hamiltonian for the unperturbed system is

$$H_0 = \frac{p_1^2}{2m} + \frac{1}{2}kx_1^2 + \frac{p_2^2}{2m} + \frac{1}{2}kx_2^2. \quad (8.5)$$

The Coulomb interaction between the atoms is

$$H' = \frac{1}{4\pi\epsilon_0} \left(\frac{e^2}{R} - \frac{e^2}{R-x_1} - \frac{e^2}{R+x_2} + \frac{e^2}{R+x_2-x_1} \right). \quad (8.6)$$

- a) Explain Equation (8.6). Assuming that $|x_1|$ and $|x_2|$ are both much less than R , show that

$$H' \cong -\frac{e^2 x_1 x_2}{2\pi\epsilon_0 R^3}. \quad (8.7)$$

- b) Show that the total Hamiltonian (eq. (8.5) plus eq. (8.7)) separates into two harmonic oscillator Hamiltonians:

$$H = \left(\frac{p_+^2}{2m} + \frac{1}{2} \left(k - \frac{e^2}{2\pi\epsilon_0 R^3} \right) x_+^2 \right) + \left(\frac{p_-^2}{2m} + \frac{1}{2} \left(k + \frac{e^2}{2\pi\epsilon_0 R^3} \right) x_-^2 \right)$$

under the change of variables $x_{\pm} \equiv \frac{1}{\sqrt{2}}(x_1 \pm x_2)$, which entails $p_{\pm} = \frac{1}{\sqrt{2}}(p_1 \pm p_2)$.

- c) The ground state energy for this Hamiltonian is evidently

$$E = \frac{1}{2}\hbar(\omega_+ + \omega_-), \quad \text{where } \omega_{\pm} = \sqrt{\frac{k}{m} \mp \frac{e^2}{2\pi\epsilon_0 m R^3}}.$$

Without the Coulomb interaction it would have been $E_0 = \hbar\omega_0$, where $\omega_0 = \sqrt{k/m}$. Assuming that $k \gg e^2/(2\pi\epsilon_0 R^3)$, show that

$$\Delta V \equiv E - E_0 \cong -\frac{\hbar}{2m^2\omega_0^3} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{1}{R^6}.$$

Conclusion: There is an attractive potential between the atoms, proportional to the inverse sixth power of their separation. This is the van der Waals interaction between two neutral atoms.

- d) Now do the same calculation using second-order perturbation theory. *Hint:* The unperturbed states are of the form $\psi_{n_1}(x_1)\psi_{n_2}(x_2)$, where $\psi_n(x)$ is a one-particle oscillator wave function with mass m and spring constant k ; ΔV is the second-order correction to the ground state energy, for the perturbation in equation (8.7) (notice that the *first-order* correction is zero).

Problem 8.6 Quadratic Stark Effect

Consider a one-electron atom in an uniform electric field in z -direction. The Hamiltonian of the problem is given by

$$H = \frac{P^2}{2m} - \frac{e^2}{r} + V = \frac{P^2}{2m} - \frac{e^2}{r} - e|\mathbf{E}|z,$$

where the electric field makes up the perturbation. Assume here that you can ignore spin, and that the energy levels of the unperturbed problem are known and not degenerate (as in the ground state of the hydrogen atom).

- a) Using symmetry (parity) show that the first-order energy shift vanishes.
 b) What is the expression for the second order shift $\Delta_2 E$? Evaluate an upper limit to the polarizability of the ground state of the hydrogen atom $\tilde{\alpha}$, defined by $\Delta_2 E = -\frac{1}{2}\tilde{\alpha}|\mathbf{E}|^2$.
Hint: Use $-E_0^{(0)} + E_k^{(0)} \geq -E_0^{(0)} + E_1^{(0)}$ to make the sum over all states $k \neq 0$ be k -independent.

Problem 8.7 Relativistic Corrections for the Hydrogen Atom

The so-called fine structure lifts the degeneracy of the hydrogen atom. One of the contributions is a relativistic correction.

a) Show that an expansion of the relativistic expression of the kinetic energy

$$T = \sqrt{c^2 P^2 + (mc^2)^2} - mc^2$$

leads to an additional term in the Hamiltonian of the form:

$$H_{\text{rel}} = -\frac{P^4}{8m^3c^2}.$$

b) Calculate the shift of the energy levels to first order in the perturbation H_{rel} : First show that the energy shift can be expressed as

$$\Delta E_{\text{rel}} = -\frac{1}{2mc^2} \langle (E - V)^2 \rangle,$$

where V is the Coulomb potential. Then evaluate this expression by using the virial theorem, and by using the fact that (without proof)

$$\langle nlm | \frac{1}{r^2} | nlm \rangle = \frac{1}{(l + 1/2)n^3 a_0^2},$$

where a_0 denotes the Bohr radius.

Remark: The second contribution to the fine structure is spin-orbit coupling. As a result the energy levels of the hydrogen atom including fine structure are given by

$$E_{nj} = -\frac{R_y}{n^2} \left(1 + \frac{\alpha^2}{n^2} \left(\frac{n}{j + 1/2} - \frac{3}{4} \right) \right),$$

where $\mathbf{J} = \mathbf{L} + \mathbf{S}$ is the total angular momentum and α the Sommerfeld fine structure constant.

Problem 8.8 Nucleus as a Homogeneous Sphere

Assume that the nucleus is a homogeneously charged sphere of radius R and charge Ze . Using first-order perturbation theory, calculate the correction as the function of the atomic number Z due to the fact that the charge of the nucleus does not behave in a point-like manner. This corresponds to energy shift of the ground state for an ion isoelectronic to the hydrogen atom (atomic number Z , one electron).

Problem 8.9 Degenerate Perturbation Calculation

Consider the three-dimensional infinite cubical well:

$$V(x, y, z) = \begin{cases} 0, & \text{if } 0 < x < a, 0 < y < a, \text{ and } 0 < z < a; \\ \infty & \text{otherwise.} \end{cases}$$

The stationary states are

$$\psi_{n_x n_y n_z}^0 = \left(\frac{2}{a} \right)^{3/2} \sin \left(\frac{n_x \pi}{a} x \right) \sin \left(\frac{n_y \pi}{a} y \right) \sin \left(\frac{n_z \pi}{a} z \right),$$

where n_x, n_y and n_z are positive integers. The corresponding allowed energies are

$$E_{n_x n_y n_z}^0 = \frac{\pi^2 \hbar^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2).$$

The first excited state is triply degenerate:

$$\psi_a \equiv \psi_{112}, \quad \psi_b \equiv \psi_{121}, \quad \text{and} \quad \psi_c \equiv \psi_{211} ,$$

all with the energy

$$E_1^0 \equiv 3 \frac{\pi^2 \hbar^2}{ma^2}$$

We introduce the perturbation

$$H' = \begin{cases} V_0, & \text{if } 0 < x < a/2, 0 < y < a/2; \\ 0 & \text{otherwise.} \end{cases}$$

a) Construct the matrix W

$$W_{ij} = \langle \psi_i^0 | H' | \psi_j^0 \rangle \quad (i, j = a, b, c) .$$

b) The perturbation will split the energy E_1^0 into three energy levels. Find them.

c) The “good” unperturbed states are linear combinations of the form

$$\psi^0 = \alpha \psi_a + \beta \psi_b + \gamma \psi_c .$$

The coefficients α, β and γ are the eigenvectors of the matrix W . Find these “good” states.

Problem 8.10 Cubical Well — Degenerate Perturbation Calculation

Consider a particle of mass m in three-dimensional infinite cubical well:

$$V(x, y, z) = \begin{cases} 0, & \text{if } 0 < x < a, 0 < y < a, \text{ and } 0 < z < a; \\ \infty & \text{otherwise.} \end{cases}$$

a) Solve the Schrödinger equation and find stationary states and energies. Write down the wave functions for two lowest energy states.

b) We introduce the perturbation

$$V'(x, y, z) = \lambda \delta \left(\frac{y}{a} - \frac{x}{a} \right) .$$

Find the corrected energies for two lowest energy states as well as the “good” unperturbed states for excited state, which are linear combinations of the form

$$\psi^0 = \alpha \psi_a + \beta \psi_b + \gamma \psi_c,$$

where the coefficients α, β and γ are the eigenvectors of the secular matrix of the problem.

c) Two non-identical particles, each of mass m , are confined *in one dimension* to same well. What are the wave functions and energies of the three lowest-energy states of the system? If an interaction potential of the form $V' = \lambda \delta(x_1 - x_2)$ is added (where x_1 and x_2 are positions of particles 1 and 2), calculate to first order in λ the energies of these three lowest states and their wave functions to zeroth order in λ .

Hint: you can use integrals

$$\int_0^a \sin \left(\frac{n\pi x}{a} \right) \sin \left(\frac{m\pi x}{a} \right) dx = \frac{a}{2} \delta_{m,n} \quad \text{and} \quad \int_0^a \sin^2 \left(\frac{n\pi x}{a} \right) \sin^2 \left(\frac{m\pi x}{a} \right) dx = \frac{a}{8} (2 + \delta_{m,n}) .$$

Problem 8.11 *Rubber-band Helium*

Although the Schrödinger equation for helium itself cannot be solved exactly, there exist “helium-like” systems that do admit exact solutions. A simple example is “rubber-band helium”, in which the Coulomb forces are replaced by Hooke’s law forces:

$$H = -\frac{\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) + \frac{1}{2}m\omega^2(r_1^2 + r_2^2) - \frac{\lambda}{4}m\omega^2|\mathbf{r}_1 - \mathbf{r}_2|^2. \quad (8.10)$$

a) Show that the change of variables from $\mathbf{r}_1, \mathbf{r}_2$, to

$$\mathbf{u} \equiv \frac{1}{\sqrt{2}}(\mathbf{r}_1 + \mathbf{r}_2), \quad \mathbf{v} \equiv \frac{1}{\sqrt{2}}(\mathbf{r}_1 - \mathbf{r}_2)$$

turns the Hamiltonian into two independent three-dimensional harmonic oscillators:

$$H = \left[-\frac{\hbar^2}{2m} \nabla_u^2 + \frac{1}{2}m\omega^2 u^2 \right] + \left[-\frac{\hbar^2}{2m} \nabla_v^2 + \frac{1}{2}(1 - \lambda)m\omega^2 v^2 \right].$$

b) What is the *exact* ground-state energy for this system?

c) If we didn’t know the exact solution, we might be inclined to apply the variational principle

$$E_{gs} \leq \langle \psi_0 | H | \psi_0 \rangle \equiv \langle H \rangle$$

where

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \left(\frac{m\omega}{\pi\hbar} \right)^{3/2} \exp \left[-\frac{m\omega}{2\hbar} (r_1^2 + r_2^2) \right]$$

is the ground state for two particles in a 3-D harmonic oscillator. Calculate $\langle H \rangle$ and compare it to the exact result.

Problem 8.12 *Perturbed Particle on a Circle*

A particle of mass m is confined to a circle of radius a , but is otherwise free. A perturbing potential $V = A \sin \varphi \cos \varphi$ is applied, where φ is the angular position on the circle. Find the correct zero-order wave functions for the two lowest states of this system and calculate their perturbed energies to second order.

Problem 8.13 *3D Harmonic Oscillator Perturbation Theory*

A particle of mass m is moving in the three-dimensional harmonic oscillator potential. A weak perturbation is applied in the form of the function

$$V'(x, y, z) = bxy + \frac{b^2}{\hbar\omega} y^2 z^2,$$

where b is a small constant. Calculate the shift in the ground and the first excited state energy to second order in b and give the first-order wave functions of the excited state in terms of the wave functions of the unperturbed three-dimensional harmonic oscillator.

8.2 Time Dependent

Problem 8.14 *Two-level System of an Atom*

Consider two atomic levels characterized by two stationary states. The ground state is denoted with $|g\rangle$, the excited state with $|e\rangle$. Both states are orthogonal and normalized, so $\langle n|m\rangle = \delta_{nm}$ with $n, m \in \{e, g\}$. The corresponding eigenvalues to the unperturbed Hamiltonian are

$$H|g\rangle = \hbar\omega_g|g\rangle; \quad H|e\rangle = \hbar\omega_e|e\rangle.$$

Now consider a perturbation which is switched on at time $t = 0$, which does not depend on time for $t > 0$. The perturbation is represented by hermitian operator W . The time dependent Schrödinger equation including W has the form

$$i\hbar|\dot{\psi}(t)\rangle = (H + W)|\psi(t)\rangle$$

We assume the most general case, where at time $t = 0$ the wavefunction is in a superposition state of the eigenstates, so

$$|\psi(0)\rangle = \sum_n |n\rangle \langle n|\psi(0)\rangle = c_g(0)|g\rangle + c_e(0)|e\rangle = \begin{pmatrix} c_g(0) \\ c_e(0) \end{pmatrix}, \quad c_n(0) = \langle n|\psi(0)\rangle.$$

- a) Display the operator $W + H$ as a matrix with respect to the basis of the eigenstates $|n\rangle$. Use the notation $W_{nm} = \langle n|W|m\rangle$.
- b) What is $|\psi(t)\rangle$? Apply the mapping $c_n(t) = b_n(t)e^{-i\omega_n t}$. Insert this expression into the time dependent Schrödinger equation. Introduce the frequency $\Omega = \omega_e - \omega_g$.
- c) For the coefficients $b_n(t)$ you get two coupled differential equations. Solve the problem with the ansatz

$$b_g(t) = Ae^{-i\omega t}, \quad b_e(t) = Be^{-i(\omega - \Omega)t}.$$

Verify the frequencies ω_{\pm} , which solve the problem. Intermediate result:

$$\omega_{\pm} = \frac{W_{gg}}{\hbar} + \frac{1}{2}\gamma \pm \sigma$$

and

$$\hbar\gamma = W_{ee} - W_{gg} + \hbar\Omega; \quad \sigma = \sqrt{\frac{1}{4}\gamma^2 + \frac{|W_{ge}|^2}{\hbar^2}}.$$

- d) Calculate $b_g(t)$ and $b_e(t)$ for the case, that at time $t = 0$ the atom is in the ground state, so $b_g(0) = c_g(0) = 1$ and $b_e(0) = c_e(0) = 0$
- e) Determine the probability to find the system in the ground state $|c_g(t)|^2$ and the excited state $|c_e(t)|^2$ for later times $t > 0$. Interpret the results.

Problem 8.15 *Time Dependent Electric Field Perturbation*

Consider a hydrogen atom in its ground state. At time $t = 0$ a spatially uniform electric field $\mathbf{E} = \mathbf{E}_0 \exp\left(-\frac{t}{\tau}\right)$ perturbs the atom. Using first order perturbation theory calculate the probability of finding the atom in the first excited state ($n = 2, l = 1, m$). The perturbing Hamiltonian reads $H' = -eE_0 z \exp\left(-\frac{t}{\tau}\right)$.

Problem 8.16 *Time-dependent Perturbation of Harmonic Oscillator*

A one-dimensional harmonic oscillator is in the ground state for $t < 0$. For $t \geq 0$ it is subjected to a time-dependent but spatially uniform *force* in x -direction

$$F(t) = F_0 e^{-t/\tau}.$$

- a) Using time-dependent perturbation theory to first order, obtain the probability of finding the oscillator in the first excited state for $t > 0$. Show that $t \rightarrow \infty$ (τ finite) limit of your expression is independent of time.
- b) Can we find higher excited states?

Hint: you may use $\langle m|x|n\rangle = \sqrt{\hbar/2m\omega} (\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1})$.

Problem 8.17 *Time-dependent Hydrogen Atom Perturbation*

The ground state of a hydrogen atom ($n = 1, l = 0$) is subjected to a time-dependent potential as follows:

$$V(\mathbf{x}, t) = V_0 \cos(kz - \omega t). \quad (8.17)$$

Using time-dependent perturbation theory, obtain an expression for the transition rate at which the electron is emitted with momentum \mathbf{p} . Show, in particular, how you may compute the angular distribution of the ejected electron (in terms of ϑ and φ defined with respect to the z -axis). For the initial wavefunction use

$$\psi_{n=1,l=0}(\mathbf{x}) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0}$$

Problem 8.18 *n -th Excited State of Harmonic Oscillator*

At some moment the electric field \mathbf{E} constant in time starts to interact with a linear harmonic oscillator that is in the ground state. Find the probability of excitation of n -th state of the oscillator, $P_n(t)$, if we switched the field on instantly.

Hint: Use the formalism of the ladder operators.

Problem 8.19 *Electric Perturbation on a Particle in a Box*

The particle with charge e is confined in the 3D rectangular box with edges of the length $2b$. The system is exposed to the electric field $\mathbf{E}(t)$:

$$\mathbf{E}(t) = \begin{cases} 0, & t \leq 0 \\ \mathbf{E}_0 e^{-\alpha t}, & t > 0 \end{cases},$$

where \mathbf{E}_0 is perpendicular to one surface of the box. In the leading order in E_0 , calculate the probability that the charged particle initially ($t = 0$) in the ground state, will be in the first excited state.

Problem 8.20 *Two Spin-coupled Fermions*

Consider a composite system made up of two spin $\frac{1}{2}$ objects. For $t < 0$, the Hamiltonian does not depend on spin and can be taken to be zero suitably adjusting the energy scale. For $t > 0$, the Hamiltonian is given by

$$H = \frac{4\Delta}{\hbar^2} \mathbf{S}_1 \cdot \mathbf{S}_2 .$$

Suppose the system is in $|+-\rangle$ state for $t \leq 0$, where $|+\rangle$ and $|-\rangle$ refer to the eigenvectors of S_z . Find, as a function of time, the probability of being found in each of the states $|++\rangle$, $|+-\rangle$, $|-\rangle$ and $|--\rangle$:

- by solving the problem exactly;
- by solving the problem assuming the validity of first-order time-dependent perturbation theory with H as a perturbation switched on at $t = 0$. Under what condition does this give the correct results?

Problem 8.21 *Perturbation of Angular Momentum States*

Particle in some central potential is in a 4-fold degenerate state with respect to angular momentum:

$$|\psi\rangle = \alpha|00\rangle + \beta|1-1\rangle + \gamma|10\rangle + \delta|11\rangle .$$

At time $t = 0$, $\alpha = 1$ and an electric field $\mathbf{E} = E_0 \sin(\omega t) \hat{\mathbf{z}}$ is turned on. Ignoring the possibility of transitions to other than these four states, calculate the occupation probability for each of them at time t in terms of the non-zero matrix elements of z .

Hint: You can use the recursion relation for associated Legendre polynomials:

$$(l - m + 1)P_{l+1}^m(x) = (2l + 1)xP_l^m(x) - (l + m)P_{l-1}^m(x) .$$

Problem 8.22 *Protons in Magnetic Field*

Protons having magnetic momentum μ are situated in a magnetic field

$$B_x = B_0 \cos \omega t$$

$$B_y = B_0 \sin \omega t$$

$$B_z = \text{const} .$$

where $B_0 \ll B_z$. At the moment $t = 0$ all the protons are polarised in $+z$ direction.

- At which frequency ω will protons have the resonant transitions?
- What is the probability that a proton has the spin oriented in $-z$ direction at time t ?

9 Scattering

Problem 9.1 The Transfer Matrix

The scattering matrix (or S -matrix) tells you the *outgoing* amplitudes (B and F) in terms of the *incoming* amplitudes (A and G):

$$\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix}.$$

For some purposes it is more convenient to work with the transfer matrix \mathbf{M} which gives you the amplitude to the *right* of the potential (F and G) in terms of those to the *left* (A and B):

$$\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}.$$

- a) Suppose you have a potential consisting of two isolated pieces (see figure below).

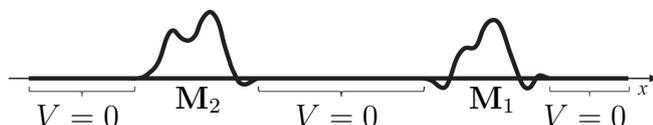


Fig. 33: A potential consisting of two isolated pieces.

Show that the M -matrix for the combination is the *product* of the two M -matrices for each section separately:

$$\mathbf{M} = \mathbf{M}_2 \mathbf{M}_1.$$

Note that this obviously generalizes to any number of pieces, and accounts for the usefulness of the M -matrix.

- b) Find the M -matrix for scattering from the double delta function potential

$$V(x) = -\alpha(\delta(x+a) + \delta(x-a)).$$

Problem 9.2 Cross Section for Spherically Symmetric Potential

Within the Born approximation calculate the differential cross section of a particle of mass m which is scattering on the potential

$$V(\mathbf{r}) = Ae^{-r^2/a^2},$$

where A is a constant.

Problem 9.3 Reflection and Scattering

Given the integral form of 1D Schrödinger equation

$$\psi(x) = \psi_0(x) - \frac{im}{k\hbar^2} \int_{-\infty}^{\infty} e^{ik|x-x'|} V(x')\psi(x') dx'$$

derive an expression for the coefficient of reflection R in the Born approximation. Using that result, calculate the transmission coefficient $T = 1 - R$ for the scattering on a finite square well and compare the obtained coefficient with the exact result.

Hint: Consider wave function in the limit $x \rightarrow \infty$.

Problem 9.4 *Scattering on a Sphere*

Calculate the amplitude of scattering on the potential

$$V(\mathbf{r}) = \begin{cases} V_0 & r \leq a, \\ 0 & r > a \end{cases}$$

in the Born approximation. Show that the total cross section is

$$\sigma \approx 4\pi \left(\frac{2ma^3V_0}{3\hbar^2} \right)^2$$

for low energies.

Problem 9.5 *Scattering on a Massive Fermion*

A particle with spin $\frac{1}{2}$, mass m and energy E is scattering on the target of infinite mass and spin $\frac{1}{2}$. If both particle and the target are not polarised, and interaction potential is

$$V(r) = \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \frac{V_0}{a^2 + r^2},$$

calculate the total cross section in the Born approximation.

Hint: Express the spin interaction in the basis \mathbf{S}^2 , \mathbf{S}_1^2 and \mathbf{S}_2^2 . Sum up the cross sections over the final states and average them over the initial spin states.

Problem 9.6 *Partial Waves Method for Coulomb Potential*

A particle is scattering on the potential

$$V(\mathbf{r}) = \frac{g}{r^2},$$

where $g > 0$ is a constant.

a) Prove that the partial waves are given by

$$\delta_l = \frac{\pi}{2} \left(l + \frac{1}{2} - \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu g}{\hbar^2}} \right).$$

b) Find the energy-dependence of the total cross section for a constant scattering angle.

c) Find the phase shifts for $\frac{2\mu g}{\hbar^2} \ll 1$ and show that the differential cross section equals

$$\frac{d\sigma}{d\vartheta} = \frac{g^2 \mu \pi^3}{2\hbar^2 E} \cot \frac{\vartheta}{2}.$$

d) Calculate the cross section for this potential in the Born approximation and compare it with results obtained from partial waves.

10 Complex and effective potentials

Problem 10.1 Ground State of Helium Atom

In this problem we will calculate the approximate ground state energy of the helium atom (its real value has been measured to be -78.975 eV). The Hamiltonian for the helium atom (ignoring small corrections) is given by:

$$H = -\frac{\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\epsilon_0} \left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \right)$$

- First ignore the electron-electron repulsion (the last term). Find the exact wave function, ψ_0 , for this Hamiltonian and the corresponding energy.
- Taking ψ_0 as the trial wave function, use the variational principle to find the ground state energy.
- A better choice of the trial function comes if instead of completely ignoring the influence of the other electron, we assume that each electron represents a cloud of negative charge which partially shields the nucleus, so that the other electron actually sees an effective nuclear charge Z that is somewhat less than 2. This suggests that we use a trial wave function of the form

$$\psi_1(\mathbf{r}_1, \mathbf{r}_2) \equiv \frac{Z^3}{\pi a^3} e^{-Z(r_1+r_2)/a}$$

where Z is to be treated as a variational parameter. Using ψ_1 find the ground state energy.

Problem 10.2 Kronig–Penney Potential

For the Kronig–Penney potential, schemed on the figure above ([source: Wikipedia](#)), take the parameters: $V_0 = 5$ eV, $a = 2$ Å i $b = 2$ Å. From the equations

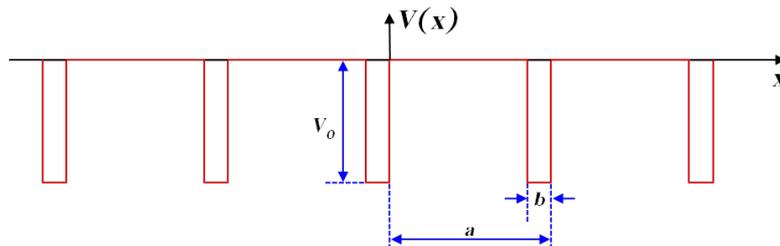


Fig. 34: A scheme of the Kronig–Penney potential.

$$\cos ql = \alpha_1 \cos kl + \beta_1 \sin kl$$

if $E < V_0$ and

$$\cos ql = \cosh 2\kappa a \cos 2kb + \frac{\epsilon}{2} \sinh 2\kappa a \sin 2kb$$

if $E > V_0$, determine the energies of the lowest bands and draw them.