Übungen zum Integrierten Kurs Quantenmechanik

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Blatt 1

Aufgabe EXP-1: *Photoeffekt*

a) Germanium (Ge) hat eine Grenzwellenlänge von $\lambda_0 = 248\,\text{nm}$. Berechnen Sie die Austrittsarbeit der Photoelektronen in eV.

b) Natrium (Na) hat eine Grenzwellenlänge von $\lambda_0 = 451\,\text{nm}$. Berechnen Sie die maximal mögliche Bremsspannung bei Bestrahlung mit Licht der Wellenlänge $\lambda = 400\,\text{nm}$.

Aufgabe EXP-2/TH-1: *Compton Streuung*

a) Ein Photon γ mit dem Viererimpuls $k^\mu = (E, E, 0, 0)$ wird an einem ruhenden Elektron e^- mit Masse m_e gestreut. Nach der Streuung hat das Photon den Viererimpuls $k'^\mu = (E', E' \cos\Theta, E' \sin\Theta, 0)$. Man zeige, daß die Energie E' des gestreuten Photons gegeben ist durch

$$E' = \frac{E}{1 + \frac{E}{m_e}(1 - \cos\Theta)} \quad .$$

Geben sie auch die kinetische Energie des Elektrons nach dem Stoß an.

b) Ein ^{37}Cs Isotop emittiert γ-Strahlen einer Wellenlänge von $1.878\,\text{pm}$. Diese werden an einem NaCl Kristall gestreut. Unter einem Winkel von $60°$ wird gestreutes Licht mit einer Wellenlänge von $3.091\,\text{pm}$ gemessen. Berechnen Sie die Compton Wellenlänge des Elektrons, sowie die Plancksche Konstante $\hbar$.

Aufgabe EXP-3/TH-2: *Hohlraumstrahlung*

In einem Hohlraum mit Wandtemperatur T herrscht im thermodynamischen Gleichgewicht ein elektromagnetisches Strahlungsfeld mit der spektralen Energiedichte

$$u(\nu, T) = \frac{8\pi}{c^3} \frac{h\nu^3}{e^{h\nu/kT} - 1} \quad .$$

a) In einer Wand des Hohlraums befindet sich ein kleines Loch der Fläche ΔA, und im Winkel Θ zur Flächennormalen geneigt ist in großem Abstand ein Detektor aufgestellt. Der Detektor überdeckt nur eine kleine Raumwinkelöffnung $\Delta\Omega \ll 4\pi$. Während der Zeit Δt wird im Frequenzintervall $[\nu, \nu + d\nu]$ die Strahlungsenergie

$$\Delta E d\nu = L(\nu, T) d\nu \Delta A \Delta\Omega \Delta t$$

registriert.

Wie hängt $L(\nu, T)$ mit $u(\nu, T)$ zusammen? Stellen Sie auch einen Zusammenhang für die in den gesamten Halbraum $\Delta\Omega = 2\pi$ ausgestrahlte Energie her, d.h. bestimmen Sie $L_{\text{ges}}(\nu, T)$.

b) Das Wiensche Verschiebungsgesetz besagt, daß die Wellenlänge λ_{max}, bei der maximale Strahlungsemission des schwarzen Körpers erfolgt, umgekehrt proportional zur Temperatur T ist. Bestimmen Sie zunächst $u(\lambda, T)$ und daraus die Proportionalitätskonstante in Abhängigkeit von $\hbar$.

c) Zeigen Sie ausgehend vom Planckschen Strahlungsgesetz die Gültigkeit des Stefan-Boltzmannschen Gesetzes

$$S = \frac{c}{4} \int_0^\infty u(\nu, T) d\nu = \sigma T^4$$

für die gesamte Strahlungsintensität des schwarzen Körpers bei einer Temperatur T. Bestimmen Sie die Proportionalitätskonstante σ in Abhängigkeit von $\hbar$.

d) Leiten Sie aus dem Planckschen Strahlungsgesetz das Rayleigh-Jeans, sowie das Wiensche Strahlungsgesetz als Grenzfälle ab.

Aufgabe EXP-4: *Sonne als "Schwarzer Strahler"*

Die Sonne kann in guter Näherung als "Schwarzer Strahler" angesehen werden ($T \simeq 6000\,\text{K}$). Berechnen Sie

a) die gesamte auf die Erde einfallende Strahlungsleistung und

b) den Prozentsatz der im sichtbaren Spektralbereich liegenden Strahlungsleistung.

Angaben: Abstand Erde-Sonne: $1.5 \times 10^8\,\text{km}$, Erdradius: $6.37 \times 10^3\,\text{km}$, Sonnenradius: $694.33 \times 10^3\,\text{km}$, sichtbarer Spektralbereich: $4 \times 10^{14}\,\text{Hz} - 7 \times 10^{14}\,\text{Hz}$

Aufgabe TH-4: *Wiederholung: δ-Distribution*

Die Diracsche δ-Distribution ist ein linearer Integraloperator, der durch seine Wirkung auf einen geeigneten Raum von Testfunktionen $f(x)$, die bei $x = 0$ stetig sind, gemäß

$$\int_{-\infty}^{\infty} f(x)\delta(x) = f(0)$$

definiert ist. Die Delta-"Funktion" läßt sich als Grenzfall einer Folge von Funktionen $\delta_n(x)$ auffassen, die ein stark ausgeprägtes Maximum bei $x = 0$ aufweisen und die Eigenschaften

$$\int_{-\infty}^{\infty} \delta_n(x) = 1 \text{ bzw. } \lim_{n\to\infty} \int_{-\infty}^{\infty} \delta_n(x) = f(0)$$

erfüllen.

a) Bestimmen Sie die Vorfaktoren g_n, für die die Funktionenfolgen

(1) $\delta_n(x) = g_n \begin{cases} 1 & : \; -1/n \leq x \leq 1/n \\ 0 & : \; \text{sonst} \end{cases}$

(2) $\delta_n(x) = g_n/(1 + nx^2)$

(3) $\delta_n(x) = g_n \exp(-nx^2)$

die oben genannten Bedingungen erfüllen.

b) Sei $h(x)$ eine Funktion mit einfachen Nullstellen x_i ($i = 1, \dots, n$), deren Ableitung $h'(x)$ bei $x = x_i$ stetig ist. Zeigen Sie

$$\delta(h(x)) \sum_{i=1}^{n} \frac{1}{|h'(x_i)|} \delta(x - x_i) \quad .$$

c) Definieren Sie die Ortsableitung $\delta\prime(x)$ der Delta Distribution über ihre Wirkung auf eine Testfunktion $f(x)$.

Aufgabe EXP-5: *Wirkung*

a) Erklären Sie die Bedeutung der Wirkung hinsichtlich der klassischen/quantenmechanischen Behandelbarkeit physikalischer Probleme.

b) Entscheiden Sie damit, ob ein Federpendel der Masse $m = 1\,\mathrm{kg}$, maximaler Auslenkung $x = 0.2$ m und Schwingungsperiode $T = 1\,\mathrm{s}$ klassisch behandelt werden kann.

c) Was gilt in dieser Hinsicht für die Streuung eines α Teilchens mit einer Energie von 40 MeV und einer Masse von 6.7×10^{-27} kg an einem Kupfer-Kern mit Radius $5.6\,\mathrm{fm}$?

d) Betrachten Sie das Bohrsche Atommodell im Bereich hoher Anregungen, d.h. für $L = n\hbar \gg \hbar$. Können Sie hier eine Parallele zur klassischen Behandlung des Elektrons auf einer Kreisbahn und der dadurch bedingten Abstrahlung eines Photons ziehen?

Aufgabe TH-5: *Wiederholung: Fourier-Transformation*

Die Fourier-Transformierte $\hat{f}(k)$ einer Funktion $f(x)$ ist definiert durch

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

(sofern dieses Integral existiert).

a) Zeigen Sie:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(k) e^{ikx} dk \quad .$$

b) Berechnen Sie die Fourier-Transformierte der Ableitung $f'(x)$ in Abhängigkeit der Fourier-Transformierten $\hat{f}(k)$ von f.

c) Berechnen Sie die Fourier-Transformierte von $h(x) = f(x)g(x)$ in Abhängigkeit der Fourier-Transformierten von f und g.

Exercises in Quantum Mechanics – Integrated Course

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Sheet 2

Ex. TH-2.1: *Matrix representation*

a) Consider two kets $|\alpha\rangle$ and $|\beta\rangle$. Suppose $\langle a_i|\alpha\rangle$ and $\langle a_i|\beta\rangle$ are all known, where $\{|a_i\rangle\}$ form a complete set of base kets. Find the matrix representation of the operator $|\alpha\rangle\langle\beta|$ in that basis.

b) We now consider a spin-1/2 system and let $|\alpha\rangle$ and $|\beta\rangle$ be $|s_z;+\rangle$ and $|s_x;+\rangle$, respectively. Write down explicitly the square matrix that corresponds to $|\alpha\rangle\langle\beta|$ in the usual ($\hat{S}_z$ diagonal) basis. What if $|\alpha\rangle = |s_y;-\rangle$ and $|\beta\rangle = |s_x;-\rangle$?

Ex. TH-2.2: *Null and projection operators*

Consider a ket space spanned by the eigenkets $\{|a_i\rangle\}$ of a Hermitian operator $\hat{A}$. There is no degeneracy.

a) Prove that

$$\prod_i (\hat{A} - a_i)$$

is the null operator.

b) What is the significance of

$$\prod_{j\neq i} \frac{(\hat{A} - a_j)}{(a_i - a_j)}\ ?$$

c) Check that the operator $\hat{P}_i = |a_i\rangle\langle a_i|$ is a *projection operator*, i.e. is Hermitian and idempotent ($\hat{P}_i^2 = \hat{P}_i$).

d) Illustrate (a) and (b) using $\hat{A}$ set equal to $\hat{S}_z$ of a spin-1/2 system.

Ex. TH-2.3: *Commutation relations*

Let's introduce the shorthand notation $|\pm\rangle \equiv |s_z;\pm\rangle$. Using the orthonormality of $|+\rangle$ and $|-\rangle$, prove

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\, S_z.$$

Ex. TH-2.4: *Spin operator in arbitrary direction*

Find the eigenkets of the spin operator in an arbitrary direction, i.e. the operator $\hat{\mathbf{S}}\cdot\mathbf{n}$, where $\hat{\mathbf{S}}$ is the vector operator $(\hat{S}_x, \hat{S}_y, \hat{S}_z)$ and $\mathbf{n}$ is the unit vector $(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$.

Ex. TH-2.5: *Energy levels of a simple two-state system*

A two-state system is characterized by the Hamiltonian

$$\hat{H} = H_{11}|1\rangle\langle 1| + H_{22}|2\rangle\langle 2| + H_{12}\left(|1\rangle\langle 2| + |2\rangle\langle 1|\right)$$

where H_{11}, H_{22}, H_{12} are real numbers with the dimension of energy, and $|1\rangle$ and $|2\rangle$ are eigenkets of some operator different from $\hat{H}$. Use the results of the previous question to find the energy eigenvalues and eigenstates.

Ex. TH-2.6: *Dispersion*

A spin-1/2 system is prepared in an eigenstate of $\hat{\mathbf{S}}\cdot\mathbf{n}$, where $\mathbf{n}$ is the unit vector $(\sin\theta, 0, \cos\theta)$.

a) Suppose s_x is measured. What is the probability of getting $+\hbar/2$?

b) Evaluate the dispersion in s_x on an ensemble of identically prepared states, i.e.

$$\left\langle \left(\hat{S}_x - \langle \hat{S}_x \rangle\right)^2 \right\rangle.$$

Ex. TH-2.7: *Sequence of Stern-Gerlach magnets*

A beam of spin-1/2 atoms goes through a series of Stern-Gerlach-type magnets with the following setup:

a) The first magnet is oriented in the $+z$ direction, and the $-\hbar/2$ component of the beam is directed into a beam dump.

b) The second magnet is aligned at an angle θ with respect to the z axis and the $-\hbar/2$ component is dumped.

c) The third magnet is oriented in the $+z$ direction, and the $+\hbar/2$ component is dumped. What is the intensity of the final $s_z = -\hbar/2$ beam with respect to the initial beam intensity? How must the second magnet be oriented in order to maximize the intensity of the final $s_z = -\hbar/2$ beam?

Ex. TH-2.8: *Schwarz inequality and uncertainty principle*

a) In the lecture we left out the proof of the uncertainty relation

$$\left\langle (\Delta\hat{A})^2 \right\rangle \left\langle (\Delta\hat{B})^2 \right\rangle \geq \frac{1}{4}\left|\left\langle [\hat{A}, \hat{B}] \right\rangle\right|^2.$$

Work out the proof with the help of Sakurai (Sec. I.4). Provide also a proof of the Schwarz inequality

$$\langle \alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2.$$

b) Show that the equality sign in the uncertainty relation holds if the state $|\alpha\rangle$ satisfies

$$\Delta\hat{A}|\alpha\rangle = \lambda\Delta\hat{B}|\alpha\rangle$$

with λ purely imaginary.

Ex. EXP-2.1: *Wave-packet*

The normalized one-dimensional wave-packet of a free particle of mass m is given by

$$\Psi(x,t) = \sqrt{\frac{m\Delta k}{\sqrt{\pi}\left(m + i\hbar t\Delta k^2\right)}}\, e^{-\frac{x^2 m\Delta k^2}{2(m+i\hbar t\Delta k^2)}}.$$

Determine the width Δk in such a way that the probability density $|\Psi(x,t)|^2$ is limited to a region of $\Delta x = 10^{-8}$cm at $t = 0$. How long does it take until Δx is equal to the distance between earth and sun for an electron?

Ex. EXP-2.2: *Group velocity dispersion*

Given is the electromagnetic wave packet (e.g. a laser pulse)

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} A(k)\, e^{i[kx-\omega(k)t]} dk,$$

the function $A(k)$ being non-zero only in a small region Δk around a mean wavenumber-vector k_0.

a) Express the wave-packet $\Psi(x,t)$ by the Fourier transform $A(y) \equiv \frac{1}{\sqrt{2\pi}} \int A(k)\, e^{iky} dk$ of the function $A(k)$. Use the dispersion relation $\omega(k)$ for photons in the vacuum. How does the shape of the wave-packet change with time?

b) With the help of optical spectral analysis the width of a laser pulse was measured to be $\Delta\lambda = 200$nm (around a mean wave length of $\lambda_0 = 800$nm). What is the duration Δt of the pulse, assuming a Gaussian shape $A(k) = e^{-(k-k_0)^2/(\Delta k)^2}$? What is the connection between $\Delta\lambda$ and Δk?

c) Propagating through a medium, each spectral component of of the pulse has a different velocity (*dispersion*). Assuming a quadratic dispersion relation

$$\omega_D(k) = \omega_0 + \omega_1(k-k_0) + \omega_2(k-k_0)^2$$

with the constants $\omega_0 = \omega(k_0)$, $\omega_1 = v_g(k_0)$ and $\omega_2 = \frac{1}{2}\, dv_g(k)/dk|_{k=k_0}$ ("*group velocity distribution*", GVD), compute $\Psi(x,t)$ for the Gaussian profile of b).

d) What is the time-dependence of the laser pulse in c) for non-zero ω_2?

e) Discuss the problems for transmitting short pulses in the presence of GVD. Try to find an arrangement of two prisms which can remove the GVD.

Ex. EXP-2.3: *Hydrogen atom and uncertainty principle*

Classically, an atom in its ground state is treated as point-like particle. Using the uncertainty principle, calculate its dimensions in the ground state by first proving the equation

$$\langle p^2 \rangle = (\Delta p)^2$$

and assuming $\langle r \rangle \approx \Delta r$ (small values of r).

Ex. EXP-2.4: *Stern-Gerlach with electrons?*

Is it possible to use electrons in a Stern-Gerlach like experiment? Discuss with the help of information from publications and the Internet!

Ex. EXP-2.5: *Quantization of angular momentum*

Show

$$\vec{J}^2 = j\,(j+1)\,\hbar^2$$

from

$$\left\langle J_z^2 \right\rangle = \frac{1}{2j+1} \sum_{m=-j}^{m=j} (m\hbar)^2$$

and

$$\vec{J}^2 = J\left\langle J_z^2 \right\rangle$$

Ex. EXP-2.6: *Paramagnetic gas*

The ground state of the Sodium atom (Z=11) has the angular momentum quantum number $j = 1/2$ and the g-factor $g = 2$. The sodium gas is located in a homogeneous magnetic field B applied in the z-direction.

a) Calculate $\vec{J}^2$ and $J_\perp$ and present the m-states of the sodium atom in the vector model.

b) Calculate the energy E_m of the Zeeman-states (in eV) for $B = 1T$.

c) Calculate the magnetization $\vec{M}$ (mean magnetic moment per volume) of the sodium gas in thermal equilibrium at temperature T, as a function of B and particle number density n (mean number of particles per volume). Express the result by the parameter

$$b \equiv \frac{\mu_B B}{kT}$$

with the Bohr Magneton μ_B and the Boltzmann constant k.
Hint: The mean *Besetzungszahl* of a m-state is proportional to $e^{-E_m/kT}$.

d) Give the limits of c) for the cases $kT \ll \mu_B B$ and $kT \gg \mu_B B$.

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Sheet 3

Ex. TH-3.1: *Operators depending on a parameter*

Consider an Operator $\hat{A}$ which depends on a real parameter η (for instance, time). Then we can define the derivative w.r.t. η as

$$\frac{d\hat{A}(\eta)}{d\eta} = \lim_{\varepsilon \to 0} \frac{\hat{A}(\eta+\varepsilon) - \hat{A}(\eta)}{\varepsilon} \quad .$$

Let the operators $\hat{A} = \hat{A}(\eta)$ and $\hat{B} = \hat{B}(\eta)$ both depend on η. Show that

a) $\dfrac{d}{d\eta}(\hat{A}\,\hat{B}) = \dfrac{d\hat{A}}{d\eta}\hat{B} + \hat{A}\dfrac{d\hat{B}}{d\eta}$

b) $\dfrac{d}{d\eta}\hat{A}^n = \displaystyle\sum_{i=1}^{n} \hat{A}^{i-1}\frac{d\hat{A}}{d\eta}\hat{A}^{n-i}$ where $n = 1, 2, 3, \ldots$

c) $\dfrac{d}{d\eta}\hat{A}^{-1} = -\hat{A}^{-1}\dfrac{d\hat{A}}{d\eta}\hat{A}^{-1}$.

Ex. TH-3.2: *Functions of operators*

In general a function $f(\hat{A})$ of an operator $\hat{A}$ can be defined as a power series (f_n denotes the coefficients of the expansion)

$$f(\hat{A}) = \sum_{n=0}^{\infty} f_n \hat{A}^n$$

(we shall not consider the problems concerning the convergence of the series, etc.). When $|a\rangle$ is an eigenket of $\hat{A}$ with eigenvalue a, $|a\rangle$ is also an eigenket of $f(\hat{A})$ with the eigenvalue $f(a)$. For example, the function $e^{\hat{A}}$ of the operator $\hat{A}$ is defined by

$$e^{\hat{A}} = \sum_{k=0}^{\infty} \frac{1}{k!}\hat{A}^k \quad .$$

Consider, for the moment, two operators $\hat{A}$ and $\hat{B}$ which fulfil

$$[\hat{A}, [\hat{A}, \hat{B}]] = 0 \quad \text{and} \quad [\hat{B}, [\hat{A}, \hat{B}]] = 0 \quad .$$

Show that

a) $e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}]$ (this is a special case of the *Baker-Hausdorff relation*).

b) $e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}}e^{[\hat{A},\hat{B}]/2}$ (this is the so-called *Glauber formula*).

c) From now on we do not assume that $[\hat{A},[\hat{A},\hat{B}]] = 0$ and $[\hat{B},[\hat{A},\hat{B}]] = 0$. Show by induction that
$$[\hat{A},\dots[\hat{A},[\hat{A},\hat{B}]]\dots] = \sum_{l=0}^{n}(-1)^l \binom{n}{l} \hat{A}^{n-l}\hat{B}\hat{A}^l$$
for the n-fold commutator.

d) Start with the series expansion of $e^{s\hat{A}}\hat{B}e^{-s\hat{A}}$ around $s=0$, s is a real parameter, to prove that
$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \dots + \frac{1}{n!}[\hat{A},\dots[\hat{A},[\hat{A},\hat{B}]]\dots] + \dots \quad .$$
(standard version of the *Baker-Hausdorff relation*).

Ex. TH-3.3: *Trace of operators*

Prove that

a) $\mathrm{tr}(\hat{X}\hat{Y}) = \mathrm{tr}(\hat{Y}\hat{X})$, where $\hat{X}$ and $\hat{Y}$ are operators

b) $\mathrm{tr}(\hat{X})$ of an operator $\hat{X}$ is independent of the representation.

Ex. TH-3.4: *Commutators of three linear operators*

$\hat{A}$, $\hat{B}$, $\hat{C}$ are linear operators with $[\hat{A},\hat{B}] = 0$ and $[\hat{B},\hat{C}] = 0$.
Does this imply that also $[\hat{A},\hat{C}] = 0$?

Ex. TH-3.5: *Anticommuting operators*

Two Hermitian operators anticommmute:
$$\{\hat{A},\hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A} = 0 \quad .$$
Is it possible to have a simultaneous eigenket of $\hat{A}$ and $\hat{B}$? Prove or illustrate your assertion!

Ex. TH-3.6: *Dispersion and uncertainty relation*

Find the linear combination of $|+\rangle$ and $|-\rangle$ kets that maximize the uncertainty product
$$\left\langle (\Delta\hat{S}_x)^2 \right\rangle \left\langle (\Delta\hat{S}_y)^2 \right\rangle \quad .$$
Verify explicitly that for the linear combination you found, the uncertainty relation for $\hat{S}_x$ and $\hat{S}_y$ is not violated.

Ex. TH-3.7: *Two-dimensional ket space*

Consider a two-dimensional ket space with base kets $|\phi_1\rangle$ and $|\phi_2\rangle$. Acting with an operator $\hat{A}$ on these kets gives
$$\hat{A}|\phi_1\rangle = -|\phi_2\rangle \quad \text{and} \quad \hat{A}|\phi_2\rangle = -|\phi_1\rangle \quad .$$

a) Express $\hat{A}$ with outer products $|\phi_i\rangle\langle\phi_j|$.

b) Check if $\hat{A}$ is Hermitian.

c) Calculate $\hat{A}\hat{A}^\dagger$, $\hat{A}^\dagger\hat{A}$, and $\hat{A}^2$.

d) What are the eigenvalues and eigenkets of $\hat{A}$?

Ex. TH-3.8: *Three-dimensional ket space*

Consider a three-dimensional ket space. If a certain set of orthonormal kets, say, $|1\rangle$, $|2\rangle$, and $|3\rangle$, are used as the base kets, the operators $\hat{A}$ and $\hat{B}$ are represented by

$$\hat{A} \doteq \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix}, \qquad \hat{B} \doteq \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix},$$

where a, b are both real.

a) Show that $\hat{A}$ exhibits a degenerate spectrum. Does $\hat{B}$ also exhibit a degenerate spectrum?

b) Calculate $[\hat{A}, \hat{B}]$.

c) Find a new set of orthonormal kets which are simultaneous eigenkets of both $\hat{A}$ and $\hat{B}$. Specify the eigenvalues of $\hat{A}$ and $\hat{B}$ for each of the three eigenkets. Does your specification completely characterize each eigenket?

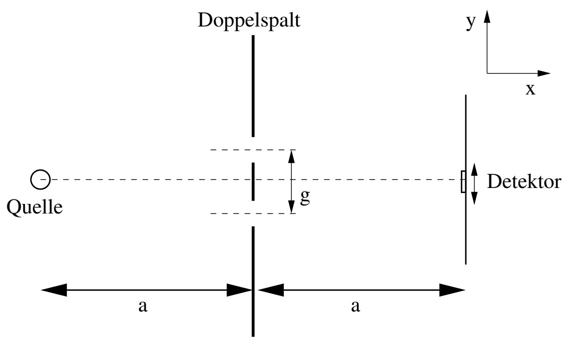
Ex. TH-3.9: *Transformation matrix*

Construct the transformation matrix that connects the $\hat{S}_z$ diagonal basis to the $\hat{S}_x$ diagonal basis. Show that your result is consistent with the general relation

$$U = \sum_n |b^{(n)}\rangle\langle a^{(n)}| \quad .$$

Ex. EXP-3.1: *Double-slit experiment and uncertainty relation*

Consider the diffraction of electrons with momentum p at a double slit structure (slit distance g). The electron source and the detector which can be moved in the y-direction are both located at a distance a from the slit. Assume $a \gg g$.

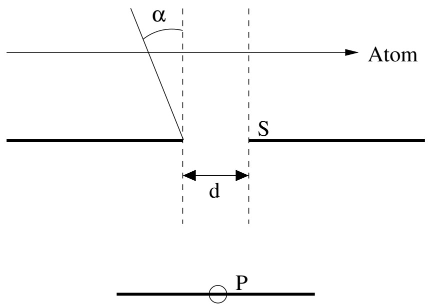


a) For a fixed double slit, determine the width of the 0^{th} order interference maximum (centered around $y = 0$), in other words the position of the 1^{st} minima of interference.

b) Now, consider the double-slit was made moveable in the y-direction, e.g. by putting it on rolls. Evaluating the momentum transfer of the scattered photon to the assembly, one can thus decide through which one of the two slits the electron travelled. Calculate the momentum transferred from the electron to the double slit assembly, and evaluate the minimum value of the uncertainty in the position of the double slit and thus the smearing of the central part of the interference maximum. What changes will be seen in the interference pattern?

Ex. EXP-3.2: *Einstein-Rupp experiment*

The following experiment seems to indicate an inconsistence between wave- and particle picture:



An atom in an excited state (velocity v) passes a slit S with width d parallel to a screen. The monochromatic light of frequency ν emitted from the atom and travelling through the slit is observed by a spectroscope at P. As the light of the atom can only reach point P in the short period t (the time the atom requires to pass the slit), the wave train observed in P has a finite length. Thus, its frequency will not be monochromatic any more and in P one will detect a broadening $\Delta\nu$ of the sharp line with frequency ν, in contradiction to the description by light quanta, where the atom emits monochromatic light.
The mistake in these considerations has been found by Bohr and is linked to the neglect of the Doppler effect and the scattering of the photon at the slit (photons travelling from the atom to P can not only be emitted perpendicularly, but also under an angle α due to the scattering).
Discuss quantitatively by calculating $\Delta\nu$!

Ex. EXP-3.3: *Pound-Rebka experiment; Einstein's "clock in the box"*

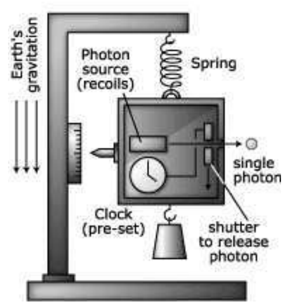
a) The principle of equivalence is the basic principle of the theory of relativity. A consequence is the equality of inertial and heavy mass. Show that the frequency of a photon falling a distance L in a gravitational field is shifted by

$$\frac{\Delta\nu}{\nu} = \frac{gL}{c^2} \quad .$$

b) Calculate this effect for a 14.4keV photon (^{57}Fe source) and $L = 22.6$m. How would you design an experimental setup (source, detector etc.)? The natural line width in this case is $\frac{\Gamma}{\nu} = 1.13 \cdot 10^{-12}$.

c) Einstein always felt uneasy about the consequences of quantum mechanics, and thus he proposed a number of thought experiments which should disprove the uncertainty principle.

Einstein's Light Box
(after a drawing by Bohr)



Discuss the following suggestion: A box filled with radiation can be opened for an arbitrarily short time Δt by a clock inside it. The energy of the escaped photon can be measured very accurately by weighing the box before and after opening it, in contradiction to $\Delta E \Delta t \geq h$. What is the problem in these considerations?

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Sheet 4

Ex. TH-4.1: *Coordinate and momentum operators*

a) Let x and p_x be the coordinate and linear momentum in one dimension. Evaluate the classical Poisson bracket $[x, F(p_x)]_{\text{classical}}$.

b) Let $\hat{x}$ and $\hat{p}_x$ be the corresponding quantum-mechanical operators this time. Evaluate the commutator $[\hat{x}, \exp(i\hat{p}_x a/\hbar)]$.

c) Using the results obtained in b), prove that $\exp(i\hat{p}_x a/\hbar)|x\rangle$ is an eigenstate of the coordinate operator $\hat{x}$. What is the corresponding eigenvalue?

Ex. TH-4.2: *Commutators of functions of coordinate and momentum operators*

a) Verify that for all functions F and G that can be expressed as power series in their arguments

$$[\hat{x}_i, G(\hat{\mathbf{p}})] = i\hbar\,\frac{\partial G}{\partial p_i}, \qquad\qquad [\hat{p}_i, F(\hat{\mathbf{x}})] = -i\hbar\,\frac{\partial F}{\partial x_i}.$$

b) Evaluate $[\hat{x}^2, \hat{p}^2]$. Compare your results with the classical Poisson bracket $[x^2, p^2]_{\text{classical}}$.

Ex. TH-4.3: *Gaussian wave packet*

Consider a Gaussian wave packet, whose position-space wave function is

$$\langle x|\alpha\rangle = \frac{1}{\sqrt{d\sqrt{\pi}}}\exp\left(ikx - \frac{x^2}{2d^2}\right).$$

a) Compute the expectation values of the operator $\hat{p}$ and $\hat{p}^2$.

b) Repeat the calculation using the momentum-space wave function

$$\langle p|\alpha\rangle = \sqrt{\frac{d}{\hbar\sqrt{\pi}}}\exp\left(-\frac{(p-\hbar k)^2 d^2}{2\hbar^2}\right).$$

Ex. TH-4.4: *Coordinate operator in momentum space*

a) Prove that

$$\langle p|\hat{x}|\alpha\rangle = i\hbar\frac{\partial}{\partial p}\langle p|\alpha\rangle,$$
$$\langle \beta|\hat{x}|\alpha\rangle = \int dp\,\langle\beta|p\rangle\, i\hbar\frac{\partial}{\partial p}\langle p|\alpha\rangle.$$

b) What is the physical significance of the operator $\exp(i\hat{x}p_0/\hbar)$, where p_0 is some number with the dimension of momentum?

Ex. TH-4.5: *Translation operator*

The translation operator for a finite (spatial) displacement is given by $\hat{\mathcal{T}}(\mathbf{l}) = \exp\left(-\frac{i\,\hat{\mathbf{p}}\cdot\mathbf{l}}{\hbar}\right)$.

a) Evaluate $\left[\hat{x}_i, \hat{\mathcal{T}}(\mathbf{l})\right]$.

b) Demonstrate how the expectation value of $\hat{x}$ changes under translation.

c) Using $[\hat{\mathbf{x}}, \hat{\mathcal{T}}(d\mathbf{x})] = d\mathbf{x}$ and $[\hat{\mathbf{p}}, \hat{\mathcal{T}}(d\mathbf{x})] = 0$, prove that under an infinitesimal translation $\langle\hat{\mathbf{x}}\rangle \to \langle\hat{\mathbf{x}}\rangle + d\mathbf{x}$ and $\langle\hat{\mathbf{p}}\rangle \to \langle\hat{\mathbf{p}}\rangle$

Ex. TH-4.6: *Commutator of momentum operators*

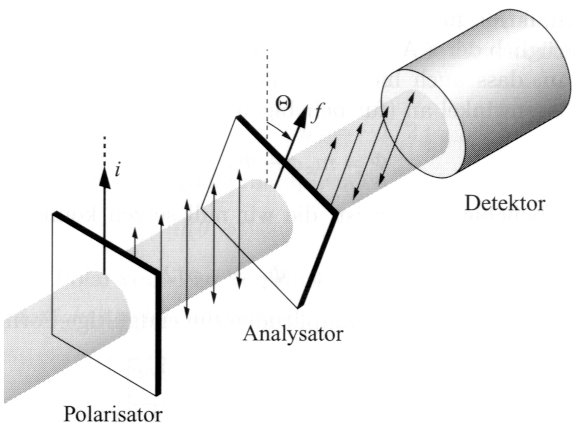
Prove that $[\hat{p}_i, \hat{p}_j] = 0$.

Ex. TH-4.7: *Ice pick in the balance*

Estimate the order of magnitude of the time that an ice pick can be balanced on its point if the only limitation is that set by the Heisenberg uncertainty principle. Assume that the point is infinitely sharp and hard and that it is sitting on an infinitely hard and smooth surface. Assume reasonable values for the dimensions and weight of the ice pick.

Ex. EXP-4.1: *Malus's law*

With the help of a polarizer, a beam of monochromatic light is converted into a linearly polarized beam (direction of polarization i). This beam hits an analyzer with direction of polarization f which is rotated by an angle θ with respect to the polarizer (see figure). Finally, a photomultiplier detects the photons in the transmitted beam.



a) Calculate the projection probability $P\,(f \leftarrow i)$ as a function of the angle θ, where i and f indicate states of photons polarized linearly in direction i or f, respectively.
Hint: Use the Poynting-vector

$$S\,(z,t) = \frac{1}{\mu_0} E\,(z,t)\,B\,(z,t) = \frac{1}{\mu_0 c} E^2\,(z,t)$$

We now measure, for different values of the angle θ, the number Z' of photons detected in the photomultiplier after a fixed time of exposition t_0. The results are given in the following table:

θ	Z'
$0°$	5056
$30°$	3750
$45°$	2598
$90°$	74

b) Using the data from the table above, calculate the ratio of the number of photons in the incident beam and in the transmitted beam $(Z_f(\theta)/Z_i)$ for the angles $\theta = 30°$ and $\theta = 45°$.
Hint: Assume $Z'(90°)$ was the mean extent of the background radiation and $Z'(0°)$ the mean number of photons in the incident beam.

c) Determine the statistical errors for the results in b) and compare the results with the respective projection probabilities of a).

Ex. EXP-4.2: *Elliptical polarization*

A monochromatic plane em-wave in free space propagates in the z-direction of a Cartesian coordinate system. The **E**-field of a general wave of this kind is of the form

$$\begin{aligned} E_x(z,t) &= E_{0x}\cos(kz - \omega t) \\ E_y(z,t) &= E_{0y}\cos(kz - \omega t + \epsilon) \\ E_z(z,t) &\equiv 0 \end{aligned}$$

a) Show that **E** describes an ellipse in every plane z =const. (*elliptically* polarized wave). Set up the equation of the ellipse in the coordinate system (x', y') of the principal axes of the ellipse.

b) For what parameter values is is the wave *linearly* polarized?

c) For what parameter values is the wave polarized left- or right*circularly*?

d) Show that a general elliptically polarized wave can be expressed as a superposition of two waves with polarization

   - to the basis (x, y)
   - to the basis (R, L).

   Hint: For the case of the basis (R, L) use the coordinate system of the principal axes of the ellipse.

e) Using the results of d), calculate the projection probabilities $P(x \leftarrow p)$, $P(y \leftarrow p)$ and $P(R \leftarrow p)$, $P(L \leftarrow p)$, where p is a state of elliptical polarization, and verify the completeness relation with respect to the bases (x, y) and (R, L).

Ex. EXP-4.3: *Spin "1"*

The spin quantum number of an atom in its ground state be $j = 1$.

a) Formulate the completeness relation with respect to the z-component $\mathbf{J}_z$ of the angular momentum!

b) Formulate the respective orthogonality relations, expressed by the projection probabilities!

c) Give an outline of an experiment that can be used to test the results of a) and b)!

<u>Ex. EXP-4.4</u>: *Distance between photons in interference experiments*

Assume a laser beam in a quantum interference experiments has a mean intensity of $N \approx 10^3$ photons/sec. What is the mean distance d between two photons?

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<u>Ex. TH-5.1</u>: *Spin precession*

The Hamiltonian of a spin-1/2 particle with charge q and mass m in a static magnetic field is given by

$$\hat{H} = -\frac{q}{mc}\,\hat{\mathbf{S}} \cdot \mathbf{B}$$

Suppose B points in the z direction and that at a time $t = 0$ the particle is in a generic pure state.

a) Find out the expectation values of the operators $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$. What happens if the initial state is an eigenstate of $\hat{S}_z$? And if it is an eigenstate of $\hat{S}_x$?

b) Write down the Heisenberg equations of motions for the time-dependent operators $\hat{S}_x(t)$, $\hat{S}_y(t)$, $\hat{S}_z(t)$ and solve them to obtain the expectation values.

<u>Ex. TH-5.2</u>: *Coordinate operators at different times*

Let $\hat{x}(t)$ be the coordinate operator for a free particle in one dimension in the Heisenberg picture. Evaluate $[\hat{x}(t), \hat{x}(0)]$.

<u>Ex. TH-5.3</u>: *Quantum virial theorem*

Consider a particle in three dimensions whose Hamiltonian is given by

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}})$$

By calculating $[\hat{\mathbf{x}} \cdot \hat{\mathbf{p}}, \hat{H}]$ obtain

$$\frac{d}{dt}\langle \hat{\mathbf{x}} \cdot \hat{\mathbf{p}} \rangle = \left\langle \frac{\hat{\mathbf{p}}^2}{m} \right\rangle - \langle \hat{\mathbf{x}} \cdot \nabla \hat{\mathbf{V}} \rangle$$

To identify the preceding relation with the quantum-mechanical analogue of the virial theorem it is essential that the left-hand side vanish. Under what conditions would this happen?

<u>Ex. TH-5.4</u>: *Time evolution of a two-state system*

Let $|a_1\rangle$ and $|a_2\rangle$ be nondegenerate eigenstates of a Hermitian operator $\hat{A}$ with eigenvalues a_1 and a_2. The Hamiltonian is

$$\hat{H} = |a_1\rangle \delta \langle a_2| + |a_2\rangle \delta \langle a_1|,$$

where δ is a real number.

a) Find the energy eigenstates and eigenvalues.

b) Write down the state vector $|a(t)\rangle$ in the Schrödinger picture for $t > 0$ if $|a(0)\rangle = |a_1\rangle$.

c) What is the probability of finding the system in $|a_1\rangle$ at a time $t > 0$?

d) Can you think of a physical situation corresponding to this problem?

Ex. TH-5.5: *Sum rule for a one-dimensional system*

Consider a particle in one dimension whose Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

By calculating $[[\hat{H}, \hat{x}], \hat{x}]$ prove that

$$\sum_j \left|\langle E_i|\hat{x}|E_j\rangle\right|^2 (E_j - E_i) = \frac{\hbar^2}{2m}$$

where $|E_i\rangle$ are the energy eigenkets.

Ex. TH-5.6: *Time evolution of the variance of a wave packet*

Consider a free-particle wave packet in one dimension. Initially it satisfies the minimum uncertainty relation. Using the Heisenberg picture, obtain $\langle \Delta\hat{x}^2(t)\rangle$, when $\langle \Delta\hat{x}^2(0)\rangle$ is given. (Hint: take advantage of the result of Ex. TH-2.8 b).

Ex. TH-5.7: *Harmonic oscillator*

The Hamiltonian for the single harmonic oscillator is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2$$

where ω is the angular frequency of the classical oscillator.

a) Recall the classical equations of motions, i.e., $x(t)$ and $p(t)$.

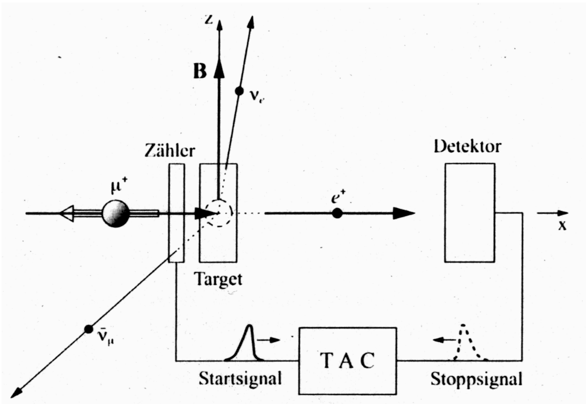
b) Derive the equations of motion for the operators $\hat{x}(t)$ and $\hat{p}(t)$ in the Heisenberg picture and demonstrate that the expectation values fulfill the classical equations of motion.

c) Does this also hold for a potential of the form $V(x) = kx^4$, with $k =$ const.?

Ex. TH-5.8: *One-dimensional box*

Consider the one-dimensional movement of a particle in a box, $x \in [-a, a]$, in position space, described by a discrete set of Schrödinger wave functions $\psi_n(x)$. What are the boundary conditions for $\psi_n(x)$ such that $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ is a Hermitian operator?

Ex. EXP-5.1: *μSR-experiment*



The decay rate of muons as a function of their lifetime t is given by

$$Z(t) = Z_0 e^{-t/\tau}\left[1 - \frac{1}{3}\cos\left(\frac{\Delta E_B}{\hbar}t\right)\right]$$

with ΔE_B being the splitting of the energy of the muon in the magnetic field and $\tau \equiv \tau_\mu$ its mean lifetime.

a) Calculate the number $N(E; t_1, t_2)$ of decays of the muon in the time interval $t_1 \leq t \leq t_2$ as a function of its energy for the cases

   i) $0 \leq t \leq \tau$ and

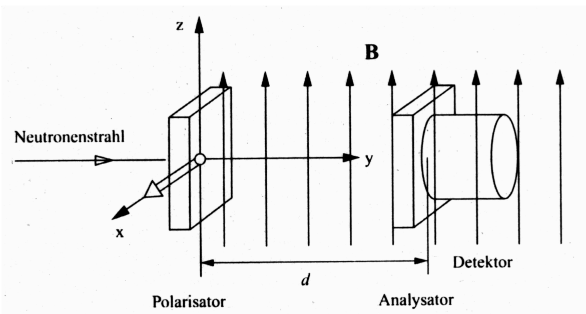
   ii) $\tau \leq t \leq \infty$.

b) Determine for the cases i) and ii) the probability of a decay of the muon as a function of its energy E:

$$P(E; t_1, t_2) = \frac{N(E; t_1, t_2)}{\int_{t_1}^{t_2} Z_0\, e^{-t/\tau} dt}$$

Ex. EXP-5.2: *Neutrons in a magnetic field*

A monochromatic beam of neutrons (de Broglie wavelength $\lambda = 1.55\,\text{Å}$, spin$= 1/2$, g-factor$= -3.83$, proton-mass $m_p = 938\ \text{MeV}/c^2 \simeq$ neutron-mass m_n) is polarized by a polarizer in x-direction and enters a region with a homogeneous magnetic field oriented in the z-direction ($B = 1.55 \cdot 10^{-3}$T).



In the distance d from the polarizer an analyzer movable in the y-direction is permeable for neutrons polarized in the x-direction. The passing neutrons are counted by an attached detector as a function of the distance d.

Calculate the probability of detection $P(d)$ of a neutron entering the magnetic field as a function of the distance d and sketch it. The decay of neutrons may be neglected.

<u>Ex. EXP-5.3</u>: *Quantum amplitudes and phases*

In the lecture, you have learned about quantum amplitudes $\langle R|r\rangle$ between linear and circular polarized light that form the basis of projection probabilities. Show that the quantum amplitude

$$\langle R|r\rangle = \langle R|x\rangle\langle x|r\rangle + \langle R|y\rangle\langle y|r\rangle$$

cannot be real but must be complex. Then, show that the respective phase can be chosen arbitrarily.

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Ex. TH-6.1: *Density operator (I)*

a) Convince yourself that the density operator ρ for a mixed ensemble fulfills $\mathrm{Tr}(\rho^2) < 1$.

b) The matrix representations of the operators A, B, and C in the $|\pm\rangle$ basis read

$$A = \begin{pmatrix} 3 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad B = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad , \quad c = \begin{pmatrix} 0 & 2i \\ -2i & 0 \end{pmatrix} \quad .$$

The following ensemble averages have been measured on a spin system:

$$[A] = 2 \ , \ \ [B] = \frac{1}{2} \ , \ \ [C] = 0 \ .$$

Use this information to construct the density matrix of the spin system and check if it is a pure or a mixed ensemble.

Ex. TH-6.2: *Density operator (II)*

A Stern-Gerlach apparatus is oriented in the direction of

$$\vec{n} = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta) \ ,$$

i.e., it can be used to prepare spin states

$$|\vec{n}; +\rangle = \begin{pmatrix} \cos(\vartheta/2) \\ e^{i\varphi}\sin(\vartheta/2) \end{pmatrix} \quad , \quad |\vec{n}; -\rangle = \begin{pmatrix} -\sin(\vartheta/2) \\ e^{i\varphi}\cos(\vartheta/2) \end{pmatrix}$$

(given in the usual $|\pm\rangle$ basis). Consider a mixed ensemble of the two spin states with probabilities w_+ and w_-.

a) Show that the density matrix in the $|\pm\rangle$ basis is given by

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + (w_+ - w_-)\cos\vartheta & (w_+ - w_-)e^{-i\varphi}\sin\vartheta \\ (w_+ - w_-)e^{i\varphi}\sin\vartheta & 1 - (w_+ - w_-)\cos\vartheta \end{pmatrix} \quad .$$

b) Calculate the ensemble averages

$$P_i \equiv [\sigma_i] = \mathrm{Tr}(\rho\sigma_i) \quad \text{where} \quad i = x, y, z \quad ,$$

and show that ρ can be written as

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + P_z & P_x - iP_y \\ P_x + iP_y & 1 - P_z \end{pmatrix} = \frac{1}{2}(1 + \vec{P}\cdot\vec{\sigma}) \quad .$$

Ex. TH-6.3: *Orthogonality of bound-state solutions*

$\Psi_1(x)$ and $\Psi_2(x)$ are bound-state solutions (real valued) of the Schrödinger equation with energy eigenvalues E_1 and $E_2 \neq E_1$, respectively. Show with the help of the Wronski determinant that $\Psi_1(x)$ and $\Psi_2(x)$ are orthogonal.

Ex. TH-6.4: *"Theorem about oscillations"*

In the lecture we have discussed the "Theorem about oscillations" stating that for two bound-state solutions of the Schrödinger equation $\Psi_{1,2}(x)$ with eigenvalues $E_2 > E_1$ at least one zero of Ψ_2 has to be found in the x interval spanned by two successive zeros of Ψ_1. Find a proof of this assertion (hint: proof by contradiction).

Ex. TH-6.5: *Particle in a one-dimensional potential*

Consider a particle of mass m in a one-dimensional potential of the form

$$V(x) = \begin{cases} V_1 > 0 & & -\infty < x \leq -x_0 \\ 0 & \text{for} & -x_0 < x < x_0 \\ V_3 > V_1 > 0 & & x_0 \leq x < \infty \end{cases} \quad .$$

Consider only energies in the range $0 \leq E < V_1$ (bound-states).

a) Specify the Schrödinger equation for each of the three different regions using

$$k^2 = \frac{2m}{\hbar^2}E \ , \ \kappa_{1,3}^2 = \frac{2m}{\hbar^2}(V_{1,3} - E) \ .$$

Specify the conditions following from the continuity of the wave function and their first derivative.

b) Show that the energy spectrum can be determined from the condition

$$1 = e^{-4ikx_0}\frac{V_3}{V_1}\left(\frac{k + i\kappa_1}{k - i\kappa_3}\right)^2$$

(if necessary you can use Maple or Mathematica to solve the system of equations).

c) Discuss why the energy spectrum is discrete [graphical discussion of the result in b)].

Ex. TH-6.6: *Double-δ-potential*

Consider a particle of mass m in a potential of the form

$$V(x) = -V_0\delta(x + x_0) - V_0\delta(x - x_0) \ \text{with} \ V_0 > 0 \ .$$

Compute the normalized eigenfunction for all bound-states. How many bound-states exist as a function of V_0? What happens for $x_0 \to 0$?

Ex. TH-6.7: *Scattering off a combined δ/rigid wall potential*

Consider an incoming wave $\Psi_{\text{in}} = e^{ik_0x}$, $k_0^2 = (2m/\hbar^2)E$, from $-\infty$ scattering off a potential of the form

$$V(x) = \begin{cases} \frac{\hbar^2 V_0}{2m}\delta(x + x_0) & \text{for} \quad x \leq 0, x_0 > 0 \\ +\infty & \text{for} \quad x > 0 \end{cases} \quad .$$

Compute the *amplitude* of the reflected wave as a function of the energy E. What happens for $V_0 = 0$ and $V_0 = \infty$?

Ex. EXP-6.1: *two-level atom and photon*

a) Inform yourselves on the concept of creation- and annihilation operators!

b) Investigate the interaction of a photon with a two-level atom with the Hamilton-operator

$$H = E_1 a_1^+ a_1 + E_2 a_2^+ a_2 + \hbar\omega b^+ b + G a_2^+ a_1 b + G a_1^+ a_2 b$$

with $E_2 - E_1 = \hbar\omega$. a_j^+, a_j are the creation- and annihilation operators for electrons, b^+, b for photons, respectively. In this context it is sufficient to treat a^+, a analogous to the operators b^+, b. ϕ_0 be the combined vacuum state. For the wave function, use

$$\psi = c_1(t)\, a_1^+ b^+ \phi_0 + c_2(t)\, a_2^+ \phi_0.$$

Verify the following rules:

$$\begin{aligned} a_1^+ a_1 \cdot a_1^+ b^+ \phi_0 &= a_1^+ b^+ \phi_0 \\ a_2^+ a_2 \cdot a_1^+ b^+ \phi_0 &= 0 \\ a_2^+ a_1 b \cdot a_1^+ b^+ \phi_0 &= a_2^+ \phi_0 \\ a_1^+ a_2 b^+ \cdot a_1^+ b^+ \phi_0 &= 0 \\ a_1^+ a_1 a_2^+ \phi_0 &= 0 \\ a_2^+ a_2 a_2^+ \phi_0 &= a_2^+ \phi_0 \\ a_2^+ a_1 a_2^+ \phi_0 &= 0 \\ a_1^+ a_2 b^+ a_2^+ \phi_0 &= a_1^+ b^+ \phi_0 \end{aligned}$$

Ex. EXP-6.2: *Hilbert space*

Prove that the spin wave functions constitute a Hilbert space!

Ex. EXP-6.3: *entanglement*

Show that the wave function

$$\psi(1,2) = \frac{1}{\sqrt{2}} \left(|\downarrow\rangle |\downarrow\rangle + |\uparrow\rangle |\uparrow\rangle \right)$$

can be written as an entanglement of the wave functions

$$\varphi_1(1) = d_1 |\downarrow\rangle_1 + d_2 |\uparrow\rangle_1, |d_1|^2 + |d_2|^2 = 1, \varphi_2(2) = d_2^* |\downarrow\rangle_2 - d_1^* |\uparrow\rangle_2.$$

Ex. EXP-6.4: *local realistic theories; EPR experiments; Bell inequality*

We try to define a local realistic theory as a substitute for quantum theories.

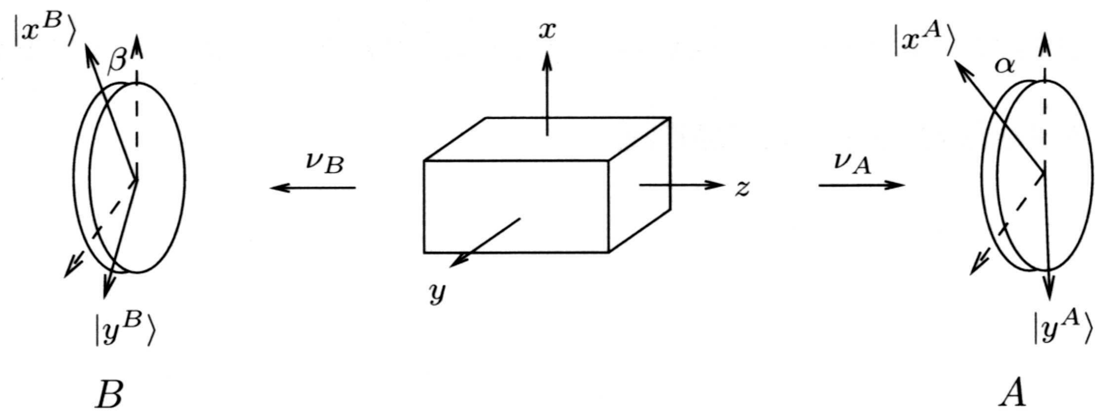
a) What does local-realistic theory mean in contrast to quantum theory? In what way is quantum theory considered to be "incomplete"?

b) In a local realistic theory we consider a source that produces particles characterized by a set of parameters λ. Particles (e.g. photons) are produced with a probability density $\rho(\lambda)$, with

$$\int \rho(\lambda)\, d\lambda = 1, \rho(\lambda) \leq 0.$$

In places A and B the polarization of the emitted photons is measured, and the result is well-defined, ± 1:

$$S_A^{\lambda}(\delta_1) = (+1, -1), S_B^{\lambda}(\delta_2) = (+1, -1)$$



The classical correlation coefficient is defined as

$$\epsilon(\delta_1, \delta_2) = \int \rho(\lambda)\, S_A^{\lambda}(\delta_1)\, S_B^{\lambda}(\delta_2)\, d\lambda.$$

In our special case, the experimentally verified complete correlation for the special case of identical orientation δ of the polarizers shall be fulfilled:

$$\epsilon^{kl}(\delta, \delta) = \int \rho(\lambda)\, S_A^{\lambda}(\delta)\, S_B^{\lambda}(\delta)\, d\lambda = 1$$

Show how one can get the result

$$\left|\epsilon^{kl}(\delta_1, \delta_2) - \epsilon^{kl}(\delta_1, \delta_3)\right| = 1 - \epsilon^{kl}(\delta_2, \delta_3).$$

(Bell inequality) out of these assumptions!

c) Does quantum theory comply with the Bell inequality, or is there a conflict?

d) Do experimental results argue for local realistic theories or for quantum theories?

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Sheet 7

<u>Ex. TH-7.1</u>: *Wave packet at a potential step*

Study "complement J_I" of Cohen-Tannoudji on the behavior of a wave packet at a potential step and discuss it in the tutorials.

<u>Ex. TH-7.2</u>: *Two-dimensional infinite well and degeneracies of energy eigenvalues*

Consider a particle of mass m restricted to the $x - y$ plane inside a "square box" of edge a; its potential energy $V(x, y)$ becomes infinite when either x or y are outside of the interval $[0, a]$. Give the energy eigenvalues and the normalized wave functions. It turns out that the same energy eigenvalue can be obtained for different combinations of the relevant quantum numbers, i.e., for different wave functions (*degeneracy*). Which of the degeneracies are caused by the symmetry of the problem? Are there also "accidental" degeneracies?

<u>Ex. TH-7.3</u>: *α-decay*

An α particle in a nucleus approximately "feels" a potential of the form

$$V(r) = \begin{cases} -V_0 & 0 < r < R \\ \frac{Z Z_\alpha e^2}{4\pi\varepsilon_0 r} & r > R \end{cases} ,$$

where r is the distance from the centre, R denotes the radius of the nucleus, and $V_0 \approx \mathcal{O}(10^7\,\mathrm{eV})$. Z is the charge of the nucleus and $Z_\alpha = 2$.

a) The decay has an exponential behavior $\sim \exp(-\lambda t)$ with the decay rate given by $\lambda = \lambda_0 T$, where

$$T = e^{-\frac{2}{\hbar}\int_R^b \sqrt{2m_\alpha(V(r)-E)}dr}$$

$(V(b) = E > 0)$. T is the transmission coefficient through a barrier derived in the lecture. Discuss why $\lambda_0 \simeq v_0/(2R)$, with v_0 the velocity of the α particle, is a good approximation for λ_0.

b) Compute the integral in the exponent of T and expand the result in the limit of small energies of the α particle: $0 < E \ll V(R)$.

c) How does $\ln(\lambda)$ scale with Z and E? This is the so-called *Geiger-Nuttal relation*.

Ex. TH-7.4: *Periodic potential a la Kronig and Penney*

Consider the following one-dimensional periodic arrangement of potential wells

$$V(x) = \sum_{n=-\infty}^{\infty} V_P(x - nL) \quad \text{with} \quad V_P(x) = \begin{cases} 0 & 0 < x < a \\ V_0 = \text{const.} > 0 & a < x < L \end{cases} .$$

Solutions are given by linear combinations of Bloch wavefunctions which have the property

$$\Psi^{(\alpha)}(x + L) = \Psi^{(\alpha)}(x)e^{i\alpha}$$

with a real phase α.

a) Show that the solutions $\Psi^{(\alpha)}(x)$ for $E < V_0$ fulfill

$$\cos(ka)\cosh(\kappa b) - \frac{\kappa^2 - k^2}{2\kappa k}\sin(ka)\sinh(\kappa b) = \cos(\alpha)$$

with $k = \sqrt{2mE}/\hbar$, $\kappa = \sqrt{2m(V_0 - E)}/\hbar$, and $b = L - a$.

b) What are the energy levels $E = E_n^{(\alpha)}$ $(n = 0, 1, 2, \dots)$ in the limit $V_0 \to \infty$ for fixed α?

c) Compute in this limit to first non-vanishing approximation the "bandwidth" of the energy spectrum, i.e.,

$$\Delta E_n = \max\left(E_n^{(\alpha)}\right) - \min\left(E_n^{(\alpha)}\right)$$

for fixed n and $\alpha \in [0, 2\pi]$.

Ex. TH-7.5: *Properties of the Hermite polynomials*

The Hermite polynomials $H_n(x)$ can be defined by their generating function $F(s,x) = \exp(-s^2 + 2sx)$:

$$F(s,x) = \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(x) \quad .$$

a) First show that

$$\begin{aligned} H_n'(x) &= 2nH_{n-1}(x) \quad , \\ H_{n+1}(x) &= 2xH_n(x) - 2nH_{n-1}(x) \quad , \end{aligned}$$

and then derive the differential equation

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0$$

obeyed by the Hermite polynomials.

b) Show with the help of the generating function $F(s,x)$ that

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

and compute H_n for $n = 0, 1, 2$.

Ex. TH-7.6: *Parity operator*

Show that the operator

$$\Pi = \exp\left[i\pi\left(\frac{p^2}{2\alpha} + \frac{\alpha}{2\hbar^2}x^2 - \frac{1}{2}\right)\right]$$

acts like the parity operator. α is a positive and real constant.

Ex. TH-7.7: *Matrix representation of the harmonic oscillator*

Give the matrix representation of the operators a, $a^\dagger$, x, and p for the base kets $\{|n\rangle\}$ and calculate $[x, p]$.

Ex. TH-7.8: *Expectation values and time development of the harmonic oscillator*

a) Compute the expectation values of x, x^2, p, p^2, and $\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle$. Choose the most convenient system of base kets to perform these calculations!

b) Consider now the time development of the harmonic oscillator in the Heisenberg picture, i.e., compute $x(t)$ and $p(t)$. Construct for $t = 0$ a linear combination of the ground state $|0\rangle$ and the first excited state $|1\rangle$ such that $\langle x\rangle$ is as large as possible. What is the state vector for $t > 0$. Evaluate the expectation value $\langle x\rangle$ and $\langle(\Delta x)^2\rangle$ as a function of t.

Ex. TH-7.9: *Coherent (Glauber) state*

In this exercise we want to construct a superposition of energy eigenstates that most closely imitates the classsical oscillator, i.e., we want a wave packet that bouces back and forth without spreading in shape. This superposition is called a coherent or Glauber state and plays an important role in laser physics.

a) Construct a normalized eigenstate

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle$$

of the annihilation operator a with complex eigenvalue α, i.e., $a|\alpha\rangle = \alpha|\alpha\rangle$.

b) Compute the expectation values of x, x^2, p, p^2, and $\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle$ in the state $|\alpha\rangle$.

c) What about an analogous construction for $a^\dagger$?

d) Now consider the unitary operator

$$D(\alpha) = e^{\alpha a^\dagger - \alpha^* a} \quad .$$

Show that (recall $\exp(A + B) = \exp(A)\exp(B)\exp(-\frac{i}{2}[A, B])$)

$$D(\alpha) = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} e^{-\alpha^* a} \quad .$$

With the help of this result find the coordinate space representation of the coherent state

$$\Psi_\alpha(x) \equiv D(\alpha)\Psi_{n=0}(x) = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \Psi_n(x) \quad .$$

e) Express $(\alpha a^\dagger - \alpha^* a)$ by x and p to show that

$$D(\alpha) = \exp\left(\frac{(\alpha^*)^2 - \alpha^2}{4}\right) \exp\left(\frac{i}{\hbar} p_\alpha x\right) \exp\left(-\frac{i}{\hbar} x_\alpha p\right)$$

where

$$x_\alpha \equiv \sqrt{\frac{2\hbar}{m\omega}} \mathrm{Re}(\alpha) \quad \text{and} \quad p_\alpha \equiv \sqrt{2\hbar m\omega}\, \mathrm{Im}(\alpha) \quad .$$

f) Use the result of section e) to show that (hint: recall the translation operator)

$$\Psi_\alpha(x) = \exp\left(\frac{(\alpha^*)^2 - \alpha^2}{4}\right) \exp\left(\frac{i}{\hbar} p_\alpha x\right) \Psi_0(x - x_\alpha) \quad .$$

g) For $t = 0$ we prepare the system to be in the coherent state $\Psi(x, 0) = \Psi_{\alpha_0}(x)$. Show that for $t > 0$

$$\Psi(x, t) = \Psi_{\alpha(t)} \exp\left(-\frac{i}{2}\omega t\right) \quad \text{where} \quad \alpha(t) = \alpha_0 e^{-i\omega t} \quad .$$

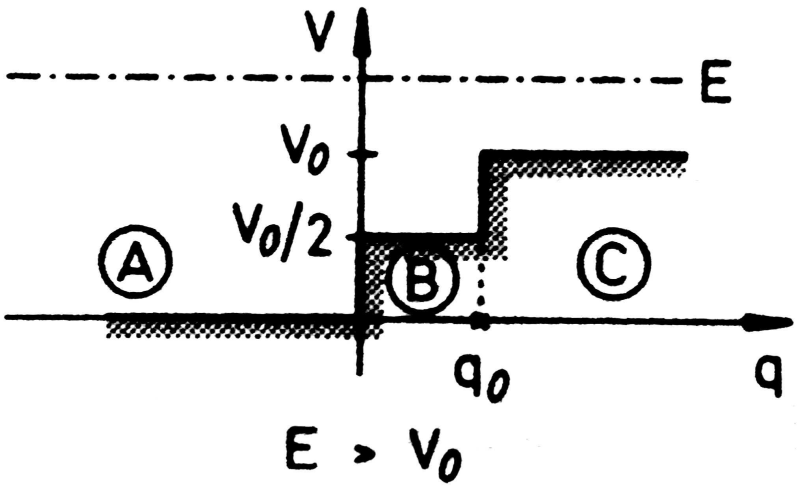
Plot $|\Psi(x, t)|^2$ for $\omega t = 0, \pi/2, \pi$ (choose $\alpha_0 = \sqrt{8}$). Compare the behavior of $|\Psi(x, t)|^2$ with the one of a wave packet describing a free particle.

Ex. EXP-7.1: *double-step potential*

A particle wave propagating from left to right hits a potential

$$V(q) = \begin{cases} 0 & \text{for} \quad q \leq 0 \\ \frac{V_0}{2} & \text{for} \quad 0 < q < q_0 \\ V_0 & \text{for} \quad q_0 \leq q \end{cases}$$

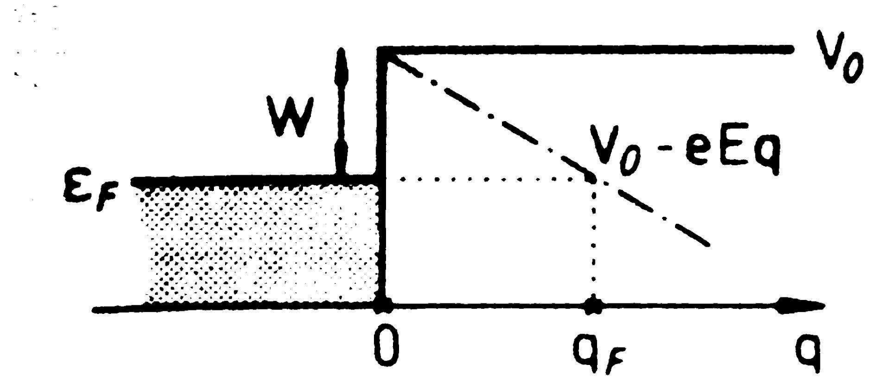
(see figure).



Give the wave functions in the three regions and calculate the transmission- and reflection coefficients! Are they larger or smaller compared to a single potential step?

Ex. EXP-7.2: *field emission*

Inside a metal, the quasi-free conduction electrons have a smaller potential energy than outside. Thus, the conduction electrons cannot leave the metal. Due to the Pauli-principle, a certain energy level can be populated by no more than two electrons (with opposite spin). At $T = 0$, they fill the conduction band up to the Fermi-energy ε_F. The energetic difference to the outer space with potential V_0 is called work function W $(= V_0 - \varepsilon_F)$.



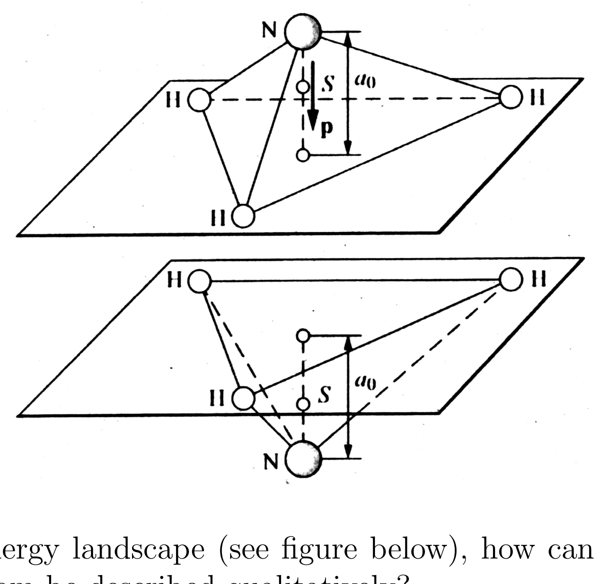
On applying a homogeneous electric field perpendicular to the metal's surface, this field does not enter the metal but changes the electrons' potential outside the metal from $V_0 = \text{const.}$ to

$$V(q) = V_0 - eEq$$

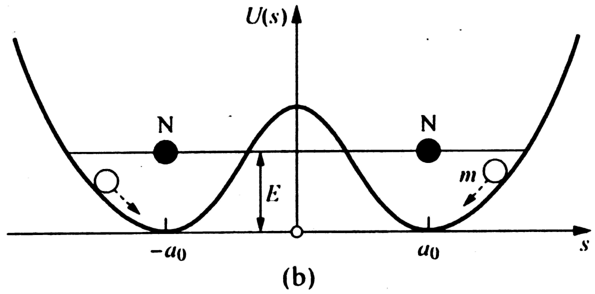
$(e < 0)$. Thus quantum mechanical tunnelling becomes possible (*field emission*).
What current j_d can be measured outside the metal after applying the field? Assume that due to the shortest tunnelling length only electrons from the Fermi edge participate in the tunnelling process!

Ex. EXP-7.3: *NH_3*

Classically, ammonia (NH_3) exists in two different states, the nitrogen atom being located either above or below the plane of the three hydrogen atoms (see figure).

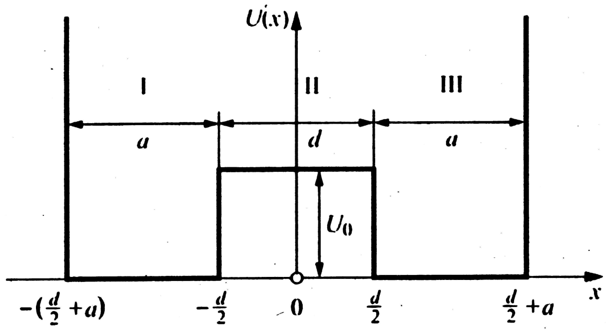


a) Looking at the energy landscape (see figure below), how can the classical movement of the nitrogen atom be described qualitatively?



(b)

A quantum mechanical treatment of the ammonia molecule is based on the potential energy of the nitrogen atom. We approximate the potential by the one shown in the figure below. We are looking for stationary states with energy E.



b) Obviously, the problem has a rotational symmetry relative to $x = 0$. What can thus be said about the parity of the solutions?

c) We concretize the above potential by setting $d = a$.
Formulate the wave functions for the three different regions. Determine parameters by taking into account boundary conditions and the normalization of the wave function. Find equations that can be used to determine the energy states.
Hint: introduce variables

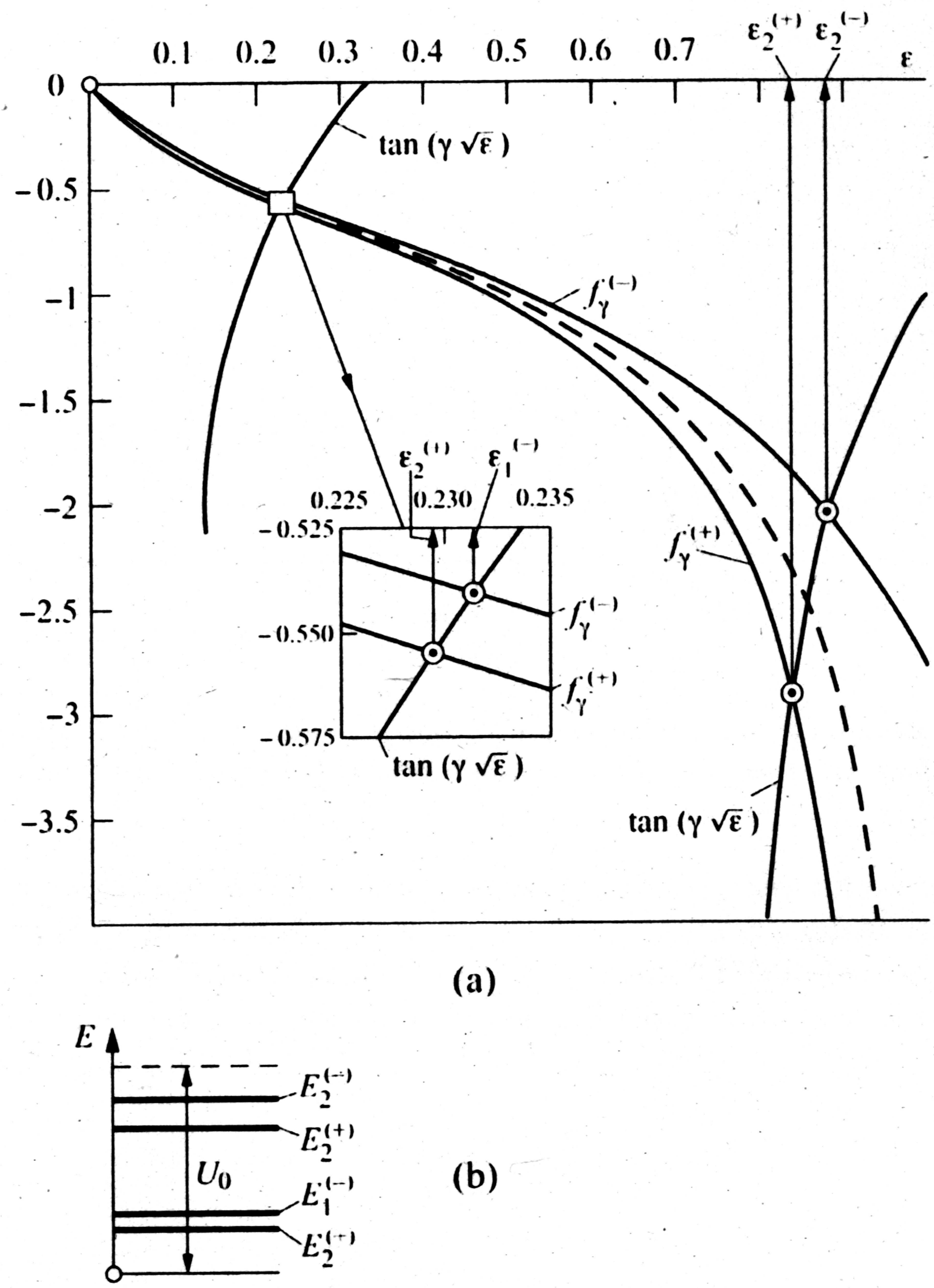
$$\epsilon := \frac{E}{U_0}; 0 \leq \epsilon \leq 1$$

and

$$\gamma := \frac{a}{\hbar}\sqrt{2mU_0}.$$

The mass of the nitrogen atom is $15 \cdot 1.66 \cdot 10^{-27}$kg. The combination of $a\,(= d)$ and U_0 be chosen in a way so that $\gamma = 5.5$.

d) Determine the energy states of ammonia. The equations found in exercise c) are somewhat difficult, thus you can solve them graphically. The graph below might help you.

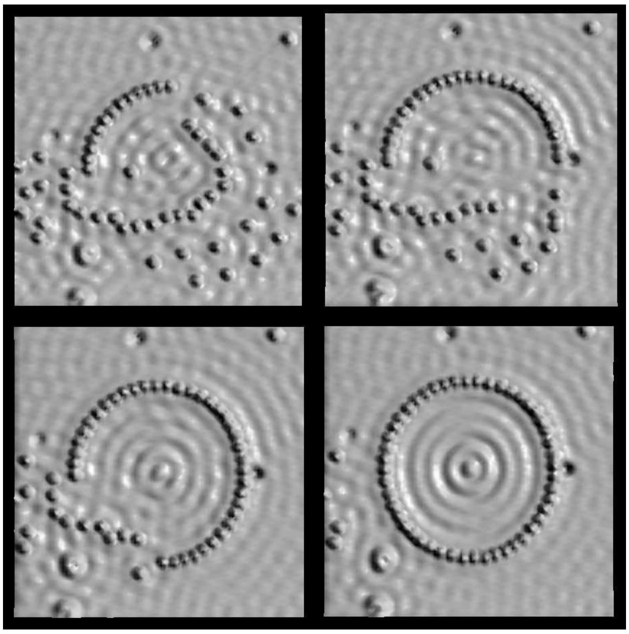


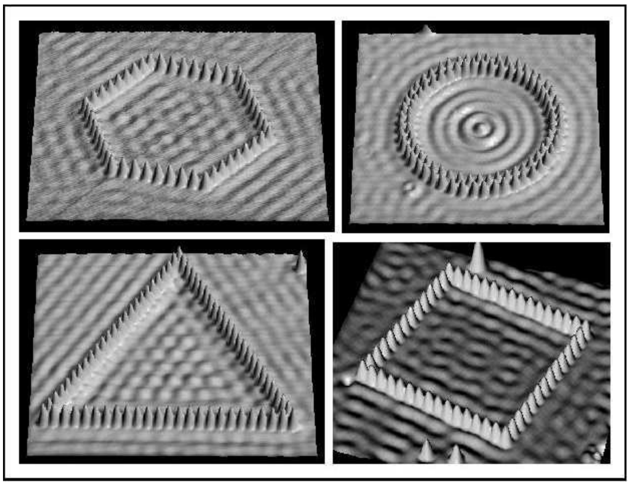
e) Now determine the wave functions of these stationary states. As the energy eigenvalues lie closely together, it is sufficient to chose the mean value of their energy parameters. What is the main difference between these wave functions and the classical states?

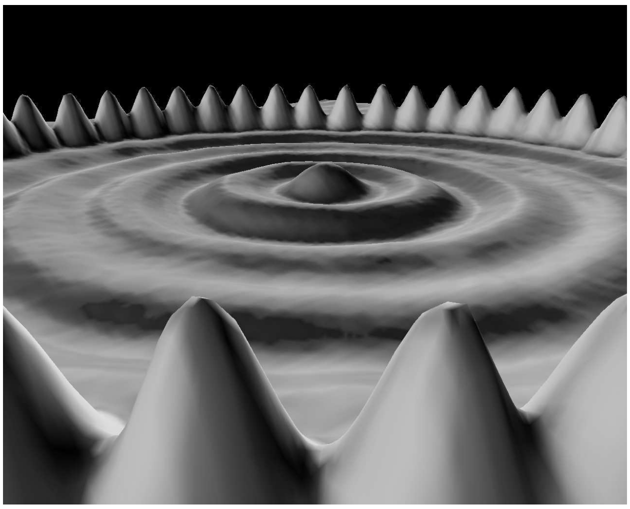
f) Formulate linear combinations of the wave functions from exercise e) that are closer to the classical solution. What is the problem with these new states? What kind of behavior would you thus expect for ammonia molecules?

Ex. EXP-7.4: *Quantum corrals*

In STM experiments it was possible to arrange 48 Fe adatoms in a ring (”corral”) on a Cu(111) surface (see pictures). The diameter of the ring was $72\mathring{A}$. In the following exercise, the quantum states of an electron in a circular 2D quantum well shall be investigated.







a) Give the 2D Laplace operator $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2$ in polar coordinates $\{r, \phi\}$ with $x = r\cos\phi$ and $y = r\sin\phi$.

b) Now investigate an electron in the 2D potential

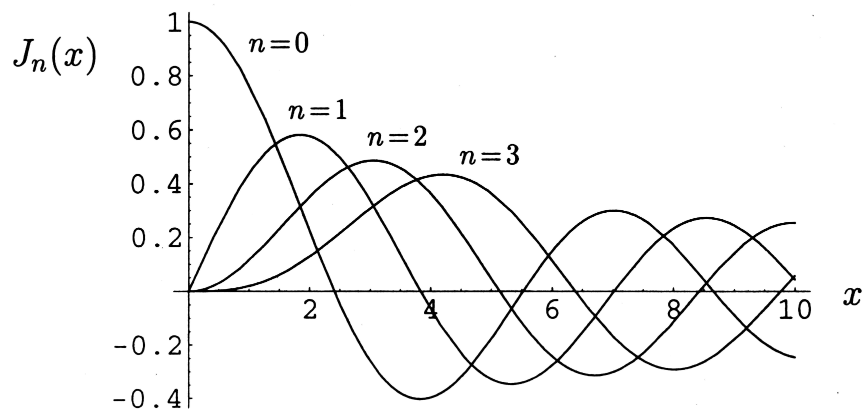
$$V(r) = \begin{cases} 0 & \text{for} \quad r < R \\ \infty & \text{for} \quad r \geq R \end{cases}$$

What values can the quantum number of angular momentum, n, assume if one takes the separational approach $\psi(r,\phi) = J(kr)\,e^{in\phi}$ for a wave function to the energy eigenvalue $E = \hbar^2 k^2/2m$?

c) Show by insertion of this separational approach into the Schrödinger equation that $J(x)$ complies with the Bessel differential equation

$$x^2 J''(x) + xJ'(x) + \left(x^2 - n^2\right) J(x) = 0$$

for $x < kR$. Its four first solutions are depicted in the figure below.



d) By which postulation are the discrete energy eigenvalues $E = \hbar^2 k^2/2m$ determined? With help of the figure above, give the three lowest energy eigenvalues for $n = 0$.

e) What do the lines defined by $\psi = 0$ look like? Compare to the respective lines you would expect if the Fe adatoms were aligned in a rectangle!

f) What changes (qualitatively) if the infinite potential walls are replaced by a finite barrier

$$V(r) = \begin{cases} 0 & \text{for} \quad r < R \\ V_0 & \text{for} \quad R \le r \le R + d \ ? \\ 0 & \text{for} \quad r > R + d \end{cases}$$

Exercises in Quantum Mechanics – Integrated Course

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Summer semester 2005
Sheet 8

Ex. TH-8.1: *Potential well of arbitrary shape and quantum properties of a particle in an arbitrary periodic structure*

Read through complements N_{III} and O_{III} of Cohen-Tannoudji and discuss the idea of a transmission matrix, S matrix, and iteration matrix in the tutorials.

Ex. TH-8.2: *One-dimensional harmonic oscillator in thermodynamic equilibrium*

Study the physical properties of a one-dimensional harmonic oscillator in thermodynamic equilibrium with a reservoir at temperature T. Such a system is not in a pure state but can be described as a statistical mixture of stationary states $|n\rangle$ with weights proportional to $\exp(-E_n/kT)$. Recall from the lectures that the corresponding density matrix is given by

$$\rho = Z^{-1} \exp(-H/kT)$$

where Z is the partition function $Z = \mathrm{Tr}\,[\exp(-H/kT)]$.

a) Show that the partition function is given by

$$Z = \frac{e^{-\hbar\omega/(2kT)}}{1 - e^{-\hbar\omega/(kT)}} \quad .$$

b) Show that the ensemble average $[H]$ is given by

$$[H] = \mathrm{Tr}(H\rho) = kT^2 \frac{1}{Z}\frac{dZ}{dT} = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\hbar\omega/(kT)} - 1} \quad .$$

c) Compare the result of b) with that for a classical oscillator, $[H]_{\mathrm{cl}} = kT$, as a function of T.

Ex. TH-8.3: *Particle in a central potential*

Consider a particle of mass m in a central potential of the form

$$V(r) = \frac{c}{r^2} + \frac{1}{2}m\omega^2 r^2 \quad , \quad c > 0 \quad .$$

a) Study only the radial part of the stationary Schrödinger equation: discuss the asymptotic behavior for $r \to 0$ and $r \to \infty$ and show that

$$u(r) = rR(r) = r^\kappa e^{-\gamma r^2} g(r)$$

is a suitable ansatz for the radial solution.

b) Find a differential equation for $g(r)$ and use the ansatz

$$g(r) = \sum_k a_k r^k$$

to solve it.

c) Why does the series in b) terminate at some finite $k = n$? Determine the allowed energy eigenvalues from this condition.

Ex. TH-8.4: *Particle in a potential with cylindrical symmetry*

a) Give the stationary Schrödinger equation in cylindrical coordinates, $x = r\cos\varphi,\ \ y = r\sin\varphi$, and $z = z$.

b) Consider a potential of the form

$$V(\vec{r}) = V(r) = -\frac{c}{r^\alpha}\ \ ,\alpha > 1,\ c > 0$$

and use the ansatz $\Psi(\vec{r}) = R(r)f(\varphi)g(z)$ to derive equations for the radial, the axial, and the angular motion of a particle. What are the solutions for the axial and the angular equations?

c) Consider now the radial equation: use the ansatz $R(r) = r^n u(r)$ to show that it can be cast into the form

$$\left(\frac{d^2}{dr^2} + \frac{2n+1}{r}\frac{d}{dr} + \frac{n^2}{r^2} - F(r)\right)u(r) = 0\ \ .$$

Specify F(r) and give the most convenient choice of n?

d) The potential of a molecule stretched along the z direction is approximately given by

$$V(\vec{r}) = V(r) = -\frac{Ze^2}{r}\quad .$$

Try to find the energy eigenvalues of an electron bound in this potential using the standard steps as, e.g., in example TH-8.3.

Ex. TH-8.5: *Pöschl-Teller potential*

Consider the one-dimensional stationary Schrödinger equation for a potential of the form

$$V(x) = \frac{V_0}{\cos^2(\alpha x)}$$

with a positive constant $V_0 = \frac{\hbar^2}{2m}\alpha^2\lambda(\lambda-1)$, i.e., $\lambda > 1$. Use $y = \sin^2(\alpha x)$ to derive a differential equation for $u(y)$. Demonstrate that with the help of $u = (1-y)^{\lambda/2}f(y)$ one arrives a hypergeometric differential equation for f:

$$y(1-y)\frac{d^2 f}{dy^2} + \left[\frac{1}{2} - (\lambda+1)y\right]\frac{df}{dy} + \frac{1}{4}\left(\frac{k^2}{\alpha^2} - \lambda^2\right)f = 0$$

where $k^2 = 2mE/\hbar^2$. What is the general solution of this equation in terms of ${}_2F_1(a,b,c;z)$?

Ex. TH-8.6: *Virial theorem, Kramers relation, and expectation values $\langle r^\lambda \rangle$ for the H-atom*

a) The virial theorem for a Hamilton operator $H = T + V$ with $T = \vec{p}^{\,2}/(2m)$ and $V = V(\vec{r})$ has the form

$$2\langle T \rangle = \langle \vec{r} \cdot \vec{\nabla} V(\vec{r}) \rangle$$

where the expectation values are taken with respect to eigenstates of H. Use this relation to calculate the expectation values $\langle 1/r \rangle_{nl}$ for the hydrogen atom.

b) Derive Kramers relation

$$\frac{\lambda+1}{n^2}\langle r^\lambda \rangle_{nl} - (2\lambda+1)a_B\langle r^{\lambda-1}\rangle_{nl} + \frac{\lambda}{4}((2l+1)^2 - \lambda^2)a_B^2\langle r^{\lambda-2}\rangle_{nl} = 0 \ ,$$

where a_B is the Bohr radius, and use the result of a) to compute $\langle r \rangle_{nl}$ and $\langle r^2 \rangle_{nl}$.

Ex. TH-8.7: *Laguerre polynomials*

The Laguerre polynomials are defined by

$$L_p(z) = e^z \frac{d^p}{dz^p}\left(z^p e^{-z}\right) \quad p = 0, 1, 2, \ldots$$

or with the help of a generating function

$$\frac{1}{1-t}\exp\left(-z\frac{t}{1-t}\right) = \sum_{p=0}^{\infty} L_p(z)\frac{t^p}{p!} \ .$$

The *associated* Laguerre polynomials (which show up in the Coulomb problem) are given by

$$L_p^k(z) \equiv \frac{d^k}{dz^k}L_p(z) \ , \quad k \le p \ .$$

a) Show that $L_p^p(z) = (-1)^p p!$.

b) Derive the recurrence relations

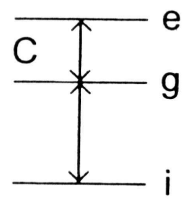
$$\begin{aligned} L_{p+1}(z) - (2p+1-z)L_p(z) + p^2 L_{p-1}(z) &= 0 \\ \frac{d}{dz}L_p(z) - p\left(\frac{d}{dz}L_{p-1}(z) - L_{p-1}(z)\right) &= 0 \ . \end{aligned}$$

c) Use b) to derive the *Laguerre differential equations*

$$\begin{aligned} \left[z\frac{d^2}{dz^2} + (1-z)\frac{d}{dz} + p\right] L_p(z) &= 0 \\ \left[z\frac{d^2}{dz^2} + (k+1-z)\frac{d}{dz} + (p-k)\right] L_p^k(z) &= 0 \ . \end{aligned}$$

Ex. EXP-8.1: *non-destructive detection of a photon in a cavity resonator*

Normally, a photon is destroyed upon detection. Thus it is impossible to detect the same photon twice. Nevertheless, by manipulating atomic states in a cavity resonator it was possible to detect a photon without destroying it, making use of a very strong interaction between matter and radiation.
In a cavity resonator, only specific modes with discrete energy can exist. Such a mode can be occupied by $n = 0, 1, 2, ...$ photons. Here, we regard such a mode C, and $n = 0$ or $n = 1$. The investigated atom has three energy levels, e, g, i, where the transition between e and g be resonant with the mode C but not with the transition between g and i (see figure).



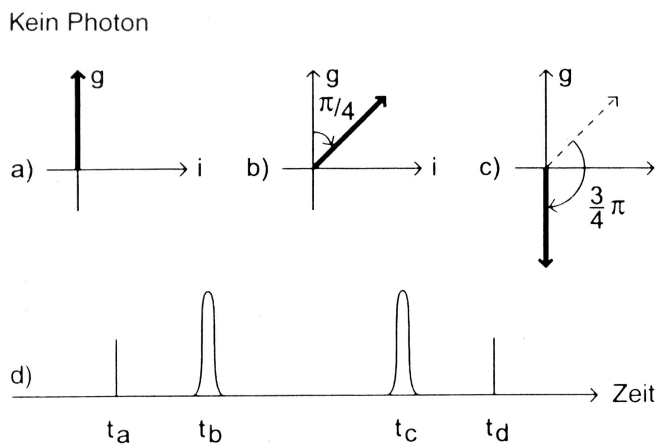
The system performs a Rabi oscillation between the states $|g, 1\rangle$ and $|e, 0\rangle$. At time t, the system is in the coherent superposition state

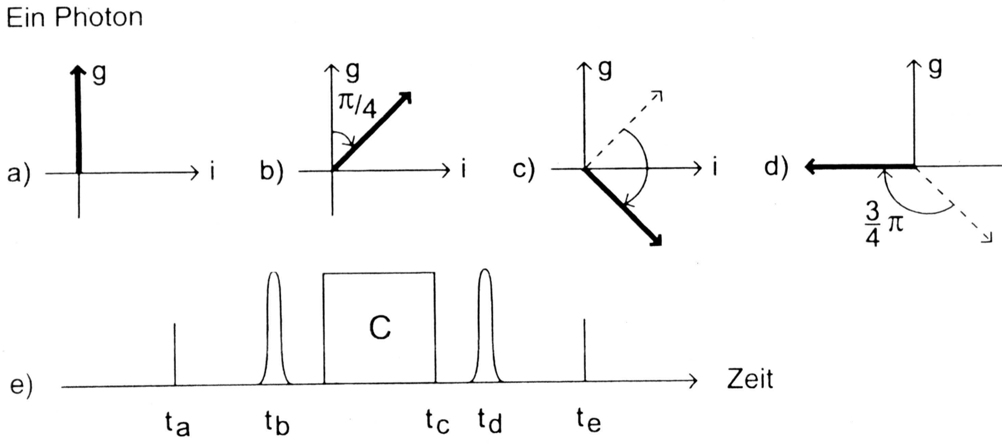
$$\psi = \cos(\Omega t/2)\,|g, 1\rangle + \sin(\Omega t/2)\,|e, 0\rangle\,.$$

a) What behavior do you expect for an interaction of duration $t = 2\pi/\Omega$, in the cases that a photon is present or not?

b) What happens by including the states $|i, 1\rangle$ and $|i, 0\rangle$ into your considerations?

c) Now two fields are applied that change the "angle" of the superposed states between the states g and i (see figures). Explain what happens here and how this behavior can be used for the non-destructive detection of a photon.





d) In exercise Exp-6.1 you have investigated a two-level atom. How can the states and rules studied in that exercise be applied to the system examined here?

Exercises in Quantum Mechanics – Integrated Course

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Summer semester 2005
Sheet 9

Ex. TH-9.1: *Electron-positron system in a uniform magnetic field*

The spin-dependent Hamiltonian of an electron-positron system in the presence of a uniform magnetic field in the z-direction can be written as

$$H = A\vec{S}^e \cdot \vec{S}^p + \left(\frac{eB}{mc}\right)(S_z^e - S_z^p) \quad .$$

Suppose the spin function of the system is given by $\chi_+^e \chi_-^p$. Note that the operator $\vec{S}^e$ acts only on the electron state spinor χ_+^e, and similarly, the operator $\vec{S}^e$ acts only on the positron state spinor χ_-^p.

a) Is this an eigenfunction of H in the limit $A \to 0$ and $eB/mc \neq 0$? If it is, what is the energy eigenvalue? If it is not, what is the expectation value of H?

b) Same problem when $eB/mc \to 0$ and $A \neq 0$.

Ex. TH-9.2: *Infinitesimal rotation of an angular-momentum eigenstate* (optional)

An angular-momentum eigenstate $|j, m = m_{\max}\rangle$ is rotated by an infinitesimal angle ε about the y-axis. Obtain an expression for the probability for the new rotated state to be found in the original state up to terms of order ε^2.

Ex. TH-9.3: *Particle in a spherically symmetric potential*

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

$$\Psi(\vec{r}) = (x + y + 3z) f(r) \quad .$$

a) Is Ψ an eigenfunction of $\vec{L}^2$? If so, what is the l value? If not, what are the possible values of l we may obtain when $\vec{L}^2$ 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 $\Psi(\vec{r})$ is an energy eigenfunction with eigenvalue E. Indicate how we may find the potential $V(r)$.

Ex. TH-9.4: *Recurrence relations for $|j,m\rangle$* (optional)

Verify the following recurrence relations for the angular momentum states $|j,m\rangle$:

a)

$$|j,m\rangle = \sqrt{\frac{(j+m)!}{(2j)!(j-m)!}}\left(\frac{1}{\hbar}J_-\right)^{j-m}|j,j\rangle \quad ,$$

b)

$$|j,m\rangle = \sqrt{\frac{(j-m)!}{(2j)!(j+m)!}}\left(\frac{1}{\hbar}J_+\right)^{j+m}|j,-j\rangle \quad .$$

Ex. TH-9.5: *Expectation values for J_x and J_y*

Consider a system prepared in an eigenstate of $\vec{J}^2$ and J_z: $|j,m\rangle$. Compute the expectation values $\langle J_x\rangle$, $\langle J_y\rangle$, $\langle J_x^2\rangle$, $\langle J_y^2\rangle$, and verify the uncertainty relation.

Ex. TH-9.6: *Quantum mechanical rotator*

Consider a molecule which has only two rotational degrees of freedom characterized by the polar and azimuthal angles ϑ and φ, respectively. The Hamiltonian for such a system is given by

$$H = \frac{1}{2I}\vec{L}^2 \quad , \quad I = \text{const (moment of inertia)} \quad .$$

a) Specify the eigenvalues (degeneracies?) and eigenfunctions of the system.

b) Suppose the system is prepared in the state

$$\Psi(\vartheta,\varphi) = N(\cos^2\vartheta + \sin^2\vartheta\cos(2\varphi)) \quad , \quad N = \text{const} \quad .$$

What are the probabilities the find $6\hbar^2$, $2\hbar^2$, and 0 in a measurement of $\vec{L}^2$?
Hint: you don't have to compute integrals here; try to express $\Psi(\vartheta,\varphi)$ by a suitable combination of spherical harmonics Y_{lm} first!

Ex. TH-9.7: *Spin 3/2 state*

A spin-3/2 system is prepared in a state $|\alpha\rangle$ characterized by

$$\langle\alpha|S_z|\alpha\rangle = \frac{3}{2}\hbar \quad .$$

Find out if $|\alpha\rangle$ is an eigenstate of S_z.

Ex. TH-9.8: *Nuclear magnetic resonance (NMR)*

Consider a neutral spin-1/2 particle (e.g. a neutron) in a *time-dependent* magnetic field

$$\vec{B}(t) = (b\cos(\omega t), b\sin(\omega t), B_0)$$

with b, B_0 constant (we have already discussed the case $b = 0$). The Hamiltonian is given by

$$H = -\mu\,\vec{\sigma} \cdot \vec{B}(t) \quad ,$$

where μ is the magnetic moment of the spin-1/2 particle.

a) Show that the ansatz ("rotating axis representation" by Rabi, Schwinger, and Van Vleck)

$$\begin{pmatrix} \Psi_+(t) \\ \Psi_-(t) \end{pmatrix} = \begin{pmatrix} e^{-i\omega t/2}\chi_+(t) \\ e^{i\omega t/2}\chi_-(t) \end{pmatrix}$$

leads to a Schrödinger equation with a *time-independent* Hamiltonian

$$i\hbar\frac{d}{dt}\begin{pmatrix} \chi_+(t) \\ \chi_-(t) \end{pmatrix} = \begin{pmatrix} E & V \\ V & -E \end{pmatrix}\begin{pmatrix} \chi_+(t) \\ \chi_-(t) \end{pmatrix} \quad .$$

Determine E and V.

b) Suppose $|\Psi(t=0)\rangle = |-\rangle$. What is the probability to find the system at a time $t > 0$ in the state $|+\rangle$? Discuss your result!

Ex. TH-9.9: *Runge-Lenz operator and "hidden" dynamical symmetries* (optional)

In the lectures we have discussed the degeneracies of the energy eigenvalues E_n of the Coulomb problem. From the symmetry properties of the problem (rotational symmetric potential $\Leftrightarrow$ SO(3) symmetry) we would expect a smaller degeneracy. Therefore the Coulomb problem has to have some "hidden" symmetry. A "hidden" symmetry generated by an operator $\vec{C}$ is characterized by $[H, \vec{C}] = 0$. For a rotational symmetric problem the generator of the symmetry commutes with the kinetic and potential term of the Hamiltonian separately.

a) Show that the dimensionless, hermitean Runge-Lenz operator (known from the Kepler problem in Classical Mechanics!)

$$\vec{C} = \frac{\vec{r}}{r} + \frac{1}{2Ze^2m}\left[(\vec{L}\times\vec{p}) - (\vec{p}\times\vec{L})\right]$$

is a hidden symmetry of the Coulomb problem $V(r) = -Ze^2/r$.

b) To better understand the properties of the symmetry generated by $\vec{C}$, try to show how the energy spectrum E_n can be derived from the algebraic properties of $\vec{C}$ (i.e., *without* solving the Schrödinger equation). Follow these steps:

   i) Compute the commutation relations for the set of six operators defined by $\{L_1, L_2, L_3, C_1, C_2, C_3\}$, i.e., $[L_k, C_L]$ and $[C_k, C_l]$ ($\vec{L}$ is the angular momentum operator, so you know the commutator already). You will find that the six operators form a closed algebra but the C_i are not angular momentum operators.

ii) Symmetrize the commutation relations obtained in i) by a suitable rescaling of $\vec{C}$, i.e., $\vec{N} \equiv \vec{C}/\sqrt{a}$. You should obtain something like

$$[L_k, L_l] = i\hbar\epsilon_{klm}L_m \quad , \quad [L_k, N_l] = i\hbar\epsilon_{klm}N_m \quad , \quad [N_k, N_l] = i\hbar\epsilon_{klm}L_m \quad .$$

Don't be scared to divide by the Hamiltonian H. Since H commutes with $\vec{L}$ and $\vec{C}$ we can always replace H by its eigenvalue E_n.

iii) Now we are almost there. Consider the linear combinations

$$\vec{N}^{\pm} = \frac{1}{2}(\vec{L} \pm \vec{N})$$

and show that *both* behave like angular momentum operators, i.e., you immediately know their spectrum of eigenvalues!

iv) Try to rewrite H in terms of these new operators and derive the eigenvalues E_n. To do so, take into account that $\vec{N} \cdot \vec{L} = 0$.

Remarks: Since $\vec{L} = \vec{N}^{+} + \vec{N}^{-}$ the actual symmetry group of the Coulomb problem turns out to be $SO(3) \otimes SO(3)$ (more precisely its $SU(2) \otimes SU(2)$), i.e., $SO(4)$ – the rotational group in *four* dimensions. The Coulomb wave function can be expressed as a function on a 3-sphere and obeys an integral equation which is rotational invariant in four dimensions. Now it should be obvious why such a symmetry is called a "hidden symmetry"!

Ex. EXP-9.1: *Dipole Matrix Elements*

In quantum mechanics, dipole matrix elements between two states with wave functions ψ_1 and ψ_2 are defined by

$$\mathbf{D} = \int \psi_1^* \, e\mathbf{r} \, \psi_2 \, dx \, dy \, dz \, .$$

a) Why is $\mathbf{D}$ a vector?

b) Calculate the components of $\mathbf{D}$ for the cases

i) $\psi_1 = \psi_2 = \psi_{1,0,0}$,

ii) $\psi_1 = \psi_{1,0,0}$, $\psi_2 = \psi_{2,0,0}$,

iii) $\psi_1 = \psi_{1,0,0}$, $\psi_2 = \psi_{2,1,0}$,

iv) $\psi_1 = \psi_{1,0,0}$, $\psi_2 = \psi_{2,1,\pm 1}$,

where $\psi_{n,l,m}$ is the hydrogen wave-function with quantum numbers n, l, m.

Ex. EXP-9.2: *Variational Principle in Quantum Mechanics*

We take the ground state of the hydrogen atom as an example to illustrate the variational principle in quantum mechanics.
Generally, this principle says that the wave-function ψ of the ground state of a Schrödinger-equation $H\psi = E\psi$ can (besides a direct solution of the Schrödinger-equation) be found by bringing the expectation value of the energy to a minimum by a proper choice of ψ:

$$\overline{E} = \int \psi^* \, H\psi \, dx \, dy \, dz = Min \, .$$

In addition, ψ must satisfy the constraint $\int \psi^* \psi \, dx \, dy \, dz = 1$.
This principle can also be used to approximately determine wave functions and energies.

a) Start from $\psi = N \, e^{-r^2/r_0^2}$. Determine the normalization factor N. Then, calculate $\overline{E}$ as a function of r_0. By a proper choice of r_0, bring the value of $\overline{E}$ to a minimum.

b) Do the same calculation again, this time starting from $\psi = N \, e^{-r/r_0}$.

c) Compare the results from a) and b) with the exact value of the energy!

Exotic Hydrogen Atoms

<u>Ex. EXP-9.3</u>: *Muonium*

Muonium is a hydrogen atom whose electron is replaced by a muon. In the following exercises, calculate quantum mechanically!

a) What is a muon?

b) Calculate the binding energy of a muon and a proton!

c) Calculate the expectation value of the radius of the orbit with $n = 1$!

d) Assume a transition of the muon from $n = 2$ to $n = 1$. Calculate the frequency of the emitted photon!

<u>Ex. EXP-9.4</u>: *Rydberg Atoms*

a) What are Rydberg atoms? What properties do they have?

For the excitation of Rydberg Atoms, the additive absorption of the light of two lasers is used. The first is a laser with a (fixed) photon energy of $E = 11.5\,\mathrm{eV}$.

b) What wave-lengths are required for the second laser to reach the states $n = 20$, $n = 30$, $n = 40$, $n = 50$?

c) What are the radii and the binding energies for these states?

d) What is the maximum of the spectral linewidth required to excite only one n-state?

<u>Ex. EXP-9.5</u>: *Revolutions of Electrons in an Excited Hydrogen Atom*

Estimate the number of revolutions an electron performs in an excited state n before it falls back to the state $n = 1$. Assume a mean lifetime of 10^{-8}s. Calculate the velocity of the electrons in Bohr's picture. Calculate the number of revolutions for

a) $n = 2$ and

b) $n = 15$.

Compare to the number of revolutions the earth has performed around the sun in the 4.5 billion years since its formation.

<u>Ex. EXP-9.6</u>: *Wannier Excitons*

A Wannier Exciton is a bound state of an electron and a hole in solid state. They can also be regarded as exotic hydrogen atoms. The dielectric constant of the medium and the effective masses of electron and hole have to be taken into account.

a) What are holes in solid state, esp. semi conductors?

b) Calculate the energies of the excited states $2 \leq n \leq 5$!

c) What does the absorption spectrum of these excitons look like?

Use the following data: Semi-Conductor Cu_2O, $\varepsilon_r \approx 10$, reduced mass $\mu \approx 0.7 m_e$

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Ex. TH-10.1: *Total angular momentum eigenstates for an electron*

Calculate the eigenstates of the total angular momentum of an electron

$$\vec{J} = \vec{L} + \vec{S} \quad , \quad s = \frac{1}{2}, \;\; l \geq 1 \quad ,$$

in, e.g., a hydrogen atom, i.e., proof that

$$\begin{aligned} \left| j = l \pm \frac{1}{2}, m, l, s = \frac{1}{2} \right\rangle \;\; = \;\; & \sqrt{\frac{l \pm m + (1/2)}{2l+1}} \left| l, s = \frac{1}{2}, m_l = m - \frac{1}{2}, m_s = \frac{1}{2} \right\rangle \\ \pm \;\; & \sqrt{\frac{l \mp m + (1/2)}{2l+1}} \left| l, s = \frac{1}{2}, m_l = m + \frac{1}{2}, m_s = -\frac{1}{2} \right\rangle \quad . \end{aligned}$$

Ex. TH-10.2: *Clebsch-Gordan coefficients for $j_1 = 1$ and $j_2 = 1$*

Compute all Clebsch-Gordan coefficients for the coupling

$$\vec{J} = \vec{J}_1 + \vec{J}_2 \quad , \quad j_1 = 1, \; j_2 = 1 \quad ,$$

and compare your results with the table of Clebsch-Gordan coefficients.

Ex. TH-10.3: *Inconsistencies if a half-integer l were possible for orbital angular momentum*

In the lectures we used the fact that $\vec{L}$ is the generator of rotations to show that the quantum number l has to be integer. Suppose Y_{lm} with half-integer l were possible. From

$$L_+ Y_{\frac{1}{2}\frac{1}{2}}(\theta, \varphi) = 0 \quad ,$$

we may deduce

$$Y_{\frac{1}{2}\frac{1}{2}}(\theta, \varphi) \simeq e^{i\varphi/2} \sqrt{\sin\theta} \quad .$$

Now try to construct $Y_{\frac{1}{2}\,-\frac{1}{2}}(\theta, \varphi)$ by

a) applying L_- to $Y_{\frac{1}{2}\frac{1}{2}}(\theta, \varphi)$ and by

b) using

$$L_- Y_{\frac{1}{2}\,-\frac{1}{2}}(\theta, \varphi) = 0 \quad .$$

Show that the two procedures lead to contradictory results. This gives an argument against half-integer l values for orbital angular momentum.

Ex. TH-10.4: *Useful identity for spherical harmonics* (optional)

In the lectures we have left out the proof for

$$\int d\Omega \;\; Y^*_{lm}(\theta,\varphi)\, Y_{l_1 m_1}(\theta,\varphi)\, Y_{l_2 m_2}(\theta,\varphi) =$$
$$\sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}}\langle l_1,l_2,0,0|l,m=0,l_1,l_2\rangle\langle l_1,l_2,m_1,m_2|l,m,l_1,l_2\rangle \quad .$$

Proof this identity starting from

$$D^{(j_1)}_{m_1 m_1'}(R) D^{(j_2)}_{m_2 m_2'}(R) = \sum_{j,m,m'} \langle j_1,j_2,m_1,m_2|j,m,j_1,j_2\rangle\langle j_1,j_2,m_1',m_2'|j,m',j_1,j_2\rangle D^{(j)}_{mm'}(R) \quad .$$

Find a proof for the latter identity first!

Ex. TH-10.5: *Proof of the Wigner-Eckart and projection theorems* (optional)

Work through the proof of the Wigner-Eckart and the projection theorem given in Sakurai and discuss it in the tutorials.

Ex. TH-10.6: *Quadrupole moment* (optional)

a) Write xy, yz, and (x^2-y^2) as components of a spherical irreducible tensor of rank 2.

b) The expectation value

$$Q \equiv e\langle n,j,m=j|(3z^2-r^2)|n,j,m=j\rangle$$

is known as the quadrupole moment. Evaluate

$$e\langle n,j,m'|(x^2-y^2)|n,j,m=j\rangle$$

where $m' = j, j-1, j-2, \ldots$ in terms of Q and appropriate Clebsch-Gordan coefficients.

Ex. TH-10.7: *Harmonic oscillator with a linear perturbation*

A simple, one-dimensional harmonic oscillator is subjected to a perturbation $V = bx$ where b is a real constant.

a) Calculate the energy shift of the ground-state to lowest non-vanishing order.

b) Solve the problem exactly and compare with your result obtained in a).

Ex. TH-10.8: *Anharmonic oscillator*

A simple, one-dimensional harmonic oscillator is subjected to a perturbation

$$V = \alpha\frac{m^2\omega^2}{\hbar}x^4$$

where α is a real constant. Calculate the energy shift in the first order perturbation theory.

Ex. TH-10.9: *Non-pointlike nucleus*

So far we have considered the nucleus to be pointlike, e.g., the proton in the hydrogen atom. To first order the proton can be considered as a homogeneously charged sphere of radius R. From Electrodynamics we know the potential of a homogeneously charged sphere to be

$$V(r) = \begin{cases} -\frac{e^2}{R}\left(\frac{3}{2}-\frac{1}{2}\frac{r^2}{R^2}\right) & \text{for} \quad 0 \le r \le R \\ -\frac{e^2}{r} & \text{for} \quad r \ge R \end{cases} \quad .$$

Compute to first order perturbation theory the energy shift of the ground-state.

Ex. EXP-10.1: *Mean Lifetime of Excited Atomic States: Semiclassical Treatment*

In the lectures, you have been given an expression of the overlap integral $\mathbf{p}_{if}$ for the spontaneous emission of a photon,

$$\mathbf{p}_{if} = q \int \mathbf{r}\overline{\psi_i}\left(\mathbf{r}\right)\psi_f\left(\mathbf{r}\right) d^3r \quad .$$

This can be used to define the quantum mechanical electrical dipole moment:

$$\mathbf{p}\left(t\right) = q \int \mathbf{r}\left|\psi\left(\mathbf{r},t\right)\right|^2 d^3r = 2Re\left\{\overline{a_i}\left(t\right) b_f\left(t\right)\mathbf{p}_{if}e^{i\omega_0 t}\right\}$$

In this exercise, a semi-classical approximation of the mean lifetime of an excited state shall be derived.

a) For simplicity, assume $\left|\overline{a_i}\left(t\right) b_f\left(t\right)\right| \simeq 1$ for $0 < t \leq \tau$ and $\overline{a_i}\left(t\right) b_f\left(t\right) = 0$ else.

b) Estimate the mean power radiated off by the excited atom by treating the quantum mechanical dipole moment given above as a classical dipole, oscillating with frequency ω_0.

c) Use the assumption from a) to link the total energy emitted from the oscillating dipole during the period of time τ to the energy difference between the two atomic states.

d) Derive the expression for τ.

Ex. EXP-10.2: *Laser*

a) What does population inversion mean?

b) How is population inversion normally achieved?

c) Is there a possibility to build a two-level laser?

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Ex. TH-11.1: *Gauge transformation*

The Schrödinger equation for a particle in an electromagnetic field can be obtained by the standard one

$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V\right]\psi(\vec{x},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t).$$

by replacing the momentum operator

$$-i\hbar\vec{\nabla} \to -i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}(\vec{x},t)$$

and using the scalar potential $V = e\Phi(\vec{x},t)$. Show that under a gauge transformation

$$\vec{A} \to \vec{A}' = \vec{A} + \vec{\nabla}\Lambda, \qquad \Phi \to \Phi' = \Phi - \frac{1}{c}\frac{\partial}{\partial t}\Lambda$$

the wavefunction has to acquire a position- and time-dependent phase factor in order to fulfill the Schrödinger equation.

Ex. TH-11.2: *Van der Waals' interaction*

A system is composed of two hydrogen atoms with their protons separated by a fixed distance r and their electrons at displacements $\vec{r}_1$ and $\vec{r}_2$ from the protons.

a) Show that the Hamiltonian can be written as the sum of the two Hamiltonians of the two noninteracting atoms plus a term

$$V = \frac{e^2}{r} + \frac{e^2}{|\vec{r}+\vec{r}_2-\vec{r}_1|} - \frac{e^2}{|\vec{r}+\vec{r}_2|} - \frac{e^2}{|\vec{r}-\vec{r}_1|}$$

.

b) For $r \gg a_0$ expand the perturbation V in powers of r_i/r, show that the first-order correction to the ground-state energy vanishes and that the second order correction goes as $1/r^6$.

Ex. TH-11.3: *Normalization of a perturbed ket*

Reproduce the proof of Eq. (5.1.48b) of Sakurai giving the normalization constant of a perturbed ket.

Ex. TH-11.4: *Two-dimensional square well with perturbation*

Consider a particle in a two-dimensional infinite square well:

$$V = \begin{cases} 0 & \text{if } 0 \le x \le a,\ 0 \le y \le a, \\ \infty & \text{otherwise.} \end{cases}$$

a) What are the energy eigenvalues of the three lowest states? Is there any degeneracy?

b) We now add a weak perturbating potential

$$V_1 = \lambda xy \qquad \text{if } 0 \leq x \leq a,\ 0 \leq y \leq a.$$

Obtain the energy shifts of the three lowest states accurate to order λ.

c) Draw an energy diagram with or without the perturbation (specifying which unperturbed state is connected to which perturbed state).

Ex. TH-11.5: *Two-dimensional harmonic oscillator with perturbation*

Consider an isotropic harmonic oscillator in two dimensions. The Hamiltonian is given by

$$\hat{H} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2).$$

a) What are the energy eigenvalues of the three lowest states? Is there any degeneracy?

b) We now add a weak perturbating potential

$$V_1 = \delta\omega^2 xy.$$

Find the zeroth-order eigenkets and the corresponding first-order energy shifts of the three lowest states.

c) Solve the problem exactly and compare with the result in b).

Ex. TH-11.6: *Stark effect*

Work out the Stark effect to lowest nonvanishing order for the $n = 3$ level of the hydrogen atom. Ignoring the spin-orbit force and relativistic correction (Lamb shift), obtain not only the energy shifts but also the corresponding zeroth-order eigenkets.

Ex. TH-11.7: *Zeeman effect for an arbitrary magnetic field*

In the presence of a uniform magnetic field B along the z axis, the Hamiltonian for a hydrogen atom becomes

$$H = H_0 + \frac{\mu_B B}{\hbar}(L_z + 2S_z) + \frac{2W}{\hbar^2}\vec{L}\cdot\vec{S},$$

where μ_B is the Bohr magneton, and W is a constant of order $\mu_B e^2\hbar^2/(4\pi m_e^2 a_0^3)$.

a) Show that

$$\vec{L}\cdot\vec{S} = \frac{1}{2}(L_+S_- + L_-S_+) + L_zS_z.$$

b) For an electron in a state with $l = 1$, working in the basis of the three eigenfunctions of L_z and the two eigenfunctions of S_z, give a matrix representation of the Hamiltonian and the corresponding eigenvalues.

c) Plot the energy eigenvalues as a function of B and discuss the weak field ($\mu B \ll W$) and strong field ($\mu B \gg W$) approximations.

Ex. EXP-11.1: *Spin-Orbit Coupling*

Give the relative splitting due to spin-orbit interaction of the different levels of a L-S-J multiplet for the multiplets ^3F and ^3D. Sketch their energy levels and indicate the allowed transitions!

<u>Ex. EXP-11.2</u>: *Fine Structure*

The spin-orbit splitting in a Cs atom between the states $6P_{\frac{1}{2}}$ and $6P_{\frac{3}{2}}$ leads to a difference on the wavelength of $\Delta\lambda = 422$Åfor the first pair of lines in the main series. The line with shorter wavelength has a wavelength of $\lambda = 8521$Å.
Calculate the fine structure constant!

<u>Ex. EXP-11.3</u>: *Sodium Triple Line*

In the emission spectrum of sodium, the following three neighboring lines have been found:

1. $3^2D \rightarrow 2^2P_{\frac{1}{2}}$
2. $3^2D \rightarrow 2^2P_{\frac{3}{2}}$
3. $3^2D \rightarrow 2^2P_{\frac{3}{2}}$

a) Taking into account the transition rules, give the quantum numbers of the total angular momentum of the initial D-states and calculate the splitting of the states in eV!

b) Compare the splitting to the mean kinetic energy of gas atoms at 20°C!

<u>Ex. EXP-11.4</u>: *Fine Structure of Hydrogen-like Ions*

The fine structure of hydrogen-like ions (ions with only one electron) is described by the additional term

$$E_{FS} = -\frac{hcRZ^4\alpha^2}{n^3} \cdot \left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right),$$

($\alpha = 1/137$ is Sommerfeld's fine structure constant, R the Rydberg constant and Z the atomic number) which takes into account relativistic effects and spin-orbit coupling. Thus, the total energy is given by $E_{n,l,j} = E_{n,l} + E_{FS}$.

a) Can n and j be chosen in a way so that the additional term disappears? What effect has this on the total energy?

b) In how many different energy levels do the levels $n = 3$ and $n = 4$ of simply ionized helium split due to the fine structure interaction?

c) Give the amount of the displacement of the energies relative to the "original" energies.

d) Determine the allowed transitions taking into account the selection rules!

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Ex. TH-12.1: *Time ordering operator*

Convince yourself that the formula for the time-evolution operator in the interaction picture

$$U_I(t, t_0) = T \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} V(t')\,dt'\right)$$

is correct.

a) First expand the formula to the second order and explicitly check that it corresponds to the second-order expansion of

$$U_I(t, t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} V(t')\,U_I(t', t_0)\,dt'.$$

b) Discuss by induction the validity of the formula to any order.

Ex. TH-12.2: *Hydrogen atom in time-dependent electric field*

A hydrogen atom is subject to a time-dependent homogeneous electric field

$$E(t) = \frac{A\tau}{e\pi}\frac{1}{t^2+\tau^2}$$

where A, τ are constants. Compute the probability to find the atom at time $t = +\infty$ in a 2p-state if it was initially ($t = -\infty$) in the ground state.

Ex. TH-12.3: *Adiabatic approximation* (optional)

Two states of an unperturbed atom are denoted by $|m\rangle$ and $|n\rangle$. The atom is subject to a perturbation

$$V(t) = \begin{cases} V(t) & \text{if } 0 \le t \le \tau, \\ 0 & \text{otherwise.} \end{cases}$$

a) Show that the probability for a transition $|m\rangle \to |n\rangle$ is very small if the *adiabatic approximation*

$$\omega_{nm}^{-1}\frac{d}{dt}\langle n|V(t)|m\rangle \ll |E_n - E_m|$$

is fulfilled [$\omega_{nm} = (E_n - E_m)/\hbar$].

b) What happens in the opposite case (*sudden change*) where

$$\omega_{nm}^{-1}\frac{d}{dt}\langle n|V(t)|m\rangle \gg |E_n - E_m|$$

in the short time interval when the perturbation turns on from zero to its maximum value?

Ex. TH-12.4: *Harmonic oscillator with time-dependent perturbation*

A one-dimensional harmonic oscillator is in its ground state for $t < 0$. For $t \geq 0$ it is subjected to a time-dependent but spatially uniform force in the 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 its first excited state for $t > 0$. Show that the $t \to \infty$ (τ finite) limit of your expression is independent of time. Is this reasonable or surprising?

b) Can we find higher excited states?
$\Big[$You may use $\langle n'|x|n\rangle = \sqrt{\hbar/2m\omega}\,(\sqrt{n}\,\delta_{n',n-1} + \sqrt{n+1}\,\delta_{n',n+1}).\Big]$

Ex. TH-12.5: *Spin-spin interaction*

Consider a composite system made up of two spin-half objects. For $t < 0$, the Hamiltonian does not depend on spin and can be taken to be zero. 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 $|+-\rangle$ for $t \leq 0$. Find, as a function of time, the probability for being found in each of the following states $|++\rangle$, $|+-\rangle$, $|-+\rangle$, $|--\rangle$:

a) By solving the problem exactly.

b) 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 b) give the correct result?

Ex. TH-12.6: *WKB approximation*

Compute the energy eigenvalues E_n of a one-dimensional harmonic oscillator using the WKB approximation.

Ex. EXP-12.1: *Zeeman Splitting*

Sodium vapor with a temperature of $T = 573$K enclosed in a glass container, emits light due to electron impact. In the visible range, the two Na-D-lines are observed at $\lambda_1 = 588,995$nm and $\lambda_2 = 589,592$nm.

a) Sodium has 11 electrons. In the ground state, how are these electrons distributed to the individual shells s,p,d,f (notation: $1s^2$,...)?

b) What is the spectroscopic denotation $^{\text{multiplicity}}X_J$ for the ground state of sodium?

c) From what excited states do the Na-D-lines emanate?

d) Calculate the energetic splitting in cm^{-1} from the wavelength. What determines this splitting?

e) In a magnetic field B, the energy of a state J,L,S is described by an additional energy term. The Landé-factor is

$$g_{JLS} = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

Calculate the g-factors for the three levels that take part in the formation of the Na-D-lines!

f) Sketch the energy levels with the calculated Zeeman splitting. Plot the allowed electric transitions. Denote the relevant quantum numbers unambiguously in the sketch.

g) Calculate the Zeeman splitting in cm^{-1} for $B = 2\text{T}$ for the three terms.

h) In this case, do we observe the normal or the anomalous Zeeman splitting? What is the difference between the two?

Ex. EXP-12.2: *Electron Spin Resonance (ESR)*

Electron Spin Resonance is the transition between electron states with different values of the magnetic quantum number. The degeneracy of these states is commonly broken by applying an external magnetic field. Thus, the transition frequencies are found in the microwave region.

a) What transitions can be observed with ESR? Compare to optical spectroscopy! What kind of transitions are observed in these two cases?

b) In an ESR experiment, microwaves interact with the electron in an atomic state. Calculate the resonance frequency in dependence on the microwave radiation!

c) With an external field of 10^{-1}T, what frequency is required to induce a reversal from parallel to antiparallel orientation in an electron pair, or vice versa?

Ex. EXP-12.3: *Double Resonance, Optical Pumping*

The different polarizations that occur in the normal Zeeman effect can be used to selectively "pump" electrons into different Zeeman levels, even if one does not have the required spectral resolution. In mercury vapor, one can excite the state $^3P_1$ from the ground state $^1S_0$ with linearly polarized light. The light emitted from this state is now also linearly polarized. However, using microwaves, one can now induce transitions between the different Zeeman levels. The light emitted from these states can now be used to detect the resonance of the microwave radiation with the transition between the Zeeman states.

a) Sketch the energy levels and the transitions that are described above!

b) How can this principle be applied to detect the Zeeman splitting of Sodium investigated in exercise 12.1? Sketch the energy levels and the respective transitions!

Ex. EXP-12.4: *Doppler-free Spectroscopy*

In gases, the spectral lines are broadened due to the Doppler effect. This broadening is generally larger than the natural line width. In the following, two possibilities to avoid this broadening shall be treated.

a) **Doppler-free Saturation Spectroscopy:**
Inversion in the occupation numbers of atomic states is a prerequisite for laser activity. Once lasing has started, this inversion is reduced by the process of stimulated emission. We now assume that the atoms in a gas laser have different axial velocities. The different atoms of velocity v now have their own occupation numbers $N_{1,v}$ and $N_{2,v}$.

   i) Taking into account the Maxwell distribution for the velocity in one direction, what does the distribution of occupation numbers depending on velocity look like?

ii) Now assume laser light with frequency ω and the natural line width γ hits the gas atoms. With what types v of atoms will it interact (ω_0 be the transition frequency of the resting atom)? How will this change the distribution of occupation numbers?

iii) How can this effect be used to determine the exact value of ω_0?

b) **Doppler-free two-Photon Absorption:**
In very intense laser fields it is possible that an atom absorbs tho photons at a time where the energetic difference between the two participating states corresponds to the double photon energy, i.e.

$$\Delta E = 2h\nu \equiv 2\hbar\omega.$$

How can this be used to avoid the Doppler effect? What geometry of the incident laser beams is required?

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Ex. TH-13.1: *Green function for scattering problem*

Show that

$$\left(\nabla^2 + k^2\right) G(\vec{x}, \vec{x}') = \delta^{(3)}\left(\vec{x} - \vec{x}'\right)$$

leads to

$$G_\pm(\vec{x}, \vec{x}') = -\frac{1}{4\pi} \frac{e^{\pm ik(\vec{x}-\vec{x}')}}{|\vec{x} - \vec{x}'|}.$$

Ex. TH-13.2: *Cross section*

Show that

$$\frac{d\sigma}{d\Omega} = \left| f(\vec{k}, \vec{k}') \right|^2$$

using

$$d\sigma = \frac{r^2 |\vec{j}_{\text{scatt.}}| d\Omega}{|\vec{j}_{\text{incid.}}|}.$$

Ex. TH-13.3: *Yukawa potential*

Compute $d\sigma/d\Omega$ and σ_{tot} for

$$V(r) = V_0 \frac{e^{-\mu r}}{\mu r}, \quad \mu > 0.$$

What happens in the limit $\mu \to 0$ and V_0/μ fixed?

Ex. TH-13.4: *Scattering in Born approximation*

a) Compute the scattering amplitude $f(\theta)$ for

$$V(r) = a e^{-\lambda r^2}, \quad \lambda > 0.$$

b) Compute the total cross section.

Ex. TH-13.5: *Expansion of plain wave* (optional)

Reproduce the derivation of the formula

$$e^{i\vec{k}\cdot\vec{r}} = \sum_l i^l (2l+1) j_l(kr) P_l(\cos\theta),$$

valid when $\vec{k} = k\hat{e}_z$.

Ex. TH-13.6: *Hard sphere scattering and partial wave method*

Compute σ_{tot} for the scattering off a hard sphere, i.e., off the potential

$$V(r) = \begin{cases} \infty & \text{if } r \leq a, \\ 0 & \text{otherwise,} \end{cases}$$

in the limit $ka \ll 1$ (small energies) and $ka \gg 1$ (large energies). In the latter case, express $\sin \delta_l$ by the spherical Bessel and Neumann functions at $\rho = ka$. For $\rho \gg 1$ we have

$$j_l(\rho) \approx \sin\left(\rho - \frac{l\pi}{2}\right)\frac{1}{\rho},$$
$$n_l(\rho) \approx -\cos\left(\rho - \frac{l\pi}{2}\right)\frac{1}{\rho}.$$

Combine the sum of trigonometric functions in a smart way!

Ex. TH-13.7: *S-wave scattering*

Suppose we have measured

$$\frac{d\sigma}{d\Omega} = a, \quad a > 0.$$

Assume pure s-wave scattering and derive the complex scattering amplitude $f(\theta)$.

Ex. TH-13.8: *Path-integral formalism* (optional)

a) Write down an expression for the classical action for a simple harmonic oscillator for a finite time interval.

b) Construct $\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle$ for a simple harmonic oscillator using Feynman's prescription for $t_n - t_{n-1} = \Delta t$ small. Keeping only terms up to order $(\Delta t)^2$, show that it is in complete agreement with the $t - t_0 \to 0$ limit of the propagator

$$K(x'', t : x', t_0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin[\omega(t - t_0)]}} \exp\left\{\frac{im\omega}{2\hbar \sin[\omega(t - t_0)]} \times \left[(x''^2 + x'^2)\cos[\omega(t - t_0)] - 2x''x'\right]\right\}.$$

Ex. EXP-13.1: *Energy-Levels of Helium-like Atoms*

The energy levels of He-like atoms with one electron in the ground state ($n = 1$) and the other one in an excited state ($n > 1$)can be described by

$$E = -RhcZ^2 - \frac{Rhc\,(Z-1)^2}{n^2}.$$

In this expression it is assumed that the electron in the ground state complete shields the charge of the nucleus. Discuss the plausibility of this expression. Calculate the energy levels of He for $n = 2, 3$, and 4 and compare to the experimental results. Why does the accuracy of the above expression rise with rising n?

Ex. EXP-13.2: *Sum over Quantum Numbers*

Show that the sum $\sum (2J + 1)$ over all possible values of J is equal to the product $(2L + 1)\,(2S + 1)$! Is this product of any physical relevance? Why (not)?

<u>Ex. EXP-13.3</u>: *LS- versus JJ-Coupling*

Discuss a two-electron-system with one $2p$ and one $3d$ electron for the case of jj-coupling and show that the number of allowed states and their total angular momentum j are the same as for the case of ls-coupling.

<u>Ex. EXP-13.4</u>: *Term Schemes*

a) Determine the number of allowed terms of an excited carbon atom with electron configuration $1s^2 2s^2 2p 3d$. Do not take care of spin-orbit-coupling.

b) Calculate the effective magnetic moment of an atom in the ground state $1s^2 2s^2 2p^6 3s^6 4s^2 3d^3$ if in the ground state L has the largest value that is compatible with Hund's rule and the Pauli principle.

c) Determine the ground state of atoms with electron configuration $4d5s^2$ (Y) and $4d^2 5s^2$ (Zr). [Note that completed electron shells are not noted and L is determined as in b).]

d) In its ground state, manganese ($Z = 25$) has a sub-shell that is just filled to the half with 5 atoms. Give the electron configuration and the ground state of the atom!

<u>Ex. EXP-13.5</u>: *Stern-Gerlach experiment*

a) Determine the maximum number of the components of the magnetic moments of vanadium (^4F), manganese (^6S) and iron atoms(^5D) in the direction of an external magnetic field, if the atomic beams in a Stern-Gerlach experiment are split into 4, 6, and 9 beams.

b) What term symbol has the singlet state whose overall splitting in an external magnetic field $B_0 = 0.5$ T is $\overline{\nu} = 1.4\text{cm}^{-1}$?