

PLANCKS Student Competition 2017

Problem Folder

Brought together by Matthias Werl

In this problem folder you will find 10 different exercises out of the various fields of theoretical physics. You will have 4 hours to to solve as many as possible. The problems are designed in a way to make it impossible to solve them all in the given time; which is why the teams need to work togethter and develop a strategy to solve as many as possible in the given time.

Each problem is worth 10 points which are distributed over the various tasks of each exercise. This results in a maximum score of 100 points. The team with the most points will win the competition. The exercices will be corrected and graded either by the contributing professors or by experts in the respective field.

Calculators are allowed, as long as they are not programmable and can only perform basic mathematical operations (addition, subtraction, multiplication). The calculators will be checked by the respective supervisors.

You will receive two sets of sheets of paper: one blank and the other squared. Squared sheets of paper are for notes only and will not be handed in. The blank sheets of paper will be handed in.

Please use a separate sheet for every problem. For each problem, there is only one correct solution. If more than one solution is given, the problem is marked as incorrect, so make sure **you only mark your final answer**.

Good luck!



1 Laser ionization



Laser resonance ionization of neutral atoms is a powerful technique for the study and manipulation of atomic samples. A first laser λ_1 interacts with the neutral atom bringing it from the ground state $|0\rangle$ to an exited state $|1\rangle$ with opposite parity. When excited, the neutral atom is finally ionized using a second laser λ_2 which can remove an electron via an auto-ionizing state or towards the continuum, provided that the sum of the photon energies $\lambda_1 + \lambda_2$ is greater than the ionization potential of the atom.

Questions:

- Consider an atom of ⁶³*Cu* moving with a velocity ν_x. For the ionization process to take place the wavelength of the |0⟩ to |1⟩ transition of an atom at rest is l₁ = 350 nm. If the atom is moving with ν_x = 550 m/s, calculate the value of the new wavelength in order to excite the neutral atom (permitting the transition |0⟩ to |1⟩) in:
 - (a) Figure 1
 - (b) Figure 2
 - (c) If now we consider an ensemble of atoms with a natural linewidth of 21.6 MHz for the state $|1\rangle$, confined in a hot cavity at T = 2000 K, and the laser bandwidth is negligible, what is the:
 - Einstein coefficient
 - Atomic linewidth
 - (d) If the hyperfine splitting (Consisting of 4 allow transitions) for the ground state is 11 GHz and for the excited state is 1 GHz, how many resolved peaks will appear in the full HFS scan?
- Imagine the same ensemble of atoms, this time moving in the same direction inside a supersonic gas-jet of velocity v_x and length x. What is the relation between the laser repetition rate and the velocity of the atoms in order to irradiate all the atoms in the ensemble?



2 Generalised 1D Brownian motion

This problem is about generalised one-dimensional Brownian motion, which is mathematically similar to the treatment of collisional processes in plasmas. We consider a heavy Brownian particle (dust) in a background of many light particles (molecules) where the background has temperature T. The background particles randomly hit the Brownian particle and influence its dynamics by collisions.

- 1. First consider the collisionless case for Newtonian Mechanics of a single Brownian particle of mass M at position X(t) and velocity V(t). (Hint: don't think in a complicated way)
 - (a) What are the equations of motion for X(t) and V(t) if a force F(X(t)) is acting on the particle? Write them in the form

$$\frac{d}{dt}X(t) = \dots,\tag{1}$$

$$\frac{d}{dt}V(t) = \dots \tag{2}$$

(b) If we approximate the differential timestep dt by a small but finite step Δt starting at time t, what are the approximate changes in position $\Delta X_{\text{orb}} = X(t + \Delta t) - X(t)$ and velocity $\Delta V_{\text{orb}} = V(t + \Delta t) - V(t)$ after the time Δt has passed?

$$\Delta X_{\rm orb} = \dots, \tag{3}$$

$$\Delta V_{\rm orb} = \dots \tag{4}$$

2. Now we consider an ensemble of non-interacting identical Brownian particles, still neglecting collisions with the background. In the force-free case F = 0, the evolution of their probability density f(x, v, t) in phase-space with coordinates (x, v) is given by

$$\frac{\partial f(x,v,t)}{\partial t} + v \frac{\partial f(x,v,t)}{\partial x} = 0.$$
 (5)

To distinguish the (x, v) used as an independent variables here, they are denoted by small letters. This is in contrast to the orbit quantities X(t), V(t) in the particle picture, being functions of time.

- (a) What is the mathematical and physical connection to the particle picture of 1.? (Hint: use a total time derivative of *f* with x = X(t), v = V(t) from 1a with F = 0)
- (b) What changes in Eq. (5) if we introduce a force F(x)?
- 3. If we allow collisions of the ensemble of Brownian particles with the background (not with each other), Eq. (5) is changed to

$$\frac{\partial f(x,v,t)}{\partial t} + v \frac{\partial f(x,v,t)}{\partial x} = v_c \frac{\partial}{\partial v} \left(v_T^2 \frac{\partial f(x,v,t)}{\partial v} + v f(x,v,t) \right).$$
(6)

Here, the zero on the right-hand side in Eq. (5) has been replaced by a Fokker-Planck collision operator, where the collision frequency v_c measures how frequently collisions occur in time, and the thermal velocity $v_T = \sqrt{2T/M}$ is the



average velocity magnitude of the Brownian particle ensemble if it had the same temperature T as the background.

- (a) For a homogenous system with $\partial f / \partial x = 0$, what is the stationary distribution f_{∞} for which f does not change in time anymore?
- (b) What is its physical meaning of f_{∞} ? Does ν_c appear in f_{∞} ? Why/why not? Explain mathematically and physically.
- (c) What is the stationary distribution in the general case with $\partial f / \partial x \neq 0$ with a conservative force F(x) acting as in 2b)?
- 4. Switching back from the ensemble to the particle picture, we can represent the orbit of the Brownian particle including randomisation by collisions with the background using

$$V(t + \Delta t) - V(t) = \Delta V_{\text{orb}} - \nu_c V(t) \Delta t + \sqrt{2\nu_c v_T^2 \Theta \sqrt{\Delta t}}.$$
 (7)

Here, Δt is a sufficiently small time-step, Θ is a random number between 0 and 1 and ΔV_{orb} is taken from 1b).

- (a) Based on the similar form of ΔV_{orb} of 1b), how can the second term on the right-hand side of Eq. (7) be interpreted in terms of a force acting on the Brownian particle?
- (b) Where does this so-called drag force appear in the Fokker-Planck equation? (Hint: move a term from the operator on the right-hand side to the left-hand side)
- (c) How does an increase or decrease of the collision frequency v_c affect the system's approach towards the stationary state over time?



3 Particle Physics

The following exercises concern the fundamental particles and forces of our universe. The theory we will use as underlying framework is the Standard Model of particle physics. All you will need for the following exercises are the following diagrams, and some intuition.

Figure 1 shows a sketch of the particles and the interactions within the Standard Model. Particles interacting with each other are connected by a line. Different colours represent different forces. The particles that are mediators of the forces have a larger border of the same colour as the interaction they mediate. In the interactions described by the Standard Model, one needs to conserve the following quantum numbers:

- Lepton number, where charged leptons and neutrinos have a lepton number *L_x* where x is the family (electron, muon, tau);
- Baryon number, where baryons like protons, neutrons, pions and kaons have a baryon number of 1, and anti-baryons have a baryon number of -1;



• Electric charge.

Figure 1: A graphical illustration of the SM interactions and forces.



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Figure 2 shows how different kinds of particles interact in a generalpurpose detector like the ATLAS detector, and shows a cross-section of the ATLAS detector.



Figure 2: A graphical illustration of the particle interactions taking place in the ATLAS detector, together with a cross-section of the detector itself. Source: http://atlas.ch/ and http://www.particleadventure.org/



- 1.1 The center of mass energy at which protons are collided at the Large Hadron Collider is 13 TeV. The average energy in Joule of a Wasa cracker is 60 kilo calories (source: a packet of Wasa). 1 eV is equivalent to $3.83 \ 10^{-20}$ calories. Use natural units, where *h* and *c*=1.
 - a) What is the LHC energy, in calories (assuming you could transform all of the cracker's energy in kinetic energy you could give to a proton) ?
 - b) How many Wasa crackers do you need to equate to the energy of an LHC pp collision?
 - c) Puzzled? How come the LHC is considered so powerful?
- 1.2 Classify the following particle reactions as strong, electromagnetic, weak, or impossible, based on the Standard Model interactions and conservation laws above. In each of the reactions, specify which particle mediates the force. Draw diagrams that connect initial state particles, force mediators and final state particles ("Feynman diagrams"), paying attention to the conservation laws at every junction ("vertex"). Note that the mediators of the interaction are not mentioned explicitly in the particle reactions below.
 - a) $v_e + \bar{v}_\tau \rightarrow e^- + \tau^+$
 - b) $\mu^- + p \rightarrow \nu_\mu + n$
 - c) $K^- \rightarrow \mu^- + \bar{\nu}_\mu$
 - d) $n \rightarrow p + e^{-}$
 - e) $\pi^0 \rightarrow \gamma + e^+ + e^-$
 - f) $\Sigma^0 \rightarrow \Lambda + \gamma$
 - g) $e^- \rightarrow \mu^- + \nu$
- 1.3 The ATLAS detector is one of the main multi-purpose detectors at the Large Hadron Collider, currently it is operating at a centre of mass energy of 13 TeV for pp collisions.

Figures 3-6 are graphical depictions of real collision events recorded at the Large Hadron Collider (LHC) by the ATLAS detector in 2010 and 2012. It is not possible to exactly determine what happened, but select for each figure the most likely interaction that took place from the list below (note: there does not need to be a 1:1 correspondence), explaining your reasoning behind the choice, and mention which force is involved.

- $W \rightarrow \mu + \nu_{\mu}$ candidate
- $Z \rightarrow \mu^+ + \mu^-$ candidate
- $J/\Psi \rightarrow e^+ + e^-$ candidate
- $p + p \rightarrow 2$ jets candidate (Where a jet is a collimated stream of hadrons) Hint: Ignore the underlying background processes, focus on the highlighted tracks. The dotted line refers to a track who although not observed by the detector is inferred by some energy imbalance in the event.



Caterina Doglioni & Peter Christiansen Lund University



Figure 3: A graphical illustration of the ATLAS detector for Event 14321500, showing the a 3D profile of the inner detector, magnets and muon spectrometers.



Figure 4: A graphical illustration of event 23181153. Left: view looking down the barrel, where the inner rings are the electromagnetic and hadronic calorimeters and the outer panels are the muon detectors. The tracks of interest are colored pink and the grey tracks are the background events. Top right: side view. Bottom right: energies recorded by the calorimeters against the track "angles" η .





Figure 5: ATLAS event display. Left: view along the beam pipe, showing the tracks from the event and the detector calorimeters. Bottom right: side profile. Top right: is a plot displaying the energies of the two tracks (in yellow) recorded in the calorimeters againist their "angle" η (pseudo-rapidity). Bottom right: looking down the barrel of the detector. The background tracks are colored blue.



Figure 6: ATLAS event display. This is a 3d mid-way section of the ATLAS detector, also called R - z view: what you see in shaded grey and black are the toroidal magnets and their support structures. The energy deposited in the electromagnetic and hadronic calorimeters is represented as yellow and green rectangles, of height proportional to the magnitude of the transverse momentum recorded by the calorimeters.



4 Nuclear/Neutron physics

- 1. Calculate the energy per fission of one atom of uranium 235 (^{235}U). How much energy can be obtained from one kg of ^{235}U ?
- 2. Compare this energy to the energy obtained by the fusion from a Deuterium $({}^{2}H)$ and a Tritium $({}^{3}H)$ atom. How much energy can be obtained by 1 kg of the necessary isotopes?

The most common fission products of ${}^{235}U$ are ${}^{139}Ba$ and ${}^{95}Kr$. Required masses: $m_{{}^{235}U} = 235.0439u$, $m_{{}^{139}Ba} = 138.9116u$, $m_{{}^{95}Kr} = 94.9153u$, $m_{{}^{2}H} = 2.0141u$, $m_{{}^{3}H} = 3.0160u$, $m_{{}^{4}He} = 4.0026u$, $m_{n} = 1.0087u$. $1u = 1.66057 \cdot 10^{-27} kg$.

3. Calculate the energy of a neutron scattered at a stationary nucleus with the weight A. Consider a neutron with the energy $E = \frac{mv^2}{2}$ in the laboratory (L) system incident upon a stationary nucleus of mass M. Since the relative masses are important in the kinematics, we set the mass of the neutron m = 1 and the mass of the nucleus M = A. It is convenient to convert to the center of mass (CM) system as indicated in Fig. 1, because the elastic scattering event is isotropic in the CM system. Give the energy of the neutron after the scattering process.



Figure 1: Scattering of a neutron at a nucles. Lab system (L) and Center of mass (CMS) system

5 Solid state physics

I, **Background**: The color of a substance is caused by selective, *i.e.* frequency dependent, dissipation and dispersion of electromagnetic radiation. A vector potential *A* oscillating at a frequency ω induces a current density *j* at the same frequency. This is described by the linear relation $j = i\omega\sigma(\omega)A$, where $\sigma(\omega)$ is a complex frequency dependent function called "optical conductivity" which characterizes the optical properties of the substance. Throughout this problem set you may assume for simplicity that the electrons move in a one-dimensional space. The quantum theory of matter coupled to radiation provides the following expression for the real (dissipative) part of the optical conductivity

$$\operatorname{Re}\sigma(\omega) = \operatorname{Re}\sigma(-\omega) = \frac{e^2}{V\hbar} \operatorname{Im} \int_0^\infty e^{i\omega t} \left\langle [\hat{x}(t), \hat{v}] \right\rangle dt \tag{1}$$

where *e* is the electron charge, *V* the sample volume, and $\langle \rangle$ is an ensemble average over the Hamiltonian eigenstates of the substance. The position (*x*) and velocity (*v*) operators satisfy the equation of motion

$$\hat{v}(t) = \frac{i}{\hbar} \left[\hat{H}, \hat{x}(t) \right] \tag{2}$$

At time t = 0 the Heisenberg representation yields $\hat{v}(0) = \hat{v}$ and $\hat{x}(0) = \hat{x}$. **Question I:** Show that the optical conductivity satisfies the following sum-rule

$$\int_{0}^{\infty} \operatorname{Re}\sigma(\omega)d\omega = \frac{\pi e^{2}}{2V\hbar^{2}}\operatorname{Re}\left\langle \left[\hat{x}, \left[\hat{H}, \hat{x}\right]\right] \right\rangle$$
(3)

II, **Background**: The momentum operator \hat{p} and the position operator satisfy the Heisenberg uncertainty relation

$$[\hat{x}, \hat{p}] = i\hbar \tag{4}$$

Eq. (4) remains valid in a crystalline environment, but the set of eigenvalues of \hat{p}

$$\hat{p}|q\rangle = q|q\rangle \tag{5}$$

is confined to a finite interval, $q \in \{-\hbar \pi/a; \hbar \pi/a\}$ where *a* is the lattice constant. In a metal in its simplest incarnation, one of the bands (the "conduction band") is partially occupied with electrons and all other bands are either fully occupied or completely empty. The corresponding band-energies $\epsilon_c(q)$ are the eigenvalues of the Hamiltonian operator

$$\hat{H} = \epsilon_c(\hat{p}) \tag{6}$$

which in a solid environment is usually some complicated non-linear function of the momentum operator \hat{p} . In vacuum this reduces to the familiar expression $\epsilon(\hat{p}) = \hat{p}^2/2m$, but in a solid environment the \hat{p} -dependence is different and varies strongly from one material to another. The optical conductivity has two types of contributions:

$$\sigma(\omega) = \sigma_c(\omega) + \sigma_b(\omega) \tag{7}$$

The current carried by the electrons in the conduction band described by Eq. (6) gives rise to the contribution $\sigma_c(\omega)$, which corresponds to a zero-frequency mode



with a finite width due to scattering. The finite-frequency ("bound charge") contribution defined as $\sigma_b(\omega)$, comes from optical transitions between the (fully and partly) occupied and (fully and partly) empty bands.

Question II: Assume that the substance contains a single electron, and that it occupies momentum eigenstate $|q\rangle$ in the conduction band. Leave all other bands out of consideration and show with the help of Eqs. (3), (4) and (6) that $\sigma_c(\omega)$ satisfies

$$\int_{0}^{\infty} \operatorname{Re}\sigma_{c}(\omega)d\omega = \frac{\pi e^{2}}{2V} \frac{\partial^{2}\epsilon_{c}(q)}{\partial q^{2}}$$
(8)

III, Background: The many-electron generalization of Eq. (8) is a somewhat lengthy exercise which we are not asking you to do. It has the following result

$$\int_{0}^{\infty} \operatorname{Re}\sigma_{c}(\omega)d\omega = \frac{\pi e^{2}}{2V} \sum_{k} n_{c}(k) \frac{\partial^{2} \epsilon_{c}(k)}{\partial k^{2}}$$
(9)

where $n_c(k) \in \{0, 1\}$ is the average number of conduction electrons with momentum k. In the limit of very high temperature, $n_c(k)$ tends toward a k-independent constant: $\lim_{T\to\infty} n_c(k) = n_c$.

Question III: Show that

$$\lim_{T \to \infty} \int_0^\infty \operatorname{Re}\sigma_c(\omega) d\omega = 0$$
 (10)

IV, Background: However, since electrons can be thermally excited from one band to another, the restriction to a single band is not justified at finite temperature. In fact the following sum-rule for the full conductivity ($\sigma = \sigma_c + \sigma_b$) holds for any temperature

$$\int_{0}^{\infty} \operatorname{Re}\sigma(\omega)d\omega = \frac{\pi N e^2}{2m_e V}$$
(11)

where m_e is the free electron mass and N is the total number of electrons summed over all (partly or fully) occupied bands. Bismuth-antimony alloys are very interesting materials that exhibit a topological insulating phase for certain compositions. Pure bismuth is a semimetal, for which the main characteristics of the electronic structure are displayed in Figure 1 (an additional band of heavy hole carriers is left out of consideration for simplicity). The conduction band of these materials is characterized by a large value of the inverse effective mass $1/m_c = \partial^2 \epsilon_c(q)/\partial q^2|_{q=0}$, in other words $m_c < m_e$. Since only a small number of q-states are occupied, all having $q \simeq 0$, the spectral weight of the zero-energy mode satisfies

$$\int_{0}^{\infty} \operatorname{Re}\sigma_{c}(\omega)d\omega = \frac{\pi N_{c}e^{2}}{2m_{c}V}$$
(12)

where N_c is the number of electrons in the conduction band.

Question IV: Given that $m_c < m_e$, would nature allow a situation where the conduction band (red in Figure 1) would be the only band that is (partly or fully) occupied, implying that the blue band would be absent from Figure 1 ? Explain why or why not.



Dirk van der Marel, University of Geneva



Figure 2: Left: Single crystal of bismuth. Middle panel: Schematic of the two bands close to the Fermi energy which are the most relevant ones for the optical spectrum shown in the right hand panel: The conduction band (red) crosses the Fermi energy E_F . A fully occupied band (blue) has its maximum about 0.02 eV below E_F . Right hand panel: Optical conductivity of bismuth. Note the presence of the zero-frequency mode, $\sigma_c(\omega)$, below $\hbar\omega \sim 0.02$ eV for T = 20 K (shifting to higher energy for higher temperatures). The rise in conductivity above 0.02 eV corresponds to $\sigma_b(\omega)$ and is due to optical transitions between the two bands indicated in the middle panel.



6 Two accelerating locomotives connected by a tincan-telephone

On a very long straight railway, two locomotives are about to get moving in the same direction at relativistic speeds by igniting a series of high-power fuel (Presto Logs aka Superzündis)¹, each of which will instantaneously increase their velocity by the same amount $\Delta v = \frac{3}{5}c = 0.6c$ with respect to their present inertial frame.

The two locomotives are separated by a clear space of 9m = 30 light-nanoseconds (lns) over which a rubber thread is spanned, connecting the two ends of a tin-cantelephone, which only works when the rubber thread has been stretched to its maximal length of 30 lns, but the thread would break if kept stretched any amount beyond that after the acceleration phase.²

The train drivers (Doc and Marty) are equipped with perfectly accurate and synchronized clocks. They will ignite their presto logs according to the time table given to them. The aim is that they reach more than 95% of c and that the thread between them does not break and is in place for a tin-can-communication (through which the drivers can compare their clock readings when moving peacefully at their final velocity).

It is clear (at least to Doc) that they cannot just ignite their presto logs at exactly the same time as given by their respective clocks. Explain why!

Marty, the driver in the first (front) locomotive is instructed to ignite his set of presto logs every 10 seconds after 12:00 on his clock. Work out

- (a) how many presto logs each train driver minimally needs,
- (b) exactly when the logs in the second (behind) locomotive have to be ignited by Doc,
- (c) what is the time difference that Doc and Marty find when comparing their clocks over the tin-can-telephone (assuming that they know exactly the velocity of sound in their telephone cable so that they can accurately subtract the obvious delays in their communication).

¹Back to the Future Part III

²That is, ignore the stress from shock waves caused by the sudden acceleration of the ends of the rubber thread (just assume that it never slacks and that it is also robust under any transitory local deformation that may occur when pushed or pulled from one end until everything is settled in a new inertial frame). Also neglect the size of the locomotives and consider them pointlike.



7 Carnot cycle with van-der-Waals gas

We are looking at a carnot cycle (adiabatic-isothermal thermodynamic cycle) with a van-der-Waals (vdW) gas as working medium.

At the start point (1), the gas has a reduced temperature of $T_1^r = 1.5$, its reduced (specific) volume is $v_1^r = 1$. In the first step, the gas is (isothermally) expanded to twice its starting volume, with the endpoint of the subsequent adiabatic step being on the critical isothermal line. The specific heat capacity (at constant volume) is given by $\frac{C_V}{n} = 3R$, so $c_V = 3$.

Hint:

The vdW gas equation is given by $\left(p + \frac{a}{v^2}\right)(v - b) = RT$, where a gives the average attraction between particles and b is the volume of a mole of particles. It is characterized by the critical point with coordinates (p_k, v_k, T_k) , where $T_k = \frac{8a}{27Rb}$, $p_k = \frac{a}{27b^2}$ and $v_k = 3b$. The reduced quantities are given by $T^r = \frac{T}{T_k}$, $p^r = \frac{p}{p_k}$ and $v^r = \frac{v}{v_k}$.

(a) For an adiabatic process with a vdW gas, the following relation between temperature T and specific volume v holds:

$$T^{cv}(v-b) = const \tag{1}$$

Express this equation *and* the vdW equation only as a function of the reduced quantities.

- (b) Explicitly calculte the reduced quantities in every point of the cycle.
- (c) Sketch the process *qualitatively* into the pv-diagram below. The critical point k on the critical isothermal line T_k alongside with other isothermal lines are already plotted.





In the following points, calculate with the *non-reduced* quantities:

- (d) Derive the formulae for exchanged specific heat quantities for every step. <u>*Hint:*</u> The differential for the (specific) internal energy for the vdW gas is given by: $du = c_V RT + \frac{a}{v^2} dv$. Use the first law of thermodynamics.
- (e) Give a formula for the efficiency of the thermodynamic cycle only as a function of the specific volumina v_i and temperatures T_i of the corner points. Show, that this efficient is the same as the efficient of a carnot cycle working with the *ideal gas* between the same temperature difference.





8 Crystal geometry

8.1 Part A - Cairo Tiling

For the Cairo tiling a two-dimensional plane is fully filled by pentagons. The geometry of a single pentagon is formed by four identical side lengths (blue colour) and one different side length (red colour) and angles of 90 $^{\circ}$ and 120 $^{\circ}$ (see Fig. 1).

- (a) Determine the 2D Bravais lattice of the Cairo tiling.
- (b) Draw the unit cell vectors \boldsymbol{a} and \boldsymbol{b} and the enclosed angle γ .
- (c) Give a derivation (or an argument) for the given angle γ .
- (d) How many tiles are within one unit cell?
- (e) Determine the 2 dimensional wallpaper group of the Cairo tiling. All possible wallpaper groups are given in Fig. 2

A Bravais lattice is an infinite array of discrete points which are generated by a set of discrete translation vectors which are multiples of the unit cell vectors *a* and *b*. The tiling has to be reproduced by the assignment of a set of tiles to each lattice point of the Bravais lattice.

The five existing 2D - Bravais lattices:

- cubic: a = b, $\gamma = 90^{\circ}$
- hexagonal: a = b, $\gamma = 120^{\circ}$
- rectangular: a \neq b, $\gamma = 90^{\circ}$
- rectangular centered: $a \neq b$, $\gamma = 90^{\circ}$ and two lattice points per unit cell
- oblique: a \neq b, $\gamma \neq$ 90°

Priority rules to determine 2D Bravais lattices:

- i Highest symmetry (cubic > hexagonal > rectangular > oblique)
- ii Smallest unit cell area
- iii Smallest lattice constants a and b

iv $a < b, \gamma \ge 90^{\circ}$



Roland Resel, TU Graz



Figure 1: Cairo Tiling



Figure 2: The 17 possible wallpaper groups. P...Primitive lattice C...Centered lattice



8.2 Part B - Trihex Tiling

For the triangle/hexagon tiling (TriHex) a two-dimensional plane is fully filled by two different types of tiles: one type of tile is a regular triangle and the second type of tile is a hexagon. Two different side lengths are involved: blue and red with a length ratio of 3:2, respectively. The arrangement of the tiles are given by Fig. 3.

As in Part A, determine the points (a)-(e) for the Trihex Tiling



Figure 3: TriHex Tiling



9 Spin Qubits

Hint: This problem should not be addressed by brute force. It is very useful to take into account **spin rotation invariance**.

In particular, when combining two systems described by angular momenta \vec{J}_1 and \vec{J}_2 , then one can choose a basis of eigenvectors of \vec{J}^2 and J^z , where $\vec{J} = \vec{J}_1 + \vec{J}_2$ is the total angular momentum operator. Also think how \vec{J}^2 is related to the scalar product $\vec{J}_1 \cdot \vec{J}_2$.



Figure 1: Setup consisting of four spin- $\frac{1}{2}$ particles.

Consider a qubit setup consisting of four spin- $\frac{1}{2}$ particles in a square arrangement (see Fig. 1). We work in units with $\hbar = 1$. The Hamiltonian of the system is:

$$H = \frac{1}{2} \sum_{i \neq j} J_{ij} \ \vec{S}_i \cdot \vec{S}_j \tag{1}$$

where

$$\vec{S}_j = \left(S_j^x, S_j^y, S_j^z\right) \tag{2}$$

denotes the three components of the quantum mechanical spin operator ¹ of particle *j* (*j* = 1, 2, 3, 4), and the dot "·" denotes scalar product over these components. The coupling constants J_{ij} can have the values J_A or J_B according to the figure.

Consider first the case $J_A < 0, J_B < 0$ **:**

(i) Determine the energy and degeneracy of the ground state of Hamiltonian from (1).

The system is prepared at t = 0 in a state consisting of all spins oriented in the x direction. At the same time a magnetic field, described by the Hamiltonian

$$H_B = -B \sum_{i=1}^{T} S_i^z \,. \tag{3}$$

¹We omit the [^] to indicate operators.



is applied in the z direction.

- (ii) How long does it take to the system to go back to the state with all spins oriented in the *x* direction?
- (iii) Determine the time dependence of the magnetisation M^x in the *x* direction, where

$$M^{\alpha} \equiv \left\langle S^{\alpha}_{tot} \right\rangle \qquad S^{\alpha}_{tot} \equiv \sum_{i=1}^{4} S^{\alpha}_{i} \qquad \alpha = x, y, z .$$
 (4)

and the expectation value $\langle \cdots \rangle$ is taken with respect to the above-mentioned time-dependent state.

We now go back to the hamiltonian from (1) (without magnetic field (eq. (3)))

- (iv) For the case $J_A = J_B$, determine all eigenvalues of *H* as well as their degeneracies
- (v) Consider now the case $\Delta J \equiv J_B J_A \neq 0$, but ΔJ small enough ². Determine again all eigenvalues of eq. (1) as well as their degeneracies.

From now on we consider the case $J_A > 0, J_B > 0$ and $\Delta J \neq 0$

(vi) Consider again the action of a magnetic field, (3). Determine the magnetc susceptibility

$$\chi \equiv \left. \frac{d \ M^z}{dB} \right|_{B=0} \tag{5}$$

where the expectation value in eq. (4) is carried out with respect to the ground state of $H + H_B$.

(vii) Consider now $\Delta J > 0$ and a magnetic field applied to the first spin only, described by the Hamiltonian

$$H_{\rm loc} = -b S_1^z \,. \tag{6}$$

determine the local susceptibility

$$\chi_{\rm loc} \equiv \left. \frac{dm^z}{db} \right|_{b=0} \tag{7}$$

where

$$m^{z} \equiv \left\langle S_{1}^{z} \right\rangle \tag{8}$$

and the expectation value is evaluated with respect to the ground state of $H + H_{loc}$ (no H_B !).

 $^{^{2}}$ We always consider ΔJ small enough such that there are neither level crossings nor accidental degeneracies.



Markus Koch & Andreas Hauser, TU Graz

10 Tribute to Joseph Ritter von Fraunhofer



10.1 Part A - Fraunhofer diffraction - The single slit

(a) Calculate the distribution of the electrical field E(Θ) as well as the intensity (irradiance) I(Θ) behind a single slit as function of the angle Θ in the Fraunhofer limit (R»D), according to Fig. 1. The slit width is D (*y* direction) and the slit is assumed to be indefinitely long (*z* direction). *Hint:* Use the expansion r(y) = R - ysin(Θ).



Figure 1: The single slit

(b) Sketch the intensity distribution.

10.2 Part B - Fraunhofer lines D1 and D2 - The sodium doublet

The Fraunhofer lines D1 and D2 appear as dark features (adsorption lines) in the spectrum of the sun (Fig. 2). The D1 line, which is higher in energy, is found at 589.0 nm.





Figure 2: Spectrum of the sun

The semiclassical derivation of the spin orbit coupling in atoms is based on a coordinate transformation into the rest frame of the valence electron. In this picture, an orbiting (singly charged) ion creates a field $B = -(\nu \times E)/c^2$ felt by the valence electron. In this B-field, the magnetic momentum μ of the electron, coupled to the electron spin s via $\mu = \frac{g_s \cdot \mu_b \cdot s}{\hbar}$, gives rise to an energy contribution $E_{so} = -\mu \cdot B$, which is known as spin-orbit interaction energy. A factor 0.5 needs to be added here due to the incorrect assumption of a linear motion of the electron in the transformation (Thomas-Factor).

Important quantities: $\mu_b = \frac{e\hbar}{2m}$; $g_s = 2$; $m_e = 9.10939 \cdot 10^{-31} kg$; $\varepsilon_0 = 8.85 \cdot 10^{-12} [\frac{F}{m}]$; $\hbar = \frac{h}{2\pi} = 1.0546 \cdot 10^{-34} Js$; $e = 1.6022 \cdot 10^{-19} C$

- (a) Write E_{so} as a function of the angular momentum l and the spin s of the valence electron. Introduce the total angular momentum j = l + s and try to find an expression for E_{so} where the operators can be replaced by their corresponding quantum numbers j, l and s. The radius of the *n*th orbit can be estimated via Bohrs ansatz $r_n = \frac{a_0 n^2}{z}$ with $a_0 = 0.529$ Å and z = 11.
- (b) With this formula, calculate the energy difference between the D1 and the D2 line of sodium in cm^{-1} . This splitting is a consequence of the SO-coupling in an electronically excited state of sodium where the 3p orbital is singly occupied.