

Problem 1

(4 Points)

A moving clock is running slower than a clock at rest.

- How does this effect depend on the velocity of the clock.
- How large is the velocity of the clock, if the effect amounts 1%?
- How was the effect discovered?
- The experimental proof of the effect was given for the first time with cosmic μ^- particles. Explain the experiment.

Problem 2

(4 Points)

- Sketch as a function of the wavelength the power per wavelength emitted by a black body at temperature T .
- Which laws characterize the radiation emitted by a black body?
- Explain how it was possible to conclude from the properties of thermal radiation that the energy of electromagnetic waves is quantized?
- Give the energy of the light quanta as a function of the wavelength.

Problem 3

(4 Points)

- What is the meaning of the acronym LASER?
- What is the difference between the light of a laser and the light emitted by a black body at temperature T ?
- What is the reason for this difference?
- Cr^{3+} doped Al_2O_3 is used as the active material of the ruby laser. Starting from the optical spectrum of Cr^{3+} in Al_2O_3 explain the operation principle of the ruby laser.

Problem 4

(4 Points)

The atoms of the C-O molecule can oscillate and rotate around the common center of gravity of the molecule. ($m_{\text{C}} = 12 \text{ g/mol}$, $m_{\text{O}} = 16 \text{ g/mol}$)

- Give Schrödinger's equation for the case that only oscillations of the molecule can be excited.
- What are the possible energy levels of the oscillating molecule?
- Calculate the spring constant between the atoms of the molecule, if oscillations can be excited with light of wavelength $\lambda = 4.7 \cdot 10^{-6} \text{ m}$.
- Calculate the excitation energies, if only rotations of the molecule are excited. Calculate the wave length of the corresponding radiation. Use a bond length of 100 pm for the C-O molecule.

Problem 5

(4 Points)

- a) Give Schrödinger's equation of an electron bound to a nucleus with the charge number Z .
- b) How large is the excitation energy of the electron in its first excited state?
- c) The quantum states of the electron are characterized by quantum numbers. Explain the meaning of these quantum numbers.
- d) Describe the wave functions of the electron in its first excited state.

Problem 6

(4 Points)

For Ti^{2+} there are two electrons in the 3d shell.

- a) What is the angular momentum of these electrons?
- b) The ground state of Ti^{2+} is determined by Hund's rules. Explain these rules. What is the ground state of Ti^{2+} .
- c) The total splitting of the ground-state multiplet of Ti^{2+} due to the spin-orbit coupling is 500 cm^{-1} . Determine the spin-orbit coupling constant of Ti^{2+} .

Problem 7

(4 Points)

Consider a simple cubic lattice with lattice constant $a=380 \text{ pm}$.

- a) The reciprocal lattice is also simple cubic. Calculate the lattice parameter of the reciprocal lattice.
- b) Write up the Laue criterion for x-ray scattering.
- c) Explain the relation between the Bragg condition and the Laue criterion.
- d) Sketch and explain the Ewald construction for x-ray scattering.

Problem 8

(4 Points)

- a) What is the fundamental difference between a gas of electrons and a classical ideal gas of charged particles?
- b) The Fermi energy of Cu is 7 eV. What is the meaning of the Fermi energy of a gas of electrons?
- c) What is the temperature dependence of the specific heat of the electron gas? Give reasons for your answer.
- d) The energy of conduction electrons is given by energy bands. What is the reason for these energy bands and why there are energy gaps in the band structure?

Required physical constants:

Velocity of light:

$$c = 3 \cdot 10^8 \text{ m/s}$$

Avogadro's number:

$$N_A = 6 \cdot 10^{23} \text{ mol}^{-1}$$

Planck's constant:

$$h = 6,63 \cdot 10^{-34} \text{ Js}$$

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- c) How was the effect discovered?
- d) The experimental proof of the effect was given for the first time with cosmic μ^- particles. Explain the experiment.

a)

$$t(v) = t_0 / \sqrt{1 - (v/c)^2}.$$

Thereby $t(v)$ denotes the time of the moving clock, whereas t_0 denotes the time of the clock at rest.

b) $(t(v) - t_0)/t_0 = 0.01$ und

$$\frac{1}{\sqrt{1 - (v/c)^2}} = 1.01$$

$$\left(\frac{1}{1.01}\right)^2 = 1 - (v/c)^2 \rightarrow v = 42.111 \text{ km/s}$$

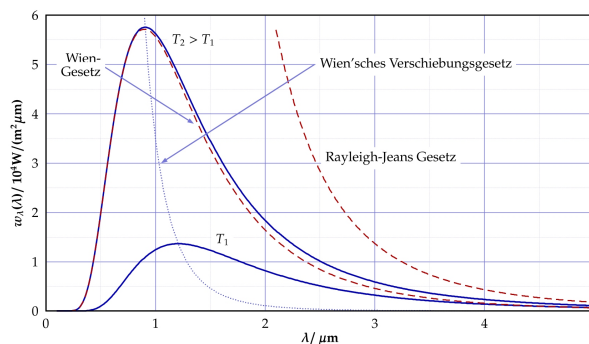
- c) The result of the Michelson Morley experiment is, that the velocity of light is a natural constant. At least for light there has to be time dilation (compare light clock). That time dilation is general has to be shown experimentally.
- d) For slow μ^- particles the life time is $\tau = 2.2 \cdot 10^{-6} \text{ s}$. The velocity of cosmic μ^- particles is in the range of the velocity of light. μ^- particles are measured by a detector equally recording the velocity and the particle number on a mountain at high altitude and on sea level at low altitude. The number of μ^- particles at sea level is much larger than expected number due to the exponential decay law using the normal time of flight. Only when time dilation is considered, the correct particle number can be calculated, i.e. the clock of the fast μ^- particles is moving slower.

Problem 2

(4 Points)

- Sketch as a function of the wavelength the power per wavelength emitted by a black body at temperature T .
- Which laws characterize the radiation emitted by a black body?
- Explain how it was possible to conclude from the properties of thermal radiation that the energy of electromagnetic waves is quantized?
- Give the energy of the light quanta as a function of the wavelength.

- Sketch of Planck's law (only blue lines)



- Thermal radiation is characterized by Planck's law, Wien's law displacement law $\lambda_{\max} = \frac{2.9 \text{ mm} \cdot \text{K}}{T}$ and the Stefan-Boltzmann law $P/A = \varepsilon \sigma T^4$.
- Planck's law can only be derived with the assumption that the energy of electromagnetic radiation is absorbed and emitted in quanta.
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$$E = h \cdot \nu$$

h denotes Planck's constant. With $\nu \cdot \lambda = c$ one gets

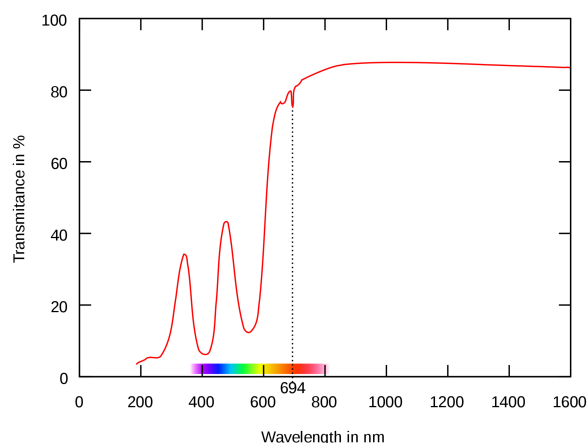
$$E = \frac{h \cdot c}{\lambda}.$$

Problem 3

(4 Points)

- a) What is the meaning of the acronym LASER?
- b) What is the difference between the light of a laser and the light emitted by a black body at temperature T ?
- c) What is the reason for this difference?
- d) Cr^{3+} doped Al_2O_3 is used as the active material of the ruby laser. Starting from the optical spectrum of Cr^{3+} in Al_2O_3 explain the operation principle of the ruby laser.

- a) Laser: light amplification by stimulated emission of radiation.
- b) The light of a laser is nearly monochromatic whereas the light of thermal radiation is distributed over a large frequency range.
- c) A selected transition is amplified by stimulated emission of radiation.
- d) Absorption spectrum of Cr^{3+} in Al_2O_3 .



Due to the strong absorption lines in the blue and green range of the spectrum excited energy levels of the Cr^{3+} ion are populated by means of a flash tube. The Cr^{3+} ion can relax without electromagnetic radiation into a lower energy level, which corresponds to the small absorption line at 694 nm. Due to the small transition probability of this level, population inversion is achieved. Stimulated emission results in a pulse of laser light.

Problem 4

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The atoms of the C-O molecule can oscillate and rotate around the common center of gravity of the molecule. ($m_C = 12 \text{ g/mol}$, $m_O = 16 \text{ g/mol}$)

- Give Schrödinger's equation for the case that only oscillations of the molecule can be excited.
- What are the possible energy levels of the oscillating molecule?
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- Calculate the excitation energies, if only rotations of the molecule are excited. Calculate the wave length of the corresponding radiation. Use a bond length of 100 pm for the C-O molecule.

- a) The Schrödinger equation is

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m_0} \frac{\partial^2 \psi(x,t)}{\partial x^2} + \frac{1}{2} D x^2 \psi(x,t)$$

or without the time dependence

$$E \psi(x) = -\frac{\hbar^2}{2m_0} \frac{\partial^2 \psi(x)}{\partial x^2} + \frac{1}{2} D x^2 \psi(x).$$

(Only one version of the equation is expected.)

Thereby $\frac{1}{m_0} = \frac{1}{m_C} + \frac{1}{m_O}$ denotes the reduced mass of the molecule and D the spring constant.

- b) The excitation energies are $E_n = \frac{1}{2} \hbar \omega (n + 1)$ mit $n = 0, 1, \dots$ und $\omega = \sqrt{\frac{D}{m_0}}$.

- c) The excitation frequency is $\nu = c/\lambda = 3 \cdot 10^8 \text{ m}/4,7 \cdot 10^{-6} \text{ m} = 6,4 \cdot 10^{13} \text{ Hz}$.
With $\nu = 6,4 \cdot 10^{13} \text{ s}^{-1} = \frac{1}{2\pi} \sqrt{\frac{D}{m_0}}$ one gets $D = (2\pi \cdot 6,4 \cdot 10^{13} \text{ s}^{-1})^2 \cdot m_0$
and with $m_0 = 6,86 \text{ g/mol}$

$$D = (2\pi \cdot 6,4 \cdot 10^{13} \text{ s}^{-1})^2 \cdot 6,86 \text{ g/mol} = 1850 \text{ kg/s}^2.$$

- d) The energy eigenvalues of the rotation are $E_\ell = h\nu_\ell = \frac{\ell(\ell+1)\hbar^2}{2m_0 r^2}$ und damit

$$E_\ell = \frac{\ell(\ell+1)\hbar^2}{2(2\pi)^2 m_0 r^2} = \ell(\ell+1) \frac{(6,63 \text{ Js} \cdot 10^{-34})^2}{2(2\pi)^2 6,86 \cdot 10^{-3} \text{ kg} / 6 \cdot 10^{23} \cdot 10^{-20} \text{ m}^2}$$

$$E_\ell = \ell(\ell+1) \cdot 4,87 \cdot 10^{-23} \text{ J} = \ell(\ell+1) \cdot h \cdot 7,34 \cdot 10^{10} \text{ Hz}$$

$$\lambda_\ell = \frac{c}{\nu_\ell} = \frac{3 \cdot 10^8 \text{ m/s}}{\ell(\ell+1) \cdot 7,34 \cdot 10^{10} \text{ Hz}} = \frac{4,1 \text{ mm}}{\ell(\ell+1)}$$

Problem 5

(4 Points)

- a) Give Schrödinger's equation of an electron bound to a nucleus with the charge number Z .
- b) How large is the excitation energy of the electron in its first excited state?
- c) The quantum states of the electron are characterized by quantum numbers. Explain the meaning of these quantum numbers.
- d) Describe the wave functions of the electron in its first excited state.

- a) The time dependent Schrödinger equation is

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m_0} \nabla^2 \psi(\vec{r}, t) + \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{r} \psi(\vec{r}, t)$$

and the time independent version

$$E\psi(\vec{r}) = -\frac{\hbar^2}{2m_0} \nabla^2 \psi(\vec{r}) + \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{r} \psi(\vec{r}).$$

- b)

$$E_n = \frac{-13.6 \text{ eV} \cdot Z^2}{n^2} \text{ mit } n = 1, 2, \dots$$

$$E_2 - E_1 = -13.6 \text{ eV} \cdot Z^2 \left(\frac{1}{2^2} - 1 \right) = 10.2 \text{ eV} \cdot Z^2$$

- c) The quantum states of the electron are characterized by the main quantum number n , the quantum numbers of the angular momentum ℓ and m , and by the quantum number of the spin m_s .
- d)
 - i) The quantum numbers of the angular momentum are $\ell = 0$ bzw. $\ell = 1$ in the first excited state of the electron.
 - ii) For $\ell = 0$ has the wave function no angular dependence. For $\ell = 1$ there are three wave functions with $\sin \theta \cdot \exp(\pm i\varphi)$ and $\cos \theta$.
 - iii) The radial part of the wave function takes a finite value $r \rightarrow 0$ and passes through zero for $\ell = 0$. For $\ell = 1$ the wave function starts at zero for $r \rightarrow 0$ and there is no change in the sign. The wave function passes over a maximum and vanishes exponentially for $r \rightarrow \infty$.

Problem 6

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For Ti^{2+} there are two electrons in the 3d shell.

- a) What is the angular momentum of these electrons?
- b) The ground state of Ti^{2+} is determined by Hund's rules. Explain these rules. What is the ground state of Ti^{2+} .
- c) The total splitting of the ground-state multiplet of Ti^{2+} due to the spin-orbit coupling is 500 cm^{-1} . Determine the spin-orbit coupling constant of Ti^{2+} .

a) The angular momentum is $\ell = 3$.

- b)
 - i) Due to the e-e repulsion the electron try to occupy different orbitals.
 - ii) L takes the maximal value of $|\sum_i m_i|$. i runs of all electrons and m_i denotes the magnetic quantum number of the orbital.
 - iii) The total spin takes the maximal possible value.
 - iv) The total angular momentum takes the quantum number $J = |L - S|$ for an electron configuration and $J = L + S$ for an hole configuration.

The ground state of Ti^{2+} is ${}^3\text{F}_2$.

- c) The Hamiltonian of the spin-orbit coupling is $\mathcal{H} = \xi \vec{L} \cdot \vec{S} / \hbar^2$ and the eigenvalues are $E_{J,L,S} = \frac{1}{2} \xi (J(J+1) - L(L+1) - S(S+1))$.
With $E_{J=4,L,S} - E_{J=2,L,S} = \frac{1}{2} \xi (4(4+1) - 2(2+1)) = 7\xi$ one gets

$$\xi = \frac{500 \text{ cm}^{-1}}{7} = 41,4 \text{ cm}^{-1}.$$

Problem 7

(4 Points)

Consider a simple cubic lattice with lattice constant $a=380$ pm.

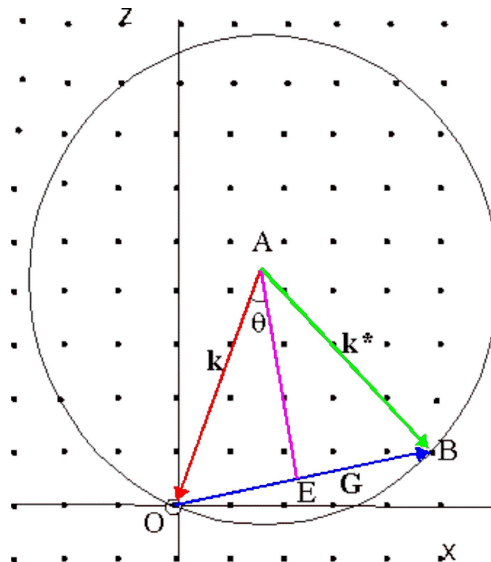
- The reciprocal lattice is also simple cubic. Calculate the lattice parameter of the reciprocal lattice.
- Write up the Laue criterion for x-ray scattering.
- Explain the relation between the Bragg condition and the Laue criterion.
- Sketch and explain the Ewald construction for x-ray scattering.

a) The lattice parameter of the reciprocal lattice is $b = \frac{2\pi}{a} = \frac{2\pi}{380 \text{ pm}} = 1.65 \cdot 10^{10} \text{ m}^{-1}$.

b) The Laue criterion is $\vec{k} - \vec{k}^* = \vec{G}$. Thereby \vec{k} denotes the wave vector of the incoming wave, \vec{k}^* the wave vector of the scattered wave and \vec{G} a vector of the reciprocal lattice.

c) \vec{G} is parallel to the normal vector of the scattering plane of the Bragg condition.

d) Sketch of the Ewald construction. The dots indicate the lattice points of the reciprocal lattice. All dots on the circle fulfill the Laue condition and indicate the direction of elastic scattering



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- a) What is the fundamental difference between a gas of electrons and a classical ideal gas of charged particles?
 - b) The Fermi energy of Cu is 7 eV. What is the meaning of the Fermi energy of a gas of electrons?
 - c) What is the temperature dependence of the specific heat of the electron gas? Give reasons for your answer.
 - d) The energy of conduction electrons is given by energy bands. What is the reason for these energy bands and why there are energy gaps in the band structure?
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- a) For electrons is the Pauli principle valid, i.e. each quantum state can be occupied only by one electron. In a classical ideal gas each state can be occupied by an arbitrary number of particles.
 - b) The Fermi energy is the highest energy of an electron within the electron gas at $T=0$.
 - c) The contribution of the electron gas to the specific heat of a metal is $\propto T$, since only a small number of electrons with their energy in a range $\approx k_B T$ around the Fermi energy can be excited thermally.
 - d) The kinetic energy of moving conduction electrons can vary continuously. The large number of quantum states for the electrons merge into energy bands. Since the electrons form matter waves, these waves are scattered by the lattice. For special directions there can be reflection and thereby the formation of standing waves. The resulting quasi-static electron density can be maximal or minimal at the place of the atoms. The energy is enhanced or reduced for these special values of the k -vectors so that an energy gap opens.