

Question 4: The band structure (25 points)

a. Which statement describes the **empty lattice approximation**? [35%]

The empty lattice approximation....

- 1. ... assumes that the periodic potential of the crystal is very strong, so that electrons are localized near ion cores.
- 2. ... treats electrons as free particles by neglecting interactions between electrons, while still keeping the periodic crystal potential that opens band gaps at Brillouin-zone boundaries.
- 3. ... describes electrons as tightly bound to individual atoms, with energy bands arising from weak overlap between neighboring atomic orbitals.
- 4. ... treats electrons as free particles by setting the crystal potential to zero, while still using the periodicity of the lattice to fold the free-electron dispersion into Brillouin zones.

b. Which of the following statements are true or false? [max. 25%, min 0%, 5% for correct answers, -5% for wrong answers] [25%]

Statement	t	f
A band gap is an energy interval in which there are no allowed electronic states.		
In the empty lattice approximation, band gaps appear at the Brillouin-zone boundaries.		
Increasing the number of unit cells in a crystal increases the number of allowed k-states in each band.		
A flatter band corresponds to a larger effective mass.		
For monovalent elements, the Fermi sphere is fully or almost-fully contained in the 1 st BZ		

c. Answer the following questions [25 %]

i. In your own words, describe what the Fermi surface represents.

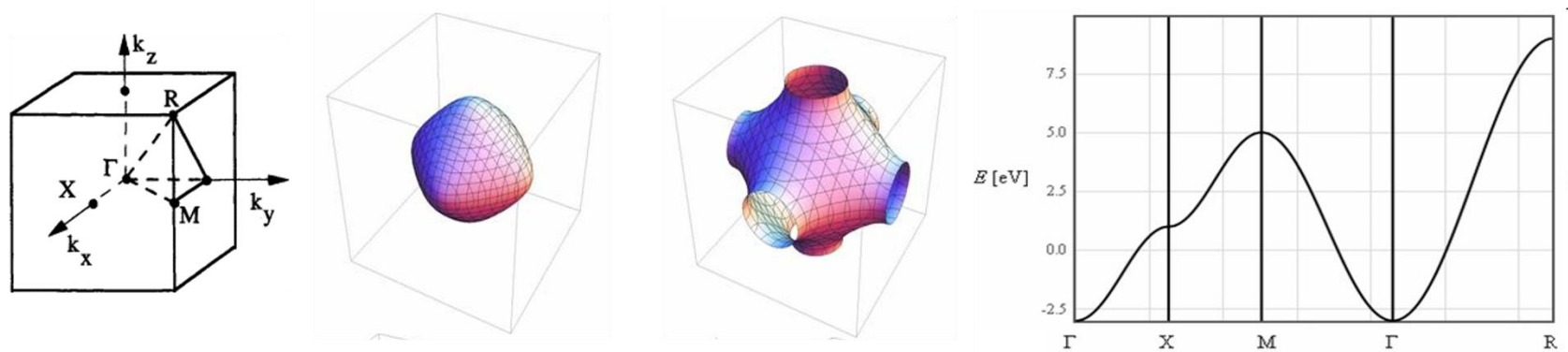
ii. How many electrons per unit cell can a single band host? Justify your reasoning.

d. The figure below shows, from left to right, the symmetry points of a simple cubic Brillouin zone, 2 different Fermi Surfaces for a simple cubic system and the band dispersion of an electronic band for a simple cubic system. Please, for the two Fermi surfaces, **mark the position of the Fermi level** in the band structure graph on the right. [15 %]

1st BZ (SC)

Fermi surf. #1

Fermi surf. #2



Molecular and Solid State Physics

Exam July 10, 2026

Name:

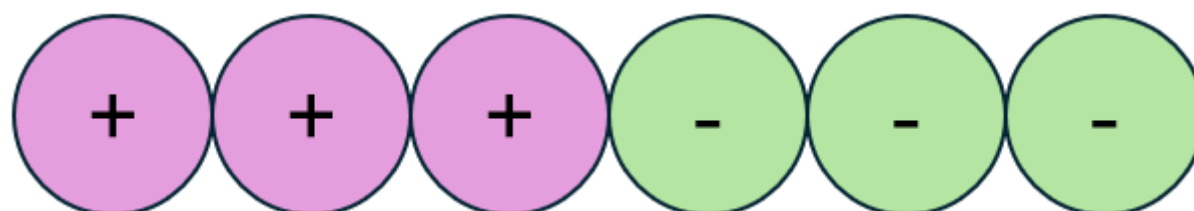
Mat. Nr:

Question 1: Schrödinger equation (25 points)

Note added after exam: The Percentages add up to more than 100%, points have been renormalized

The simplest diatomic ion is H_2^+ .

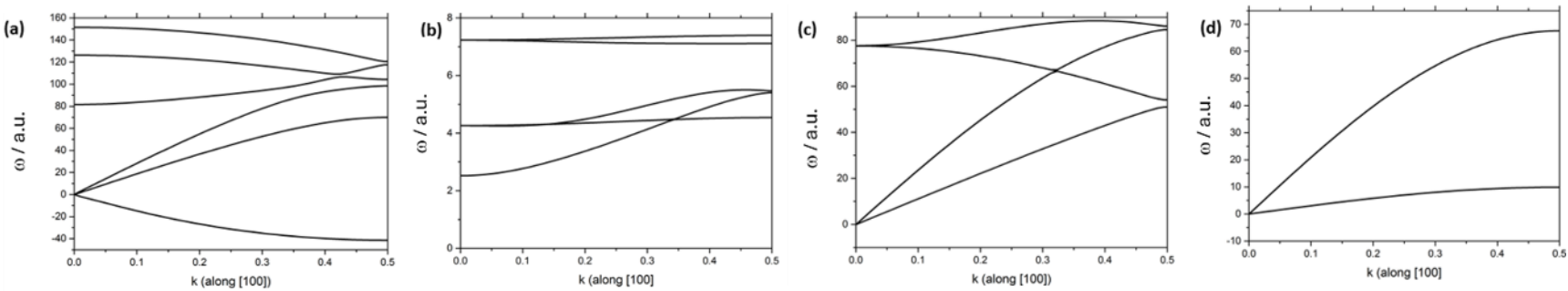
- a) Write down the full Hamiltonian for this system. How many electron-nucleus terms are there? [20%]
- b) In practice, the Schrödinger equation can be solved using the Generalized Eigenvalue Equation (aka Roothan-equations). Write down this Equation for H_2^+ using a minimal basis (1s for each of the hydrogen atoms). Write out the matrices (i.e., write down all elements) [20%]
- c) Does the bond in H_2^+ occur due to a decrease in kinetic or in potential energy? Is it a covalent or an ionic bond? Justify your reasoning. [30%]
- d) Sketch schematically the total energy curve as function of the distance between the two H atoms. Don't forget to label the axes and provide units. Indicate in this plot the bond energy (**neglecting zero-point vibration**), the forces acting on the atoms at a given distance, and the equilibrium distance. What is the **order of magnitude (+unit!)** of for the bond energy? [20%]
- e) Below you find an orbital for the linear chain of six H-atoms, consisting of s-states on each atom.. State (i) Whether this is a **σ -orbital or a π -orbital** and with respect to which atoms it is bonding/antibonding. Explain in 1 sentence each (i) how σ and π -bonds can be differentiated and (ii) how you determine whether a part of the orbital is bonding or antibonding. [30%]



Question 2: Crystal structure (25 points)

a) Draw schematically a quadratic crystal structure (**2D**) with two atoms in the basis. Clearly label the two different atoms and the lattice constant. **[40%]**

- b) In the plot below, you find four potential candidates for the **phonon dispersion** of Cesium Iodide (CsI) along the [100] direction.
- C1) How many optical and how many acoustic phonon bands should CsI have? **[10%]**
- C2) Do you expect some bands to be degenerate? Why (not)? **[5%]**
- C3) In **all** the plots, indicate which bands (if any) are acoustic and which are optic. **[10%]**
- C4) Out of the four candidates, mark the plot that corresponds to CsI. **[15%]**



c) Which of the following statements are true or false **[max. 20%, 5% for correct, -5% for wrong answers, min 0%]**

Statement	t	f
The Wigner-Seitz cell in reciprocal space is called the first Brillouin zone		
To calculate the electronic properties of a crystal, it is enough to solve the Schrödinger equation within the first Brillouin zone.		
The number of optical phonon bands depends on the choice of the unit cell		
The color of a crystal can be calculated using the Schrödinger equation, but the solution depends on the choice of the unit cell		

Question 3: Graphene in the Drude model (25 points)

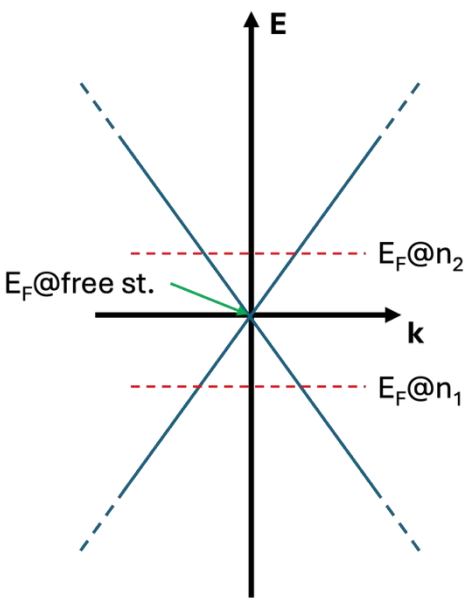
- a) **Define** the Hall coefficient (R_H) in terms of the Hall electric field ($\vec{E}_H$), current density ($\vec{j}$), and magnetic field ($\vec{H}$). Then write the **microscopic expression** for the Hall coefficient within the Drude model. What is the relevant information that can be extracted by measuring R_H ? [35%]

- b) For the Drude model, which of the following statements are true or false? [max. 25%, min 0%, 5% for correct, -5% for wrong answers] [25%]

Statement	t	f
The relaxation time τ represents the average time between electron-electron collisions		
The Drude model can explain Ohm's law microscopically		
A larger relaxation time τ leads to lower electrical conductivity σ .		
If an electromagnetic wave in the visible range, with angular frequency $\omega < \omega_p$, where ω_p is the plasma frequency, hits a metal, it is reflected off.		
The Wiedemann–Franz law states that, for a metal, the ratio of thermal-to electrical conductivity is proportional to temperature.		

- c) Free-standing Graphene (i.e. isolated graphene) is a 2-dimensional material that exhibits a linear dispersion relation, with the band crossing each other at the Fermi energy (as sketched below). This linear dispersion relation can be written as $E = \hbar c_F |\vec{k}|$, where c_F is the slope of the band structure and has the units of [m/s].
- i. **Derive** the analytic expression of the density of states $D(E)$ for Graphene. [25%]
- [hint: to derive the expression you would need to use the fact that in 2D, $\Delta k = \frac{4\pi^2}{A}$ and $D(E) = \frac{dN}{dE} \cdot \frac{dk}{dE}$]

- ii. Experimentally, it is possible to change the electron density (n) of graphene and thus the position of the Fermi level. Two possible electron densities n_1 and n_2 are indicated by the red dashed lines.



- Is **free-standing graphene** a metal, an insulator or a zero-gap semiconductor? Explain your reasoning [10%]
- What would the **sign** of the Hall coefficient be when the Fermi energy is moved at $E_F@n_2$ and $E_F@n_1$, respectively? Explain your reasoning. [5%]