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 1st BZ		

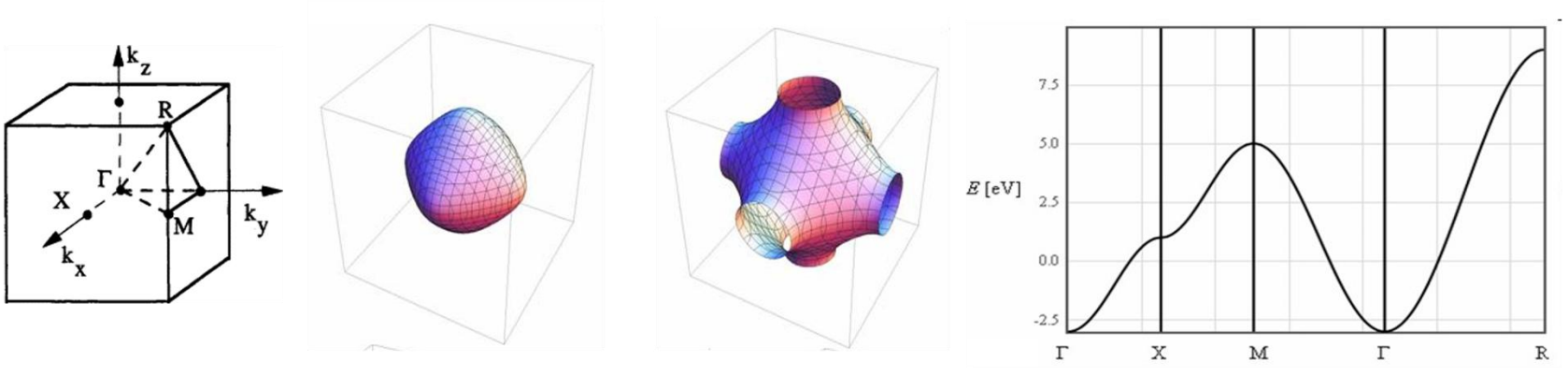
c. Answer the following questions **[25 %]**

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: Slightly modified version of the exam – void questions have been removed.

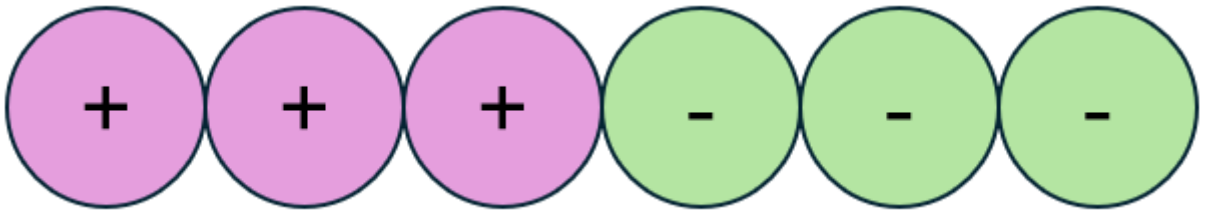
The simplest diatomic ion is H_2^+.

a) Write down the full Hamiltonian for this system. How many electron-nucleus terms are there? **[30%]**

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) 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%]

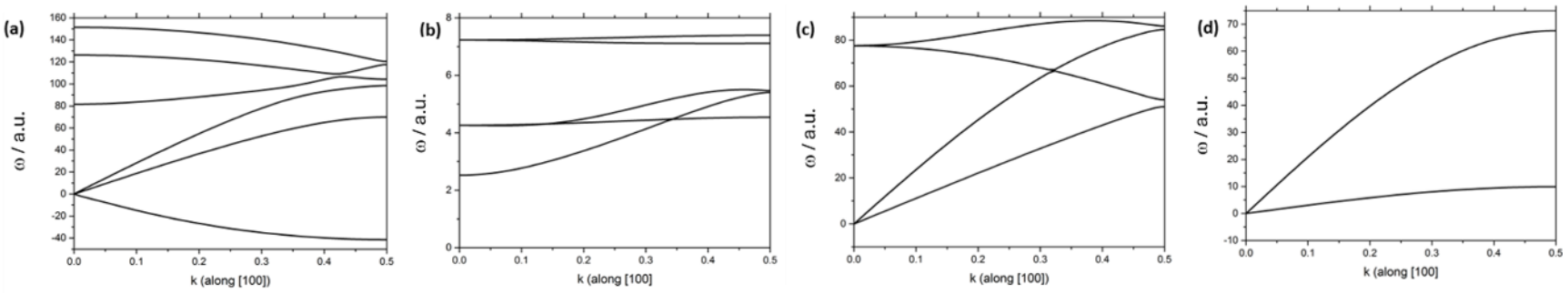
d) Below you find an orbital for the linear chain of six H-atoms, consisting of s-states on each atom.. State (i) Whether this is a **σ-orbital or a π-orbital** and with respect to which atoms it is bonding/antibonding. Explain in 1 sentence each (i) how σ and π-bonds can be differentiated and (ii) how 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%]**

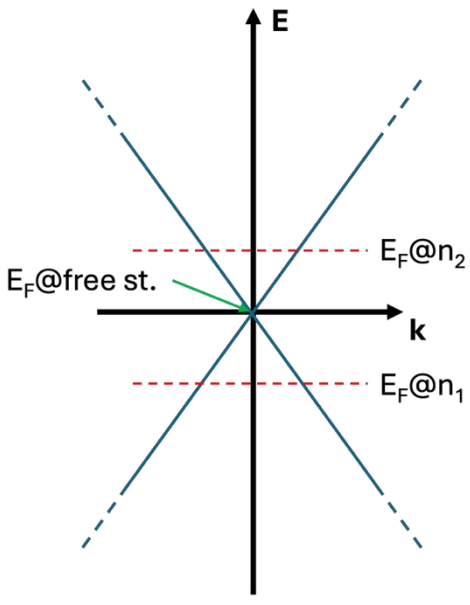
Statement	t	f
The relaxation time τ represents the average time between **electron-electron** collisions		
The Drude model can explain Ohm's law microscopically		
A larger relaxation time τ leads to lower electrical conductivity σ.		
If an electromagnetic wave in the visible range, with angular frequency $\omega < \omega_p$, 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 $D(E) = \frac{dN}{dE} \cdot \frac{dk}{dk}$]

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 n1 and n2 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 $E_F@n_2$, respectively? Explain your reasoning. **[5%]**