Assessment
Solid-state physics

Assignment 4: Heat capacity, chemistry, and 1D materials

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Due: 1700, September 18, 2023

Exercise 1 *Debye* (6 points)

(i) What are the assumptions of the Debye model?

(ii) Write an expression for the number of modes in a two-dimensional system, and thus determine the *Debye wavenumber* (the wavenumber which corresponds to the Debye frequency).

(iii) Provide a brief discussion of which elements you would expect to have a high Debye temperature, and which elements you would expect to have a low Debye temperature.

Note: your reasoning is important, not the actual elements!

Exercise 2 *Sommerfeld* (10 points)

(i) In your own words, explain what is the Fermi energy, Fermi temperature and the Fermi surface

(ii) Write an expression for the number of states for a gas of free electrons in three dimension and use this to calculate the Fermi wavenumber and Fermi Energy

(iii) Using the previous result, estimate the value of the Fermi energy for Caesium

(iv) Obtain an expression for the density of states at the Fermi surface of a **two-dimensional** free-electron gas.

(v) Using the above result, show that for a two-dimensional free-electron gas that the chemical potential μ is independent of temperature when $T \ll \mu$

Exercise 3 *Chemistry* (6 points)

(i) Explain using the simplest language you can muster why is the periodic table important?

(ii) Choose a naturally occurring element with a high atomic number and use Madelung's Rule to deduce the shell filling configuration.

For lols: the highest unique atomic number will be awarded an additional prize

(iii) Using any tools at your disposal (i.e. use a computer) produce a plot of the energy eigenstate described by $|5, 2, 0\rangle$. You must include your code and you will be partially assessed on presentation: producing content that is digestible and visually pleasing is an important part of modern science!

Exercise 4 *Bonding: not LCAO* (9 points)

(i) In you own words, explain why ionic bonds occur, and what properties one would expect from and ionic solid.

(ii) The (first) ionisation energy of sodium is roughly 5.14 eV, and the electron affinity of chlorine is roughly 3.62 eV, and the bond length between the two atoms when a sodium chloride molecule is formed is roughly 0.236 nm. Assuming that *all* of the cohesive energy is due to the Coulomb interaction, calculate the bonding energy.

(iii) The measured value of the bonding energy of sodium chloride is 4.26 eV. How does this compare to your value above? Justify your response.

(iv) In our discussion of bonding, we did not explicitly discuss van der Waals bonding. Research what is the nature of the van der Waals bond, explicitly describing the origin of the attractive force formation and reason as to why the force is of the form R^{-7}

Exercise 5 *Bonding: LCAO* (8 points)

In our formulation of the LCAO formulation we assumed that orbitals were orthogonal, with the justification that the qualitative behaviour was still going to be fine.
Assume that we introduce a trial wavefunction:

$$|\psi\rangle = \sum_{i=1}^{N} \phi_i |i\rangle$$

however, we are not going to enforce that the state be orthogonal. Rather, we define an overlap matrix $\mathcal{S}$ with elements

$$\mathcal{S}_{i,j} = \langle i|j\rangle$$

(i) Show that with the above conditions, one arrives at an *effective* Schrödinger equation

$$\mathcal{H}\phi = E\mathcal{S}\phi$$

where

$$\mathcal{H}_{i,j} = \langle i|\hat{H}|j\rangle$$

and ϕ is the vector of the coefficients for the ϕ_i.

(ii) Consider the case where N=2 (i.e. the diatomic case) and the orbitals are s ($l = 0$) orbitals. Use the above equation to solve for the energy eigenvalues of the system.

A neat treat is available for a person that can identify why we consider s states.

Exercise 6 *One-dimensional oscillations* (19 points)

(i) Explain what is meant by a *normal mode* and a *phonon*

(ii) Derive the dispersion relation for longitudinal oscillations of an infinite one-dimensional chain of identical atoms, assuming mass m, spring constant κ, and lattice spacing a

(iii) Show that a the mode with wavevector k is equivalent to the mode $k + 2\pi/a$

(iv) Assuming periodic boundary conditions, how many different modes are there?

(v) Find expressions for and plot both the group and phase velocities

(vi) Find an expression for the density of states $g(\omega)$ and plot $g(\omega)$

(vii) Using $g(\omega)$, find an expression for the heat capacity and use any tools at your disposal to plot the heat capacity versus temperature