# 513.001 Molecular and Solid State Physics

January 24, 2014

**Problem 1: Helium**

(a) Write down the Slater determinant that represents the ground state of a helium atom (Helium has two protons and two electrons).

(b) Write down the Slater determinant that represents the first excited state of helium.

(c) Explain how you would calculate the singlet-triplet splitting of the excited states.

**Problem 2: Structure factors**

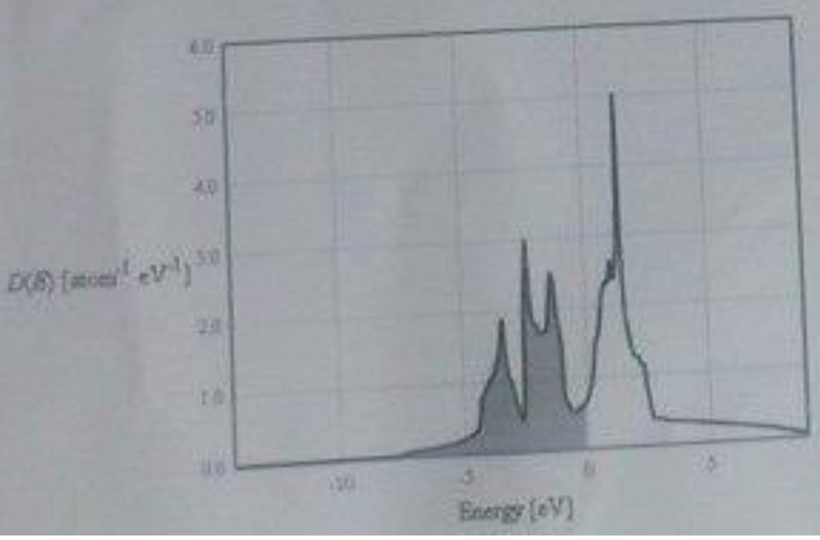
A two dimensional crystal has a rectangular Bravais lattice ($b = \sqrt{2}\, a$) and a basis of two atoms. Atom A is located at (0 ,0 ) and atom B is located at (0.25, 0.5). The electron densities of both atoms can be approximated by a delta function $n(\vec{r}) = Z_i \delta(\vec{r}_i)$ where $Z_i$ is the number of electrons of atom i and ri is the position of atom $i$ ($i$ = A,B). Explain how you could calculate the structure factors of $S(1\ 0)$, $S(0\ 1)$, $S(1\ 1)$, and $S(1\ 2)$ from this information. How could you measure the structure factors?

**Problem 3: Chrome**

The electronic density of states for chrome is shown below. The band structure calculation used to determine this density of states included the 3d and 4s bands. The electron configuration for chrome is $3d^5\,4s^1$.

(a) What is the definition of the Fermi energy and how could it be determined from the density of states?

(b) To determine the Fermi energy, you must know the electron density. The size of the conventional unit cell is 2.87 Å making the volume of the conventional unit cell $2.36 \times 10^{-29}$ m$^3$ and the volume of the primitive unit cell $1.18 \times 10^{-29}$ m$^3$. What electron density should you use to calculate the Fermi energy?



**Problem 4: Split-off band**

Silicon has an indirect bandgap of 1.1 eV. Beneath the valence band it has a split-off band. The minimum of the conduction band is along the Γ-X direction in *k*-space. The maximum of the valence band is at $k = 0$. There are light holes and heavy holes. The maximum of the split-off band is at $k = 0$ and is 0.044 eV below the maximum of the valence band.

(a) Draw the band structure of silicon.

(b) Silicon is doped with acceptors with a concentration of $10^{17}$ $cm^{-3}$. Draw the chemical potential (approximately) into the band diagram of part (a) for this case.

(c) Assuming that the maxima and the minima in the band structure can be approximated by parabolas, sketch the density of states. Indicate in this sketch the contribution of the split-off band.