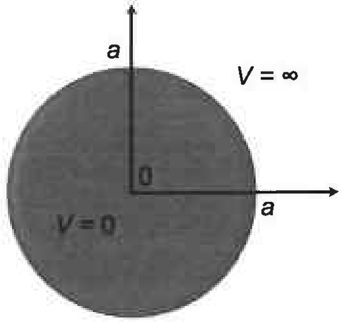
Exam Nanophysics and Nanotechnology – WBPH025-05

Friday, 12th of April 2024, 9.00-11.00

READ THIS FIRST:

- This exam has a duration of 2 hours.
- Clearly write your name and student number on each answer sheet that you use.
- On the first answer sheet, write the total number of answer sheets that you turn in.
- You are not allowed to use any notes, books and mobile devices. You can use the calculator.
- Give clear descriptions of what you calculate, explain physical arguments wherever it is needed.
- The list of constants is given on the last page.
- The full exam is 100 points. Your grade for the exam is the total score divided by 10.

Problem E1.1 [25 points]
To describe a carrier confined to a quantum dot, one can consider a model of a particle in a sphere, as schematically illustrated below.



For a sphere of radius a, the lowest-energy solution of the corresponding Schrödinger equation is:

$$\psi(r,\theta,\phi) = N\frac{\sin(\pi r/a)}{r}$$

(a) [13 points] Find the normalization factor N.
(b) [12 points] Consider an electron trapped in this well. Calculate the probability of finding the electron inside an inner sphere of radius $a/2$. Assume the same lowest-energy solution.

Hint: The infinitesimal element of volume in spherical coordinates is $\mathrm{d}V = r^2 \sin\theta \, \mathrm{d}\phi \, \mathrm{d}\theta \, dr$.

Problem E1.2 [20 points]
Calculate the energy dispersion of a two-dimensional square lattice using a simple tight-binding model in the nearest-neighbor approximation. You can use the formula:

$$E(\mathbf{k}) = E_a - A - \sum_{\mathbf{R}\neq\mathbf{0}} Be^{i\mathbf{k}\cdot\mathbf{R}}$$

where E_a is the energy of the particular atomic orbital, A and B are hopping parameters, and $\mathbf{R}$ are the nearest neighbours vectors.

(a) [4 points] Start with writing down the vectors of the nearest-neighbors.
(b) [4 points] Find the general energy dispersion.
(c) [4 points] Draw the Brillouin zone marking the high-symmetry points. Write them down in fractional coordinates in the basis of reciprocal lattice vectors.
(d) [8 points] Schematically plot the energy dispersion along the k_x direction throughout the entire (first) Brillouin zone. Make a plot for general values of E_a, A and B.

Problem E1.3 [15 points]
The figure below presents selected information downloaded from Materials Project database, namely the structure, band structure along the high-symmetry lines and the density of states of an elemental material calculated using first-principles simulations.
Based on the crystal structure:
(a) [2 points] Specify the Bravais lattice (crystal system + centering) of the material.

(b) [1 points] Find the crystal system of the reciprocal lattice.

Based on the electronic structure and density of states, respond the following questions

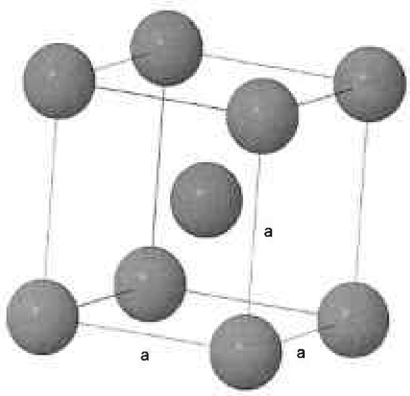
(c) [3 points] Is it a paramagnetic or ferromagnetic phase? Justify your answer.

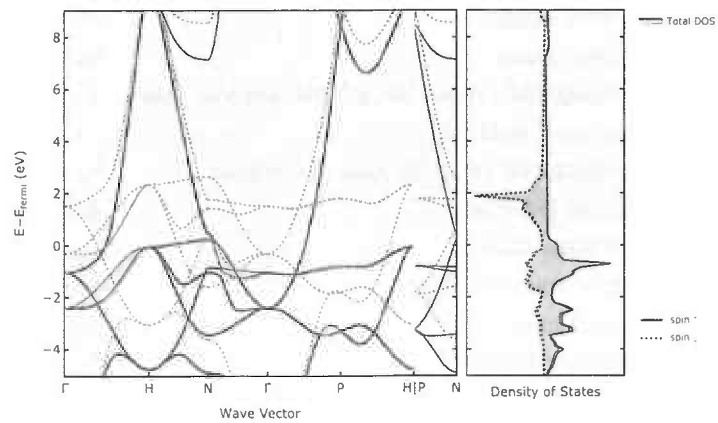
(d) [3 points] Is it insulating/semiconducting/semimetalic/metallic? Justify your answer.

(e) [3 points] Is the material half-metallic? Justify your answer.

(f) [2 points] Does the material possess a Fermi surface? Explain.

(g) [1 point] Specify the value of the band gap.





Problem E1.4 [10 points]

(a) [3 points] What are van der Waals interactions?

(b) [4 points] Which potential is often used as an approximate model for the isotropic part of a total (repulsion plus attraction) van der Waals force as a function of distance? Write the approximate formula, indicate the attractive and repulsive part.

(c) [3 points] Make a sketch of the potential as a function of distance.

Problem E1.5 [30 points]

(a) [15 points] Demonstrate that the Bohr radius expressed as:

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e q^2}$$

and de Broglie wavelength $\lambda = h/p$ are equivalent. The Bohr radius is a classical concept therefore the Coulomb force can be equilibrated with the centrifugal force. You should also consider that an integer number of wavelengths should fit in the orbit of the electron $n\lambda = 2\pi r$.

(b) [3 points] What is the de Broglie wavelength of C60 moving at 200 m/s? The mass of C is 12u.

(c) [2 points] What is your de Broglie wavelength when moving at 35 m/s? and 1000 km/h?

(d) [10 points] Using an optical microscope, you observe two point sources that are separated by 270 nm on your sample. Their emission wavelength is λ = 400 nm. The microscope's objective possesses a numerical aperture NA = 1.3. Can you resolve the nanoemitters as distinct point sources according to the Rayleigh-criterion? Explain.

NATURAL CONSTANTS AND UNITS

Speed of light in vacuum	c	$299792458\ \mathrm{ms}^{-1}$ (exact)
Planck's constant	h	$6.62607015 \cdot 10^{-34}$ Js (exact)
Planck's constant in eV s	h	$4.136 \cdot 10^{-15}$ eVs
Planck's reduced constant	$\hbar$	$1.055 \cdot 10^{-34}$ Js
Planck's reduced constant in eV s	$\hbar$	$6.582 \cdot 10^{-16}$ eVs
1 electron volt (unit 1 eV)	eV	$1.602 \cdot 10^{-19}$ J
Electron charge	$-e$	$-1.602 \cdot 10^{-19}$ C
Electron mass	m_e	$9.109 \cdot 10^{-31}$ kg
Gyromagnetic ratio for orbital angular momentum of electron	γ	$-8.794 \cdot 10^{10}\ \mathrm{s}^{-1}\mathrm{T}^{-1}$
Gyromagnetic ratio for spin of electron	γ_e	$-1.761 \cdot 10^{11}\ \mathrm{s}^{-1}\mathrm{T}^{-1}$
Electron g-factor	g_e	2.002
Bohr magneton	μ_B	$9.274 \cdot 10^{-24}\ \mathrm{JT}^{-1}$
Atomic mass constant	m_u	$1.661 \cdot 10^{-27}$ kg
Proton mass	m_p	$1.673 \cdot 10^{-27}$ kg
Avogadro constant	N_A	$6.022 \cdot 10^{23}\ \mathrm{mol}^{-1}$
Bohr radius for H atom	a_0	$5.292 \cdot 10^{-11}$ m
Rydberg unit of energy for H atom in eV	R_y	13.61 eV
Boltzmann constant	k_B	$1.380649 \cdot 10^{-23}\ \mathrm{JK}^{-1}$ (exact)
Electric permittivity of vacuum	ϵ_0	$8.854 \cdot 10^{-12}\ \mathrm{Fm}^{-1}$
Magnetic permeability of vacuum	μ_0	$1.257 \cdot 10^{-6}\ \mathrm{Hm}^{-1}$