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Exam in TFY4205 Quantum Mechanics

25. May 2005
9:00–13:00

Allowed help: Alternativ C

Approved Calculator.

K. Rottman: *Matematische Formelsammlung*

Barnett and Cronin: *Mathematical formulae*

Fundamental constants, useful relations and tips are given at the end of the exam.

This problem set consists of 4 pages.

Problem 1. Electronic transitions in one-dimensional molecules

Consider the chain polymer in the figure below.

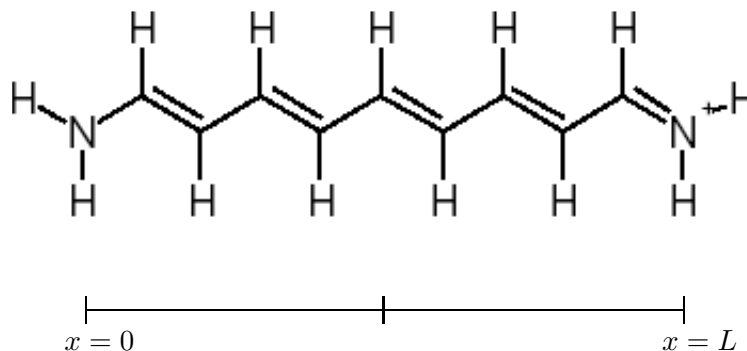


Figure 1: A chain polymer. Carbon atoms at the bond connections are not plotted for clarity.

There are 12 delocalized electrons that propagate freely in the one-dimensional chain between the nitrogen (N) atoms which act as infinite barriers. The distance between neighboring carbon atoms is $l_{C-C} = 1.40\text{\AA}$ and between carbon and nitrogen is $l_{C-N} = 1.34\text{\AA}$.

- a) The spin-1/2 delocalized electrons in the chain do not interact but they obey the **Pauli principle**. Neglect the small angles between the bonds, what is the wavelength of the first photon (smallest energy) that the chain may absorb?

- b) Substituting the hydrogen atom in the middle ($x = L/2$) with another atom or group may perturb the potential of the chain. Assume that the weak perturbing potential is given by

$$V(x) = \begin{cases} V_0 & |x - \frac{L}{2}| \leq x_0 \\ 0 & |x - \frac{L}{2}| > x_0. \end{cases} \quad (1)$$

$$0 \quad |x - \frac{L}{2}| > x_0. \quad (2)$$

Here, $V_0 = 10^{-19} J$ and $x_0 = L/4$. Find the new sixth and seventh energy level using first order perturbation theory.

Problem 2. Particle in a ring

A benzene molecule, see figure below, may be treated as an one dimensional ring with radius $R = 1.34 \text{ \AA}$ in which six delocalized electrons can move freely around. The delocalized electrons in the ring do not interact but they obey the Pauli principle.

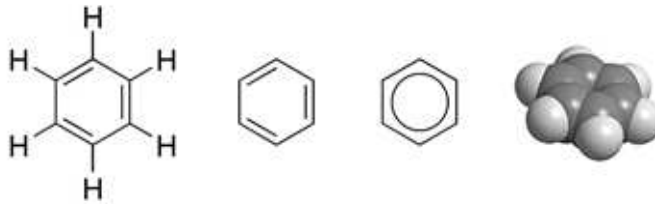


Figure 2: Miscellaneous diagrams and a figure of the benzene molecule.

- a) Find all the stationary single particle wavefunctions and their energies for the delocalized electrons.
- b) Find the angular momentum for the wavefunctions in a).

Problem 3. Addition of spin

Assume that $\vec{S} = \vec{S}_1 + \vec{S}_2 + \vec{S}_3$ is the total spin of a collection of three electrons. What are the possible eigenvalues of S^2 ?

Problem 4. Scattering problem

Consider a three-dimensional, stationary scattering problem of an electron with a large momentum $\vec{p} = \hbar \vec{k}$ hitting an aluminium atom with a Yukawa-Coulomb potential $V(\vec{r}) = U_0 e^{-\alpha r}/r$. Here, $U_0 = -13e^2/4\pi\epsilon_0$ and $1/\alpha$ is a screening length.

- a) Formulate the problem in terms of a stationary Schrödinger equation and state the boundary conditions. Propose a form of the wavefunction that is valid at distances far away from the scattering center.
- b) A formal solution of the wavefunction for the scattering problem given in a) is

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int d^3r' G(\vec{r} - \vec{r}') \frac{2m}{\hbar^2} V(\vec{r}') \psi(\vec{r}') \quad (3)$$

$$G(\vec{r} - \vec{r}') = -\frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} \quad (4)$$

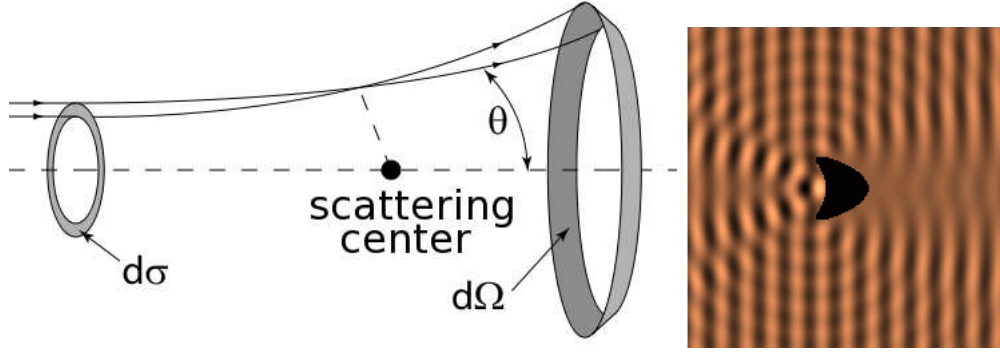


Figure 3: *Left: schematic figure of the scattering problem. Right: scattering of a plane wave against a sickle shaped potential. Note that the Yukawa-Coulomb potential has spherical symmetry.*

where $\psi_0(\vec{r})$ is the solution of the problem without the scattering potential. Use the *first order Born-approximation* and the large r approximation: i.e. $k|\vec{r}-\vec{r}'| \approx kr - \vec{k}' \cdot \vec{r}'$, $\vec{k}' = k\vec{r}/r$ and $1/|\vec{r}-\vec{r}'| \approx 1/r$ to find the differential scattering cross section for the electron expressed by fundamental constants, α and $|\vec{q}| = |\vec{k}' - \vec{k}| = 2k \sin(\theta/2)$.

Useful fundamental constants and relations:

a) Fundamental constants:

Elementary charge $e = 1.60 \times 10^{-19} C$

Electron mass $m_e = 9.11 \times 10^{-31} kg$

Planck constant $h = 6.63 \times 10^{-34} Js$

Velocity of light $c = 3.00 \times 10^8 m/s$

Permittivity $\epsilon_0 = 8.85 \times 10^{-12} C^2/Nm^2$

b) The differential equation

$$\frac{d^2}{dx^2} f(x) + k^2 f(x) = 0 \quad (5)$$

(6)

has the general solution

$$f(x) = Ae^{ikx} + Be^{-ikx} \quad (7)$$

c) Useful integral #1

$$\int dx \sin^2(x) = \frac{1}{2}x - \frac{1}{2}\sin(x)\cos(x) \quad (8)$$

d) Laplace operator in cylindrical coordinates (ρ, ϕ, z)

$$x = \rho \cos \phi \quad (9)$$

$$y = \rho \sin \phi \quad (10)$$

$$z = z \quad (11)$$

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\frac{1}{\rho} \frac{\partial f}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2} \quad (12)$$

e) Derivative operator in spherical coordinate (r, θ, ϕ)

$$x = r \sin \theta \cos \phi \quad (13)$$

$$y = r \sin \theta \sin \phi \quad (14)$$

$$z = r \cos \theta \quad (15)$$

$$\frac{\partial}{\partial x} = \sin \theta \cos \phi \frac{\partial}{\partial r} + \frac{\cos \theta \cos \phi}{r} \frac{\partial}{\partial \theta} - \frac{\sin \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \quad (16)$$

$$\frac{\partial}{\partial y} = \sin \theta \sin \phi \frac{\partial}{\partial r} + \frac{\cos \theta \sin \phi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \quad (17)$$

$$\frac{\partial}{\partial z} = \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \quad (18)$$

f) Useful Jacobians

$$\int d^3 r = \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \int_0^\infty dr r^2 \quad (19)$$

$$= \int_0^{2\pi} d\phi \int_{-1}^1 d(\cos \theta) \int_0^\infty dr r^2 \quad (20)$$

$$(21)$$

g) A vector relation

$$\vec{q} = \vec{k}' - \vec{k} \quad (22)$$

if $k = k'$ then

$$q = 2k \sin(\theta/2) \quad (23)$$

where θ is the angle between $\vec{k}$ and $\vec{k}'$.

h) Useful integral #2

$$\int_0^\infty dr e^{-\alpha r} \sin(qr) = \frac{q}{\alpha^2 + q^2} \quad (24)$$