NTNU **Institutt for fysikk**

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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.

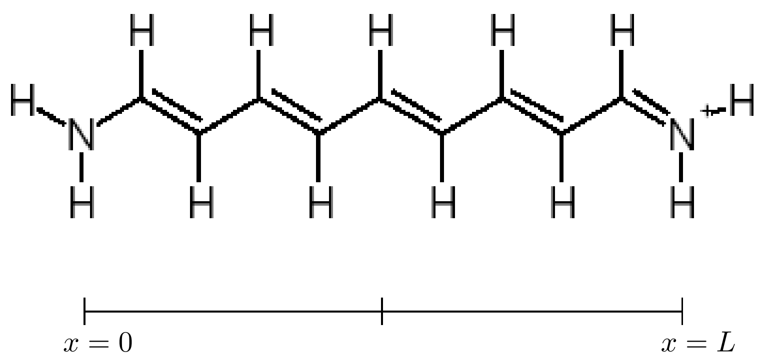

Figure 1: *A chain polymer. Carbon atoms at the bond connections are not plotted for clarity.*

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 $l_{C-C} = 1.40\text{Å}$ and between carbon and nitrogen is $l_{C-N} = 1.34\text{Å}$.

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

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

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 $R = 1.34$Å in which six delocalized electrons can move freely around. The delocalized electrons in the ring do not interact but they obey the Pauli principle.

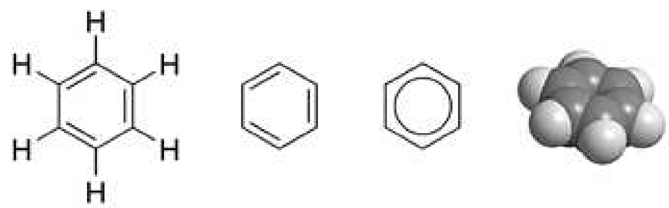

Figure 2: *Miscellaneous diagrams and a figure of the benzene molecule.*

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

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

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

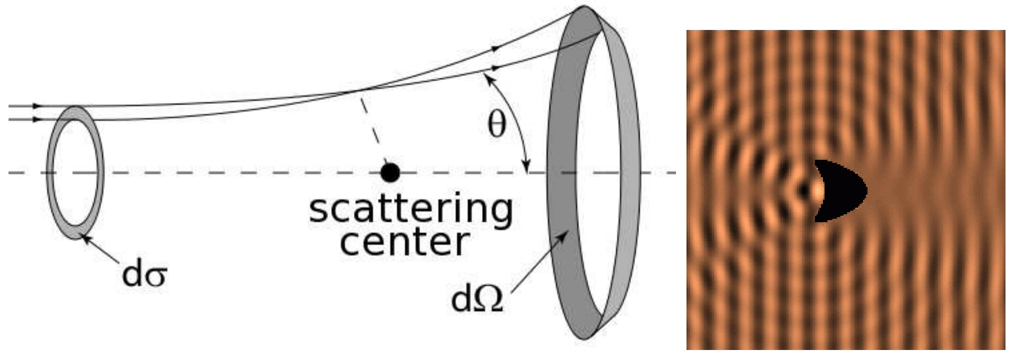

Figure 3: *Left: schematic figure of the scattering problem. Right: scattering of a plane wave against a sickle shaped potential. Note that the Yukawa-Coulomb potential has spherical symmetry.*

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 $c = 3.00 \times 10^{8} m/s$
Permitivity $\epsilon_0 = 8.85 \times 10^{-12} C^2/Nm^2$

b) The differential equation

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

$$\tag{6}$$

has the general solution

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

c) Useful integral #1

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

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

$$\begin{aligned} x &= \rho\cos\phi && (9)\\ y &= \rho\sin\phi && (10)\\ z &= z && (11)\\ \frac{\partial^2 f}{\partial x^2}+\frac{\partial^2 f}{\partial y^2}+\frac{\partial^2 f}{\partial z^2} &= \frac{1}{\rho}\frac{\partial}{\partial\rho}(\frac{1}{\rho}\frac{\partial f}{\partial\rho})+\frac{1}{\rho^2}\frac{\partial^2 f}{\partial\phi^2}+\frac{\partial^2 f}{\partial z^2} && (12) \end{aligned}$$

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

$$\begin{aligned} x &= r\sin\theta\cos\phi && (13)\\ y &= r\sin\theta\sin\phi && (14)\\ z &= r\cos\theta && (15)\\ \frac{\partial}{\partial x} &= \sin\theta\cos\phi\frac{\partial}{\partial r}+\frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta}-\frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi} && (16)\\ \frac{\partial}{\partial y} &= \sin\theta\sin\phi\frac{\partial}{\partial r}+\frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta}+\frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi} && (17)\\ \frac{\partial}{\partial z} &= \cos\theta\frac{\partial}{\partial r}-\frac{\sin\theta}{r}\frac{\partial}{\partial\theta} && (18) \end{aligned}$$

f) Useful Jacobians

$$\begin{aligned} \int d^3r &= \int_0^{2\pi} d\phi \int_0^{\pi} d\theta\sin\theta \int_0^{\infty} dr\ r^2 && (19)\\ &= \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \int_0^{\infty} dr\ r^2 && (20)\\ & && (21) \end{aligned}$$

g) A vector relation

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

if $k = k'$ then

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

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

h) Useful integral #2

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