Re-examination
Quantum Engineering (FKA132), Chalmers
2014-01-14

Time and place: 14:00-18:00 on January 14th, 2014, Johanneberg, "Maskin-salar". Registration for re-examination is mandatory.
Examinator: Elsebeth Schröder (tel 031 772 8424).
Allowed references: Dictionaries, Beta, Physics Handbook, one handwritten paper of size A4 (both sides) with own notes, and a Chalmers-approved calculator. Correct solution of each problem gives 6 points. 15 points are needed to pass.
MOTIVATE YOUR ANSWERS, answers lacking reasonable motivation will not yield full credit. Extra resources are given at the end of the set of problems.

Problem 1. (One point per question)
a) Two observables are represented by the operators $\hat{A}$ and $\hat{B}$. What does the relation $[\hat{A}, \hat{B}] = 0$ imply?
b) Using wavefunctions explain the quantum phenomena of tunneling. Give at least one example of an experiment where quantum tunneling is essential.
c) Write down a wavefunction that is a superposition and explain the meaning of its components.
d) Draw a three-dimensional structure of $Si(CH_3)_2Cl_2$ showing all valence electrons.
e) Draw a molecular orbital diagram for two interacting atomic orbitals (AOs) that belong to two different atoms. Outline how the covalent bond strength, i.e. the interaction energy, depends on the interaction between two atomic orbitals. What are the two most important parameters?
f) Write down the time-independent Schrödinger equation and explain all terms of the equation. Assume that the time-independent Schrödinger equation has the set of eigenvalues $\{E_\alpha\}$ and eigenvectors $\{\psi_\alpha\}$, then argue for the form of and write down the general solution $\psi(\mathbf{r}, t)$ to the quantum problem.

Problem 2. The Hamiltonian for a particle of mass m in a harmonic oscillator potential is given by

$$H = \frac{p_x^2}{2m} + \frac{m\omega^2 x^2}{2} \tag{1}$$

where ω is the angular frequency of the oscillator. The oscillation is subjected to a perturbation $V = bx$ where b is a real constant.
a) Use perturbation theory: Calculate to lowest non-vanishing order the energy shift of the ground state due to the perturbation.
b) Solve the problem exactly and compare to the result obtained in question a).
c) Write down the (unperturbed) Hamiltonian for the three-dimensional harmonic oscillator that has the same angular frequency ω in all spatial directions. Compared to the case of the one-dimensional harmonic oscillator in (1), what is the qualitative difference of the energy spectrum?

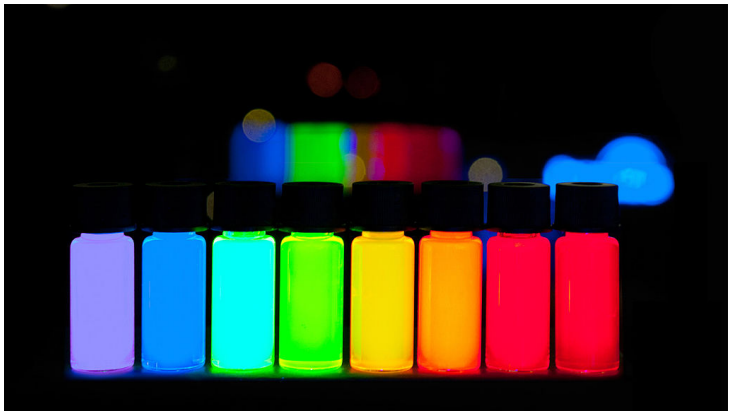

Figure 1: (Problem 4) Quantum dots with vivid colours stretching from violet to deep red are being currently manufactured at PlasmaChem GmbH at a large scale. Alexei Antipov/Wikipedia Commons.

Problem 3. A particle of mass m moves in a one-dimensional potential well given by

$$V(x) = \begin{cases} \infty & \text{for } x < 0 \\ 0 & \text{for } 0 < x < b \\ \infty & \text{for } b < x \end{cases} \tag{2}$$

The particle is initially in the ground state ψ_1 with eigenvalue (energy) E_1. At time $t = 0$ the potential is rapidly changed to double the width

$$V(x) = \begin{cases} \infty & \text{for } x < 0 \\ 0 & \text{for } 0 < x < 2b \\ \infty & \text{for } 2b < x \end{cases} \tag{3}$$

Find the probabilities that the particle is in the first, second, third and fourth excited state in this new potential when $t \geq 0$.

Problem 4. Wikipedia on Quantum dots: *A quantum dot is a nanocrystal made of semiconductor materials that are small enough to display quantum mechanical properties . . . Researchers have studied applications for quantum dots in transistors, solar cells, LEDs, and diode lasers. They have also investigated quantum dots as agents for medical imaging and as possible qubits in quantum computing.*
Electrons in quantum dots may be modelled as electrons in three-dimensional infinite square wells.
a) Qualitatively, what happens to the energy levels of the electron as the size of the dot is decreased, and why?
b) Assume that the quantum dot has the side lengths $L = 1$ nm in two directions (the x and y direction) but length $L/\sqrt{2}$ in the third direction (the z-direction). What is the ground state energy of the electron? Needed is both the expression in terms of L and a numerical result.
c) Draw a scetch of the energy levels of the ground state and the first three excited states with correct values and spacing of the energy levels.
d) What is the wavelength of the lowest energy photon that can be emitted from the quantum dot as a result of the electron decaying from one state to a state of lower energy? (Which two states are involved?)
e) What is the degeneracy of the first and second excited states?

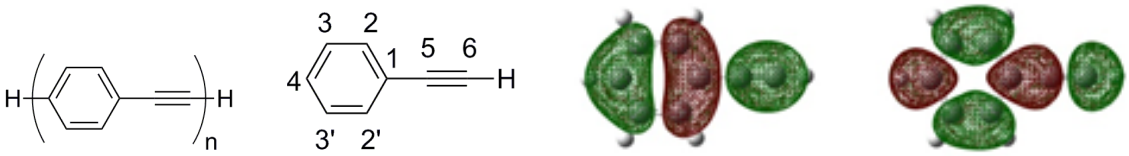

Figure 2: (Problem 5) Poly(1,4-phenylene-ethynyl), ethynylbenzene, HOMO, and LUMO.

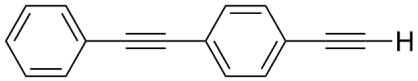

Figure 3: (Problem 5) The shortest possible polymer of ethynylbenzene.

Problem 5.
Conjugated organic molecules such as poly(1,4-phenyleneethynylene) are investigated as potential candidates to be used as molecular wires in molecular electronics and in nanotechnology. The repeating unit (building block) in the polymer is shown in Figure 2. So are the highest occupied and lowest unoccupied molecular orbitals for the monomer ethynylbenzene.

a) To which class of molecular orbitals are HOMO and LUMO designated, σ or π, and what is the definition of such an orbital?
b) Give a mathematical expression for the HOMO wave function in terms of suitable atomic orbitals φ_i, where i is the atom number shown in the structure of ethynylbenzene above. Numerical values for the constants used in your expression are not needed but the correct signs must be shown. What atomic orbital does φ_i correspond to?
c) Will the HOMO-LUMO gap increase or decrease with increasing number of repeating units in the polymer? Rationalize your answer briefly.
d) Draw the orbital shapes for the HOMO and the LUMO of the shortest possible polymer of ethynylbenzene, the dimer shown in Figure 3.
e) Compounds similar to the dimer shown in Figure 3 are also used as liquid crystals. What are the two most important intermolecular forces between molecules in assemblies of such compounds? Describe briefly the origin of each one of these two forces.

Extra resources
Depending on how you solve this set of problems you may find useful the following definition of the creation and annihilation operators in the harmonic oscillator:

$$a = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{a_0} + i\frac{\hat{p}}{p_0}\right); \qquad a^\dagger = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{a_0} - i\frac{\hat{p}}{p_0}\right); \tag{4}$$

with the properties

$$[a, a^\dagger] = 1 \tag{5}$$

and where

$$a_0 = \sqrt{\frac{\hbar}{m\omega}}\,; \qquad p_0 = \frac{\hbar}{a_0} = \sqrt{\hbar m\omega} \tag{6}$$

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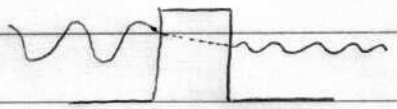
1. a) $[A, B] = 0$ observables can be measured simultaneously

b) 

"Tail" of wavefunction extends in through the barrier and a small part of the wave emerges on the other side. Sinus-waves outside barrier, exp. decay inside.

Example: STM

c) If ψ_1 & ψ_2 steady-state solutions to a problem then $\psi = a\psi_1 + b\psi_2$ with $|a|^2 + |b|^2 = 1$ is, too. $|a|^2$ and $|b|^2$ measures probability of measuring values corresponding to ψ_1 or ψ_2, respectively

d) + e) Please see separate document

f) $\hat{H}\psi_\alpha = E_\alpha \psi_\alpha$ with $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$ [kinetic energy operator + potential]

General solution $\psi(\vec{r}, t) = \sum_\alpha \psi_\alpha(\vec{r})\, e^{-E_\alpha t/\hbar}$

2 a) Perturbation, first order vanishes $\langle 0|b\hat{x}|0\rangle = b\langle 0|\frac{a_0}{\sqrt{2}}(\hat{a} + \hat{a}^+)|0\rangle = 0$

because $\hat{a}|0\rangle = 0$ and $\langle 0|\hat{a}^+ = 0$.

Second order: $E_0 = E_0^{(0)} + \sum_{k=1}^{\infty} |\langle 0|b\hat{x}|k\rangle|^2 / (E_0^{(0)} - E_k^{(0)})$

with $E_0^{(0)} = \frac{1}{2}\hbar\omega$, $E_1^{(0)} = \frac{3}{2}\hbar\omega$ and only non-vanishing term is for $k = 1$.

$E_0 = \frac{1}{2}\hbar\omega - \frac{1}{2}\frac{b^2}{m\omega^2}$

b) $\hat{H}_{tot} = \frac{\hat{p}_x^2}{2m} + \frac{m\omega^2}{2}(x - x_0)^2 - \frac{1}{2}\frac{b^2}{m\omega^2}$ with $x_0 = \frac{b}{m\omega^2}$

i.e. harm. osc. solutions with shift of energy $-\frac{1}{2}\frac{b^2}{m\omega^2}$

thus $E_0 = \frac{1}{2}\hbar\omega - \frac{1}{2}\frac{b^2}{m\omega^2}$ as in a).

c) $\hat{H}_{3D} = \frac{\vec{p}^2}{2m} + \frac{m\omega^2}{2}\vec{r}^2$

$E_{3D} = \left(\frac{3}{2} + n_x + n_y + n_z\right)\hbar\omega$ $\quad n_x, n_y, n_z = 0, 1, 2, \ldots$

Difference from 1D: Ground state $\frac{3}{2}\hbar\omega$ instead of $\frac{1}{2}\hbar\omega$

Energies degenerate (several (n_x, n_y, n_z) give same energy).

3. $P_n = |\langle \varphi_n | \psi_1 \rangle|^2$ ψ_1 old, φ_n new

$$\langle \varphi_n | \psi_1 \rangle = \int_0^b \varphi_n^* \psi_1 \, dx = \frac{\sqrt{2}}{b} \int_0^b \sin\left(\frac{n\pi}{2b}x\right) \sin\left(\frac{\pi}{b}x\right) dx$$

$$P_n = \frac{2}{\pi^2} \left| \frac{\sin\left(\frac{\pi}{2}(n-2)\right)}{n-2} - \frac{\sin\left(\frac{\pi}{2}(n+2)\right)}{n+2} \right|^2$$

$\therefore P_1 = \frac{2}{\pi^2}\frac{16}{9}$, $P_2 = \frac{1}{2}$ (use $\frac{\sin y}{y} \to 1$ when $y \to 0$), $P_3 = \frac{2}{\pi^2}\frac{16}{25}$, $P_4 = 0$

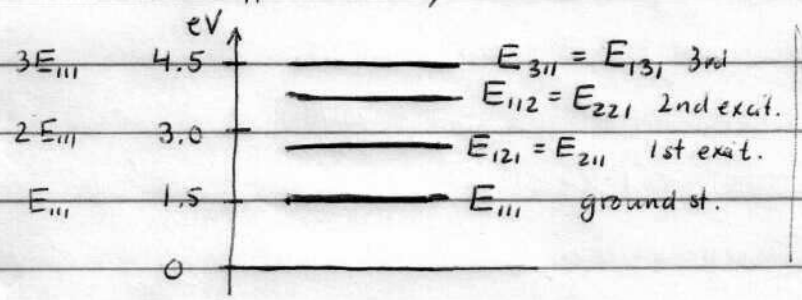
4. a) smaller dot → more spacing in energy and higher energy, $E \propto \frac{1}{D^2}$, D diameter

b) 3D box, separation of variables yields $E_{111} = \frac{\pi^2\hbar^2}{2m}\left(2 \cdot \frac{1}{L^2} + \frac{1}{(L/\sqrt{2})^2}\right)$

$$= \frac{2\pi^2\hbar^2}{mL^2} = 2.4 \cdot 10^{-9}\,\text{J} = 1.5\,\text{eV}$$

c) $E_{n_x, n_y, n_z} = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + 2n_z^2)$

$E_{111} = 1.5\,\text{eV}$, $E_{121} = E_{211} = \frac{7}{4}E_{111}$, $E_{112} = E_{221} = \frac{10}{4}E_{111}$, $E_{311} = E_{131} = \frac{12}{4}E_{111}$



d) Assuming no further states relevant, the transition from states E_{311} or E_{131} to states E_{112} or E_{221} emits the lowest energy photon, wavelength

$$\lambda = \frac{2\pi\hbar c}{E_{311} - E_{112}} = 1.7\,\mu\text{m}$$ (outside visible spectrum)

e) Degeneracy 1st excited state: 2

2nd " " : 2

(3rd " " : 2).

5) Please see separate document.