

Exam
Quantum Engineering (FKA132)
2013-10-22

Time and place: 14:00-18:00 on October 22nd, 2013, in the V building.

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.

Problem 1. (One point per question)

- a) Describe the variational approach to estimating the ground-state energy E_0 of a system and explain why this estimate will be an *upper* bound on the value of E_0 .
- b) For a simple barrier in one dimension sketch the wave function of an incoming electron that has an energy lower than the barrier.
- c) Write and sketch how you would explain spin to your neighbor's 12 year old son or daughter.
- d) Define the concept "polarizability".
- e) What are the structural requirements for the formation of a strong hydrogen bond?
- f) Calculate the de Broglie wavelength of a neutron at room temperature. Explain why the neutron may be used to determine the atomic structure of material. (The de Broglie wavelength of a particle is the wavelength in the particle wave-description)

Problem 2. A particle in a one-dimensional harmonic oscillator has the following wavefunction at time $t = 0$

$$\psi(x, t = 0) = e^{-\frac{1}{2}\alpha^2 x^2} \left(\frac{\alpha}{2\sqrt{\pi}} \right)^{\frac{1}{2}} \left(\frac{1}{2} + \alpha x + \alpha^2 x^2 \right) \quad (1)$$

Which values of the energy would be possible outcomes in a measurement at $t = 0$?

What are the probabilities of measuring each of these values?

What is the wavefunction of the particle at a later time $t = t_a$?

What is the expectation value of the energy?

Problem 3. Carbon monoxide has the molecular formula CO.

- a) Draw a correct Lewis structure for this compound. (1 point)
- b) Figure 1 shows the molecular orbital diagram for CO. The corresponding molecular orbitals (MOs) are shown to the right of the diagram. For each one of the four lowest energy levels, give a simple and approximate expression for the linear combination of two (2) atomic orbitals (AOs) that gives the best approximation of the corresponding molecular orbital (MO). Numerical values for the constants is not necessary, but for each expression indicate which one of the constants that is the largest. (2 points)
- c) Use valence bond (VB) theory to describe the CO bond in carbon monoxide. Describe the bond both in text and using drawings. Compare the VB picture (your answer) and

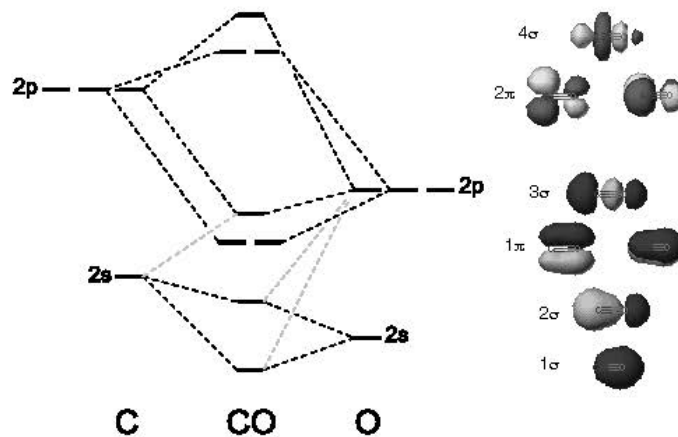


Figure 1: For problem 3 — molecular orbital diagram for CO.

the MO picture (shown in Figure 1). Relate your orbital pictures to the correct MOs shown in Figure 1. (2 points)

d) The electrons are not localized between the carbon and the oxygen, show where they are localized according to the VB theory. (1 point)

Problem 4. For a one-dimensional oscillator with oscillator mass m and angular frequency ω the lowest order relativistic correction has the form

$$H' = -\frac{p_x^4}{8m^3c^2} \quad (2)$$

where c is the velocity of light. Determine to lowest nonvanishing order in perturbation theory the change in ground state energy caused by the relativistic correction. Compare the change to the non-relativistic result when the particle is an electron and $\hbar\omega = 10$ eV. Are we sloppy when ignoring relativistic effects in that case?

Problem 5. Surface physics and the scanning tunneling microscope (STM) provide quantum systems with other symmetries than those in natural atoms and molecules. It is possible to build up atomic structures on surfaces with a very high accuracy, by moving the adsorbed atoms with the tip of the STM (see Figure 2). As the bias (difference in voltage) V is varied the current I through the STM tip is measured. A publication with participation from Chalmers reports an experiment where an STM tip is used to place three to 15 Cu atoms in straight chains on a Cu surface. Using the STM, the electron states in the chain are then measured. [Fölsch, Hyldgaard, Koch, and Ploog, *Physical Review Letters* **92** (2004) 056803]

a) The chain might be modelled as a one-dimensional square well for a negatively charged particle of effective mass m^* . Write an expression for the probability density $P_n(x)$ of the states in the well if its length is L and the walls are considered infinitely high.

b) Figure 3, right hand side, shows a spatial scan of dI/dV along a chain of 15 atoms. In the figure, dI/dV corresponds to the probability density of a state (for various values of the bias).

The distance between two Cu atoms in the chain is approximately 2.55 \AA . Sketch the

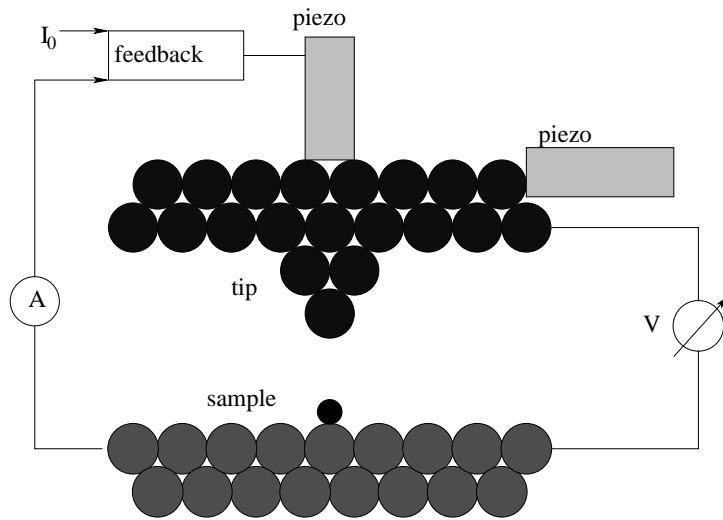


Figure 2: Sketch of an STM

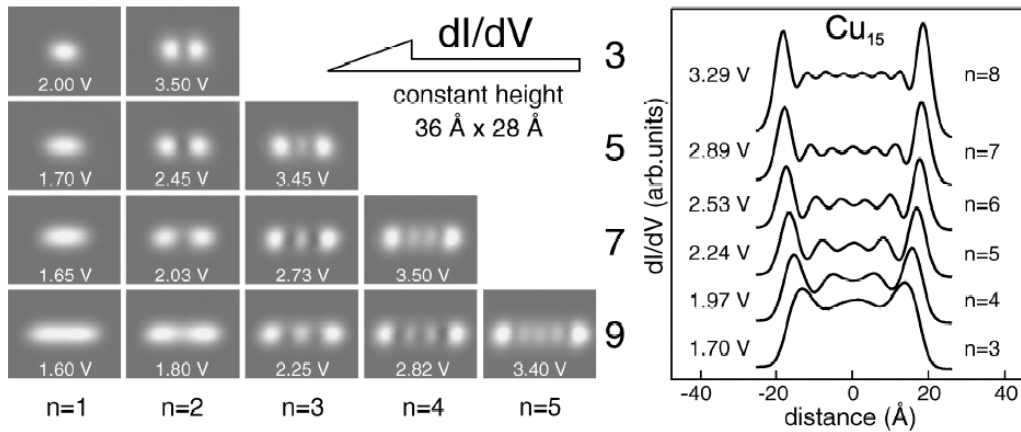


FIG. 2. Left panel: dI/dV maps measured at constant tip height showing the square of the wave function of the chain-localized states (tunneling parameters prior to opening the feedback loop: 1 nA, 1 V). Rows from top to bottom correspond to chains of three, five, seven, and nine atoms while columns include eigenstates of fixed order n (n : number of lobes). Right panel: dI/dV contours measured along a Cu_{15} chain for orders $n = 3$ to $n = 8$ taken at the same initial tunneling parameters as the dI/dV maps (left).

Figure 3: From the publication: Fölsch, Hyldgaard, Koch, and Ploog, *Physical Review Letters* **92** (2004) 056803.

probability density for the first excited state in a chain with 15 Cu atoms using the square-well assumption (indicate distances in the box). Also sketch (for the same chain) the probability density for the fourth and seventh excited state. Compare with the right hand side of Figure 3 and discuss your results.

c) In an ideal square well with infinitely high barriers there is no upper limit on the excited states: as the energy of the states grows the wavelength of the eigenstate becomes smaller. In the Cu chain the wave “lives” in a well with a certain build-in discreteness (the atoms), and the shortest possible wavelength is approximately the width of 3 atoms. Does this explain the limited number of pictures on the left hand side of Figure 3? Motivate your answer!

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Sketch of answers, physics part

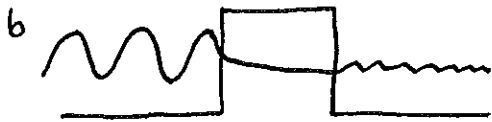
1 a Variational approach. Hamiltonian \hat{H} , unknown ground state energy E_0 , $\langle 0 | \hat{H} | 0 \rangle = E_0$ $|0\rangle$ unknown ground state.

Take any wavefunction $|\psi\rangle$, write as superposition of steady states $|0\rangle, |1\rangle, |2\rangle, \dots$, orthogonal $|\psi\rangle = \sum_j c_j |j\rangle$

$$\langle \psi | \hat{H} | \psi \rangle = \sum_j |c_j|^2 E_j \geq \sum_j |c_j|^2 E_0 = E_0$$

↑
replace E_j by E_0 , $E_j \geq E_0$

By varying $|\psi\rangle$ (e.g. parameters), upper bound on E found.



c \perp so many possibilities. Important points in general, but adjust to 12 y.o.:

- spin not classical, is inherent for the particles
- magnetic field affects particle
- could also mention that for some spins (like $1/2$) particles cannot be in the same state (Fermi repulsion).

f Room temperature $T = 300\text{K}$. Mass neutron $m = 1.67 \cdot 10^{-27}\text{kg}$

de Broglie $\lambda = h/p$, $E_{kin} = p^2/(2m) \therefore \lambda = h(2mE_{kin})^{-1/2}$

$E_{kin} = T k_B$. Thus $\lambda \cong 1.8 \text{ \AA}$. This is order of magnitude of distance between atoms in crystal. Add energy to neutron ("shoot"), then λ even smaller.

2 1D harmonic oscillator

$$\psi(x, t=0) = e^{-\frac{1}{2}\alpha^2 x^2} \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} \left(\frac{1}{2} + \alpha x + \alpha^2 x^2\right)$$

Find states that make up ψ superposition. Find ψ_0, ψ_1, ψ_2 in Physics Handb.

$$\psi = c_0 \psi_0 + c_1 \psi_1 + c_2 \psi_2, \text{ compare powers of } x$$

$$c_2 \frac{4\alpha^2 x^2}{\sqrt{8}} = \frac{1}{\sqrt{2}} \alpha^2 x^2 \quad \text{i.e.} \quad c_2 = \frac{1}{2}$$

$$c_1 \frac{1}{\sqrt{2}} 2\alpha x = \frac{1}{\sqrt{2}} \alpha x \quad \text{i.e.} \quad c_1 = \frac{1}{2}$$

$$c_0 - c_2 \frac{2}{\sqrt{8}} = \frac{1}{\sqrt{2}} \cdot \frac{1}{2} \quad \text{i.e.} \quad c_0 = \frac{1}{\sqrt{2}}$$

$$\left. \begin{array}{l} \\ \\ \end{array} \right\} \text{check } c_0^2 + c_1^2 + c_2^2 = \frac{1}{2} + \frac{1}{4} + \frac{1}{4} = 1$$

O.K.

(2) Possible energies: corresponding to ψ_0, ψ_1, ψ_2

$$E_n = (n + \frac{1}{2}) \hbar \omega \quad E_0 = \frac{1}{2} \hbar \omega \quad E_1 = \frac{3}{2} \hbar \omega \quad E_2 = \frac{5}{2} \hbar \omega$$

$$\text{Probabilities} \quad |c_0|^2 = \frac{1}{2} \quad |c_1|^2 = \frac{1}{4} \quad |c_2|^2 = \frac{1}{4}$$

$$\psi(x, t_0) = \frac{1}{\sqrt{2}} \psi_0(x) \exp(-\frac{i}{\hbar} E_0 t_0) + \frac{1}{2} \psi_1(x) \exp(-\frac{i}{\hbar} E_1 t_0) + \frac{1}{2} \psi_2(x) \exp(-\frac{i}{\hbar} E_2 t_0)$$

Expectation value of energy?

$$\langle H \rangle = \int \psi^*(x, t) \hat{H} \psi(x, t) dx, \quad \hat{H} \psi_n = E_n \psi_n$$

$$= \sum_i \sum_j c_i^* c_j e^{-\frac{i}{\hbar} (E_j - E_i) t} E_j \int \underbrace{\psi_i^*(x) \psi_j(x)}_{\delta_{ij}} dx$$

$$= \sum_i |c_i|^2 E_i$$

$$= |c_0|^2 E_0 + |c_1|^2 E_1 + |c_2|^2 E_2 = \frac{1}{2} \frac{1}{2} \hbar \omega + \frac{1}{4} \frac{3}{2} \hbar \omega + \frac{1}{4} \frac{5}{2} \hbar \omega$$

$$= \frac{5}{4} \hbar \omega$$

4 1D oscillator, mass m , frequency ω , relativistic correction

$$H' = -\frac{p_x^4}{8m^3 c^2}$$

$$H = H^{(0)} + H'$$

$$E'_{n=0} = \langle \psi_0 | H' | \psi_0 \rangle \quad \text{step operators } \hat{a} \text{ and } \hat{a}^\dagger$$

$$\hat{p}_x = -i \sqrt{\frac{\hbar m \omega}{2}} (\hat{a}^\dagger - \hat{a})$$

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

$$\hat{a} |n\rangle = \sqrt{n} |n-1\rangle$$

$$\langle 0 | p_x^4 | 0 \rangle = \left(-i \sqrt{\frac{\hbar m \omega}{2}} \right)^4 \langle 0 | (\hat{a} - \hat{a}^\dagger)^4 | 0 \rangle$$

$$\langle 0 | (\hat{a} + \hat{a}^\dagger)^4 | 0 \rangle = \langle 0 | \hat{a}^4 + \hat{a}^3 \hat{a}^\dagger + \dots | 0 \rangle$$

only combinations with $\hat{a} \hat{a} \hat{a}^\dagger \hat{a}^\dagger$ may survive in general, for the ground state first (left) operator must be \hat{a}^\dagger

$$\hookrightarrow = \langle 0 | \hat{a} \hat{a} \hat{a}^\dagger \hat{a}^\dagger + \hat{a} \hat{a}^\dagger \hat{a} \hat{a}^\dagger | 0 \rangle$$

$$= \langle 0 | 2 + 1 | 0 \rangle = 3$$

$$E'_{n=0} = -\frac{1}{8m^3 c^2} \frac{\hbar^2 m^2 \omega^2}{4} \cdot 3 = -\frac{3}{32} \frac{(\hbar \omega)^2}{mc^2} \quad \#; \quad E_{n=0}^{(0)} = \frac{1}{2} \hbar \omega$$

Change $\left| \frac{E'_{n=0}}{E_{n=0}^{(0)}} \right| = \frac{3}{16} \frac{\hbar \omega}{mc^2} \approx 4 \cdot 10^{-7}$ A very small change, can often be ignored.

$$E_{n=0} = E_{n=0}^{(0)} + E'_{n=0} = \frac{1}{2} \hbar \omega \left(1 - \frac{3}{16} \frac{\hbar \omega}{mc^2} \right)$$

5. STM measurement of chains of atoms.

Model: particle in a box



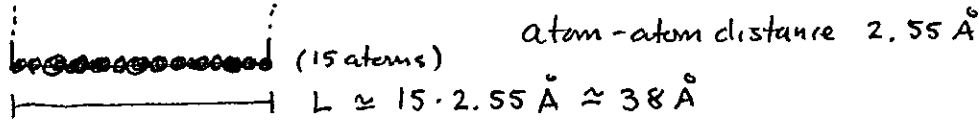
$$\Psi_n = \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}$$

a)

Probability density

$$P_n(x) = |\Psi_n(x)|^2 = \frac{2}{L} \sin^2 \frac{\pi n x}{L}, \quad n = 1, 2, 3, \dots$$

b)



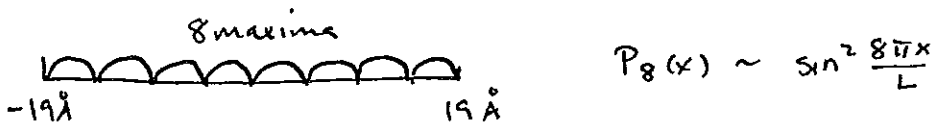
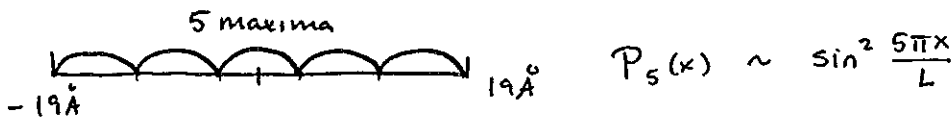
First excited state: $n=2$

$$P_2(x) = \frac{2}{L} \sin^2 \frac{2\pi x}{L} \quad \text{zero at } \frac{x}{L} = 0, \frac{1}{2}, 1; \text{ max between those}$$



Fourth and seventh excited state.

$$n=5 \text{ zero at } 0, \frac{1}{5}, \frac{2}{5}, \frac{3}{5}, \frac{4}{5}, 1$$



Besides the large probabilities at the edges, the number ^{of} and position of the zero-points (minima) fits well with experiment.

c) 3 atoms can support one full wavelength

Then 6 atoms can support ~ two full wavelengths.

• 3 atoms ~ 1 wavelength ~ first excited state is maximum possible state
i.e. $n=1$ (ground state) and $n=2$ (1st excited state)
are the only possible ~ 2 pictures, O.K.

• 7 atoms ~ a little more than 2 wavelengths ~ $n=1, 2, 3, 4$ possible.
These are the states shown for 7 Cu atoms, so fits reasonably well with experiment.

• 9 atoms ~ 3 wavelengths ~ $n=1, 2, 3, 4, 5, 6$ possible.

Only up to $n=5$ shown, i.e. fits less well for longer chains.