

Re-Exam
Quantum Engineering (FKA132), Chalmers
2015-01-05

Time and place: 10:00-14:00 on January 5, 2015, MC2.

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.

Problem 1. (One point per question)

a) Write down the Schrödinger equation for a three-dimensional system with general potential $V(\mathbf{r}, t)$. For a potential that does *not* depend on time we know that stationary states are solutions. What does the time dependence of the stationary states look like (describe or write down)?

b) The hamiltonian \hat{H} has the set of normalized and orthogonal stationary eigenstates u_n with corresponding eigenvalues E_n , for $n = 1, 2, 3, \dots$. The state $\psi(t)$ is at time $t = 0$ given by

$$\psi(t = 0) = \sqrt{\frac{11}{21}} u_1 + \frac{1}{\sqrt{7}} u_3 + \frac{1}{\sqrt{N}} u_7. \quad (1)$$

Determine N to make $\psi(t = 0)$ normalized. Write down the state $\psi(t)$ at $t > 0$, in terms of some of the E_n 's. What values of the energy may be measured, and with which probabilities?

c) \hat{x} and \hat{p} are the position and momentum operators in a one-dimensional system. The function $f(p, x) = p^2 + \alpha x/2$ is given, α is a real constant. What are the results of the following commutators? $[f(\hat{p}, \hat{x}), \hat{x}]$ and $[f(\hat{p}, \hat{x}), \hat{p}]$

d) Two identical spin- $\frac{1}{2}$ -particles are confined to a one-dimensional harmonic oscillator potential $V(x) = \frac{1}{2}kx^2$. If there is no other interaction between the particles, and the sum of the spin of the two particles is 0, what is the lowest possible energy of the system (the system energy being defined as the sum of the energies of the two particles)? If the total spin is 1, what is the lowest possible energy of the system?

e) List the basic assumptions of valence bond theory.

f) Explain the origin of π - π interactions and show by a drawing the favorable geometrical arrangement of two interacting benzene molecules.

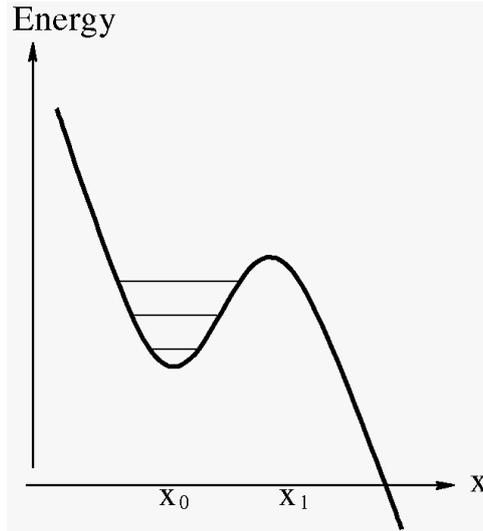


Figure 1: Sketch of the anharmonic potential $V(x) = \frac{1}{2}m\omega^2x^2 - \frac{1}{3}\lambda m\omega^2\alpha x^3$ with local minimum at x_0 and local maximum at x_1 .

Problem 2.

A one-dimensional harmonic oscillator with potential $V_0 = \frac{1}{2}m\omega^2x^2$ and hamiltonian \hat{H}_0 , is subject to a small perturbation $\hat{H}' = -\frac{1}{3}\lambda m\omega^2\alpha x^3$, with $\alpha = \sqrt{m\omega/\hbar}$. The total hamiltonian becomes $\hat{H} = \hat{H}_0 + \hat{H}'$.

a) Write the perturbation \hat{H}' in terms of the annihilation and creation operators \hat{a} and \hat{a}^\dagger , defined by

$$\hat{a} = \frac{\alpha}{\sqrt{2}}\left(\hat{x} + i\frac{\hat{p}}{\hbar\alpha^2}\right) \quad (2)$$

and its hermitian conjugate.

b) Using perturbation theory, show that the first-order correction to the energy is zero for all energy levels.

c) For the ground state energy, calculate the first non-vanishing correction in perturbation theory.

d) The anharmonic oscillator with the above hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}'$ is a good model for certain biased systems (e.g., in a SQUID). A small number of quantum states can be trapped in a local minimum, with a small but non-negligible barrier if the thermal motion is small. For the hamiltonian in this problem, find the position x_0 of the potential local minimum and the position x_1 of the position of the top of the barrier. What is the barrier height, measured from the local potential minimum? If we neglect the perturbative terms in the energy levels (is this reasonable?) and simply assume the states to be harmonic oscillator states, what are the conditions on λ for the barrier to hold at least three bound states (neglecting tunneling)?



Problem 3.

A particle is in a one-dimensional infinite square well of width L . Determine the probability of finding the particle within a distance $L/3$ from the left hand wall of the well for a particle

- a1) in the ground state
- a2) in the first excited state
- a3) in a highly excited state
- a4) for a classical particle.

Discuss your findings in a1)-a4) and how they are related.

b) In a experiment electrons with kinetic energy 100 eV are shot into a grounded metal pipe (A), continuing after a small gap into another pipe (B) that is kept at potential -50 V compared to ground. What percentage of the electrons will be reflected at the gap? Assume the change in potential between the two pipes to be sharp.

Problem 4.

Wikipedia on Scanning tunneling microscopes (STM): *A scanning tunneling microscope (STM) is an instrument for imaging surfaces at the atomic level. Its development in 1981 earned its inventors, Gerd Binnig and Heinrich Rohrer (at IBM Zürich), the Nobel Prize in Physics in 1986. For an STM, good resolution is considered to be 0.1 nm lateral resolution and 0.01 nm depth resolution. With this resolution, individual atoms within materials are routinely imaged and manipulated. The STM can be used not only in ultra-high vacuum but also in air, water, and various other liquid or gas ambients, and at temperatures ranging from near zero kelvin to a few hundred degrees Celsius.*

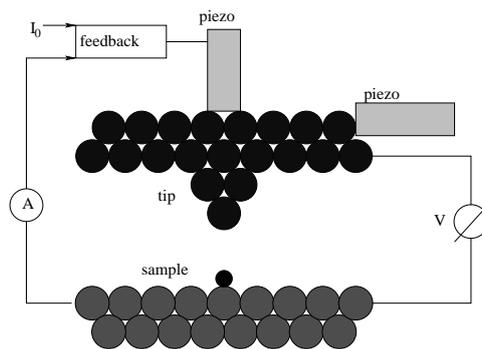


Figure 2: Sketch of an STM

a) The STM works by applying a bias (voltage difference) between the tip and the surface, to make the electrons of the surface tunnel through (what is usually) vacuum between the surface and the tip. The current across the barrier is then measured. Create a simple sketch of the tunnel barrier.

b) Write the wave function of the electron on both sides of the barrier (tip and surface)

and in the barrier. Use (unknown) coefficients A, B, \dots . Assume that the barrier is higher than the electron energy. In your sketch of the barrier, also sketch the electron wave function.

c) The STM can be scanned across the surface keeping a constant height over the surface, or with the tip changing height so as to keep the current constant. In the simple model of question a), how will a small “hill” (e.g., an added atom) on the surface affect the output current if the tip is kept at a constant height? (i.e., if z is the direction upwards, the value of z remains unchanged). A motivated, qualitative answer suffices.

Problem 5.

1,3,5,7-Cyclooctatetraene (C_8H_8) is a cyclic unsaturated hydrocarbon. X-ray diffraction data demonstrate that cyclooctatetraene exists as a non-planar “tube shaped” molecule and contains two distinct C-C bond lengths.

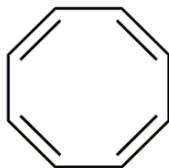


Figure 3: Cyclooctatetraene.

- Assuming that the molecule is flat, use the Hückel theory and draw an approximate π -orbital energy diagram for cyclooctatetraene.
- Show the π -electron configuration for cyclooctatetraene according to Hückel theory by adding in electrons into the π -orbital energy diagram.
- According to your π -orbital energy diagram, is the highest occupied orbital: bonding, non-bonding or antibonding?
- Explain whether cyclooctatetraene is an aromatic compound or not.
- What is the bond order for the carbon-carbon bonds in cyclooctatetraene according to the Hückel treatment?
- What is the approximate bond order for the different carbon-carbon bonds in the real “tube shaped” molecule?

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1.a $i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi$ where the hamiltonian $\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t)$
stationary states have time dependence $\sim e^{-\frac{i}{\hbar} E t}$ where E is the energy of the particular stationary state.

1.b Normalized: $\int |\psi(t=0)|^2 dr = 1$ i.e. $\frac{11}{21} + \frac{1}{7} + \frac{1}{N} = 1$ because the u_n are orthogonal and normalized ($\int u_n^* u_m dr = \delta_{nm}$).

Thus $N=3$.

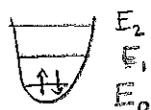
$$\psi(t) = \sqrt{\frac{11}{21}} u_1 e^{-\frac{i}{\hbar} E_1 t} + \frac{1}{\sqrt{7}} u_3 e^{-\frac{i}{\hbar} E_3 t} + \frac{1}{\sqrt{3}} u_7 e^{-\frac{i}{\hbar} E_7 t}$$

Energies E_1, E_3 and E_7 may be measured, at probabilities

$$\left| \sqrt{\frac{11}{21}} e^{-\frac{i}{\hbar} E_1 t} \right|^2 = \frac{11}{21}, \quad \left| \frac{1}{\sqrt{7}} e^{-\frac{i}{\hbar} E_3 t} \right|^2 = \frac{1}{7}, \quad \dots = \frac{1}{3}.$$

1.c $[f(\hat{p}, \hat{x}), \hat{x}] = [\hat{p}^2 + \frac{1}{2} \hat{x} \alpha, \hat{x}] = [\hat{p}^2, \hat{x}] = \hat{p} [\hat{p}, \hat{x}] + [\hat{p}, \hat{x}] \hat{p}$
 $= 2\hat{p} (-i\hbar) = -2i\hbar \hat{p}$
 $[f(\hat{p}, \hat{x}), \hat{p}] = \dots = [\frac{1}{2} \hat{x} \alpha, \hat{p}] = \frac{1}{2} (+i\hbar) \alpha = \frac{1}{2} \hbar \alpha$

1.d



total spin $\frac{1}{2} + (-\frac{1}{2}) = 0$, total energy $2 \cdot E_0 = 2 \cdot \frac{1}{2} \hbar \omega = \hbar \omega$



total spin $\frac{1}{2} + \frac{1}{2} = 1$, total energy $E_0 + E_1 = \frac{1}{2} \hbar \omega + \frac{3}{2} \hbar \omega = 2 \hbar \omega$

Fermi exclusion principle requires the two particles of $m_{s1} = \frac{1}{2}$, $m_{s2} = \frac{1}{2}$ to be in different energy states.

1.e+f see Jerker's solutions

2. $\hat{H} = \hat{H}_0 + \hat{H}'$, $\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2$, $\hat{H}' = \lambda \left(-\frac{1}{3} m \omega^2 \alpha \hat{x}^3 \right)$

a) $\hat{a} = \frac{\alpha}{\sqrt{2}} \left(\hat{x} + i \frac{\hat{p}}{\hbar \alpha} \right)$, $\hat{a}^\dagger = \frac{\alpha}{\sqrt{2}} \left(\hat{x} - i \frac{\hat{p}}{\hbar \alpha} \right)$

$\hat{x} = \frac{1}{\alpha \sqrt{2}} (\hat{a} + \hat{a}^\dagger)$. Then $\hat{H}' = -\lambda \frac{1}{3} m \omega^2 \alpha \left(\frac{1}{\sqrt{2} \alpha} \right)^3 (\hat{a} + \hat{a}^\dagger)^3$
 $= -\lambda \frac{1}{6\sqrt{2}} \frac{m \omega^2}{\alpha^2} (\hat{a} + \hat{a}^\dagger)^3 = -\lambda \frac{1}{6\sqrt{2}} \hbar \omega (\hat{a} + \hat{a}^\dagger)^3$

b) Perturbation theory, first order, $|n\rangle \sim$ unperturbed solutions.

$$E_n^{(1)} = \langle n | \hat{H}' | n \rangle = -\lambda \frac{\hbar \omega}{6\sqrt{2}} \langle n | (\hat{a} + \hat{a}^\dagger)^3 | n \rangle$$

$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$ terms $\sim \hat{a}^3, \hat{a}^2 \hat{a}^\dagger, \hat{a} (\hat{a}^\dagger)^2, (\hat{a}^\dagger)^3$ will all raise & lower the state $|n\rangle$ to a state not $|n\rangle$, which will become zero when taken with $\langle n |$.

2c Perturbation, second order, ground state:

$$E_{n=0}^{(2)} = - \sum_{\substack{k \neq n \\ (n=0)}} \frac{\langle n | H' | k \rangle \langle k | H' | n \rangle}{E_k^{(0)} - E_n^{(0)}}$$

$$\hat{a} | 0 \rangle = 0$$

$$\langle k | (\hat{a} + \hat{a}^\dagger)^3 | 0 \rangle \stackrel{\downarrow}{=} \langle k | (\hat{a} + \hat{a}^\dagger)^2 \hat{a}^\dagger | 0 \rangle = \langle k | (\hat{a} + \hat{a}^\dagger)^2 | 1 \rangle$$

$$\hat{a} \hat{a} | 1 \rangle = \hat{a} | 0 \rangle = 0$$

$$\hat{a} \hat{a}^\dagger | 1 \rangle = \sqrt{2} \hat{a} | 2 \rangle = \sqrt{2} \sqrt{2} | 1 \rangle = 2 | 1 \rangle$$

$$\hat{a}^\dagger \hat{a} | 1 \rangle = \hat{a}^\dagger | 0 \rangle = | 1 \rangle$$

$$\hat{a}^\dagger \hat{a}^\dagger | 1 \rangle = \sqrt{2} \hat{a}^\dagger | 2 \rangle = \sqrt{2} \sqrt{3} | 3 \rangle$$

$$\therefore \langle k | (\hat{a} + \hat{a}^\dagger)^3 | 0 \rangle = \langle k | (3 | 1 \rangle + \sqrt{6} | 3 \rangle)$$

Only terms $k=1$ and $k=3$ will contribute in the sum of $E_{n=0}^{(2)}$.

$$\begin{aligned} E_{n=0}^{(2)} &= - \lambda^2 \left(\frac{1}{6\sqrt{2}} \right)^2 (\hbar\omega)^2 \left\{ \frac{1}{E_{k=1}^{(0)} - E_{n=0}^{(0)}} |\langle 1 | 3 | 1 \rangle|^2 \right. \\ &\quad \left. + \frac{1}{E_{k=3}^{(0)} - E_{n=0}^{(0)}} |\langle 3 | \sqrt{6} | 3 \rangle|^2 \right\} \\ &= - \lambda^2 \frac{1}{2^3 3^2} \left\{ \frac{3^2}{\hbar\omega} + \frac{6}{3\hbar\omega} \right\} (\hbar\omega)^2 \\ &= - \lambda^2 \frac{11}{72} \hbar\omega \end{aligned}$$

i.e., $\left| \frac{E_{n=0}^{(2)}}{E_{n=0}^{(0)}} \right| = \frac{\lambda^2 \frac{11}{72} \hbar\omega}{\frac{1}{2} \hbar\omega} = \lambda^2 \frac{11}{36}$, a small part if $\lambda \ll 1$
[not asked here, but in 2.d]

2d

$$V(x) = \frac{1}{2} m\omega^2 x^2 - \lambda \frac{1}{3} m\omega^2 \alpha x^3$$

Extrema: $\frac{d}{dx} V(x) = m\omega^2 x - \lambda m\omega^2 \alpha x^2 = 0$

$$\therefore x=0 \text{ or } x = (\lambda\alpha)^{-1}$$

$$\frac{d^2}{dx^2} V(x) = m\omega^2 - \lambda 2 m\omega^2 \alpha x = \begin{cases} m\omega^2 & \text{at } x=0, \text{ i.e. minimum} \\ -m\omega^2 & \text{at } x=(\lambda\alpha)^{-1}, \text{ i.e. maximum} \end{cases}$$

Local minimum at $x_0=0$ with value $V(x_0)=0$

Local maximum at $x_1=(\lambda\alpha)^{-1}$ with value

$$V(x_1) = \frac{1}{6} \frac{1}{\lambda^2} \hbar\omega, \text{ i.e. barrier height } V(x_1) - V(x_0) = \frac{1}{\lambda^2} \frac{1}{6} \hbar\omega$$

(2d continued)

Neglect perturbative terms in the energy levels.

Reasonable? Yes, will lower the energies (seen for the ground state in 2b) slightly and thus if three bound levels are secured without the perturbative energy terms then at least three (but possibly more) states will be bound.

$$\begin{aligned} \text{Three states: } E_0 &= \frac{1}{2} \hbar \omega \\ E_1 &= \frac{3}{2} \hbar \omega \\ E_2 &= \frac{5}{2} \hbar \omega \end{aligned}$$

Must have barrier height larger than E_2 , i.e.

$$\frac{5}{2} \hbar \omega < V(x_1) - V(x_0)$$

or
$$\frac{5}{2} \hbar \omega < \frac{1}{\lambda^2} \frac{1}{6} \hbar \omega \quad \text{i.e.} \quad \lambda < \frac{1}{\sqrt{15}} \approx 0.26 \text{ is required}$$

Aside: (not asked)

We can estimate the effect of neglecting the $E_n^{(2)}$ and higher order energy terms by studying the problem:

Find requirement on λ for the well to hold at least one bound state.

Including the $E_{n=0}^{(2)}$ - term the requirement is

$$\frac{1}{2} \hbar \omega - \lambda^2 \frac{11}{72} \hbar \omega < \frac{1}{\lambda^2} \frac{1}{6} \hbar \omega$$

or

$$0 < \frac{11}{12} \lambda^4 - 3\lambda^2 + 1$$



Roots:
$$\lambda_0^2 = \frac{3 \pm \sqrt{9 - \frac{11}{3}}}{\frac{11}{6}} = \begin{cases} 2.896 & \text{"+" solution} \\ 0.3767 & \text{"-" solution} \end{cases}$$

Since λ "small" we must require $\lambda \lesssim 1$, thus only the lower branch of the solution is relevant:

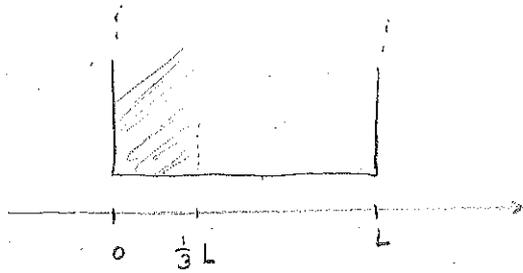
$$\lambda^2 < \frac{6}{11} (3 - \sqrt{9 - \frac{11}{3}})$$

so for one bound state we need $\lambda < 0.614$

Ignoring $E_{n=0}^{(2)}$ we find the requirement $\frac{1}{2} \hbar \omega < \frac{1}{\lambda^2} \frac{1}{6} \hbar \omega$, i.e. $\lambda < \frac{1}{\sqrt{3}} \approx 0.577$

Thus the approximate solution is reasonable here.

3.9



1D infinite quantum well,
wave functions for stationary states:

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

for $0 \leq x < L$

(and 0 outside this range)

Probability of finding particle

within $\frac{1}{3}L$ from left wall

$$P_n = \int_0^{L/3} |\Psi_n(x)|^2 dx = \frac{2}{L} \int_0^{L/3} \sin^2 \frac{n\pi x}{L} dx$$

$$= \frac{2}{L} \frac{1}{2 \left(\frac{n\pi}{L}\right)} \left[\frac{n\pi}{L} x - \sin\left(\frac{\pi n}{L} x\right) \cos\left(\frac{\pi n}{L} x\right) \right]_0^{L/3}$$

$$= \frac{1}{n\pi} \left(\frac{n\pi}{L} \frac{L}{3} - \sin\left(\frac{\pi n L}{3L}\right) \cos\left(\frac{\pi n L}{3L}\right) \right)$$

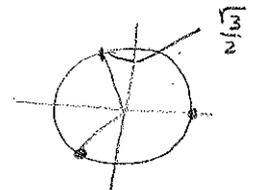
$$= \frac{1}{3} \left(1 - \frac{3}{2\pi n} \sin \frac{2\pi n}{3} \right)$$

a1) $n=1$, $P_{n=1} = \frac{1}{3} \left(1 - \frac{3}{2\pi} \frac{\sqrt{3}}{2} \right) \approx 0.196$

a2) $n=2$, $P_{n=2} = \frac{1}{3} \left(1 + \frac{3}{2\pi \cdot 2} \frac{\sqrt{3}}{2} \right) \approx 0.402$

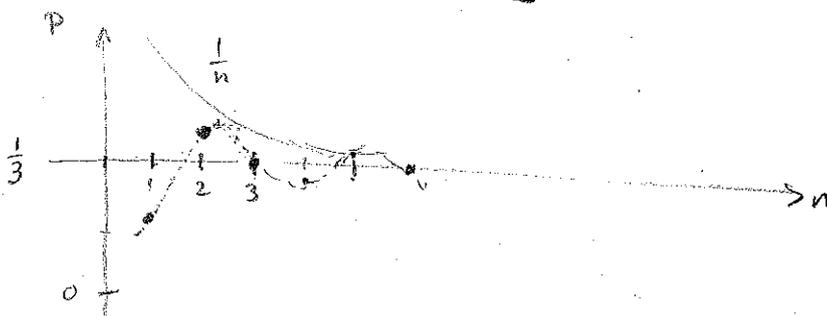
a3) $n \rightarrow \infty$, last term $\rightarrow 0$ for $\frac{2\pi n}{3} \rightarrow \infty$, thus $P_{n \rightarrow \infty} = \frac{1}{3}$

a4) Classically the probability is evenly distributed in the well,
thus $P_{\text{classically}} = \frac{1}{3}$



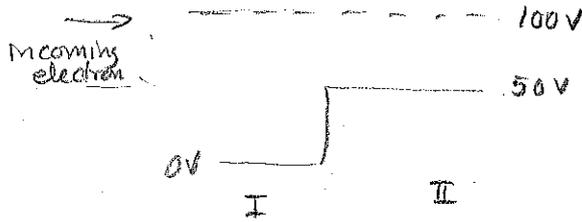
We expect high energy states (n large) to approach classical behavior, which a3 and a4 show.

P_n as a function of n oscillates around $\frac{1}{3}$ with a damped oscillation, damped by $\frac{1}{n}$



3b

For the electron with negative charge the potential is zero in A and +50V in B



$$k_I = \frac{1}{\hbar} \sqrt{(E - V_I) 2m_e} = \frac{1}{\hbar} \sqrt{2m_e E} \quad \text{because } V_I = 0$$

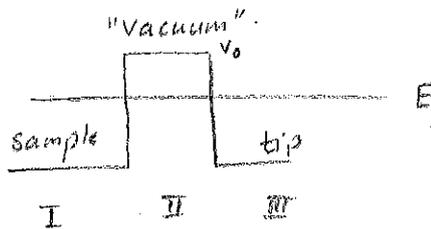
$$k_{II} = \frac{1}{\hbar} \sqrt{(E - V_{II}) 2m_e}$$

$$\text{Reflection } R = \left(\frac{k_I - k_{II}}{k_I + k_{II}} \right)^2 = \left(\frac{\sqrt{E} - \sqrt{E - V_{II}}}{\sqrt{E} + \sqrt{E - V_{II}}} \right)^2$$

$E = 2 \cdot V_{II}$ in this particular experiment

$$R = \left(\frac{\sqrt{2} - 1}{\sqrt{2} + 1} \right)^2 = 3\%$$

4.a)



b) Wave functions

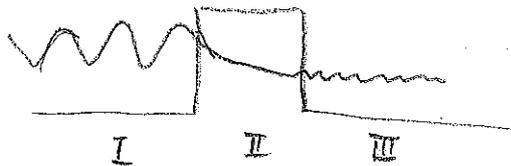
$$\psi_I = A e^{ik_I x} + B e^{-ik_I x}$$

$$k_I = \sqrt{\frac{2m E}{\hbar^2}}$$

$$\psi_{II} = C e^{kx} + D e^{-kx}$$

$$k = \sqrt{\frac{2m}{\hbar^2} (V_0 - E)}$$

$$\psi_{III} = D e^{ik_I x} + E e^{-ik_I x}$$



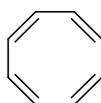
g) Hill: barrier more than, i.e. larger transmittance, thus large output current.

Exam questions in chemistry 2015-01-05

List the basic assumptions of valence bond theory.

Explain the origin of π - π interactions and show by a drawing the favorable geometrical arrangement of two interacting benzene molecules.

1,3,5,7-Cyclooctatetraene (C_8H_8) is a cyclic unsaturated hydrocarbon. X-ray diffraction data demonstrate that cyclooctatetraene exists as a non-planar "tube shaped" molecule and contains two distinct C-C bond lengths.



Cyclooctatetraene

- Assuming that the molecule is flat, use the Hückel theory and draw an approximate π -orbital energy diagram for cyclooctatetraene.
- Show the π -electron configuration for cyclooctatetraene according to Hückel theory by adding in electrons into the π -orbital energy diagram.
- According to your π -orbital energy diagram, is the highest occupied orbital bonding, non-bonding or antibonding?
- Explain whether cyclooctatetraene is an aromatic compound or not.
- What is the bond order for the carbon-carbon bonds in cyclooctatetraene according to the Hückel treatment?
- What is the approximate bond order for the different carbon-carbon bonds in the real "tube shaped" molecule?

Answers to exam questions

- List the basic assumptions of valence bond theory.

Answer:

A covalent bond is formed by the overlapping of two half-filled valence atomic orbitals (AOs) of two different atoms. The overlap may also be between one empty AO and one half-filled or filled AO.

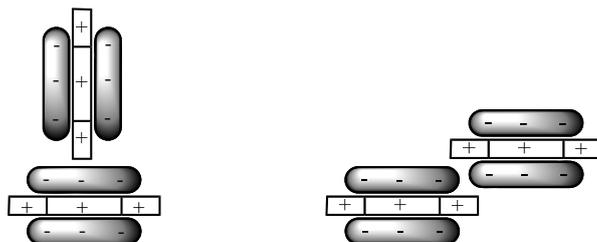
The electrons in the overlapping orbitals get paired and confined between the nuclei of two atoms.

Linear combination of AOs *at the same atom* (hybridization) is applied to harmonize with observed coordination geometry around the central atom

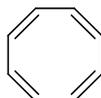
- Explain the origin of π - π interactions and show by a drawing the favorable geometrical arrangement of two interacting benzene molecules.

Answer:

The π -electrons are located above and below the plane of the molecule leaving behind a slightly electron deficient (positive) σ -system. This interacts with the π -electron cloud of another benzene.



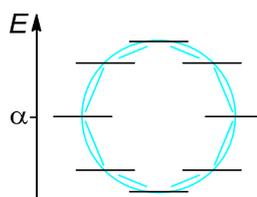
3. 1,3,5,7-Cyclooctatetraene (C_8H_8) is a cyclic unsaturated hydrocarbon. X-ray diffraction data demonstrate that cyclooctatetraene exists as a non-planar “tube shaped” molecule and contains two distinct C-C bond lengths.



Cyclooctatetraene

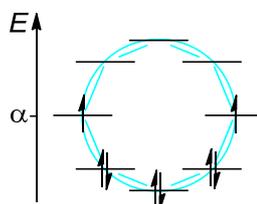
- a. Assuming that the molecule is flat, use the Hückel theory and draw an approximate π -orbital energy diagram for cyclooctatetraene.

Answer:



- b. Show the π -electron configuration for cyclooctatetraene according to Hückel theory by adding in electrons into the π -orbital energy diagram.

Answer:



- c. According to your π -orbital energy diagram, is the highest occupied orbital bonding, non-bonding or antibonding?

Answer:

Non-bonding

- d. Explain whether cyclooctatetraene is an aromatic compound or not.

Answer:

Cyclooctatetraene is not aromatic. Eight π -electrons is not a Hückel number ($4n + 2$).

- e. What is the bond order for the carbon-carbon bonds in cyclooctatetraene according to the Hückel treatment?

Answer:

Bond order (B.O.) = (# electrons in bonding orbitals – # electrons in antibonding)/2. It has to be scaled by the number of bonds in the cyclic structure. $B.O. = (6 - 0)/2 = 3$. These three π -bonds are evenly distributed between eight carbons in cyclooctatetraene. Thus, there is $3/8$ π -bond, in addition to the σ -bond, between each pair of carbons. $B.O. = 1.375$

- f. What is the approximate bond order for the different carbon-carbon bonds in the real “tube shaped” molecule?

Answer:

Eight π -electrons yields an anti-aromatic compound if planar. The compound is forced out of planarity disrupting the conjugation. Cyclooctatetraene therefore have alternating single and double bonds in its most favorable conformation.