# **1** Theoretical questions

(answer them in short and clear sentences including the necessary formulas when needed)

1. According to (classical) electrodynamics an accelerating charge loses energy by radiation. Explain why does the electron not radiate energy in a stationary state of an atom. Is (classical) electrodynamics wrong?

# Solution:

*Electrodynamics is correct, however the electron does not accelerate in stationary states.* 

2. "Although the electron is either a wave or a particle at any given time, but when we perform a measurement we force the electron to randomly jump into either one of these states." – Is this statement true or not? Explain!

#### Solution:

The electron is neither a wave nor a particle independent of any measurements. Measurements determine what properties of the electron we observe.

3. Define the Fermi energy for a system of electrons!

# Solution:

The Fermi energy is the energy up to which at T = 0K all energy levels are occupied but above which all are empty.

4. Enumerate the phenomena that lead to the development of quantum physics.

# Solution:

- Black body radiation
- (external) Photoelectric effect
- Compton effect
- Stability of atoms
- Line spectrum of atoms
- Frank-Hertz experiment
- 5. Give the time independent Schrödinger equation of a one dimensional linear harmonic oscillator and sketch the wave functions for the first 3 energy states! Solution:

$$-\frac{\hbar}{2m_e}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}m_e\,\omega^2\,\psi(x) = i\,\hbar\,\frac{d\psi(x)}{dt}$$

6. How can we determine the solution of the time-dependent Schrödinger equation from the solutions of the stationary equation?

## Solution:

The eigenfunctions of the time dependent Schrödinger equation are the product of the eigenfunctions of the corresponding stationary Schrödinger equation and the function  $e^{-E/\hbar t}$ . Therefore the solution of the time dependent equation may be written as a linear combination of such products. In 1D e.g.:

$$\psi(x,t) = \sum_{E} \phi_E(x) e^{-E/\hbar t}$$



Figure 1: Wave function and probability densities for the linear harmonic oscillator

7. How many ways can the orbital angular momentum of an electron on the 2p shell be positioned ?

## Solution:

The total angular momentum on a p shell is  $\ell = 1$  independently of the principal quantum number, therefore it can be positioned in  $2 * \ell + 1 = 3$  ways only.

8. In a double slit experiment let the wave function of an electron going through slit number 1 be  $\psi_1(\mathbf{r},t)$  and for the one through slit 2 be  $\psi_2(\mathbf{r},t)$ . What is the probability that the electron hits a given point  $P(\mathbf{r}, t)$  of the screen? Solution:

The probability is  $|\psi_1(\mathbf{r},t) + \psi_2(\mathbf{r},t)|^2$ .

9. In a double slit experiment we determine which slit an electron went through by illuminating it with light. Let the wave function of an electron going through slit number 1 be  $\psi_1(\mathbf{r}, t)$  and for the one through slit 2 be  $\psi_2(\mathbf{r}, t)$ . What is the probability that the electron hits a given point  $P(\mathbf{r}, t)$  of the screen?

#### Solution:

The probability is  $|\psi_1(\mathbf{r},t)|^2 + |\psi_2(\mathbf{r},t)|^2$ .

10. In the double slit experiment let the wave function of an electron be  $\psi_1(\mathbf{r},t)$ when slits #1 is blocked and  $\psi_2(\mathbf{r}, t)$  when slit #2 is blocked. Is the statement "The probability that the electron hits a given point of the screen when both splits are open is  $|\psi_1(\mathbf{r},t)|^2 + |\psi_2(\mathbf{r},t)|^2$ ." true or false and why? Explain!

## Solution:

False. The probability is  $|\psi_1(\mathbf{r},t) + \psi_2(\mathbf{r},t)|^2$ , because the probability is not the sum of the individual probabilities.

11. "In the double slit experiment let the wave function of an electron going through slit number 1 is  $\psi_1(\mathbf{r}, t)$  and for the one through slit 2 is  $\psi_2(\mathbf{r}, t)$ . Then the probability that the electron hit a given point of the screen is  $|\psi_1(\mathbf{r},t)|^2 +$  $|\psi_2(\mathbf{r},t)|^2$ ." – Is this statement true or not? Explain!

# Solution:

False. The probability is  $|\psi_1(\mathbf{r},t) + \psi_2(\mathbf{r},t)|^2$ .

12. In the photoelectric effect if we increase the frequency of the incident light the number of the emitted electrons will or will not change?

## Solution:

The number of emitted electrons will not change, only the velocities of the emitted electrons changes

13. In the photoelectric effect if we increase the intensity of the incident light the velocity of the emitted electrons will or will not change?

Solution:

The velocity of the emitted electrons will not change, only the number of the emitted electrons changes.

14. Is it always true that the wave function of a system of electrons must be antisymmetric for the exchange of the coordinates of two electrons? Explain. Solution:

False. The total wave function (including the spin) of a system of electrons must always be antisymmetric to the exchange of the coordinates of two electrons. This wave function can be written as a product of two functions. One that depend on the spatial coordinates of the electrons the other one depends on their spin. So when the spin dependent part is antisymmetric the spatial coordinate dependent part must be symmetric.

15. Is there a contradiction between electrodynamics and the electron not radiating in a stationary state in an atom? – Explain!

## Solution:

There is no contradiction. Electrodynamics is applicable, but the electron does not accelerate in stationary states.

16. Is there any system in which the eigenvalues of the Schrödinger equation are not discrete? If you answer "yes" give an example, if you answer "no" explain it why!

## Solution:

Yes, there is. For free electrons the energy spectrum is continuous. (For electrons enclosed even in a very big potential box the energy states are discrete, however this discreteness cannot be measured if the dimensions of the box are large enough.)

17. Is the statement "Because a black-body absorbs all radiation it will always look black, darker than any other object." true or false? Explain!

## Solution:

False. The color depends on the temperature and at any given temperature the black-body is brighter than non black-bodies

18. What is the difference between the behavior of a classical particle and a wave? What is the wave-particle duality?

#### Solution:

A classical particle has a well defined position and velocity (momentum), i.e. a well defined trajectory. A classical wave presents diffraction and interference phenomena. Wave particle duality - under suitable circumstances the quantum mechanical particle behaves like either a wave or a particle.

Background info: the particle's behavior is described by a probability (density) wave whose absolute square gives the probabilities. When in a process the probabilities can be added to get the resultant probability (example: two electrons in two separate atoms, when the electronic wave functions do not interlap) then the particle behaves like a classical particle, and when the amplitudes of the waves must be added to get the resulting amplitude (example: 2 slits experiment) we got diffraction. 19. What is the ratio of population between two energy levels in thermal equilibrium?

Solution: 
$$n_i$$

$$\frac{n_i}{n_j} = \frac{g_i}{g_j} \cdot e^{-\frac{\Delta \mathcal{E}}{k_B T}}$$

20. Is the statement "The electron is either a wave or a particle depending on the measurement we perform." true or false? Explain!

## Solution:

The electron is neither a wave nor a particle independent of any measurements. Measurements determine what properties of the electron we observe.

21. "Observable electron interference patterns are formed only when there are many electrons present in a system at the same time and they interact with each other. A series of non-interacting single electrons does not create an interference pattern, no matter how many electrons are used" – Is this statement true or not? Explain!

#### Solution:

False. Interference patterns are formed, because every electron has a wave like state function. It doesn't matter how many electrons are simultaneously present, every electron interfere with itself.

22. Select the right hand side of the one dimensional (time dependent) Schrödinger equation from the following:

$$a)\frac{\hbar}{i}\frac{\partial E}{\partial x}, \qquad b)\frac{\hbar}{i}\frac{\partial \psi}{\partial x}, \qquad c)i\hbar E, \qquad d)i\hbar\frac{\partial \psi}{\partial t}$$

## Solution:

d)

23. Select the right hand side of the one dimensional time dependent Schrödinger equation from the following:

$$a)i\hbar\frac{\partial\psi}{\partial t}, \qquad b)\frac{\hbar}{i}\frac{\partial E}{\partial x}, \qquad c)i\hbar E, \qquad d)\frac{\hbar}{i}\frac{\partial\psi}{\partial x},$$

## Solution:

a)

24. What is tunneling? Give the most important characteristics. Solution:

Tunneling is the phenomena when a particle, with a total energy less than the potential in a region of space still may pass through this region, although in classical mechanics this would be impossible. In 1D the transition probability decreases fast when either the width of the region or the height of the potential barrier increases.

25. What physical quantity do we call "potential" in quantum mechanics Solution:

The "potential" in quantum mechanics is called the potential energy in classical physics.

26. Sketch the radial part of the wave function of the hydrogen atom for n=1 and n = 2!.



27. "The black-body absorbs all radiation therefore it will always look black" – Is this statement true or not? Explain!

## Solution:

False. The color depends on the temperature and at any given temperature the black-body is brighter than non black-bodies

28. "The eigenvalues of the Schrödinger equation are always discreet." – Is this statement true or not? Explain!

## Solution:

False. For free electrons the energy spectrum is continuous.

29. "The electron is a particle which has some wave characteristics." – Is this statement true or not? Explain!

## Solution:

False. The electron is a quantum mechanical object which has characteristics of both classical waves and particles.

30. The electron is characterized by the wave function. Can we measure the wave function itself or if not what do we measure then?

#### Solution:

We do not measure the wave function. We measure physical quantities like position, momentum, energy, etc. The absolute square of the wave function determines the probability of the result of a position measurement.

31. The electron is characterized by the wave function, but we do not measure the wave function itself. What do we measure then? Explain!

Solution:

We measure physical quantities like position, momentum, energy, etc. We can also measure the absolute square of the wave function when we measure the position of the electron.

32. The electron is characterized by the wave function, but we never measure the wave function itself. What do we measure then? Explain!

# Solution:

We measure physical quantities like position, momentum, energy, etc. We can measure the absolute square of the wave function when we measure the position of the electron.

- 33. "The electron is either a wave or a particle, depending on the type of the actual interactions with the environment."
  - Is this statement true or not? Explain!

## Solution:

False. The electron is neither a wave nor a particle independent of any interactions. It is a quantum mechanical object which has characteristics of both of these classical notions.

- 34. "The energy of a bound electron (i.e. an electron restricted in space) in quantum mechanics is always discreet."
  - Is this statement true or not? Explain!

## Solution:

True. Bound states means the wave function must vanish toward infinity. This restricts the possible energy values. For free electrons no such condition exists.

- 35. "The energy of an electron in quantum mechanics is always discreet."
  - Is this statement true or not? Explain!

## Solution:

False. For free electrons the energy spectrum is continuous.

- 36. "The (ideal) black body got its name for only absorbing but not emitting electromagnetic radiation."
  - Is this statement true or false? Explain!

## Solution:

The statement is false: black bodies are called "black" only to show that they absorb all electromagnetic radiations. In thermal equilibrium they emit the same amount of radiation they absorb.

37. We know all of the stationary  $\phi_n(\mathbf{r})$  eigenfunctions and  $E_n$  eigenvalues of a Hamiltonian and we know the actual  $\psi(\mathbf{r}) = \psi(\mathbf{r}, 0)$  function of a system at

## t = 0. Write the formula for the time dependent $\psi(r, t)$ wave function! Solution:

The known  $\psi(\mathbf{r})$  function is a linear combination of the  $\phi_n(\mathbf{r})$  eigenfunctions of the Hamiltonian.

$$\psi_n(\mathbf{r}) = \sum_n C_n \, \phi_n(\mathbf{r})$$

Each  $\phi_n(\mathbf{r})$  solutions of the stationary Schrödinger equation when multiplied by  $e^{-E_n/\hbar t}$  becomes the solution of a time-dependent Schräinger equation. So to get the time dependent wave function corresponding to  $\psi_n(\mathbf{r}, t)$  we have to write:

$$\psi_n(\mathbf{r},t) = \sum_n C_n \,\phi_n(\mathbf{r}) e^{-\frac{E_n}{h}t}$$

# 38. What are selection rules and what do they mean?

## Solution:

Selection rules constrain the possible transitions of a system. They can be formulated for electronic, vibrational or rotational transitions. Examples: for electronic transitions the total angular momentum difference between the initial and final states must be an integer multiple of  $\hbar$ . Transitions prohibited by a selection rule may still happen by allowing other kind of interactions taking place. Usually these transitions have a much smaller probability than the one prohibited by the selection rule.

39. What are the assumptions of the Bose-Einstein and of the Fermi-Dirac statistics?

Both statistics are valid for indistinguishable particles. Fermi-Dirac statistics is valid for half-spin particles called fermions (like electrons) where no two particle may occupy the same quantum state, while Bose-Einstein statistics is valid for particles of integer spin (bosons), where any number of particles may be in the same quantum state.

40. What are the possible values of the total angular momentum for a single electron on an s shell?

> Solution:  $\ell = 0, m = 0, s = -\frac{1}{2}, \frac{1}{2} \Rightarrow J = L + S : -\frac{1}{2}, \frac{1}{2}$

41. What are the possible values of the total angular momentum for a single electron on a p shell?

. .

## Solution:

Solution:  

$$\ell = 1, m = -1, 0, 1, s = -\frac{1}{2}, \frac{1}{2} \implies J = L + S : -1\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, 1\frac{1}{2}$$
  
and the values  $-\frac{1}{2}, \frac{1}{2}$  correspond to degenerate levels  $(-\frac{1}{2} = -1 + \frac{1}{2})$   
 $or -\frac{1}{2} = 0 - \frac{1}{2})$ 

42. What do we call an atomic orbital? What is a molecular orbital?

## Solution:

An atomic orbital is the wave function of the electron inside the atom. The molecular orbital is the same for a molecule. (In chemistry the same term may be applied to the region of space where the electron is found with suitable high (e.g. 90%) probability.) Background info:

43. What is Raman scattering?

## Solution:

Raman scattering is the inelastic scattering of light on particles much smaller than their wavelengths. The wavelength of the scattered light is different from that of the incident light.

44. What is Rayleigh scattering?

# Solution:

Rayleigh scattering is the elastic scattering of light on particles much smaller than their wavelengths. The wavelength of the scattered light is the same as that of the incident light.

## 45. What is hybridization?

# Solution:

Hybridization means the mixing of atomic orbitals to create orbitals which qualitatively describe the atomic bonding in molecules. Their name is derived from the corresponding atomic orbitals used. Example: an  $sp^3$  orbital is the linear combination of one s and 3 p orbitals (like in  $CH_4$ )

46. What is quantum tunneling?

# Solution:

It is enough to give either the definition or a drawing A microscopic particle (e.g. an electron) may travel through a region (potential wall) where the potential is higher than the total energy of the particle if the width of the wall is sufficiently small.

$$ln(Probability of transfer) \approx -2 \frac{\sqrt{2 m_e V_o - \mathcal{E}}}{\hbar} (width of wall)$$



Figure 2: Quantum tunneling

47. What is the Fermi energy?

# Solution:

For a system of electrons in a box it is the energy up to which all energy levels are occupied and above which all are empty at T = 0K.

48. What is the Raman and what is the Rayleigh scattering?

#### Solution:

Raman scattering is the inelastic scattering of light on particles much smaller than their wavelengths. Rayleigh scattering is the elastic scattering.

49. What is the difference between the behavior of a classical particle and a wave? What is the wave-particle duality?

## Solution:

A classical particle has a well defined position and velocity (momentum), i.e. a well defined trajectory. A classical wave presents diffraction and interference phenomena. Wave particle duality - under suitable circumstances the quantum mechanical particle behaves like either a wave or a particle.

Background info: the particle's behavior is described by a probability (density) wave whose absolute square gives the probabilities. When in a process the probabilities can be added to get the resultant probability (example: two electrons in two separate atoms, when the electronic wave functions do not interlap) then the particle behaves like a classical particle, and when the amplitudes of the waves must be added to get the resulting amplitude (example: 2 slits experiment) we got diffraction.

50. What is the meaning of the term "spin-orbit interaction"?

# Solution:

In electronic states with non zero angular momentum there is a non zero B(L) magnetic field in the coordinate system attached to the electron. This magnetic field interacts with the magnetic momentum that corresponds to (and proportional to) the electron spin S. The interaction energy therefore  $E_{SL} = \text{const}\mathbf{SL}$ .

51. What is the physical meaning of the wave function?

The absolute square of the wave function integrated over an interval gives the probability the electron is found in that interval. Therefore the integral of the absolute square of the wave function for the whole space is 1.

52. What is the physical meaning of the wave function (Coppenhagen interpretation) ?

#### Solution:

Integrating the absolute square of the wave function of a particle over an interval gives the probability of finding the particle in that interval. (Therefore the integral of the wave function for the whole of space is equal to 1.

53. What is the physical reason of the spin-orbit interaction (or spin-orbit coupling) ?

## Solution:

The coupling of the magnetic moments associated to the spin ad the orbital angular momentum.

54. What is the spin-orbit interaction (or spin-orbit coupling) ?

## Solution:

It is the coupling of the magnetic moments associated to the spin and the orbital angular momentum.

55. What is tunneling? Give the most important characteristics.

## Solution:

Tunneling is the phenomena when a particle, with a total energy less than the potential in a region of space still may pass through this region, although in classical mechanics this would be impossible. In 1D the transition probability decreases fast when either the width of the region or the height of the potential barrier increases.

56. What physical quantity do we call "potential" in quantum mechanics Solution:

The "potential" in quantum mechanics is called the potential energy in classical physics.

57. Where is the Fermi level in an a) intrinsic, b) extrinsic semiconductor at T=0K?

#### Solution:

In intrinsic semiconductors in the middle of the energy gap, in extrinsic semiconductors in the middle between the impurity (donor or acceptor) levels and the nearest band edge (conduction and valence band respectively).

58. Which of the following appears on the right hand side of the one dimensional (time dependent) Schrödinger equation:

$$a)\frac{\hbar}{i}\frac{\partial E}{\partial x}, \qquad b)\frac{\hbar}{i}\frac{\partial \psi}{\partial x}, \qquad c)i\hbar E, \qquad d)i\hbar\frac{\partial \psi}{\partial t}$$

## Solution:

d)

59. Why is state 2s called a *metastable* state in a hydrogen atom? Solution:

The transition  $2s \rightarrow 1s$  is forbidden because in the first order (dipole) approximation only transitions between states whose angular momentum difference is  $(\pm 1\hbar)$  are allowed (the photon has a spin of 1) and states 2s and 1s have the same l = 0 angular momentum. This transition may nevertheless occur, albeit with a far smaller probability, because higher order (non dipole) processes may also take place.

60. Write down the 1 dimensional time dependent Schrödinger equation and explain the various terms!

Solution:

$$-\frac{\hbar}{2m_e}\frac{d^2}{dx^2}\psi(x) + V(x)\,\psi(x) = i\,\hbar\,\frac{d\psi(x)}{dt}$$

61. Write the length of the electron spin!

Solution:  
$$|S| = \sqrt{\frac{1}{2} \cdot (\frac{1}{2} + 1)} \cdot \hbar = \frac{\sqrt{3}}{2} \cdot \hbar$$

62. Write the length of the orbital angular momentum in a d state!

#### Solution:

In a d state the maximum of the z-component of the angular momentum is  $\ell = 2 |L| = \sqrt{2 \cdot (2+1)} \cdot \hbar = \sqrt{6} \cdot \hbar$ 

63. question here

## Solution:

solution here

64. Give the formulas of the photon density of states  $g(\nu)$  and the average energy density  $u(\nu, T)$  in a cavity.

Solution:

$$g(\nu) = \frac{8\,\pi\,V}{c^3}\,\nu^2 \tag{1.1}$$

$$u(\nu,T) = \frac{8\pi h}{c^3} \frac{\nu^3}{e^{h\,\nu/k_B T} - 1} \tag{1.2}$$

## 2 Problems

Useful constants :

: Planck's constant:  $h = 6.63 \, 10^{-34} \, Js$ , elementary charge :  $e = 1.6 \, 10^{-19} \, C$ , electron mass :  $m_e = 9.1 \, 10^{-31} kg$ , Stefan - Boltzman constant :  $\sigma = 5.670373(21) \cdot 10^{-8} \, Wm^{-2} \, K^{-4}$ , Rydberg energy :  $1 \, Ry = 13.6 \, eV$ Avogadro's constantL  $6.022 \cdot 10^{23} \, 1/mol$ 

65. Calculate the distance between the 4th and 5th rotational levels in an  $O_2$  molecule! The mass of the O atom is  $m_o = 1.33 \, 10^{-23} g$  and the internuclear distance between the atoms in the molecule is  $r_o = 1.2 \, 10^{-10} m$ 

$$\begin{split} \mathcal{E}_{rot}^{\ell} &= \frac{\hbar^2}{2\Theta} \,\ell \left(\ell + 1\right) \qquad now \,\ell = 4\\ \Delta \mathcal{E} &= \mathcal{E}_{rot}^{\ell+1} - \mathcal{E}_{rot}^{\ell} = \frac{\hbar^2}{2\Theta} \left[ \left(\ell + 1\right) \left(\ell + 2\right) - \ell \left(\ell + 1\right) \right] \\ &= \frac{\hbar^2}{\Theta} \left(\ell + 1\right) = 5 \,\frac{\hbar^2}{\Theta} \\ \Theta &= \frac{m_O}{2} \,r_o^2 = 9.58 \,10^{-44} kgm^2 \end{split}$$

Therefore  $\Delta \mathcal{E}_{rot}^4 = \frac{5*\hbar^2}{9.58 \cdot 10^{-44}} = 5.81 \cdot 10^{-25} J = 3.62 \cdot 10^{-6} eV$ 66. An electron gun emits electrons with energies between 3.2 keV and 3.3 keV.

What is the minimum uncertainty of the position of the electrons?

Solution:

Because

$$U = \frac{p^2}{2 m_e e}$$
$$p = \sqrt{2 m_e e U}$$

and

$$\Delta p \Delta x \geq \frac{\hbar}{2}$$

and

$$\begin{split} \Delta p &= p_2 - p_1 = \sqrt{2 \, m_e \, e \, U} - \sqrt{2 \, m_e \, e \, U} \\ &= 3.1036419 \, 10^{-23} - 3.0562553 \, 10^{-23} = 4.74 \, 10^{-25} \, kg \, m^2/s^2 \\ \Delta x &= \frac{\hbar}{2 \, \Delta p} = 1.11 \, 10^{-10} \, m \end{split}$$

Using h/2 instead of  $\hbar/2$  would give  $6.99 \, 10^{-10}$  m, while with h this would be  $1.39 \, 10^{-9}$  m.

67. An electron is confined in a 3D potential box with sides  $10\mu m$ ,  $20\mu m$  and  $30 \mu m.$  Give the energy and degeneracy of the 3 lowest states.

## Solution:

The possible energy levels in one direction:

$$E_n = \frac{h^2}{8 m_e L^2} n^2$$

therefore in 3D

$$E_{n_1,n_2,n_3} = \frac{h^2}{8 m_e} \left( \frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2} \right)$$
  
= 6.02 10<sup>-28</sup>  $\left( \frac{n_1^2}{1} + \frac{n_2^2}{4} + \frac{n_3^2}{9} \right) [J]$   
= 3.76 10<sup>-9</sup>  $\left( \frac{n_1^2}{1} + \frac{n_2^2}{4} + \frac{n_3^2}{9} \right) [eV]$ 

The 3 lowest lying energy states can be determined by trying out different combinations of the 3 numbers and selecting the 3 smallest values

cara a c				
$n_1$	$n_2$	$n_3$	factor	
1	1	1	1.36	
1	1	2	1.47	
1	$\mathcal{Z}$	1	1.61	From this table the indices for the 2 lowest
2	1	1	2.36	Tront titls tuble the thuices for the 5 towest
2	$\mathcal{Z}$	1	2.61	
1	$\mathcal{Z}$	2	1.72	
1	1	3	1.58	

 $1 \mid 1 \mid 3 \mid 1.50$ levels are: (1,1,1), (1,1,2) and (1,2,1).

The corresponding energies and degeneracies:

Energy level	$E(\times 10^{-28} J)$	$E(\times 10^{-9} eV)$	degeneracy
$E_{111}$	8.20	5.11	1
$E_{112}$	8.87	5.53	1
$E_{121}$	12.7	7.94	1
$E_{113}$	13.6	8.46	1
$E_{122}$	14.7	9.19	1
$E_{211}$	26.3	16.39	1
$E_{212}$	28.3	17.7	1
$E_{221}$	30.8	19.2	1
$E_{222}$	32.8	20.47	1

68. An electron is confined in a three dimensional cubic potential box with sides of  $L = 3200 \, nm$ . What is the wavelength of the photon emitted during an electronic transition between level 3 and the ground state?

How would this value change if the size of the box was doubled?

# Solution:

For a cubic potential box (3 D problem) the wave function can be written as the product of 3 one dimensional wave functions, each along one coordinate axis, therefore the total energy can be written as the sum of 3 energy values for the 3 axes. In a one dimensional potential box for the wave function at the n-th level

$$\begin{split} L &= n \frac{\lambda}{2} \Rightarrow \lambda = 2 \frac{L}{n} \Rightarrow \\ p &= \frac{h}{\lambda} = \frac{h}{2L} n \quad n = 1, 2, 3... \\ \mathcal{E}_n &= \frac{p^2}{2m} = \frac{h^2}{8 m L^2} n^2 \end{split}$$

Therefore in 3D

$$\mathcal{E}_{n} = \frac{h^{2}}{8 \, m \, L^{2}} \, \left( n_{x}^{2} + n_{y}^{2} + n_{z}^{2} \right)$$

For a cubic box in 3 dimensions all but the ground level is degenerate. In the ground state  $(E_1)$  all of  $n_x, n_y, n_z$  must be 1. On level 3  $(E_3)$  any two of them must be 2, i.e. the degeneracy of level 3 is 3.

(On level 2 one of  $n_x, n_y, n_z$  is 2, the others are 1.)

$$\begin{aligned} \mathcal{E}_1 &= \frac{h^2}{8 \, m \, L^2} (1+1+1) = 1.76 \cdot 10^{-26} \, J = 1.1 \cdot 10^{-7} \, eV \\ \mathcal{E}_3 &= \frac{h^2}{8 \, m \, L^2} (2^2+2^2+1) = \frac{9}{3} \, \mathcal{E}_1 = 5.295 \cdot 10^{-26} J = 3.3 \cdot 10^{-7} \, eV \\ h \, \nu &= \mathcal{E}_3 - \mathcal{E}_1 = \frac{h^2}{8 \, m \, L^2} (9-3) = \\ &= \left(\frac{9}{3} - 1\right) \, \mathcal{E}_1 = 3.53 \cdot 10^{-26} \, J = 2.2 \cdot 10^{-7} \, eV \\ \lambda &= \frac{c}{\nu} = \frac{8 \, m \, L^2 \, c}{6 \, h} = 5.627 \, m \end{aligned}$$

If L, the size of the box, is doubled according to the formula for  $\lambda$  the wavelength is quadrupled.

 $\lambda=22.5m$ 

69. A spherical body with a radius of  $R = 1 \ cm$  has a constant absorption coefficient in the whole spectral range. What is the absorption coefficient if it emits  $2.7 \cdot 10^{20} eV$  in every second? at  $T = 1000 \ K$ ?

# Solution:

The total energy emitted per unit time by black-bodies is given by the Stefan-Boltzmann law:  $E_{tot} = A\sigma T^4$ , Kirchoff's law states that e/a = const, where a = 1 for black-bodies, therefore for a body with a < 1 the emitted energy is less by the same factor:

$$E_{tot} = a \, 4 \, \pi \, R^2 \, \sigma \, T^4 = a \cdot 4 \, \pi \, 10^{-4} \cdot 5.670373 \cdot 10^{-8}$$
$$= a \cdot 71.33 J/s = a \cdot 4.5 \cdot 10^{20} eV/s = 2.7 \cdot 10^{20} eV/s$$
$$a = 0.6$$

70. Calculate the momentum and diameter (position uncertainty) for a dust particle with mass of  $730 \cdot 10^{-4} ng$ , if its velocity uncertainty is  $1.45 \cdot 10^{-18} \frac{m}{s}$ . Solution:

71. Calculate the momentum and velocity uncertainty for a dust particle of diameter  $500 \,\mu$  and mass of about  $730 \cdot 10^{-4} \, ng$ , which is at rest.

Solution:

If the particle is at rest then the position uncertainty  $\Delta x$  equals to its size. Therefore

$$\begin{split} \Delta x &= 5 \cdot 10^{-4} \, m, \\ \Delta p &= \frac{\hbar}{2 \cdot \Delta x}, \\ \Delta v &= \frac{\hbar}{2 \cdot m \cdot \Delta x}, \end{split} \qquad \Delta p &= 1.06 \cdot 10^{-31} \, kg \, \frac{m}{s} \\ \Delta v &= 1.45 \cdot 10^{-18} \, \frac{m}{s} \end{split}$$

72. Calculate the wavelength of the light emitted by the electron in a hydrogen atom during the  $E_3 \rightarrow E_2$  transition! Solution:

$$\begin{split} \nu &= \frac{E_3 - E_2}{h} \\ \underline{\lambda} &= \frac{c}{\nu} = \frac{c \cdot h}{E_3 - E_2} = \frac{3 \cdot 10^8 \ m/s \cdot 6.64 \cdot 10^{-34}}{(-13.6) \ 1.6 \cdot 10^{-19} \ \left(\frac{1}{9} - \frac{1}{4}\right)} = 6.564 \cdot 10^{-7} \ m \\ \underline{\lambda} &= \frac{656 \ nm}{or \ with \ the \ value \ of \ \nu} \\ \nu &= \frac{-13.6 \ eV \ 1.6 \cdot 10^{-19} \ J/eV}{6.64 \cdot 10^{-34}} \ \left(\frac{1}{9} - \frac{1}{4}\right) = 4.567 \cdot 10^{14} \ 1/s \\ \lambda &= \frac{c}{\nu} = \frac{3 \ 10^8 \ m/s}{4.567 \cdot 10^{14} \ 1/s} = 6.564 \cdot 10^{-7} \ m = 656 \ nm \end{split}$$

73. Calculate the wavelength of the light emitted by the electron in a hydrogen atom during the  $E_4 \rightarrow E_2$  transition!

Solution:

$$\nu = \frac{E_4 - E_2}{h} = \frac{-13.6 \cdot 1.6 \cdot 10^{-19}}{h} \left(\frac{1}{16} - \frac{1}{4}\right) = 6.16 \cdot 10^{14} Hz$$
(2.1)
$$\lambda = \frac{c}{\nu} = 487 \ nm$$
(2.2)

74. Consider an isotropic harmonic oscillator in 2 dimensions! The Hamiltonian is given by

$$H_o = \frac{p_x^2}{2\,m} + \frac{p_y^2}{2\,m} + \frac{m\,\omega^2}{2}\,(x^2 + y^2)$$

Create a table of the energies and degeneracy of the four lowest lying states **Solution:** 

A one-dimensional linear harmonic oscillator may have an energy of

$$\mathcal{E}_n = h \nu (\frac{1}{2} + n), \text{ where } n = 0, 1, 2, 3, \dots$$

In two dimensions

$$\mathcal{E}_n = h \nu (1 + n_x + n_y), \text{ where } n = 0, 1, 2, 3, \dots$$

The energy and the degeneracy of the 4 lowest lying states are

Level	$\mathbf{n_x}$	$ \mathbf{n_y} $	degeneracy
$\mathcal{E}_o = h  \nu$	0	0	non-degenerate
$\mathcal{E}_1 = 2  h  \nu$	1	0	2
	0	1	
$\mathcal{E}_2 = 3  h  \nu$	2	0	
	0	2	3
	1	1	
$\mathcal{E}_3 = 4  h  \nu$	3	0	
	0	3	
	2	1	4
	1	2	

- 75. Consider the following hypothetic wave function for a particle confined in the region  $7 \le x \le 10$ :  $\psi(x) = A(70 + 3xx^2)$  inside the region and 0 outside it
  - (a) Sketch the wave function

Inverted parabola with peak 72.25 \* A at position 1.5

(b) Normalize the wave function over the range the particle is confined in **Solution:** 

Normalization means the determination of A so that the absolute square integral of the wave function is 1.

$$1 = \int_{-7}^{10} |\psi(x)|^2 dx =$$
  
=  $|A|^2 \int_{-7}^{10} (70 + 3x - x^2)(70 + 3x - x^2)dx =$   
=  $|A|^2 \int_{-7}^{10} (4900 + 9x^2 + x^4 + 420x - 140x^2 - 6x^3)dx =$   
=  $|A|^2 \left[ 4900x + \frac{1}{5}x^5 + 210x^2 - \frac{131}{3}x^3 - \frac{6}{4}x^4 \right]_{-7}^{10} =$   
=  $|A|^2 \cdot (31333.33 - 15995.23) = 47328.57 \cdot |A|^2$   
 $A = 1/\sqrt{47328.57} = 1/217.55 = 4.5966 \cdot 10^{-3}$ 

(c) Determine the expectation value  $\langle x \rangle$  using the normalized wave function

#### Solution:

The expectation value of a physical quantity O which depends on x is  $\int \psi^*(x) \hat{O}(x) \psi(x) dx$ 

$$< x > = A^2 \int_{-7}^{10} (4900x + x^5 + 420x^2 - 131x^3 - 6x^4) dx =$$
  
= 2.113 \cdot 10^{-5} \left[ 2450x^2 + \frac{1}{6}x^6 + 130x^3 \frac{131}{4}x^4 - \frac{6}{5}x^5 \right]\_{-7}^{10} =   
= 1.5 \end{tabular}

(d) Again, using the normalized wave function, calculate the expectation value of the kinetic energy of the particle

$$\langle E_{kin} \rangle = \int_{-7}^{10} \psi^*(x) \hat{E_{kin}}(x) \psi(x) dx = \int_{-7}^{10} \psi^*(x) \frac{\hat{p}^2}{2m_e}(x) \psi(x) dx =$$
$$= \int_{-7}^{10} \psi^*(x) \left( -\frac{\hbar^2}{2m_e} \frac{d^2}{dx^2} \right) (x) \psi(x) dx =$$
$$= A^2 \left( -\frac{\hbar^2}{2m_e} \int_{-7}^{10} (70 + 3xx^2) \cdot (-2) dx \right) =$$
$$= 2.113 \cdot 10^{-5} \left[ -140x - 3x^2 + 2/3x^3 \right]_{-7}^{10} = 9.7377 \cdot 10^{-34} J$$
$$= 6.07 \cdot 10^{-15} eV$$

76. Prove the following commutation relationships of operators  $\hat{A}$ ,  $\hat{B}$  and  $\hat{C}$ 

$$\begin{split} & [\hat{A} + \hat{B}; \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}] \\ & [\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}] \end{split}$$

#### Solution:

Substitute into the definition of the commutator:  $[\hat{A}, \hat{B}] = \hat{A} \cdot \hat{B} - \hat{B} \cdot \hat{A}$ :

$$\begin{split} [\hat{A} + \hat{B}, \hat{C}] &= (\hat{A} + \hat{B})\hat{C}\hat{C}(\hat{A} + \hat{B}) \\ &= \hat{A}\hat{C} + \hat{B}\hat{C}\hat{C}\hat{A}\hat{C}\hat{B} \\ &= (\hat{A}\hat{C}\hat{C}\hat{A}) + (\hat{B}\hat{C}\hat{C}\hat{B}) \\ &= [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}] \\ [\hat{A}, \hat{B}\hat{C}] &= \hat{A}(\hat{B}\hat{C})(\hat{B}\hat{C})\hat{A} = \hat{A}(\hat{B}\hat{C}) + \hat{B}(\hat{A}\hat{C}) - \hat{B}(\hat{A}\hat{C}) - (\hat{B}\hat{C})\hat{A} \\ &= (\hat{A}\hat{B})\hat{C}(\hat{B}\hat{A})\hat{C} + \hat{B}(\hat{A}\hat{C}) - \hat{B}(\hat{C}\hat{A}) \\ &= [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{C}, \hat{A}] \end{split}$$

77. Determine the work function of potassium in electron volts knowing that when illuminated by a light with a wavelength of  $\lambda = 350nm$  it emits electrons with a velocity of 710 km/s!Solution:

$$W = h\nu - \frac{1}{2}m_e v^2 = h\frac{c}{\lambda} - \frac{1}{2}m_e v^2 = 3.38 \cdot 10^{-19}J = 2.11\,eV$$

78. Determine the work function of potassium in electron volts knowing that when illuminated by a light with a wavelength of  $\lambda = 400nm$  it emits electrons with a velocity of 591 km/s!Solution:

$$W = h\nu - \frac{1}{2}m_e v^2 = h\frac{c}{\lambda} - \frac{1}{2}m_e v^2 = 3.38 \cdot 10^{-19}J = 2.11\,eV$$

79. Determine the work function of potassium in electron volts knowing that when illuminated by a light with a wavelength of  $\lambda = 580nm$  it emits electrons with a velocity of 100 km/s!

$$W = h\nu - \frac{1}{2}m_e v^2 = h\frac{c}{\lambda} - \frac{1}{2}m_e v^2 = 3.38 \cdot 10^{-19}J = 2.11\,eV$$

80. The ground state energy of the H atom is  $\mathcal{E}_1 = 13.6 eV$ . What is the wavelength of a photon emitted during the transition  $\mathcal{E}_4 > \mathcal{E}_2$ ? Solution:

$$\mathcal{E}_n = \mathcal{E}_1 \frac{1}{n^2} \qquad n = 1, 2, 3...$$
  

$$h\nu = \Delta \mathcal{E} = \mathcal{E}_2 - \mathcal{E}_4 = \mathcal{E}_1 (1/4 - 1/16) = 2.55 eV = 4.09 \, 10^{-19} J$$
  

$$\lambda = \frac{c}{\nu} = c * h/4.09 \, 10^{-19} = 4.86 \, 10^{-7} m = 486 nm$$

- 81. The W work function of a metal may be measured by applying an external U voltage on it to prohibit the emission of electrons. Determine W if, at
  - $\lambda_1 = 281 nm$  this voltage is  $U_1 = 0.66V$ , while for  $\lambda_2 = 245 nm U_2 = 1.26V$ Solution:

 $h\nu(=h\frac{c}{\lambda}) = W + \frac{1}{2}m_e v^2$  When electron emission is prohibited by an external U voltage, then v = 0, and the energy above W is  $\mathcal{E} = -e U$ . The two equations are

$$h\frac{c}{\lambda_1} = W - e U_1$$
$$h\frac{c}{\lambda_2} = W - e U_2$$

I.e.

$$W = \frac{1}{2} \left[ \left( h \frac{c}{\lambda_1} + e U_1 \right) + \left( h \frac{c}{\lambda_2} + e U_2 \right) \right] = 1.51 \, 10^{-18} J = 9.47 eV$$

82. The Zeeman components of a 500 nm spectral line are 0.0116 nm apart when the magnetic field is 1.00 T. Find the  $e/m_e$  ratio for the electron from these data.

#### Solution:

The magnitude of the energy shift from the given  $\Delta \lambda$  value is

$$\Delta E_B = h \,\Delta \nu = h \,\left(\frac{c}{\lambda_2} - \frac{c}{\lambda_1}\right) = \frac{c \,h}{\lambda_1 \,\lambda_2} (\lambda_1 - \lambda_2) = -\frac{c \,h \,\Delta \lambda}{\lambda_1 \,\lambda_2}$$

Where  $\lambda_{1,2} = \lambda \pm \Delta \lambda/2$ . But  $\Delta \lambda \ll \lambda$  therefore in the denominator  $\lambda_1 \lambda_2 \approx \lambda^2.$ 

$$|\Delta E_B| = \frac{h c \Delta \lambda}{\lambda^2} = \frac{6.63 \cdot 10^{-34} \cdot 3 \cdot 10^8 \cdot 0.0116 \cdot 10^{-9}}{(500 \cdot 10^{-9})^2} = 9.22 \, 10^{-24} J$$

For the Zeeman effect

$$\Delta E_B = \frac{e}{2m_e} \mathbf{L} \cdot \mathbf{B}$$
$$\frac{e}{m_e} = \frac{2 \left| \Delta E_B \right|}{L \cdot B}$$

Substituting  $\Delta E_B$  and taking L and B parallel, B = 1 T and  $L = 1 \hbar$ 

$$\frac{e}{m_e} = \frac{2 \cdot 9.22 \cdot 10^{-24}}{1.05 \cdot 10^{-34}} = 1.748 \, 10^{11}$$

The exact value is  $1.76 \, 10^{1}$ 

83. The absorption coefficient for a spherical body with a radius of  $R = 1 \ cm$  is 0.6 in the whole spectral range. How much energy will it emit at  $T = 1000 \ K$ ? Solution:

The total energy emitted per unit time by black-bodies is given by the Stefan-Boltzmann law:  $E_{tot} = A\sigma T^4$ , Kirchoff's law states that e/a = const, where a = 1 for black-bodies, therefore for a body with a = 0.6 the emitted energy is less by the same factor:

$$E_{tot} = a \, 4 \, \pi \, R^2 \, \sigma \, T^4 = 0.6 \cdot 4 \, \pi \, 10^{-4} \cdot 5.670373 \cdot 10^{-8} = 42.8 \, J/s = 2.7 \cdot 10^{20} \, eV/s$$

84. The un-normalized wave function of an electron is  $\psi(x) = 12x^2 - 8x$  Calculate the kinetic energy of this electron.

#### Solution:

The kinetic energy is determined from the formula:

$$\langle E_{kin} \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x) \frac{\hat{p}^2}{2m_e} \psi(x) dx}{\int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx}$$

where the denominator contains the normalization factor. For our wave function both integrals are infinite, so this function is not a physical wave function in the whole space. After integration the numerator contains 3rd an 2nd powers of x, while the one in the denominator (the normalization factor) contains 5th and 4th power of x too. If we now set the limits of the integration to  $\pm a$  and calculate the limit of this fraction as a tends to  $\infty$  we may see that the denominator goes faster to infinity than the numerator does, i.e. the value of kinetic energy tends to 0.

85. What is the acceleration voltage in an electron gun, if the average wavelength of the emitted electrons is 3.1 nm?

## Solution:

$$p = \frac{h}{\lambda}, \quad E = \frac{p^2}{2m_e} = e\Delta U \quad \Rightarrow \Delta U = \frac{p^2}{2m_e e} = \frac{h^2}{2m_e e \lambda^2}$$
$$\Delta U = \frac{(6.63 \, 10^{-34})^2}{2 \cdot 9.1 \, 10^{-31} \cdot 1.6 \, 10^{-19} \cdot (3.1 \, 10^{-9})^2} = 0.16V$$

86. What is the energy in eV and the momentum of a photon with a wavelength of

 $a)\lambda = 0,600\,\mu$  (visible light)

- $b\lambda = 0,100 nm$  (X-ray)
- c) $\lambda = 0,001 nm$  (gamma ray)
- What are the de Broglie-wavelengths and energies of electrons which have the same momentum as these photons?

For the photon:  $E = h\nu = h\frac{c}{\lambda}$ , and the momentum  $p = h\frac{\nu}{c} = \frac{h}{\lambda}$  therefore for photons

$a)\mathcal{E}$	$= 3.311 \cdot 10^{-19} \ J = \underline{2.066 \ eV},$	$p = 1.104 \cdot 10^{-27} \ kgm/s$
$b)\mathcal{E}$	$= 1.987 \cdot 10^{-15} \ J = \underline{1.240 \cdot 10^4 \ eV},$	$p = 6.626 \cdot 10^{-24} \ kgm/s$
$c)\mathcal{E}$	$= 1.987 \cdot 10^{-13} \ J = \underline{1.240 \cdot 10^6} \ eV,$	$p = 6.626 \cdot 10^{-22} \ kgm/s$

For an electron the de Broglie-wavelength is given by the same formula,  $\lambda = \frac{h}{p}$ , as for photons, therefore when photons and electrons have the same momentum, they have the same wavelength as well. However the energies of electrons and photons will be different:  $\mathcal{E}_e = \frac{p^2}{2 m_e} = \frac{h^2}{2 m_e \lambda^2}$ , and  $\mathcal{E}_{ph} = c \cdot p = \frac{c \cdot h}{\lambda}$  $a) E_e(0,600 \mu m) = 6.694 \cdot 10^{-25} J = 4.178 \cdot 10^{-6} eV$  $a) E_e(0,100nm) = 2.410 \cdot 10^{-17} J = 1.504 \cdot 10^2 eV$  $a) E_e(0,001nm) = 2.410 \cdot 10^{-13} J = 1.504 \cdot 10^6 eV$ 

87. You have a system of 7 half-spin particles (Fermions) with energy levels  $\mathcal{E}_n = n \cdot \mathcal{E}$  (n = 0,1,2,3,...). How many microstates are there for the seven particles if the macrostate has a total energy of 14  $\mathcal{E}$ 

Every level may be occupied by maximum 2 electrons of opposite spins, therefore only the following 14 configurations are possible: level | Configuration |

	1	2	3	4	5	6	7	8	9	10
8	•									
$\gamma$		•								
6			•	•	•					
5						••	•	•	•	•
4			•				•	•		
3		•		••	•		•		••	•
2	••	•	•		••	•		••	•	••
1	••	••	••	••	•	••	••	•	•	••
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1 1		7 C			1					

ievei	C	Jonjig	urano	n
	11	12	13	14
8				
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4	••	••	•	•
3	•		••	••
2	•	••	••	•
1	•	••		••
0	••	•	••	•

88. You have a system of six half-spin particles (Fermions) with energy levels  $\mathcal{E}_n = n \cdot \mathcal{E}$  (n = 0,1,2,3,...). How many ways can you distribute the six particles so that the total energy of the system is  $12 \cdot \mathcal{E}$ 

spins, 1	there f	fore or	ily the	e folla	wing	18 co	nfigur	ration	s are	possib
level				C	Config	uratio	n			
	1	2	3	4	5	6	$\gamma$	8	9	10
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Every level may be occupied by maximum 2 electrons of opposite spins, therefore only the following 18 configurations are possible: