Problems in Quantum Mechanics for Electrical and Chemical Engineers

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Contents

The problems presented here together with their solutions help the deeper understanding of the lectures. Similar problems may be given in the tests. We tried to give a very detailed solution for every one of them, however in the tests you need not give so much details. This material will be refreshed from time to time, so please check the date on the title page!

Chapter 1

Formulas used in the solutions

1.1 Quantum mechanics

Wien's displacement law

$$\lambda_{max} \cdot T = 2.8977721(26) \cdot 10^{-3}\, K\, m \tag{1.1.1}$$

If we use frequency as the parameter instead of wavelength the shape of the emission curve changes: the frequency ν_{max} at the location of the maximum does not correspond to simply c/λ_{max}. Here ν_{max} is the frequency that corresponds to the maximum of the emission *per unit frequency*. For this case Wien's law becomes:

$$\frac{\nu_{max}}{T} = 5.879 \cdot 10^{10}\, Hz\, K^{-1}$$

The Stefan-Boltzmann law states that the total energy emitted by a black-body per unit surface area is proportional to the 4th power of the absolute temperature:

$$\mathcal{P}_A = \sigma\, T^4 \tag{1.1.2}$$

where $\sigma = 5.670373(21) \cdot 10^{-8}\, W m^{-2}\, K^{-4}$ is the Stefan–Boltzmann constant.

Photo effect

$$h\,\nu = \frac{1}{2}\, m_e\, v^2 + W \tag{1.1.3}$$

where v is the velocity of the electron and W is the work function.

Compton effect The quantity

$$\frac{h}{m_e\, c} = 2.43 \cdot 10^{12}\, m \tag{1.1.4}$$

is known as the *Compton wavelength* of the electron. The amount $\Delta\lambda = \lambda' - \lambda$ the wavelength changes by is called the *Compton shift*. It is between zero (for $\theta = 0^o$) and twice the Compton wavelength of the electron (for $\theta = 180^0$). The total energy in a 3D potential box:

$$\mathcal{E}_{nml} = \frac{\hbar^2 \pi^2}{2\, m_e} \left(\frac{n^2}{L_x^2} + \frac{m^2}{L_y^2} + \frac{l^2}{L_z^2} \right) \tag{1.1.5}$$

The probability of the transition between states "1" and "2" is

$$W(1 \to 2) = |C_2(t)|^2 = \frac{1}{\hbar^2} \left| \int_0^t K_{21}(\tau)\, e^{i\,\omega_{21}\,\tau}\, d\tau \right|^2 \tag{1.1.6}$$

Electron in a 1 dimensional potential box.

$$\varphi_n(x) = A_n\, sin\, k_n\, x, \text{ where } k_n = \frac{n\,\pi}{L} \tag{1.1.7a}$$

$$p_n = \hbar\, k_n = \frac{\hbar\,\pi}{L} n \quad n = 1, 2, 3... \tag{1.1.7b}$$

$$\mathcal{E}_n = \frac{p_n^2}{2\, m_e} = \frac{\pi^2\, \hbar^2}{2\, m_e\, L^2} n^2 \quad n = 1, 2, 3... \tag{1.1.7c}$$

$$\text{or } \mathcal{E}_n = n^2\, \mathcal{E}_1, \quad \text{where} \quad \mathcal{E}_1 = \frac{\pi^2\, \hbar^2}{2\, m_e\, L^2} = \frac{h^2}{8\, m_e\, L^2} \tag{1.1.7d}$$

See section for Uncertainty relations

The operator of the angular momentum and its z component in spherical polar coordinates

$$\Delta \equiv \nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial \phi^2}. \tag{1.1.8}$$

The sum of the second and third parts contains the operator of the square of the length of the angular momentum:

$$\frac{1}{\hbar^2\, r^2} \hat{L}^2 \equiv \frac{1}{r^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right]. \tag{1.1.9}$$

Miller indices The distance d_{hkl} between adjacent lattice planes is

$$d_{hkl} = \frac{2\pi}{|\mathbf{g}_{hkl}|} = \frac{1}{\sqrt{\frac{h^2}{a_1^2} + \frac{k^2}{a_2^2} + \frac{l^2}{a_3^2}}} \tag{1.1.10}$$

Problem 1.

The effective temperature of the Sun is 5778 K. What is the value of λ_{max} for the Sun if the Sun is a black-body?

Solution:

$$\lambda_{max} = 2.90 \cdot 10^{-3}/5778 = 5.02 \cdot 10^{-7} m = 502\, nm$$

This corresponds to the wavelength of green light near the peak sensitivity of the human eye.

Problem 2.

According to theory, approximately a second after its formation the Universe was a near-ideal black-body in thermal equilibrium at a temperature above $10^{10}\, K$. The temperature decreased as the Universe expanded and the matter and radiation in it cooled. The cosmic microwave background radiation observed today is "the most perfect black-body ever measured in nature" as it has an anisotropy less than 1 part per 100,000. Now, some 15 billion years after the Big Bang the peak of the observed *cosmic background radiation* is at $1.07\, mm$. What is the temperature of the cosmos?

Solution:

$$T = 2.898\, 10^{-3}/\lambda_{max} = 2.7\, K$$

Problem 3.

A human body also radiates energy. Calculate the total energy needs for an adult to keep the body temperature constant. Because the mid- and far-infrared emissivity of skin and most clothing is near unity we may approximate the human body with a black-body. The average total skin area of an adult human being is about $2m^2$, and in an ambient temperature of $20\, ^oC$ the temperature of the bare skin is about 33^oC, while under the clothing it is about $28\, ^oC$.

Solution:

From Wien's law (equations (1.1.1)) the peak wavelength of the thermal radiation of a naked human body is is about $9.5\, \mu m$[1]. To calculate the energy needed to keep the temperature of the body constant can be obtained from the Stefan-Boltzmann law (1.1.2). The radiated power is the difference between the power absorbed from the environment (which is also considered a black-body) and the one emitted by the body:

$$\begin{aligned} \mathcal{P}_{body} &= \mathcal{P}_{absorption} - \mathcal{P}_{emission} = \sigma\, (T^4_{environ} - T^4_{body})\, A \\ &= -95.10\, W \end{aligned}$$

[1]Therefore thermal imaging devices are tuned to be most sensitive in the 7–14 micron range. But the human body emits at much larger wavelengths too. New imaging devices used in some border stations or airports use wavelengths in the 1 cm–1 mm (terrahertz) range. These are most suited to detect people smuggled in trucks.

The total energy requirement for a whole day therefore is

$$\mathcal{E} = -\mathcal{P}_{body} \cdot 24 \cdot 3600 = 8.216\, MJ = 1965\, kcal$$

Problem 4.

Let us model the Earth with a perfect spherical black-body without an atmosphere! Determine the *effective* or average surface temperature if the *solar constant* I_o, i.e. the amount of incoming solar electromagnetic radiation per unit area – that is incident on a plane perpendicular to the rays, at a distance of one astronomical unit (AU) (roughly the mean distance from the Sun to the Earth) – was $1361 W/m^2$!

Solution:

In the stationary state the "model 'Earth" absorbs the same amount of energy from the Sun as it emits. The Earth-Sun distance is so large that the rays of sunshine are almost parallel when they reach us. Half of the Earth surface is illuminated all the time by the Sun. The total energy absorbed by the Earth as a black-body, therefore equals to the solar constant multiplied by the cross section of the Earth perpendicular to the Earth-Sun direction[2] and by the duration Δt

$$\mathcal{E}_{tot,absorbed} = R^2 \pi \cdot I_o \cdot \Delta t$$

If the surface temperature is T then the total radiated energy from the Earth according to the Stefan-Boltzmann law is

$$\mathcal{E}_{tot,rad} = 4\,\pi\, R^2 \sigma\, T^4 \cdot \Delta t$$

In a stationary state these two energies must be equal:

$$\mathcal{E}_{tot,absorbed} = \mathcal{E}_{tot,rad}$$

from which

$$T = \sqrt[4]{\frac{I_o}{4\,\sigma}} = 278.3\, K = 5.3\, ^oC$$

The real effective temperature of the Earth is higher, because of the atmosphere.

Problem 5.

The *albedo* or *reflection coefficient* of the Earth is 0.3. This means that 30% of the solar radiation that hits the planet gets scattered back into space without absorption.
a) In the previous example what would be the temperature if the absorption coefficient of the Earth was $a = 0.7$ instead of 1?

[2]The sunlight I is perpendicular to the surface only at the point nearest to the Sun. Let us take a cross section of the sunlight with an area of A at this point. At a θ angle to the direction of the Sun this part of the sunlight hits a larger area $A' = A \cdot cos\Theta$, but only the component perpendicular to the surface is absorbed, which is $I' = I_o/cos\theta$. The total absorbed radiation flux therefore $P = A \cdot cos\Theta \cdot I/cos\theta = IA$ is the same at every point of the illuminated surface with a perpendicular surface area of A.

b) In climate calculations it is sometimes assumed that regardless to reflection the Earth still emits like a black-body (this contradicts Kirchoff's law). What would the temperature be with this assumption?

Solution:

a)

If $a = 0.7$ then the absorbed energy is $I_a = I_o\, a$, a times as much as above, and according to Kirchoff's law the emission must be lower by the same factor, i.e. $E'_{tot,rad} = a\, E_{tot,rad}$, therefore the temperature is the same as was in the previous example, namely $5.3\,^oC$.

b)

In this case

$$\mathcal{E}_{tot,absorbed} = 0.7\, R^2\pi \cdot I_o \cdot \Delta\, t\mathcal{E}_{tot,rad} = 4\,\pi\, R^2\sigma\, T^4 \cdot \Delta\, t$$

and the temperature

$$T = \sqrt[4]{\frac{0.7\, I_o}{4\,\sigma}} = 254.58\, K = -18.58\,^oC$$

Problem 6.

Determine the work function of potassium in electronvolts knowing that when illuminated by a light with a wavelength of $\lambda = 560nm$ it emits electrons with a velocity of $190\, km/s$!

Solution:

From equation (1.1.3)

$$W = h\,\nu - \frac{1}{2}\, m_e\, v^2 = h\,\frac{c}{\lambda} - \frac{1}{2}\, m_e\, v^2 = 3.38 \cdot 10^{-19} J = 2.21\, eV$$

Problem 7.

Determine the maximum speed of a photoelectron emitted from a chromium surface when illuminated with light of a wavelength of 180 nm, from knowing that at a wavelength of $150\, nm$ the maximum photoelectron energy is $3.92\, eV$? How large is the work function? ($m_e = 9.1.10^{-31} kg$)

Solution:

Let $\lambda_1 = 1.8 \cdot 10^{-7}\, m$ and $\lambda_2 = 1.5 \cdot 10^{-7}\, m$ and the maximum photoelectron kinetic energy at λ_2 $\mathcal{E}_{kin}(\lambda_2) = 3.92\, eV$. From equation (1.1.3) and using $\nu = c/\lambda$ the work function can be determined:

$$W = h\,\frac{c}{\lambda_2} - \mathcal{E}_{kin}(\lambda_2) = 6.96 \cdot 10^{-19} J = 4.35\, eV$$

Therefore the maximum velocity at λ_1:

$$v(\lambda_1) = \sqrt{\frac{2}{m_e}\left(h\,\frac{c}{\lambda_1} - W\right)} = 945,970\, m/s$$

Problem 8.

Calculate the scattering angle and the energy transferred to the electron compared to the energy of the incoming photon in a Compton effect, if at wavelength $\lambda = 0.01\,nm$ $\Delta\lambda = 0.0024\,nm$.

Solution:

From (1.1.4) the Compton angle is

$$cos\,\theta = 1 - \frac{m_e\,c\,\Delta\lambda}{h} = 0.01084 \quad \Rightarrow \quad \theta = 89.379^{\,o}$$

The energy transferred to the electron is

$$\mathcal{E}_e = h\,c\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right) \qquad = h\,c\left(\frac{1}{\lambda} - \frac{1}{\lambda + \Delta\lambda}\right) = 3.84 \cdot 10^{-15} J = 24\,keV$$

The energy of the incoming photon according to the theory of (special) relativity is $E_{ph} = h\,\nu = h\,c\,/\lambda = 1.99 \cdot 10^{-14}\,J$, i.e $\dfrac{\mathcal{E}_e}{E_{ph}} = 0.19$.

Problem 9.

What will be the momentum of the Compton electron if for $\lambda = 0.005\,nm$ the photon scattering angle is 90^o?

Solution:

If the Compton angle is 90^o then $cos\,\theta = 0$ and

$$\lambda' = \lambda + \frac{h}{m_e c} = 7.426 \cdot 10^{-12} m = 0.007426\,nm$$

Because of the momentum conservation the total momentum of the electron after the collision equals to the total momentum difference between the incoming and outgoing photons. The photon momentum and energy is connected by the formula $p_{photon} = \mathcal{E}_{photon}/c = h\,\nu/c$. Therefore

$$\Delta\,p_e = \frac{h\,\nu}{c} - \frac{h\,\nu'}{c} = \frac{h}{\lambda} - \frac{h}{\lambda'} = 4.33 \cdot 10^{-23}\,kg\,m\,s^{-1}$$

Problem 10.

The *ground state* and the *first excited state* (the stationary states with the smallest and the next lowest energy) in a hydrogen atom have an energy of $\mathcal{E}_0 = -13.6\,eV$ and $\mathcal{E}_1 = -3.4\,eV$ respectively relative to the energy of the free electron. What is the frequency of the photon that, when absorbed, can excite the electron from the ground state to the first excited state? What will be the frequency of a photon emitted during the $\mathcal{E}_1 \rightarrow \mathcal{E}_0$ transition?

Solution:

For a photon to be absorbed the photon energy must equal to the energy difference of the two states in question:

$$h\,\nu = \mathcal{E}_1 - \mathcal{E}_0 = 10.2\,eV = 1.634 \cdot 10^{-18}\,J \quad \Rightarrow$$
$$\nu = 2.47 \cdot 10^{+15} Hz$$

The frequency of the photon emitted in the reverse transition must be the same as that of the absorbed photon.

Problem 11.

Determine the wavelength of an electron that is accelerated through a voltage U. What magnitude of voltage must be used to have a wavelength comparable to atomic distances around 0.05-10 nm in solids?

Solution:

The kinetic energy of an electron of momentum p is $\mathcal{E}_{kin} = \dfrac{p^2}{2\,m_e}$. If the electron is accelerated through a U voltage $\mathcal{E}_{kin} = e\,U$ (e is the elementary charge). The corresponding momentum is

$$p = \sqrt{2\,m_e\,e\,U}$$

The de Broglie wavelength

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2\,m_e\,e\,U}}$$

Therefore the accelerating voltage for λ is

$$U = \frac{h^2}{2\,m_e\,e\,\lambda^2}$$

For wavelengths $0.05\,nm$ and $10\,nm$ the required voltages are:

$$U(0.05\,nm) = 601.7\,V \text{ and } U(10\,nm) = 0.015\,V$$

Problem 12.

What is the momentum and velocity uncertainty for a) a dust particle of diameter $500\,\mu$ and mass of about $5.4 \cdot 10^{-4}\,mg$, b) an ammunition bullet with a size of about 7×40 mm and mass 5.2 g, c) a 75 kg 1.8 m $\times$ 40 cm $\times$ 20 cm object if all of them are seemingly at rest.

Solution:

If these objects are at rest then the position uncertainty equals to their size. Therefore

$$\Delta\,p = \frac{\hbar}{2 \cdot size}, \quad \Delta\,v = \frac{\hbar}{2 \cdot m \cdot size}$$

a) $\Delta x = 5 \cdot 10^{-4}\, m,$ $\Delta p = 1.06 \cdot 10^{-31} kg\, \frac{m}{s}$
$\Delta v = 1.95 \cdot 10^{-25} \frac{m}{s}$

b) $\Delta x_1 = 7 \cdot 10^{-3}\, m,$ $\Delta p_1 = 7.54 \cdot 10^{-33} kg\, \frac{m}{s}$
$\Delta v_1 = 1.45 \cdot 10^{-30} \frac{m}{s}$

$\Delta x_2 = 40 \cdot 10^{-4}\, m,$ $\Delta p_2 = 1.31 \cdot 10^{-33} kg\, \frac{m}{s}$
$\Delta v_2 = 2.54 \cdot 10^{-31} \frac{m}{s}$

c) $\Delta x = 1.8\, m,$ $\Delta p = 2.93 \cdot 10^{-35} kg\, \frac{m}{s}$
$\Delta v = 3.91 \cdot 10^{-37} \frac{m}{s}$

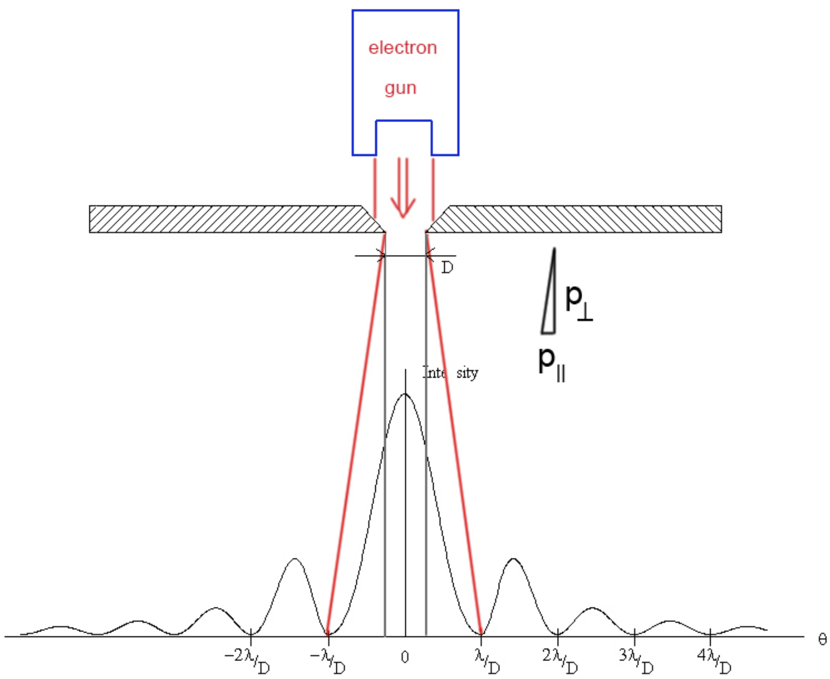
$\Delta x_1 = 0.4\, m,$ $\Delta p_1 = 1.32 \cdot 10^{-34} kg\, \frac{m}{s}$
$\Delta v_1 = 1.75 \cdot 10^{-36} \frac{m}{s}$

$\Delta x_2 = 0.2\, m,$ $\Delta p_2 = 2.63 \cdot 10^{-34} kg\, \frac{m}{s}$
$\Delta v_2 = 3.52 \cdot 10^{-36} \frac{m}{s}$

As you can see the momentum and velocity uncertainties are to small to be measured. That is the reason why we may say these objects are at rest.

Problem 13.

An electron gun emits electrons with a velocity of $v_\perp = 1m/s$ perpendicular[3] to a thin metal plate which has a hole of diameter $D = 1\, mm$ (see figure). Determine the size minimum of the spot on a screen $l = 1$ cm behind the hole.



[3]This is only an approximation, because an exactly 0 momentum component would require an infinitely large position uncertainty in the parallel direction.

Solution:

The electrons arrive at the slit with a velocity and momentum perpendicular to the slit, so the component of their momentum parallel with the slit is $p_{\|} = 0$. The slit restricts the diameter of the electron beam to D, therefore right after the slit the position uncertainty of the electrons will be D. This means an uncertainty in the $p_{\|}$ momentum of

$$\Delta p_{\|} \geq \frac{\hbar}{2\,D} = 5.27 \cdot 10^{-32}\, kg\, m/s$$

and a velocity uncertainty of

$$\Delta\, v_{\|} \geq \Delta\, p_{\|}/m_e = 0.058\, m/s$$

The electrons need $\Delta\, t = l/v_{\perp}$ time to reach the screen, during which the maximum parallel distance they may travel is $\Delta\, d = v_{\|}\,\Delta\, t$. The minimal size of the spot on the screen is therefore:

$$d_{min} = 2\, v_{\|}\, l/v_{\perp} + D = 2.2mm$$

Problem 14.

What is the wavelength of the photon emitted by an electron transition from the 4^{th} to the 3^{rd} level in a 1 dimensional potential box of size $100\, nm$?

Solution:

From (1.1.7c) the energy difference between level 4 and 3 is

$$\underline{\underline{\Delta\,\mathcal{E}}} = \mathcal{E}_4 - \mathcal{E}_3 = \frac{\hbar^2\,\pi^2}{2\,m_e\,L^2}\,(4^2 - 3^2) = \frac{1.1121 \cdot 10^{-68}\, J^2 s^2 \times \pi^2}{2 \times 9.1 \cdot 10^{-31}\, kg \times (10^{-7}\, m)^2} \times 7$$
$$= \underline{\underline{4.217 \cdot 10^{-23}\, J}}\ (= 2.632 \cdot 10^{-4}\, eV)$$

and the photon frequency is

$$\nu = \frac{\Delta\,\mathcal{E}}{h} = \frac{4.217 \cdot 10^{-23}}{6.62\, 10^{-34}} = 6.365 \cdot 10^{10}\, Hz$$

The wavelength of the emitted photon then

$$\lambda = \frac{c}{\nu} = 4.710 \cdot 10^{-3}\, m = 4.710\, mm.$$

Problem 15.

Determine the first 3 energy levels in a *cubic* potential box whose size is $a = 10\,\mu m$.

Solution:

Substituting $L = L_x = L_y = L_z = 10\,\mu m$ into (1.1.5) we get

$$\mathcal{E}_{n_x,n_y,n_z} = \frac{\hbar^2\,\pi^2}{2\,m_e\,L^2}(n_x^2 + n_y^2 + n_z^2) \qquad n_x, n_y, n_z = 1, 2, 3, \ldots$$
$$\mathcal{E}_{n_x,n_y,n_z} = 6,02 \cdot 10^{-26}(n_x^2 + n_y^2 + n_z^2) \qquad n_x, n_y, n_z = 1, 2, 3, \ldots$$

Because the result depends on the sum of the squares of the three numbers, the same energy values will result for all permutations of the same three numbers:

n	m	l	$\mathcal{E}$ ($\mathcal{E}_1 := 1.81 \cdot 10^{-27} J$)	$\mathcal{E}$ $\times 10^{-27}\, J$
1	1	1	$3 \cdot \mathcal{E}_1$	1.807
1	1	2		
1	2	1	$6 \cdot \mathcal{E}_1$	3.61
2	1	1		
2	2	1		
2	1	2	$9 \cdot \mathcal{E}_1$	5.42
1	2	2		
2	2	2	12	7.23
1	1	3		
1	3	1	$11 \cdot \mathcal{E}_1$	6.63
3	1	1		

Problem 16.

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 4 lowest lying states.

Solution:

The possible energy levels are

$$\mathcal{E}_{n_x,n_y,n_z} = \frac{\hbar^2\, \pi^2}{2\, m_e\, L^2}(n_x^2 + n_y^2 + n_z^2) \qquad n_x, n_y, n_z = 1, 2, 3, ...$$

n	m	l	$\mathcal{E}(\times 10^{-27} J)$
1	1	1	1.36
1	1	2	1.47
1	2	1	1.61
2	1	1	2.36
2	2	1	2.61
2	1	2	2.47
1	2	2	1.72
2	2	2	2.72
1	1	3	1.58
1	3	1	1.86
3	1	1	3.36
1	2	3	1.83
2	1	3	2.58
2	3	1	2.86
3	2	1	3.61
3	1	2	3.47
2	2	3	2.83
2	3	2	2.97
3	2	2	3.72
1	3	3	2.08
3	1	3	3.58
3	3	1	3.86
2	3	3	3.08
3	2	3	3.83
3	3	2	3.97
3	3	3	4.08

$$\begin{aligned}\mathcal{E}_{n_x,n_y,n_z} &= \frac{h^2}{8\,m_e}\left(\frac{n^2}{L_x^2} + \frac{m^2}{L_y^2} + \frac{l^2}{L_z^2}\right)\\ &= 6.02\,10^{-28}\left(\frac{n_x^2}{1} + \frac{n_y^2}{4} + \frac{n_z^2}{9}\right)[J]\end{aligned}$$

The 4 lowest lying energy states can be determined by trying out different combinations of the numbers 1,2 and 3 and selecting the ones with the 4 smallest energy values.

From the table we can see that there are no degenerate states for this physical object and the indices for the 4 lowest lying levels sorted by energy in ascending order are: (1,1,1), (1,1,2), (1,1,3) and (1,2,1).

Problem 17.

In an aluminum–aluminum oxide–aluminum layer structure a current of electrons with energies of $1\,eV$ flows through the $0.5\,nm$ thick insulating oxide boundary, which we represent as a square potential barrier with $V_0 = 10\,eV$. What is the probability of an electron to pass through the barrier?

Solution:

Notations: $a = 5 \cdot 10^{-10} m$, $\mathcal{E} = 1\,eV$

$$\begin{aligned} q &= \frac{\sqrt{2\,m_e\,(V_0 - E)}}{\hbar} = \frac{\sqrt{2 \cdot 9.1 \cdot 10^{-31} \cdot (10-1) \cdot 1.6 \cdot 10^{-19} \cdot}}{1.055 \cdot 10^{-34}} \\ &= 1.537 \cdot 10^{10} m^{-1} \\ q\,a &= 7.685 \\ T \approx e^{-2\,q\,a} &= 2.114 \cdot 10^{-7} \end{aligned}$$

Problem 18.

Determine the transition probability in a 1 dimensional two level system under the influence of en external electromagnetic field. In this case the perturbation is of the form:

$$K(x,t) = \mathcal{K}(x) \cdot cos\omega\,t,$$

where ω is very close to ω_{21} in the sense[4] that

$$\omega_{21} + \omega \gg |\omega_{21} - \omega|$$

and both are in the optical range ($\approx 10^{14}\,Hz$). What is the range of validity of the perturbation theory in this case? What interesting behavior will you find and why?

Solution:

From (1.1.6)

$$W(1 \to 2) = \frac{1}{\hbar^2} \left| \int_0^t \mathcal{K}_{21} cos(\omega\,\tau)\, e^{i\,\omega_{21}\,\tau}\, d\tau \right|^2$$

where $\omega_{21} = (\mathcal{E}_2 - \mathcal{E}_1)/\hbar$ and $\mathcal{K}_{21} \equiv \int_{-\infty}^{\infty} \varphi_2^*(x)\,\mathcal{K}\,\varphi_1^*(x)\,dx$. Because $cos\,\omega\,\tau = \left(e^{i\,\omega\,\tau} + e^{-i\,\omega\,\tau}\right)/2$

$$\begin{aligned} W(1 \to 2) &= \frac{|\mathcal{K}_{21}|^2}{2\,\hbar^2} \left| \int_0^t \left(e^{i\,(\omega_{21}+\omega)\,\tau} + e^{i\,(\omega_{21}-\omega)\,\tau}\right) d\tau \right|^2 = \\ &= \frac{|\mathcal{K}_{21}|^2}{4\,\hbar^2} \left| \frac{e^{i\,(\omega_{21}+\omega)\,t} - 1}{\omega_{21} + \omega} + \frac{e^{i\,(\omega_{21}-\omega)\,t} - 1}{\omega_{21} - \omega} \right|^2 \end{aligned}$$

[4]This is not a serious limitation, because perturbations with other frequencies have a negligible probability to cause a transition anyway.

Now because of our assumptions for ω and ω_{21} the first term in the absolute sign may be neglected as it is much smaller than the second one (the numerator is of the same magnitude, while the denominator of the first term is much greater than in the second one)

$$\begin{aligned} W(1\to 2) &\approx \frac{|\mathcal{K}_{21}|^2}{4\,\hbar^2}\left|\frac{e^{i\,(\omega_{21}-\omega)\,t}-1}{\omega_{21}-\omega}\right|^2 = \\ &= \frac{|\mathcal{K}_{21}|^2}{4\,\hbar^2}\left|\frac{e^{i\,(\omega_{21}-\omega)\,t/2}}{\omega_{21}-\omega}\right|^2\cdot\left|e^{i\,(\omega_{21}-\omega)\,t/2}-e^{i\,(\omega_{21}-\omega)\,t/2}\right|^2 = \\ &= \frac{|\mathcal{K}_{21}|^2}{\hbar^2}\frac{sin^2[(\omega_{21}-\omega)\,t/2]}{(\omega_{21}-\omega)^2} \end{aligned}$$

If $|\omega_{21}-\omega| \ll 1$ then the sine can be approximated with its argument and the maximum of $W \propto |\mathcal{K}\,t/\hbar^2$ which increases with t. However the assumption that this is a small perturbation will become invalid long before this maximum reaches 1. Therefore our result is only valid for relatively small t.

The most interesting feature of this solution is that the transition probability *oscillates* sinusoidally as a function of time between 0 and a maximum value which is still much less than 1, otherwise this would not be a *small* perturbation. When $t = \dfrac{2\,\pi\,n}{|\omega_{21}-\omega|}$, where $n = 1, 2, 3, ...$ the particle will be back in the lower state.

The reason for this behavior is that although ψ_1 and ψ_2 are eigenfunctions (i.e. stationary states) of the non-perturbed system they are not eigenfunctions of the perturbed system.

Problem 19.

We define some operators with the formulas:

$\hat{O}_1\mathbf{v}(t) := v_x$ - x coordinate of the velocity vector

$\hat{O}_2 f(t) := A\,sin f(t)$ - sine of a time dependent function, e.g $f(t) = \omega\,t$

$\hat{O}_3 f(k) := \dfrac{1}{\sqrt{2\,\pi}}\displaystyle\int_{-\infty}^{\infty} f(k)\,e^{-i\,k\,x}dk$ -Fourier transform of $f(k)$

$\hat{O}_4 f(x) := \sqrt[3]{f(x)}$

Which of these are the linear operators?

Solution:

$\hat{O}_1$ and $\hat{O}_3$

Problem 20.

Determine the adjoint of the operators $\hat{p}, \hat{x}$ and $\hat{H}$!

Solution:

a) adjoint of the momentum operator

According to the definition of the adjoint operator:

$$\langle \hat{p}^\dagger \varphi_2 \,|\, \varphi_1 \rangle = \langle \varphi_2 \,|\, \hat{p}\, \varphi_1 \rangle \quad \text{i.e.}$$

$$\langle \hat{p}^\dagger \varphi_2 \,|\, \varphi_1 \rangle = \langle \varphi_2 | \frac{\hbar}{i} \frac{d\,\varphi_1}{d\,x} \rangle$$

$$\int_{-\infty}^{\infty} (\hat{p}^\dagger\, \varphi_2)^* \cdot \varphi_1 \, dx = \int_{-\infty}^{\infty} \varphi_2^* \cdot (\hat{p}\, \varphi_1)\, dx \text{ or}$$

$$\int_{-\infty}^{\infty} (\hat{p}^\dagger\, \varphi_2)^* \cdot \varphi_1 \, dx = \int_{-\infty}^{\infty} \varphi_2^* \cdot \frac{\hbar}{i} \frac{d\,\varphi_1}{d\,x}\, dx$$

The right hand side can be calculated with integration by parts:

$$\int_{-\infty}^{\infty} \varphi_2^* \cdot \frac{\hbar}{i} \frac{d\,\varphi_1}{d\,x}\, dx = \frac{\hbar}{i}\, \left[\varphi_2^* \cdot \varphi_1\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\hbar}{i} \frac{d\,\varphi_2^*}{d\,x} \cdot \varphi_1 \, dx$$

Because both φ_1 and φ_2 are physical wave functions they must be square integrable, therefore they must vanish when $x \to \infty$, so the first term is zero

$$\int_{-\infty}^{\infty} (\hat{p}^\dagger\, \varphi_2)^* \cdot \varphi_1 \, dx = -\int_{-\infty}^{\infty} \frac{\hbar}{i} \frac{d\,\varphi_2^*}{d\,x} \cdot \varphi_1 \, dx$$

Because $(p^\dagger \varphi)^* = (p^\dagger)^*\, \varphi^* = \left(-\frac{\hbar}{i}\, \frac{d}{dx}\right)^*\, \varphi^*$:

$$\hat{p}^\dagger \equiv \frac{\hbar}{i} \frac{d}{d\,x} = \hat{p}$$

The momentum operator is *self-adjoint*.

b) adjoint of the position operator

This is much simpler, because $\hat{x} \equiv x\cdot$ is a multiplication with a real number (or vector in 3 dimensions) and it commutes with the wave functions, therefore

$$\hat{x}^\dagger = \hat{x}$$

The position operator is self adjoint too.

c) the Hamiltonian

The Hamiltonian is a linear combination of the operators $\hat{p^2} = -\hbar^2 \frac{d^2}{dx^2}$ and $V(x) = V(x)\cdot$. It is easy to prove that the product and sum of self-adjoint operators is also a self-adjoint operator.

Because the operator of the potential is a multiplication with a function it is self-adjoint, and $\hat{p^2} = \hat{p}\,\hat{p}$ is a product of the self-adjoint $\hat{p}$ with itself, the Hamiltonian is also self-adjoint:

$$\hat{H}^\dagger = \hat{H}$$

Problem 21.
Determine the eigenfunctions and eigenvalues for the 3D momentum operator!
Solution:

$$\hat{\mathbf{p}}\,\varphi_{\mathbf{p}}(\mathbf{r}) = \mathbf{p}\,\varphi_{\mathbf{p}}(\mathbf{r})$$

$$\frac{\hbar}{i}\nabla\,\varphi_{\mathbf{p}}(x,y,z) = \mathbf{p}\,\varphi_{\mathbf{p}}(x,y,z)$$

$$\frac{\hbar}{i}\left(\frac{\partial, \varphi_{\mathbf{p}}(x,y,z)}{\partial\,x}, \frac{\partial, \varphi_{\mathbf{p}}(x,y,z)}{\partial\,y}, \frac{\partial\varphi_{\mathbf{p}}(x,y,z)}{\partial\,z},\right) = (p_x, p_y, p_z)\,\varphi_{\mathbf{p}}(x,y,z)$$

$$\varphi_{\mathbf{p}}(x,y,z) = e^{i(p_x\,x + p_y\,y + p_z\,z)/\hbar} = e^{i\,\mathbf{p}\,\mathbf{r}/\hbar}$$

i.e. the eigenfunctions of the $\hat{\mathbf{p}}$ operator are plane waves with eigenvalues corresponding to a continuous set of exact momenta. Because these functions are not quadratically integrable, they can not describe any physical state of the system separately. As we saw (Section 1.1) we must use wave packets created as a linear combination of an infinite number of these eigenstates ($\Rightarrow$ Fourier transformation.) to describe a physical state.

Problem 22.
Determine whether there exists an uncertainty formula for the different components of the angular momentum operator.
Solution:
An uncertainty formula between two physical quantities exists only if their commutator is not 0. Let us calculate $[\hat{L}_x, \hat{L}_y]$! This requires simple algebra and not higher mathematics. We do not even have to know the concrete form of the operators, because their commutators show exactly how their products can be rearranged.

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= \hat{L}_x\,\hat{L}_y - \hat{L}_y\,\hat{L}_x = \\
&= (\hat{y}\,\hat{p}_z - \hat{z}\,\hat{p}_y)\,(\hat{z}\,\hat{p}_x - \hat{x}\,\hat{p}_z) - (\hat{z}\,\hat{p}_x - \hat{x}\,\hat{p}_z)\,(\hat{y}\,\hat{p}_z - \hat{z}\,\hat{p}_y) = \\
&= \underset{------}{\hat{y}\,\hat{p}_z\,\hat{z}\,\hat{p}_x} - \underset{======}{\hat{y}\,\hat{p}_z\,\hat{x}\,\hat{p}_z} - \underset{\sim\sim\sim\sim}{\hat{z}\,\hat{p}_y\,\hat{z}\,\hat{p}_x} + \underset{++++++}{\hat{z}\,\hat{p}_y\,\hat{x}\,\hat{p}_z} - \\
&\quad - \underset{------}{\hat{z}\,\hat{p}_x\,\hat{y}\,\hat{p}_z} + \underset{\sim\sim\sim\sim}{\hat{z}\,\hat{p}_x\,\hat{z}\,\hat{p}_y} + \underset{======}{\hat{x}\,\hat{p}_z\,\hat{y}\,\hat{p}_z} - \underset{++++++}{\hat{x}\,\hat{p}_z\,\hat{z}\,\hat{p}_y}
\end{aligned}$$

where the different "underlines" mark terms from which common factors may be pulled out, because some or all of the operators in them commute and therefore their order is not important. E.g. $\hat{y}\,\hat{p}_z\,\hat{z}\,\hat{p}_x \equiv \hat{y}\,\hat{p}_x\,\hat{p}_z\,\hat{z}$, because $\hat{p}_x$ commutes with all other operators in this term. But the order of $\hat{z}$ and $\hat{p}_z$ is important as they do not commute.

$$
\begin{aligned}
[\hat{L}_x, \hat{L}_y] = {} & (\underset{-----------}{\hat{y}\,\hat{p}_x\,\hat{p}_z\,\hat{z} - \hat{y}\,\hat{p}_x\,z\,\hat{p}_z}) + (\underset{===========}{\hat{x}\,\hat{y}\,\hat{p}_z\,\hat{p}_z - \hat{x}\,\hat{y}\,\hat{p}_z\,\hat{p}_z}) + \\
& (\underset{\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim\sim}{\hat{z}\,\hat{z}\,\hat{p}_y\,\hat{p}_x) - \hat{z}\,\hat{z}\,\hat{p}_y\,\hat{p}_x}) + (\underset{++++++++++++}{\hat{x}\,\hat{p}_y\,\hat{z}\,\hat{p}_z - \hat{x}\,\hat{p}_y\,\hat{p}_z\,\hat{z}}) = \\
& = \hat{y}\,\hat{p}_x\,(\hat{p}_z\,\hat{z} - \hat{z}\,\hat{p}_z) + 0 + 0 + \hat{x}\,\hat{p}_y\,(\hat{z}\,\hat{p}_z - \hat{p}_z\,\hat{z}) = \\
& = (\hat{x}\,\hat{p}_y - \hat{y}\,\hat{p}_x)\,(\hat{z}\,\hat{p}_z - \hat{p}_z\,\hat{z})
\end{aligned}
$$

Because $(\hat{x}\,\hat{p}_y - \hat{y}\,\hat{p}_x) = \hat{L}_z$ and $(\hat{z}\,\hat{p}_z - \hat{p}_z\,\hat{z}) = [\hat{z}, \hat{p}_z] = i\hbar$

$$[\hat{L}_x, \hat{L}_y] = i\,\hbar\,\hat{L}_z \tag{1.1.11a}$$

Similar formulas could be derived for the commutator of any two components:

$$[\hat{L}_y, \hat{L}_z] = i\,\hbar\,\hat{L}_x \tag{1.1.11b}$$

$$[\hat{L}_z, \hat{L}_x] = i\,\hbar\,\hat{L}_y \tag{1.1.11c}$$

Because their commutator is not zero, the different components of the angular momentum may not be determined with arbitrary accuracy simultaneously. There is an uncertainty relation between them.

Problem 23.

Determine the eigenvalues and eigenfunctions of $\hat{L}_z$!

Solution:

This problem is best dealt with in a spherical polar coordinate system. The form of the $\hat{L}_z$ operator in spherical polar coordinates is (see Appendix 1.1)

$$\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\,\phi} \tag{1.1.12}$$

In such a system the form of the eigenvalue equation of $\hat{L}_z$ becomes

$$\frac{\hbar}{i}\,\frac{d\,\varphi}{d\,\phi} = \lambda\,\varphi \quad \Rightarrow \quad \varphi(\phi) = C\,e^{\frac{i}{\hbar}\,\lambda\,\phi},$$

where the C normalization constant is determined from the equation

$$\int_0^{2\pi} |\varphi(\phi)|^2 \, d\phi = 1$$

$$\int_0^{2\pi} |C|^2 \, d\phi = 2\pi \, |C|^2 = 1$$

$$C = \frac{1}{\sqrt{2\pi}}$$

and because φ is periodic in ϕ:

$$\varphi(\phi + 2\pi) = \varphi(\phi)$$

$$e^{\frac{i}{\hbar}\lambda 2\pi} = 1$$

$$\frac{\lambda}{\hbar} = m, \qquad \text{where } m \text{ is an integer, i.e.}$$

$$\lambda = m\,\hbar, \qquad m = 0, \pm 1, \pm 2, \pm 3, ...$$

Problem 24.

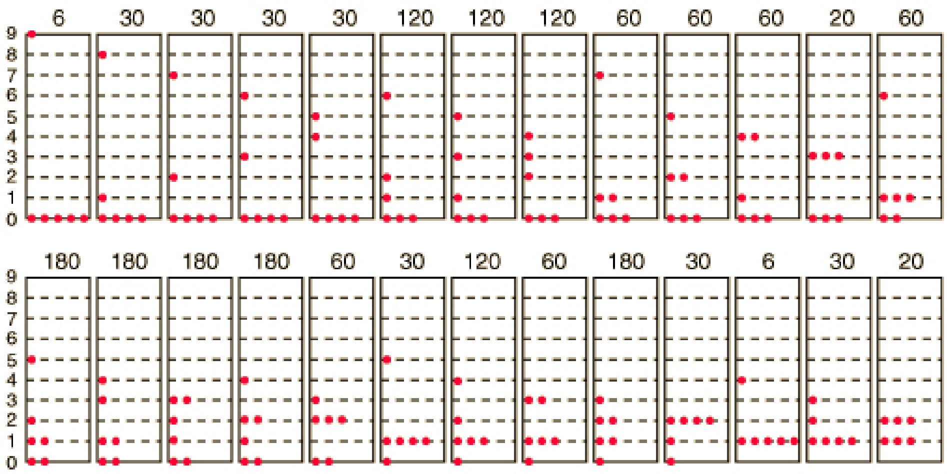
In a system with equidistant energy levels how many ways can you distribute 9 units of energy among 6 *identical. distinguishable* particles? The energy of the ground state (i=0) is 0, and the levels are one unit of energy distant from each other.

Solution:

In this case the observable different *macrostates* give the number of particles on every level, while the *microstates* are the possible ways to achieve a given macrostate.

Because we must distribute 9 units of energy among the particles and the energy of the ground state is 0, we have to use 10 energy levels.

The number of macrostates are so few (in this case 26) they can easily be counted. The figure shows all macrostates with a total energy of 9 units, together with the number of the microstates that correspond to the same macrostate. The first macrostate in the first row have $\frac{6!}{5!} = 6$ microstates, the second one $\frac{6!}{4!\,1!\,1!} = 30$, while the first one in the second row have $\frac{6!}{2!\,2!\,1!\,1!} = 180$, etc. The total number of microstates is 2002.



Problem 25.

Graph the distribution for Problem 24 and compare it with the Maxwell-Boltzmann distribution function!

Solution:

We have to graph the n_i vs $\mathcal{E}$ discrete function of Problem 24. The average occupation numbers for the levels are

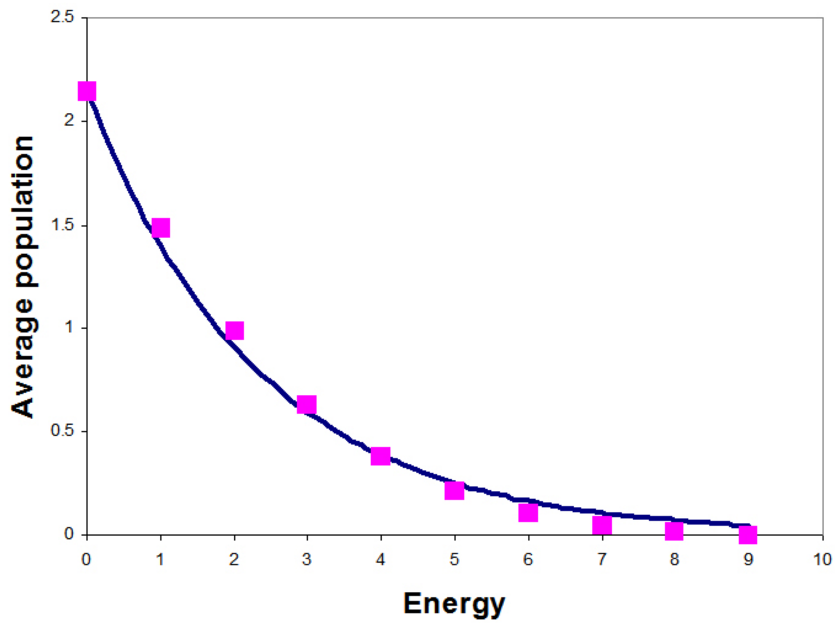
$$\langle n_i \rangle = \frac{\sum_{\ell=1}^{26} w_i(\ell)\, n_i(\ell)}{\sum_{n}^{26} w_i}$$

where the summation goes from 1 to the number of all possible macrostates, and $w_i(\ell)$ is the number of the microstates that results in the ℓ-th macrostate. The denominator is the total number of microstates, which is 2002 as we have shown previously in Problem 24. So for instance for $i = 0$

$$n_0 = \frac{6 \cdot 5 + 4 \cdot 30 \cdot 4 + (3 \cdot 120 + 3 \cdot 60 + 20) \cdot 3 + (2 \cdot 60 + 4 \cdot 180) \cdot 2}{2002} + \frac{(30 + 120 + 60 + 180 + 30) \cdot 1 + (30 + 6 + 30 + 20) \cdot 0}{2002} = 2.143$$

The average occupation numbers or *average population* of the levels:

Energy level	0	1	2	3	4	5
$\langle n_i \rangle$	2.143	1.484	0.989	0.629	0.378	0.210
Energy level	6	7	8	9		
$\langle n_i \rangle$	0.104	0.045	0.015	0.003		



while in the figure you can see the results compared to that of the continuous Maxwell-Boltzmann distribution function.

As you can see the distribution for even as few as 6 particles closely approximates the Maxwell-Boltzmann distribution function.

Problem 26.

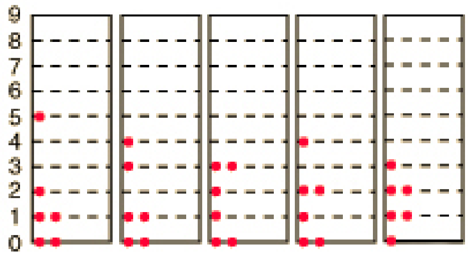
In a system with equidistant energy levels how many ways can you distribute 9 units of energy among 6 fermions? The energy of the ground state (i=0) is 0, and the levels are one unit of energy distant from each other. Calculate and graph the distribution and compare it both with the Fermi-Dirac distribution function and with the Maxwell-Boltzmann distribution and distribution function!

Solution:

Like in Problem 24 the observable different *macrostates* give the number of particles on every level, while the *microstates* are the possible ways to achieve a given macrostate.

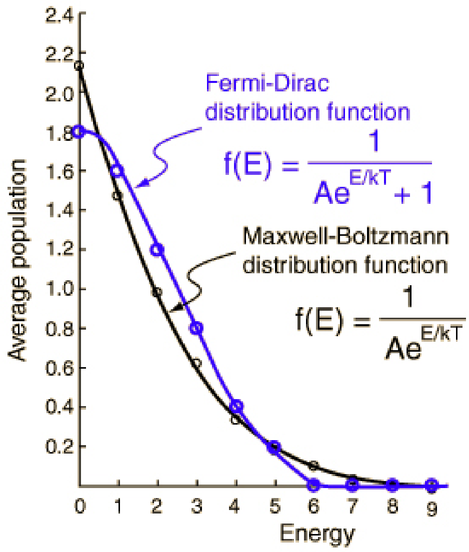
Because we must distribute 9 units of energy among the particles and the energy of the ground state is 0, we have to use 10 energy levels.

Because fermions are indistinguishable, obey the Pauli exclusion principle and have a half-integer spin there may be maximum 2 particles of opposite spins in each state:



Whereas there were 26 possible configurations for distinguishable particles (see Problem 24), these are reduced to the 5 states which have no more than two particles in each state. The average occupation numbers or *average population* of the levels are easier to calculate in this case. In the table we compared these numbers with the ones we got for the Maxwell-Boltzmann distribution.

Energy level	$\langle n_i^{FD} \rangle$	$\langle n_i^{MB} \rangle$
0	1.8	2.143
1	1.6	1.484
2	1.2	0.989
3	0.8	0.629
4	0.4	0.378
5	0.2	0.210
6	0.0	0.105
7	0.0	0.045
8	0.0	0.015
9	0.0	0.003



In the figure we used A for the factor e^{α} we got from our conditional maximum calculation. For the Maxwell-Boltzmann distribution $A \equiv Z$, for the Fermi-Dirac distribution $A \equiv e^{-\mathcal{E}_F/k_B T}$.

Low energy states are less probable with Fermi-Dirac statistics than with the Maxwell-Boltzmann statistics while mid-range energies are more probable. This difference is dramatic for large number of particles and for low temperatures as you will see later.

Problem 27.

In a system with equidistant energy levels how many ways can you distribute 9 units of energy among 6 bosons? The energy of the ground state (i=0) is 0, and the levels are one unit of energy distant from each other. Calculate the distribution and compare it with both the Maxwell-Boltzmann and Fermi-Dirac distribution!

Solution:

Like in Problem 24 the observable different *macrostates* give the number of particles on every level, while the *microstates* are the possible ways to achieve a given macrostate.

We must distribute 9 units of energy among the particles and the energy of the ground state is 0, we have to use 10 energy levels.

Because any number of bosons can be in the same state (as is the case of the classical distinguishable particles of the Maxwell-Boltzmann distribution), the total number of macrostates is again 26. (See the corresponding figure at page 18.) But now the number of microstates is also 26, because bosons are indistinguishable particles, so the exchange of two bosons does not lead to a different microstate. In the next table we compared the average occupation numbers or *average population* of the levels with the ones we got for the other two distributions, but only graph the Bose-Einstein and Maxwell-Boltzmann curves.

Energy level	$\langle n_i^{BE} \rangle$	$\langle n_i^{FD} \rangle$	$\langle n_i^{MB} \rangle$
0	2.269	1.8	2.143
1	1.538	1.6	1.484
2	0.885	1.2	0.989
3	0.538	0.8	0.629
4	0.269	0.4	0.378
5	0.192	0.2	0.210
6	0.115	0.0	0.105
7	0.077	0.0	0.045
8	0.038	0.0	0.015
9	0.038	0.0	0.003