RAČUNALNIŠKE TEHNOLOGIJE – EXERCISES

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1 OSCILLATIONS AND WAVES

♥ EX. 1.1

Instead of using equation $x = A \sin(\omega t + \phi)$ the displacement in harmonic oscillation can be generally written as a sum of sine and cosine parts:

$$x = A_1 \sin(\omega t) + A_2 \cos(\omega t)$$

Calculate partial amplitudes A_1 and A_2 in the case $A = 8$ cm and $\phi = \pi/6$.

With the use of the formula $\sin(\alpha + \beta) = \sin\alpha \cos\beta + \cos\alpha \sin\beta$, we obtain: $A_1 = A \cos\phi = 6{,}93$ cm, $A_2 = A \sin\phi = 4$ cm. ♠

♥ EX. 1.2

Find direct connection between displacement $x = x_0 \cdot \sin(\omega t + \phi)$ and velocity. What part of maximum velocity has the pendulum at the moment, when the displacement value is a quarter of the amplitude?

Let’s write again the displacement and velocity:

$$x = x_0 \sin(\omega t + \phi)$$

$$v = \dot{x} = \omega x_0 \cos(\omega t + \phi) = v_0 \cos(\omega t + \phi)$$

Here the velocity amplitude $v_0 = \omega x_0$ has been introduced. Divide first equation by x_0, second equation by v_0, then square both of them and sum. We obtain:

$$\left(\frac{x}{x_0}\right)^2+\left(\frac{v}{v_0}\right)^2=1$$

In the case $x = x_0/4$ we obtain:

$$\frac{v}{v_0}=\pm\sqrt{1-\left(\frac{x}{x_0}\right)^2}=\pm\frac{\sqrt{3}}{2}$$

Both signs are sensible since the pendulum can move to the left or right. ♠

♥ EX. 1.3

The equation for displacement in the case of damped harmonic oscillation is:

$$x = A\exp(-t/\tau)\sin(2\pi t/T+\phi)$$

T is time period and τ is relaxation (characteristic damping) time, supposed to be known. Express parameters A and ϕ with initial conditions: $x(0) = x_0$, $v(0) = v_0$.

First we express velocity:

$$v=\dot{x}=A\exp(-t/\tau)\left[-(1/\tau)\sin(2\pi t/T+\phi)+(2\pi/T)\cos(2\pi t/T+\phi)\right]$$

Next we use initial conditions:

$$x(0)=A\sin\phi=x_0$$

$$v(0)=A\left[-(1/\tau)\sin\phi+(2\pi/T)\cos\phi\right]=v_0$$

Parameter A is eliminated by dividing equations and then rearranging to obtain ϕ:

$$\phi=arc\cot\left[\frac{T}{2\pi}\left(\frac{v_0}{x_0}+\frac{1}{\tau}\right)\right]$$

Finally we calculate amplitude: $A = x_0/\sin\phi$.

For comparison, we solve the problem with complex numbers. Using Euler formula $\exp(\mathrm{i}\varphi) = \cos\varphi + \mathrm{i}\sin\varphi$ we can set displacement x as an imaginary part of complex number z: $x = \mathrm{Im}(z)$. Thus we use complex displacement, where parameters A and ϕ remain real:

$$z=A\exp\left[\mathrm{i}(-t/\tau+2\pi t/T+\phi)\right]$$

$$z = A\exp\left[\mathrm{i}((-1/\tau + 2\pi/T)t + \phi)\right]$$

The complex velocity V is:

$$V = \dot{z} = A\mathrm{i}(-1/\tau + 2\pi/T)\exp\left[\mathrm{i}((-1/\tau + 2\pi/T)t + \phi)\right]$$

Use initial conditions:

$$x(0) = \mathrm{Im}[z(0)] = \mathrm{Im}[A\exp(\mathrm{i}\phi)]$$

$$x(0) = A\sin\phi = x_0$$

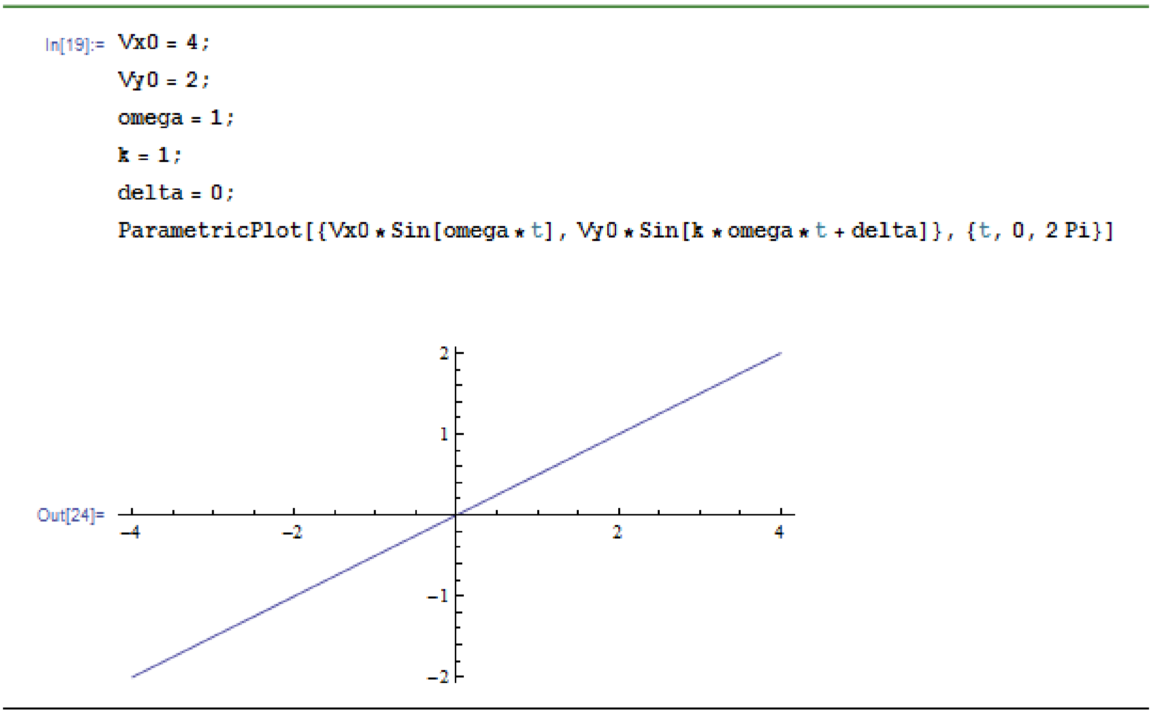
$$v(0) = \mathrm{Im}[V(0)] = \mathrm{Im}[A\mathrm{i}(-1/\tau + 2\pi/T)\exp(\mathrm{i}\phi)] \equiv \mathrm{Re}[A(-1/\tau + 2\pi/T)\exp(\mathrm{i}\phi)]$$

$$v(0) = A[-(1/\tau)\sin\phi + (2\pi/T)\cos\phi] = v_0$$

We obtain the same equations for A and ϕ as above. ♠

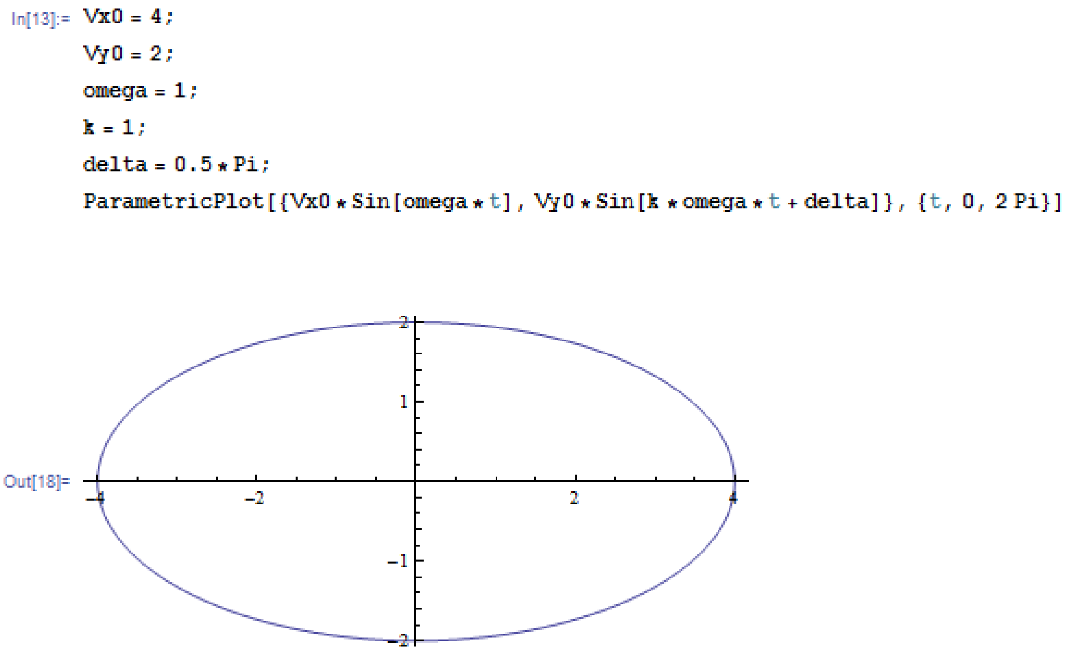
♥ EX. 1.4

We can use oscilloscope to track time evolution of two voltages simultaneously. One of them is presented at horizontal axis, the other at vertical axis; we obtain the corresponding diagrams. Let's take: $V_x = V_{x0} \cdot \sin(\omega\, t)$, $V_y = V_{y0} \cdot \sin(k\ \omega\, t + \delta)$, where k is rational number. Some examples are shown on Figs. R1, and the code in Mathematica is added.



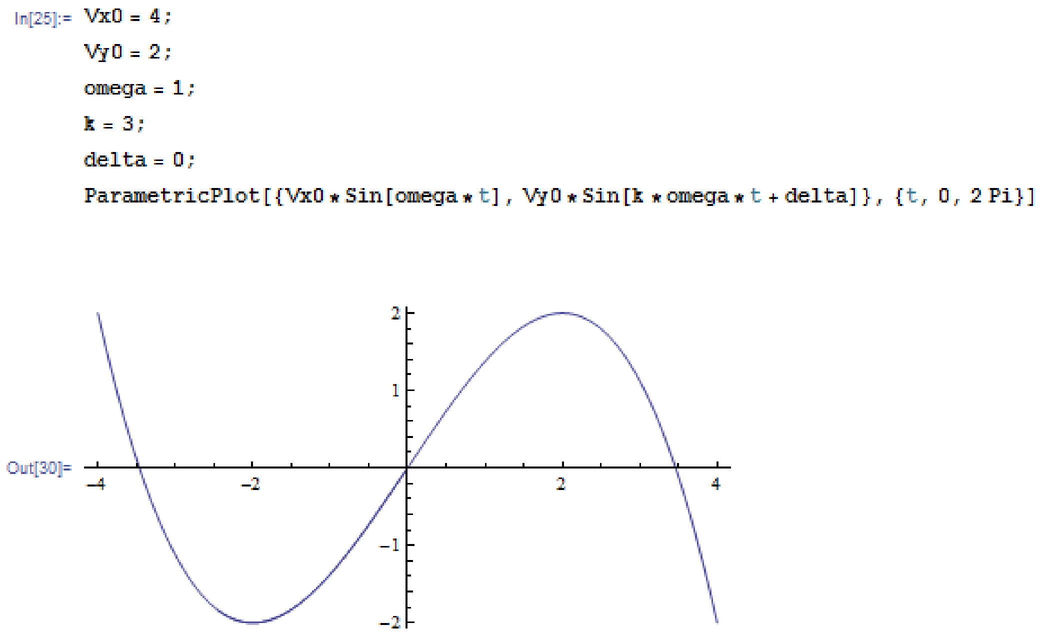
```
In[19]:= Vx0 = 4;
         Vy0 = 2;
         omega = 1;
         k = 1;
         delta = 0;
         ParametricPlot[{Vx0 * Sin[omega * t], Vy0 * Sin[k * omega * t + delta]}, {t, 0, 2 Pi}]
```

Fig. R1 a: Graph of $V_y(V_x)$ for $V_{x0} = 2V_{y0}$, $k = 1$ and $\delta = 0$ → 1D case



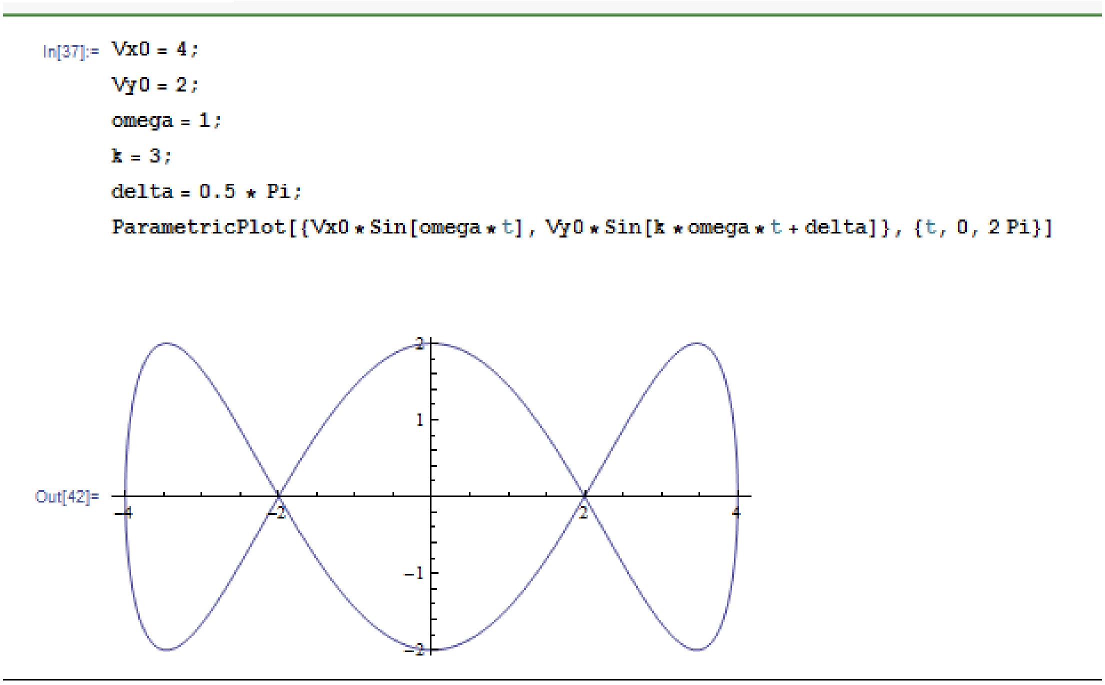
```
In[13]:= Vx0 = 4;
         Vy0 = 2;
         omega = 1;
         k = 1;
         delta = 0.5 * Pi;
         ParametricPlot[{Vx0 * Sin[omega * t], Vy0 * Sin[k * omega * t + delta]}, {t, 0, 2 Pi}]
```

Fig. R1 b: Graph of $V_y(V_x)$ for $V_{x0} = 2V_{y0}$, $k = 1$ and $\delta = \pi/2$ → ellipse



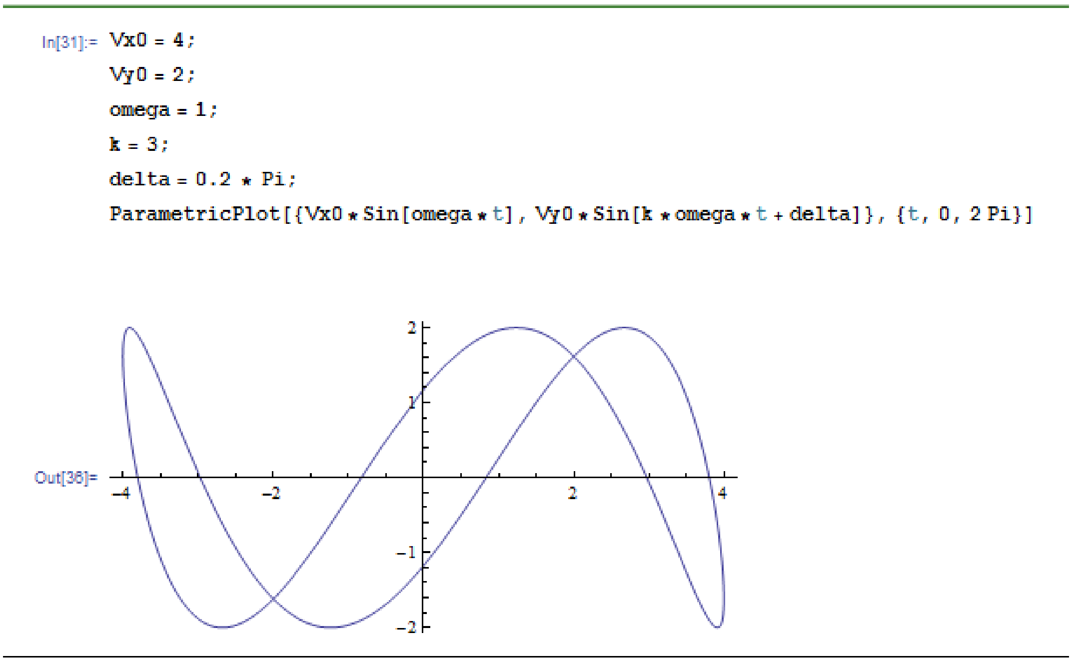
```
In[25]:= Vx0 = 4;
         Vy0 = 2;
         omega = 1;
         k = 3;
         delta = 0;
         ParametricPlot[{Vx0 * Sin[omega * t], Vy0 * Sin[k * omega * t + delta]}, {t, 0, 2 Pi}]
```

Fig. R1 c: Graph of $V_y(V_x)$ for $V_{x0} = 2V_{y0}$, $k = 3$ and $\delta = 0$ → cubic function $V_y = (V_x/2)\cdot [3 - 4(V_x/V_{x0})^2]$



```
In[37]:= Vx0 = 4;
         Vy0 = 2;
         omega = 1;
         k = 3;
         delta = 0.5 * Pi;
         ParametricPlot[{Vx0 * Sin[omega * t], Vy0 * Sin[k * omega * t + delta]}, {t, 0, 2 Pi}]
```

Fig. R1 č: Graph of $V_y(V_x)$ for $V_{x0} = 2V_{y0}$, $k = 3$ and $\delta = \pi/2$ → symmetrical closed curve



```
In[31]:= Vx0 = 4;
         Vy0 = 2;
         omega = 1;
         k = 3;
         delta = 0.2 * Pi;
         ParametricPlot[{Vx0 * Sin[omega * t], Vy0 * Sin[k * omega * t + delta]}, {t, 0, 2 Pi}]
```

Fig. R1 d: Graph of $V_y(V_x)$ for $V_{x0} = 2V_{y0}$, $k = 3$ and $\delta = \pi/5$ → asymmetrical closed curve ♠

♥ EX. 1.5

Calculate oscillation time of pendulum with mass m for small values of displacement around equilibrium position $x = 0$, if the dependence of potential energy (potential) on coordinate is hyperbolic cosine: $V(x) = V_0 \cosh(k\,x)$.

We use the Taylor series. Hyperbolic functions $\cosh x$ and $\sinh x$ are derivatives of each other: $(\cosh x)' = \sinh x$, $(\sinh x)' = \cosh x$. Therefore, the Taylor series is:

$$\cosh x = \cosh 0 + \frac{1}{1!}\sinh 0 \cdot x + \frac{1}{2!}\cosh 0 \cdot x^2 + \frac{1}{3!}\sinh 0 \cdot x^3 + \frac{1}{4!}\cosh 0 \cdot x^4 + \ldots$$

There also holds $\cosh 0 = 1$ and $\sinh 0 = 0$, so we obtain:

$$\cosh x = 1 + \frac{1}{2} \cdot x^2 + \frac{1}{24} \cdot x^4 + \ldots$$

The potential is thus:

$$V(x) = V_0 \left[1 + \frac{1}{2} \cdot (kx)^2 + \frac{1}{24} \cdot (kx)^4 + \ldots \right]$$

The force is the negative derivative of potential with respect to coordinate x:

$$F(x) = -V'(x) = -V_0 \left[k^2 x + \frac{1}{6} k^4 x^3 + \ldots \right]$$

In the case of small x (more exactly $kx \ll 1$) we keep only the first term: $F \approx -k^2 V_0 x$. From Newton law $ma = F$ the differential equation follows:

$$\ddot{x} + \frac{k^2 V_0}{m} x = 0$$

This is equation for harmonic oscillation with squared angular frequency: $\omega^2 = k^2 V_0 / m$. The time $T = 2\pi/\omega$ is:

$$T = \frac{2\pi}{k}\sqrt{\frac{m}{V_0}}$$ ♠

♥ EX. 1.6

Rotational pendulum (swing-wheel with spring) oscillates according to: $\varphi = \varphi_0 \cdot \sin(2\pi t/T)$. Damping is neglected. Here φ denotes the angle of deflection of any pendulum point out of equilibrium, with amplitude $\varphi_0 = 120° = 2\pi/3$. Period time T depends on inertial moment J and on spring coefficient D: $T = 2\pi(J/D)^{1/2}$. Let the swing-wheel be steel cylinder with radius $R = 10$ cm, height $h = 2$ cm and density $\rho = 7{,}8$ kg/dm^3, its moment is $J = mR^2/2$. The spring coefficient is defined as $D = M_1/\varphi_1$, where M_1 is some external torque needed to deform the spring by the angle φ_1. Let's take $\varphi_1 = \varphi_0 = 2\pi/3$, $M_1 = 2$ N m. Calculate T. Draw together the dimensionless graphs of time dependence of coordinates x and y of some point at the edge of cylinder. This point is on the x axis at rest, so $x = R\cos\varphi$, $y = R\sin\varphi$.

Data:

$\varphi_0 = \varphi_1 = 2\pi/3$

$R = 10$ cm

$h = 2$ cm

$\rho = 7{,}8$ kg/dm^3

$M_1 = 2$ N m

$T = ?$

Calculate T first:

$$T = 2\pi\sqrt{\frac{J}{D}} = 2\pi\sqrt{\frac{mR^2\varphi_0}{2M}} = 2\pi\sqrt{\frac{(\rho\pi R^2 h)R^2\varphi_0}{2M}} = \sqrt{\frac{2\pi^3\rho h\varphi_0}{M}} \cdot R^2 = 1\ \mathrm{s}$$

Equations for coordinates are: $x = R\cos[\varphi_0 \cdot \sin(2\pi t/T)]$, $y = R\sin[\varphi_0 \cdot \sin(2\pi t/T)]$. We have obtained slightly unusual periodic functions (Figs. R2).

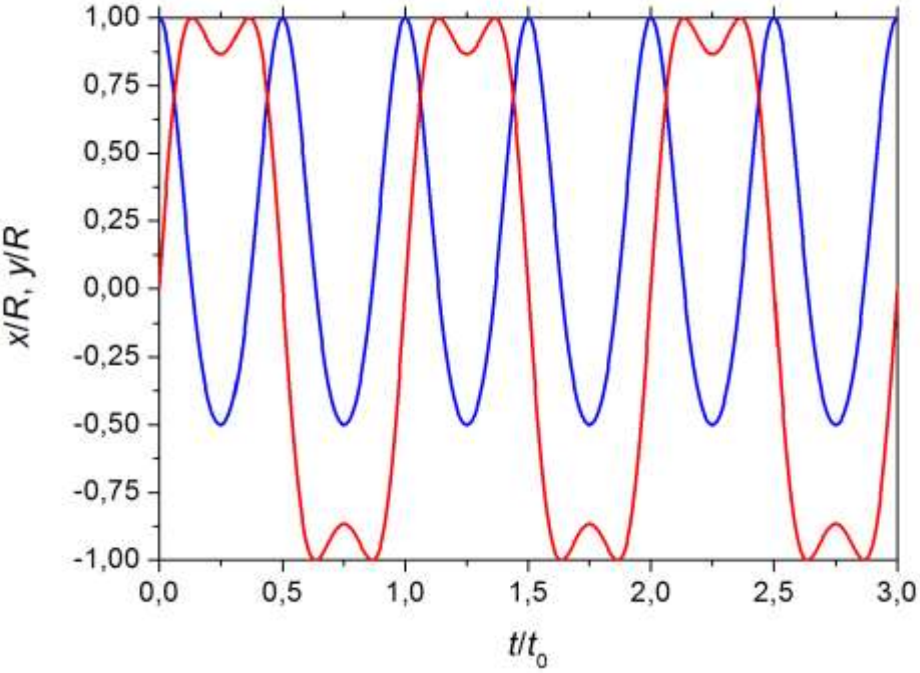


Fig. R2: Graphs of $x(t)$ (blue) and $y(t)$ (red) in dimensionless form

Try to understand by yourself why the function x/R does not reach minimum value -1 and why the curve y/R includes »small valleys« in maxima and minima. ♠

♥ EX. 1.7

Physical pendulum is made of two equal sticks with length L joined to form the letter T. Axis (Os) of oscillation is at the upper end (Fig. R3). What's the oscillation time?

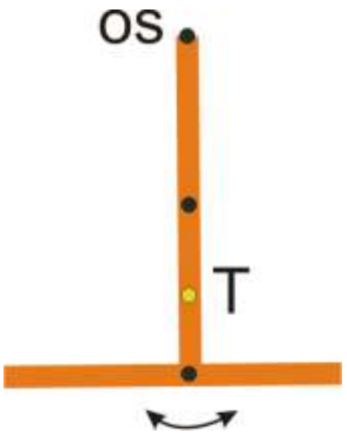


Fig. R3: Pendulum in the shape of T

First we find the position of the mass center (point T) of the composition of sticks:

$$r^* = \frac{my_1 + my_2}{2m} = \frac{1}{2}\left(\frac{L}{2} + L\right) = \frac{3}{4}L$$

Inertial moment is the sum of both moments, but we must also use Steiner rule:

$$J = 2J^* + my_1{}^2 + my_2{}^2 = 2 \cdot \frac{1}{12}mL^2 + m\left(\frac{L}{2}\right)^2 + mL^2 = \frac{1}{2}mL^2$$

Oscillation time:

$$T = 2\pi\sqrt{\frac{J}{mgr^*}} = 2\pi\sqrt{\frac{2L}{3g}}$$

Equation reminds us of the mathematical pendulum; we only have additional factor 2/3 under the square root. This similarity is typical for all physical pendulums made of homogeneous material. ♠

♥ EX. 1.8

Futuristic engineers have thought of some train for long distances that is driven by the gravity. Initial (ZP) and finial (KP) stations (with no intermediate stations) are connected by straight evacuated tunnel (Fig. R4). How long does it take from ZP to KP?

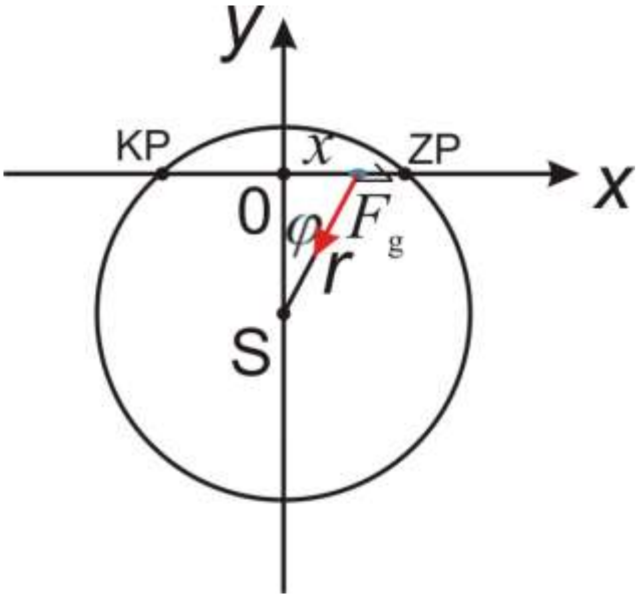


Fig. R4: Position of train at the moment (blue point) and the gravitation force

Equilibrium point halfway between both stations is denoted by 0, and the center of Earth by S. The position of the train at the moment is given by coordinate x, but the distance between the train and the center of Earth is r. We suppose that the acceleration of gravity inside the Earth is linear with r: $g = g_0 r/R$, where g_0 is its value at the surface of Earth and R is the Earth's radius. The train feels the gravity force $F_g = mg_0 r/R$ towards the center S. But we must take its component in the direction of x (along the tunnel), while friction and air resistance are neglected. The equation is: $ma = F_{gx} = -\, mg_0 r/R \cdot \sin \varphi = -\, mg_0 x/R$. So we got the equation for harmonic oscillation:

$$\ddot{x} + \frac{g_0}{R} x = 0$$

We have: $\omega^2 = g_0/R$, and for oscillation time $T = 2\pi/\omega$:

$$T = 2\pi\sqrt{\frac{R}{g_0}}$$

We must take half of this:

$$t = \pi\sqrt{\frac{R}{g_0}} = 42 \text{ min}$$

We have inserted: $g_0 = 9{,}8$ m/s^2, $R = 6400$ km. ♠

♥ EX. 1.9

Electric oscillation circuit is composed of flat capacitor with plates of area 1 dm^2 at distance 1 mm, and of the coil with length 10 cm, 200 turnings and cross-section 1 cm^2. What's the frequency of oscillation of this circuit? What's the initial energy of oscillations if the capacitor has been loaded at the voltage 15 V? After how many oscillations does the energy fall to 1 % of the initial value, if the circuit contains Ohm resistance so that the coefficient of damping is $\beta = \omega/10$?

Data:

$S_1 = 1$ dm^2

$d = 1$ mm

$l = 10$ cm

$N = 200$

$S_2 = 1$ cm^2

$U_0 = 15$ V

$\beta = \omega/10$

$W/W_0 = 1$ %

$\nu = ?$

$W_0 = ?$

$N_{\mathrm{nih}} = ?$

The capacity of the capacitor is $C = \varepsilon_0 S_1/d$, with $\varepsilon_0 \approx 8{,}85 \cdot 10^{-12}$ As/Vm. The inductivity of the coil is $L = \mu_0 N^2 S_2/l$, with $\mu_0 = 4\pi \cdot 10^{-7}$ Vs/Am. The angular frequency is then:

$$\omega = \frac{1}{\sqrt{LC}} = \frac{1}{\sqrt{\varepsilon_0 \mu_0 N^2 \frac{S_1 S_2}{dl}}} = 1{,}5 \cdot 10^7 \text{ s}^{-1},$$

The frequency is: $\nu = \omega/(2\pi) = 2{,}4$ MHz. The energy is the initial electric energy of the capacitor, because electric and magnetic energy are repeatedly transformed into each other:

$$W = \frac{CU_0{}^2}{2} = \frac{\varepsilon_0 S_1 U_0{}^2}{2d} = 9{,}96 \text{ nJ}$$

Lastly we have:

$$W = W_0 e^{-\beta t} \rightarrow t = \frac{1}{\beta} \ln \frac{W_0}{W} = \frac{10}{\omega} \ln 100 = 3{,}07 \ \mu\text{s}$$

The corresponding number of oscillations is:

$$N_{nih} = \frac{t}{T} = \frac{1}{\beta} \ln \frac{W_0}{W} \cdot \frac{\omega}{2\pi} = \frac{10}{2\pi} \ln 100 = 7{,}33$$

In reality, when the damping is present, the angular frequency is not exactly the same as calculated above, but a little smaller. However, the difference is not significant for $\beta \ll \omega$. Some comment about β: it was defined here so that the equation for oscillating physical quantity, such as electric current in our case, includes also exponential factor $\exp(-\beta t/2) \equiv$

$\exp(-t/\tau)$. Twice larger exponent in the equation for energy comes from the fact that the energy is proportional to the square of the amplitude of the electric current. ♠

♥ EX. 1.10

Prove that the following relations hold for the operation of conjugating complex numbers: a) $(z_1 \pm z_2)^* = z_1^* \pm z_2^*$, b) $(z_1z_2)^* = z_1^*z_2^*$, c) $(z_1/z_2)^* = z_1^*/z_2^*$! Prove the following rules for absolute values of complex numbers: č) $\leq \big||z_1| - |z_2|\big| \leq |z_1 \pm z_2| \leq |z_1| + |z_2|$, d) $|z_1z_2| = |z_1| \cdot |z_2|$, e) $|z_1/z_2| = |z_1|/|z_2|$!

Take complex numbers $z_1 = a_1 + b_1\mathrm{i}$, $z_2 = a_2 + b_2\mathrm{i}$. Conjugation changes the sign of imaginary component, say $z_1^* = a_1 - b_1\mathrm{i}$.

Proofs:

a) $(z_1 + z_2)^* = (a_1 + b_1\mathrm{i} + a_2 + b_2\mathrm{i})^* = ((a_1 + a_2) + (b_1 + b_2)\mathrm{i})^* = a_1 + a_2 - (b_1 + b_2)\mathrm{i} = (a_1 - b_1\mathrm{i}) + (a_2 - b_2\mathrm{i}) = z_1^* + z_2^*$. Similarly for the difference!

b) $(z_1z_2)^* = ((a_1 + b_1\mathrm{i}) \cdot (a_2 + b_2\mathrm{i}))^* = (a_1a_2 - b_1b_2 + (a_1b_2 + a_2b_1)\mathrm{i})^* = a_1a_2 - b_1b_2 - (a_1b_2 + a_2b_1)\mathrm{i} = (a_1 - b_1\mathrm{i}) \cdot (a_2 - b_2\mathrm{i}) = z_1^*z_2^*$

c) It is enough to take only the special case, $(1/z)^* = 1/z^*$, since the rule (b) can be consequently use to generalize the rule:

$$(\frac{1}{z})^* = (\frac{1}{a+b\mathrm{i}})^* = (\frac{a-b\mathrm{i}}{a^2+b^2})^* = \frac{a+b\mathrm{i}}{a^2+b^2} = \frac{1}{a-b\mathrm{i}} = \frac{1}{z^*}$$

Next, $|z|^2 = zz^*$. Let's prove the rule (d), since the proof of (e) is similar: $|z_1z_2|^2 = (z_1z_2)(z_1z_2)^* = (z_1z_2)\, z_1^*z_2^* = z_1z_1^*z_2z_2^* = |z_1|^2\,|z_2|^2 \rightarrow |z_1z_2| = |z_1| \cdot |z_2|$. Rule (č) is slightly more complicated:

$$|z_1 + z_2|^2 = (a_1 + a_2)^2 + (b_1 + b_2)^2 = a_1^2 + a_2^2 + b_1^2 + b_2^2 + 2(a_1a_2 + b_1b_2)$$

$$(|z_1| + |z_2|)^2 = |z_1|^2 + |z_2|^2 + 2|z_1| \cdot |z_2| = a_1^2 + a_2^2 + b_1^2 + b_2^2 + 2|z_1| \cdot |z_2|$$

Let the difference of both expressions be Δ:

$$\Delta = 2(\sqrt{a_1^2 + b_1^2} \cdot \sqrt{a_2^2 + b_2^2} - (a_1a_2 + b_1b_2))$$

The positivity of Δ can be checked by comparing the two terms; the exercise is left for the student. If the rule holds generally for $z_1 + z_2$, it also holds for $z_1 - z_2$; we only have to substitute $z_2 \rightarrow -z_2$. This was the way for proving the right non-equality; the proof for the left non-equality goes similarly. ♠

♥ EX. 1.11

Prove Euler relation exp(iθ) = cos θ + i sin θ with Taylor series for all the three functions.

Taylor series for exponential function: $e^x = 1 + x + x^2/2 + x^3/6 + \ldots$ In our case:

$$e^{i\theta} = 1 + (i\theta) + \frac{1}{2!}(i\theta)^2 + \frac{1}{3!}(i\theta)^3 + \frac{1}{4!}(i\theta)^4 + \frac{1}{5!}(i\theta)^5 + \frac{1}{6!}(i\theta)^6 \ldots$$

$$e^{i\theta} = 1 + (i\theta) - \frac{1}{2!}\theta^2 - i\frac{1}{3!}\theta^3 + \frac{1}{4!}\theta^4 + i\frac{1}{5!}\theta^5 - \frac{1}{6!}\theta^6 \ldots$$

We write separately the real and imaginary part of this:

$$\operatorname{Re} e^{i\theta} = 1 - \frac{1}{2!}\theta^2 + \frac{1}{4!}\theta^4 - \frac{1}{6!}\theta^6 \ldots$$

$$\operatorname{Im} e^{i\theta} = \theta - \frac{1}{3!}\theta^3 \frac{1}{5!}\theta^5 \ldots$$

But these are just Taylor series for cosine and sine functions. ♠

♥ EX. 1.12

Oscillation of atoms in the aligned molecule CO_2 can be treated with mechanical model. There is a carbon atom with mass *m* in the middle, and to the left and right from it oxygen atoms each with mass *M* are positioned. There is a spring between carbon and each oxygen atom, its coefficient being *k* (Fig. R5). Equilibrium distance C – O is *a* (however, this piece of data will play no role in the calculation) which corresponds to the length of un-stretched spring. Consider linear oscillations of these atoms.

Let's denote the displacement of the left oxygen atom from its equilibrium to the right by x_L, the displacement of the right oxygen atom by x_D, and of carbon atom by y (positive values all mean displacement to the right). Let's imagine increasing displacements to the right: $x_L < y < x_D$. Then both springs are elongated, so that they tend to shrink again and correspondingly act with forces and atoms (see figure). Let's write the second Newton law for all three atoms:

$$M\ddot{x}_L = k(y - x_L)$$

$$m\ddot{y} = -k(y - x_L) + k(x_D - y) = k(x_L + x_D - 2y)$$

$$M\ddot{x}_D = k(y - x_D)$$

As regards the oxygen atom, we have to consider both springs: one of them pulls to the left (negative force), the other to the right (positive force). We expects all the atoms to oscillate with the same frequency, but with different amplitude and phase shift. It's appropriate to write the displacements in complex: $x_L = A\exp(i\omega t)$, $y = B\exp(i\omega t)$, $x_D = C\exp(i\omega t)$, where also the amplitudes *A*, *B* and *C* may be complex numbers. We also divide equations by masses and define the following angular frequencies: $\omega_M = (k/M)^{1/2}$, $\omega_m = (k/m)^{1/2}$. Oxygen atoms have larger mass than carbon, $M > m$, so we have $\omega_M < \omega_m$. The upper differential equations turn to usual algebraic equations for *A*, *B* and *C*:

$$-\omega^2 A = \omega_M{}^2 (B - A)$$

$$-\omega^2 B = \omega_m{}^2 (A + C - 2B)$$

$$-\omega^2 C = \omega_M{}^2 (B - C)$$

This is the system of three homogeneous linear equations, rewritten as:

$$(\omega^2 - \omega_M{}^2)A + \omega_M{}^2 B + 0 = 0$$

$$\omega_m{}^2 A + (\omega^2 - 2\omega_m{}^2)B + \omega_m{}^2 C = 0$$

$$0 + \omega_M{}^2 B + (\omega^2 - \omega_M{}^2)C = 0$$

In fact, besides the coefficients A, B and C also the angular frequency ω is unknown, but it can be treated as a parameter rather as an unknown. Homogeneous system of linear equations has solutions which are not trivial (exactly zero) only when the determinant of the matrix is zero:

$$\det\begin{bmatrix} \omega^2 - \omega_M{}^2 & \omega_M{}^2 & 0 \\ \omega_m{}^2 & \omega^2 - 2\omega_m{}^2 & \omega_m{}^2 \\ 0 & \omega_M{}^2 & \omega^2 - \omega_M{}^2 \end{bmatrix} = 0$$

We obtain an equation of the third degree in ω^2:

$$\omega^2\left[\omega^4 - 2(\omega_M{}^2 + \omega_m{}^2)\omega^2 + \omega_M{}^2(\omega_M{}^2 + 2\omega_m{}^2)\right] = 0$$

First solution, $\omega^2 = 0$, means only the translation of the molecule as whole, and it is of no interest. We can easily check that it corresponds to equal displacements: $A = B = C$. The other two solutions are significant and simple:

$$\omega_1{}^2 = \omega_M{}^2$$

$$\omega_2{}^2 = \omega_M{}^2 + 2\omega_m{}^2$$

Since the angular frequency is taken as positive by definition, we finally obtain:

$$\omega_1 = \omega_M$$

$$\omega_2 = \sqrt{\omega_M{}^2 + 2\omega_m{}^2}$$

Physical interpretation of both solutions is easy when we insert both frequencies in the upper system of equations and express the corresponding relations between the coefficients. In the first case, where $\omega = \omega_1 = \omega_M$, we find: $C = -A$, $B = 0$. This means that the carbon atom is at rest, while the oxygen atoms oscillate in the opposite phase; this is correct since the mass center of the whole molecule remains still in this case. In the second case, $\omega = \omega_2$, all the atoms vibrate: $C = A$, $B = -2(\omega_m{}^2/\omega_M{}^2)A = -2(M/m)A$. Now, the oxygen atoms oscillate in the same phase, but the carbon atom moves in the opposite direction with larger amplitude. Again the mass center of the molecule is at rest: $AM + Bm + CM = 0$.

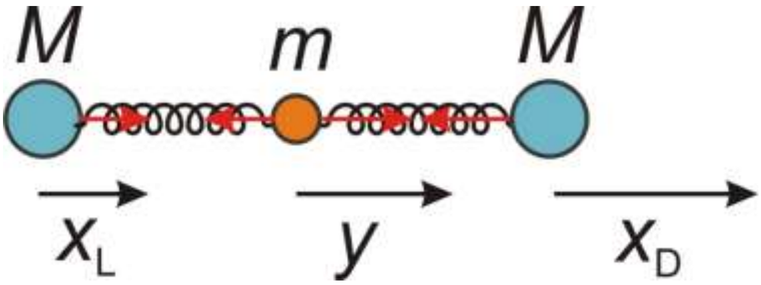


Fig. R5: Molecule CO_2 as a system of three bodies and two springs; displacements to the right are shown. But this is allowed in reality only if the translation of the whole molecule is also included. The forces of the springs are shown with red arrows.

Although the frequencies ω_1 and ω_2 cannot be calculated directly because we don't know the coefficient k or atomic forces, their ration is independent of k:

$$\frac{\omega_2}{\omega_1} = \sqrt{1 + 2\frac{{\omega_m}^2}{{\omega_M}^2}} = \sqrt{1 + 2\frac{M}{m}}$$

This ratio which can be checked experimentally, for instance with absorption of electromagnetic waves with appropriate wavelengths, depends only on the known masses of both types of atoms in the molecule:

$$\frac{\omega_2}{\omega_1} = \sqrt{1 + 2 \cdot \frac{16}{12}} = 1{,}91$$ ♠

♥ EX. 1.13

Show that the common function $\psi(x, t) = \psi_1(x - ct) + \psi_2(x + ct)$ really satisfies the wave equation: $\frac{\partial^2 \psi}{\partial t^2} = c^2 \cdot \frac{\partial^2 \psi}{\partial x^2}$ for any functions ψ_1 and ψ_2.

We'll use the fact that the functions ψ_1 and ψ_2 are usual functions of intermediate parameters (phases) $\varphi_1 = x - ct$ and $\varphi_2 = x + ct$. Let's calculate step by step all necessary derivatives (take care about signs for usual and partial differentiations!):

$$\frac{\partial \psi}{\partial t} = \frac{\mathrm{d}\psi_1}{\mathrm{d}\varphi_1} \cdot \frac{\partial \varphi_1}{\partial t} + \frac{\mathrm{d}\psi_2}{\mathrm{d}\varphi_2} \cdot \frac{\partial \varphi_2}{\partial t} = \frac{\mathrm{d}\psi_1}{\mathrm{d}\varphi_1} \cdot (-c) + \frac{\mathrm{d}\psi_2}{\mathrm{d}\varphi_2} \cdot c$$

$$\frac{\partial^2 \psi}{\partial t^2} = \frac{\mathrm{d}^2\psi_1}{\mathrm{d}{\varphi_1}^2} \cdot (-c)^2 + \frac{\mathrm{d}^2\psi_2}{\mathrm{d}{\varphi_2}^2} \cdot c^2 = c^2 \left(\frac{\mathrm{d}^2\psi_1}{\mathrm{d}{\varphi_1}^2} + \frac{\mathrm{d}^2\psi_2}{\mathrm{d}{\varphi_2}^2}\right)$$

$$\frac{\partial \psi}{\partial x} = \frac{\mathrm{d}\psi_1}{\mathrm{d}\varphi_1} \cdot \frac{\partial \varphi_1}{\partial x} + \frac{\mathrm{d}\psi_2}{\mathrm{d}\varphi_2} \cdot \frac{\partial \varphi_2}{\partial x} = \frac{\mathrm{d}\psi_1}{\mathrm{d}\varphi_1} \cdot 1 + \frac{\mathrm{d}\psi_2}{\mathrm{d}\varphi_2} \cdot 1$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\mathrm{d}^2\psi_1}{\mathrm{d}{\varphi_1}^2} \cdot 1^2 + \frac{\mathrm{d}^2\psi_2}{\mathrm{d}{\varphi_2}^2} \cdot 1^2 = \frac{\mathrm{d}^2\psi_1}{\mathrm{d}{\varphi_1}^2} + \frac{\mathrm{d}^2\psi_2}{\mathrm{d}{\varphi_2}^2}$$

Both second partial derivatives really satisfy the wave equation above. ♠

♥ EX. 1.14

Derive the wave equation and the corresponding speed for the transversal wave on the string which is loaded with the longitudinal force F. The string is homogeneous: its cross-section is S and the density of the material is ρ.

Consider the forces that act on the short section of the string with length dx and mass dm = ρSdx. Axis x is directed along the non-deformed string (Fig. R6). To keep the geometrical imagination we denote the displacement of the string by coordinate y. We stress in advance that the shape (curvature) of the string is relevant here, rather than the (average) displacement itself or the (averaged) angle with the x axis. The shown piece has the shape of convex increasing function, so that the inclination of its left end, tan $\alpha(x) \equiv \partial y/\partial x(x)$, is smaller than that at the right end, tan $\alpha(x + \mathrm{d}x) \equiv \partial y/\partial x(x + \mathrm{d}x)$. What's about (non)equilibrium of forces on such piece? Usually the displacement are small so that the angle α Is also small everywhere. The component of the force F in x direction is $F_\mathrm{x} = F\cos\,\alpha \approx F$. Therefore, in regard to x direction we have practically equilibrium and we can disregard the movement in this direction. It's different about y direction: the difference of the components of the forces at both ends is: $\Delta F_y = F\sin\,\alpha(x + \mathrm{d}x) - \mathrm{F}\sin\,\alpha(x)$. According to Newton law d$m \cdot a_y = \Delta F_y$ it follows:

$$\mathrm{d}m \cdot \frac{\partial^2 y}{\partial t^2} = F \cdot \left[\sin\alpha(x+dx) - \sin\alpha(x)\right]$$

Since α is small, we can take sin $\alpha \approx$ tan α = $\partial y/\partial x$:

$$\rho S\mathrm{d}x \cdot \frac{\partial^2 y}{\partial t^2} = F \cdot \left[\frac{\partial y}{\partial x}(x+dx) - \frac{\partial y}{\partial x}(x)\right]$$

At last, we divide with mass dm = ρSdx and take into account that dividing the difference of the first derivative at nearby points by dx on the right side of equation actually means the second derivative:

$$\frac{\partial^2 y}{\partial t^2} = \frac{F}{\rho S} \cdot \frac{\partial^2 y}{\partial x^2}$$

Indeed, we got the wave equation with the wave speed:

$$c = \sqrt{\frac{F}{\rho S}}$$

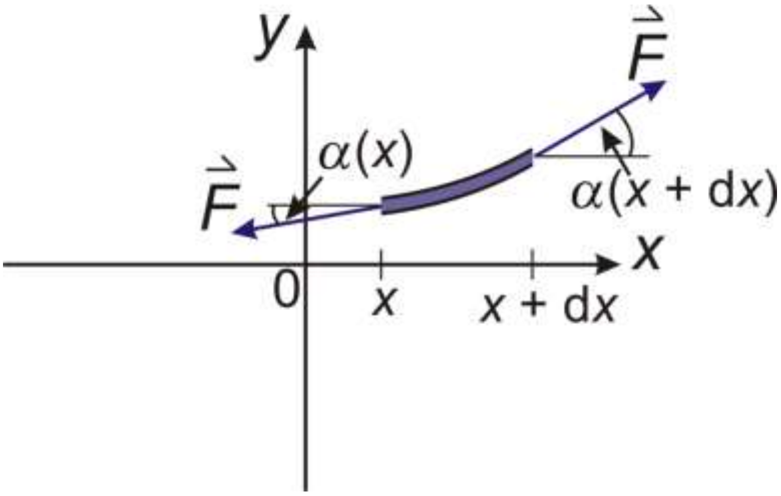


Fig. R6: Forces in the derivation of the wave equation; the shown displacements and angles are exaggerated for the sake of evidence. ♠

♥ EX. 1.15

Steel string of length 80 cm has the diameter 0,2 mm. The density of steel is 7,8 kg/dm^3. What force must we use to stretch the string in order to achieve the fundamental frequency 400 Hz?

Data:

l = 80 cm

r = 0,1 mm

ρ = 7,8 kg/dm^3

ν_1 = 400 Hz

F = ?

The speed of wave is expressed in two ways:

$$c = \lambda_1 \nu_1 = 2l\,\nu_1$$

$$c = \sqrt{\frac{F}{\rho \pi r^2}}$$

We can eliminate c to calculate the force:

$$F = 4\pi\rho \cdot l^2 r^2 \nu_1^{\ 2} = 100{,}4\ \text{N}$$ ♠

♥ EX. 1.16

What's the mechanical energy of oscillation of the string tied at both ends in the n-th wave mode? The equation for displacement is: $\psi_n = A_n \sin(k_n x) \sin(\omega_n t)$, where the coordinate x has values in the interval $0 \le x \le L$. It doesn't matter for the time factor whether we choose sine or cosine function. Express energy with the data for amplitude A_n, force F, length L, density ρ and thickness (diameter) D.

Mechanical energy of oscillation (standing wave) at any moment is the sum of elastic and kinetic terms. In practice, it can be calculated as the maximum elastic energy (at limiting position) or as maximum kinetic energy (when string passes the equilibrium position). The most direct way is the calculation of the latter. But first the velocity in transverse direction for every piece of the string must be expressed: $v = \partial\psi/\partial t = \omega_n A_n \sin(k_n x) \cos(\omega_n t)$. At time $t = 0$ we have the maximum of the velocity: $v_0 = \omega_n A_n \sin(k_n x)$, but this still depends on coordinate x, where the piece is positioned. The entire kinetic energy is calculated by the following integral:

$$E_n = \frac{1}{2}\int_m \mathrm{d}m v_0^{\ 2} = \frac{1}{2}\int_0^L (\rho S \mathrm{d}x)\left[\omega_n A_n \sin(k_n x)\right]^2$$

$$E_n = \frac{\rho S \omega_n^{\ 2} A_n^{\ 2}}{2}\int_0^L \sin^2(k_n x)\mathrm{d}x$$

We needn't bother much with this integral, since it is known that integrating the square of sine or cosine function over the interval L, which is the multiple of half-period (what is true in our case), gives simply the result $L/2$. The angular frequency is: $\omega_n = 2\pi\nu_n = 2\pi c/\lambda_n = 2\pi c/(2L/n) = n\pi c/L$. So, the energy is:

$$E_n = \frac{\rho S A_n^{\ 2}}{2}\cdot\left(\frac{n\pi c}{L}\right)^2\cdot\frac{L}{2} = \frac{\rho S A_n^{\ 2} n^2 \pi^2}{4L}\cdot\frac{F}{\rho S} = \frac{n^2\pi^2 F}{4L}\cdot A_n^{\ 2}$$

In the case of fundamental wave mode ($n = 1$) we have: $E_1 = (\pi^2/4) F A_1^{\ 2}/L \approx 2{,}47\ F A_1^{\ 2}/L$. Although in fact the string vibrates in several wave modes simultaneously (this depends on initial conditions), the energy of the first mode strongly prevails in most cases, because the amplitude A_1 is usually much larger than others. ♥

♥ EX. 1.17

This example is served as a confirmation of the calculation of maximum kinetic energy and the entire energy in the previous case. Let’s calculate the true elastic energy in “null” position and in simplified limiting position for $n = 1$, where we take triangular shape instead of sine function (Fig. R7). The difference between the elastic energies in both positions can be the guide for the maximum kinetic energy.

We can take the elastic energy of linear spring: $E_{\mathrm{pr}} = Kx^2/2 = F^2/(2K)$, if the force on spring is F and its elongation is x. We have used the symbol K for the spring coefficient instead of k, to avoid confusion with the wave vector. Straight wire with the Young modulus E is not a spring, but nevertheless the analogy between them may be used to find the relation between the force and elongation: $F = Kx$ for the spring and $F = ESx/L_0$ for the wire (string). Thus we can introduce $K = ES/L_0$, where L_0 is the length of the wire before stretching. Thus, the elastic energy of the string is: $E_{\mathrm{pr}} = Kx^2/2 = ESx^2/(2L_0)$ ali $E_{\mathrm{pr}} = F^2/(2K) = F^2L_0/(2ES)$. It holds: $L > L_0$. We then write: $L = L_0 + x_0$, where x_0 means the string elongation in null position, »null« elastic energy is then $E_{\mathrm{pr0}} = ESx_0^2/(2L_0)$. Next, we displace the string so that the perpendicular displacement at the middle is A. We look at the isosceles triangle and find for the new string length: $L' = (L^2 + 4A^2)^{1/2}$. New elongation is then $x = L' - L_0$ and the new elastic energy is $E_{\mathrm{pr}} = ESx^2/(2L_0)$. Their difference is:

$$\Delta E_{\mathrm{pr}} = \frac{ES}{2L_0}(x^2 - x_0{}^2) = \frac{ES}{2L_0}\left[(L'-L_0)^2 - (L-L_0)^2\right] = \frac{ES}{2L_0}\left[L'^2 - L^2 - 2L_0(L'-L)\right]$$

$$\Delta E_{\mathrm{pr}} = \frac{ES}{2L_0}\left[4A^2 - 2L_0(\sqrt{L^2+4A^2} - L)\right]$$

Take $A << L$ and $(1 + \varepsilon)^{1/2} \approx 1 + \varepsilon/2$ for $\varepsilon << 1$, and we find:

$$\Delta E_{\mathrm{pr}} \approx \frac{2ES}{L_0}(1 - \frac{L_0}{L})A^2 = \frac{2ESx_0}{L_0 L}A^2 = \frac{2ES}{L_0 L}\cdot\frac{FL_0}{ES}\cdot A^2 = \frac{2F}{L}\cdot A^2$$

The final result remind us of that in the previous exercise for $n = 1$, but now we have the factor 2 instead of 2,47 because of the different string shapes.

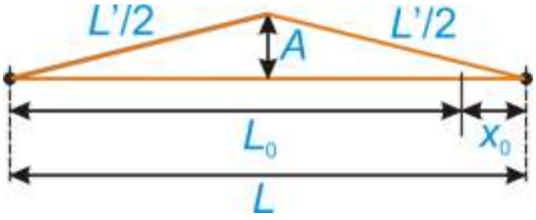


Fig. R7: Elongation of the string ♠

♥ EX. 1.18

Derive wave equation and the speed for sound as longitudinal wave in matter. Solid matter has the modulus of compressibility K and the density ρ. The modulus K is defined so: if the small piece of the material with the volume V is additionally compressed with external contact forces (so we have negative change of its volume, ΔV), additional pressure appears in the material, proportional with the relative volume change: $\Delta p = -K\Delta V/V$.

Take a look at forces acting on the piece of matter with length dx and mass dm = ρSdx (see Fig. R8). Here, S is optional cross-section of the matter. This time the displacement of the pieces of matter from equilibrium at x for every point is denoted by ψ. What about the (non)equilibrium of the forces? The difference of the pressure at both ends of the piece is relevant! This difference is proportional to the resultant force. Let in our case the "left" force $F_L = S\Delta p(x)$ be larger than the "right" force $F_D = S\Delta p(x + \mathrm{d}x)$; the forces act in opposite directions. This also means that additional pressure is larger on the left side, i. e., the matter is more compresse on the left side (only at the given moment!). The Newton law d$m \cdot a = F_L - F_D$ gives:

$$\mathrm{d}m \cdot \frac{\partial^2 \psi}{\partial t^2} = S \cdot \left[\Delta p(x) - \Delta p(x + dx)\right]$$

Take the definition of the K modulus:

$$\rho S\mathrm{d}x \cdot \frac{\partial^2 \psi}{\partial t^2} = SK \cdot \left[-\frac{\Delta V}{V}(x) + \frac{\Delta V}{V}(x + dx)\right]$$

Here, we must be careful about the interpretation of relative volumes on the right side of the last equation. For instance, the symbol V now does not represent the entire volume of the piece in the figure, but only its much smaller part, on the left and right side; the similar holds for the change ΔV. Suppose that the matter does not move in the transverse directions (this is also an approximation and is not self-evident!). Therefore, the changes in the volume appear only due to displacement in x direction: $\Delta V/V = \Delta b/b \equiv \partial\psi/\partial x$. Thus:

$$\rho S\mathrm{d}x \cdot \frac{\partial^2 \psi}{\partial t^2} = SK \cdot \left[\frac{\partial \psi}{\partial x}(x + dx) - \frac{\partial \psi}{\partial x}(x)\right]$$

Divide equation by mass dm = ρSdx:

$$\frac{\partial^2 \psi}{\partial t^2} = \frac{K}{\rho} \cdot \frac{\partial^2 \psi}{\partial x^2}$$

We've really got wave equation and the wave speed is:

$$c = \sqrt{\frac{K}{\rho}}$$

Finally, we mention that for fluids and gasses we can use K (for adiabatic change), but for elastic solid matter we must substitute K with Young modulus E.

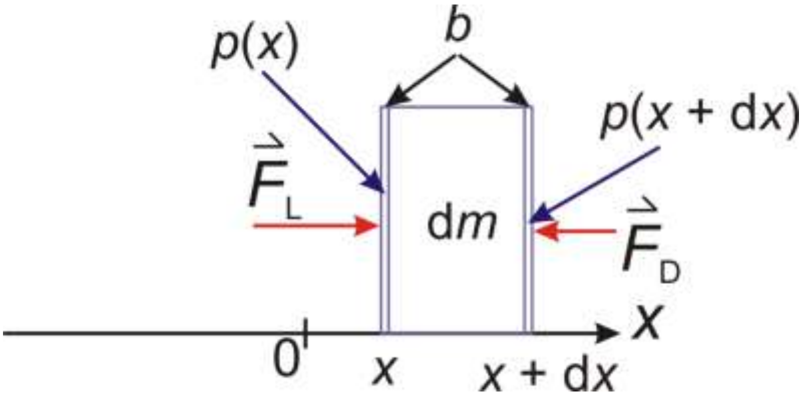


Fig. R8: Forces on the piece of matter with regard to sound♠

♥ EX. 1.19

Consider sound wave in the ideal gas. To calculate the modulus K_{ad} for adiabatic compression use the adiabatic relation: $pV^{\kappa} = C$, where p is pressure, V volume, C some constant (given by mass and type of the gas, not relevant here) and $\kappa = c_p/c_V$ is the ratio of specific heats at constant pressure and volume, respectively. Calculate the sound speed in nitrogen at 273 K. Write expressions for oscillations of position, pressure and density.

Let write equation $\Delta p = -K_{ad}\Delta V/V$ in differential form: $\mathrm{d}p = -K_{ad}\mathrm{d}V/V$. In this way, the modulus K can be calculated by:

$$K_{ad} = -V\cdot\frac{\mathrm{d}p}{\mathrm{d}V} = -V\cdot\frac{\mathrm{d}(CV^{-\kappa})}{\mathrm{d}V} = -V\cdot(-\kappa CV^{-\kappa-1}) = \kappa CV^{-\kappa} = \kappa p$$

Therefore, the adiabatic modulus for ideal gas can be expressed directly with pressure. We also use $pV = (m/M)RT$, where m is the mass of gas, M kilomole mass, T absolute temperature and R = 8314 J/(kmol K) the gas constant. From this equation the density follows: $\rho = m/V = Mp/(RT)$. The sound speed is:

$$c = \sqrt{\frac{K_{ad}}{\rho}} = \sqrt{\frac{\kappa RT}{M}}$$

The nitrogen molecule N_2 contains two atoms with atomic mass 14, so M = 28 kg/kmol. For two-atomic gasses we have κ = 1,4. The speed of sound at 273 K is then 337 m/s. We also mention, that the kinetic theory of gases gives the following average speed of individual gas molecules:

$$v_{\mathrm{RMS}} = \sqrt{\frac{3RT}{M}}$$

This is 493 m/s for nitrogen at 273 K. Thermal speed of molecules and the sound speed are thus of the same order for gasses. If we are more exact: the average speed expressed above is in fact the square root of the statistical mean value of the square of the speed; that's why we have used the symbol RMS (root mean square).

Consider now the sound in the gas as a harmonic wave and write the equation for the displacement of the parts of air from their equilibrium positions as:

$$\psi = \psi_0 \sin(\omega t - kx)$$

If the part of the gas with some mass m experiences the increment of the volume by some small proportion, its density is simultaneously decreased by the same relative proportion; in differential form: $\mathrm{d}\rho/\rho = -\mathrm{d}V/V$. This can be easily proved from $\rho = m/V$ with the use of differential. In the previous example (derivation of the speed of sound in the matter) we have used the following relation: $\Delta V/V = \partial\psi/\partial x$. Use this for the density now:

$$\frac{\Delta\rho}{\rho_0} = -\frac{\partial\psi}{\partial x} = -k\psi_0 \cos(\omega t - kx)$$

Here $\Delta\rho$ is meant as the deviation of the gas density from its equilibrium (mean) value ρ_0, i. e., the density without sound perturbation. The actual density is thus varied as:

$$\rho = \rho_0 + \Delta\rho = \rho_0 - k\psi_0\rho_0 \cos(\omega t - kx) = \rho_0 + k\psi_0\rho_0 \sin(\omega t - kx - \pi/2)$$

The amplitude in the density variation is $(\Delta\rho)_0 = k\rho_0\psi_0$, while the phase shift is $\pi/2$, the quarter of the oscillation. The pressure oscillates with the phase of density:

$$\Delta p = K_{\mathrm{ad}} \frac{\Delta\rho}{\rho_0} = \kappa p_0 k\psi_0 \sin(\omega t - kx - \pi/2)$$

In total:

$$p = p_0 + \Delta p = p_0 + \kappa p_0 k\psi_0 \sin(\omega t - kx - \pi/2)$$

The pressure oscillation amplitude is also proportional to the amplitude of displacements: $(\Delta p)_0 = \kappa k p_0 \psi_0$.

Let's say something about the sound energy. The energy flux density in the flat mechanical wave is $j = P/S = (1/2)\rho\omega^2\psi_0^2 c$. In the case of sound, ρ is the gas density, $\omega = 2\pi\nu$, c is the sound speed, ψ_0 the displacement amplitude; the quantity j is also called the intensity of sound. Take again nitrogen, $p = 1$ bar $= 10^5$ Pa, $T = 273$ K. Let the frequency be $\nu = 1$ kHz, and the intensity $j = 10^{-12}$ W/m^2, this is typically at the threshold of human sound perception. We calculate: $\psi_0 \approx 10^{-11}$ m, $(\Delta\rho)_0 \approx 2 \cdot 10^{-10}$ kg/m^3, $(\Delta p)_0 \approx 3 \cdot 10^{-5}$ Pa $= 3 \cdot 10^{-10}$ bar. These are extremely small values which demonstrate the sensitivity of human ear. By the way, we have also used the relation for the wave vector: $k = 2\pi/\lambda = 2\pi\nu/c$. ♠

♥ EX. 1.20

Displacement in the harmonic wave is: $\psi(x, t) = A\cos[2\pi(x/\lambda - t/T)]$, where λ is the wavelength, and $T = 5$ ms oscillation time. Find positive solutions for time t, such that the displacement at $x = \lambda/4$ has the value $\psi = A/2$.

Let's make an arrangement for ψ at $x = \lambda/4$: $\psi = A\cos(\pi/2 - 2\pi t/T) = A\sin(2\pi t/T)$. Two of the solutions are obtained as:

$$\frac{2\pi t}{T} = \arcsin\frac{\psi}{A} = \arcsin\frac{1}{2}$$

The first solution is: $2\pi t_1/T = \pi/6 \rightarrow t_1 = T/12$, another one is: $2\pi t_2/T = 5\pi/6 \rightarrow t_2 = 5T/12$. All other solution are obtained by adding the integer multiple of oscillation time. For positive solutions we have: $T/12$, $5T/12$, $13T/12$, $17T/12$ … ♠

♥ EX. 1.21

A pair of synchronized sound speakers produces sound with frequency 100 Hz. The speed of sound is 340 m/s. What should be the distance between the sound speakers in order to find the first order sound amplification at the angle 40° with respect to the symmetry axis? What are the angles for amplification of higher orders?

Data:

$\nu = 100$ Hz

$c = 340$ m/s

$\beta_1 = 40°$

$a = ?$

$\beta_2, \ldots = ?$

The task is simple:

$$a \sin\beta_1 = \lambda = \frac{c}{\nu} \to a = \frac{c}{\nu \sin\beta_1} = 5{,}29 \text{ m}$$

Other angles can be calculated directly from the first one:

$$\sin\beta_N = N \sin\beta_1$$

But there no other solutions for our data. This is also seen from:

$$N_{\max} = \frac{a}{\lambda} = \frac{1}{\sin\beta_1} = 1{,}56 \rightarrow 1$$

If we want to have at least the second solution, we should have $\beta_1 < 30°$. ♠

♥ EX. 1.22

Derive the dependence of the light intensity on the angle β with respect to symmetry axis in the Young experiment with N elongated thin slits in equal distances a. Use the expression for the spherical wave from each slit: $\psi_j = \exp(ikr_j)$, $j = 1 - N$, where $k = 2\pi/\lambda$, r_j is the distance between each slit and the point on the screen (Fig. R9).

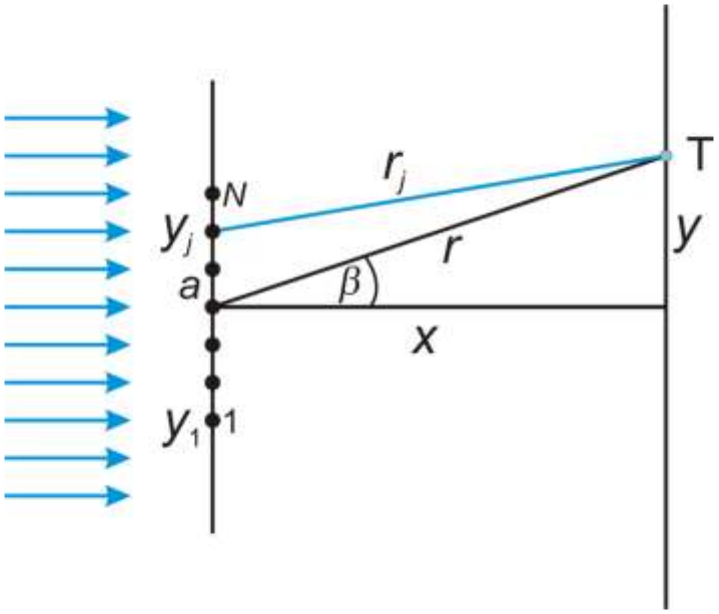


Fig. R9: Geometry of the interference experiment with *N* slits with equal spacing; the slits are shown as point sources of waves (black circles), but in reality they are elongated in the direction perpendicular to the plane of drawing.

The time part of the wave function was omitted since we consider the coherent wave which hits the piece with slits. So the time factor is equal for all the slits and cancels in the final expression for the intensity. The common function for all the slits is (at point T):

$$\psi = \sum_{j=1}^{N} \exp(\mathrm{i}kr_j)$$

In order to simplify the calculation we must write the distances r_j as simply as possible. Let the size of the piece with slits be small as compared to coordinates x and y which determine the point T on the distant screen. Denote: $r = (x^2 + y^2)^{1/2}$. Vertical coordinates with respect to the centre of the piece are denoted by y_j. Continue with r_j:

$$r_j = \sqrt{x^2 + (y - y_i)^2} \approx \sqrt{x^2 + y^2 - 2yy_i} = \sqrt{r^2 - 2yy_i} = r\sqrt{1 - 2yy_i / r^2}$$

We have neglected the smallest term y_i^2. We use the old trick $(1 \pm \varepsilon)^{1/2} \approx 1 \pm \varepsilon/2$:

$$r_j \approx r(1 - yy_j / r^2) = r - y_j \cdot y / r = r - y_j \cdot \sin\beta$$

The wave function is:

$$\psi = \sum_{j=1}^{N} \exp\left[\mathrm{i}k(r - y_j \sin\beta)\right]$$

Summing over the index j can be made simpler if we write all y-coordinates of slits with respect to the coordinate of the first slit: $y_j = y_1 + (j - 1)a$. Go on:

$$\psi = \sum_{j=1}^{N} \exp\left[\mathrm{i}k(r - (y_1 + (j-1)a)\sin\beta)\right] = \exp\left[\mathrm{i}k(r - y_1 \sin\beta)\right] \cdot \sum_{j=1}^{N} \exp\left[-\mathrm{i}ka(j-1)\sin\beta\right]$$

The factor in front of the sum has the absolute value 1 and has no effect on the final results, so we omit it:

$$\psi = \sum_{j=1}^{N} \exp\left[-\mathrm{i}ka(j-1)\sin\beta\right]$$

This is the sum of terms of geometric series: $1 + q + q^2 + \ldots + q^{N-1}$, where $q = \exp(-\mathrm{i}ka \sin\beta)$. This sum is $(q^N - 1)/(q - 1)$, in our case:

$$\psi = \frac{\exp(-N\mathrm{i}ka\sin\beta) - 1}{\exp(-\mathrm{i}ka\sin\beta) - 1}$$

Intensity of light at some place is proportional to the square of the absolute value of the complex wave function. We are not going to deal with the factor of proportionality since the wave function itself was not normalized in an appropriate way. So we prefer to write:

$$I = I_0 \psi\psi^* = I_0 \cdot \frac{\exp(-N\mathrm{i}ka\sin\beta) - 1}{\exp(-\mathrm{i}ka\sin\beta) - 1} \cdot \frac{\exp(+N\mathrm{i}ka\sin\beta) - 1}{\exp(+\mathrm{i}ka\sin\beta) - 1}$$

Multiply and consider Euler, ($\exp(\mathrm{i}z) = \cos z + \mathrm{i}\sin z$), to get:

$$I = I_0 \cdot \frac{2 - 2\cos(Nka\sin\beta)}{2 - 2\cos(ka\sin\beta)}$$

Cancel 2, take $\sin^2\alpha = (1 - \cos(2\alpha))/2$, then $k = 2\pi/\lambda$ and we land at the expression:

$$I = I_0 \cdot \left[\frac{\sin(\frac{1}{2} Nka\sin\beta)}{\sin(\frac{1}{2} ka\sin\beta)} \right]^2 = I_0 \cdot \left[\frac{\sin(N\pi \frac{a}{\lambda} \sin\beta)}{\sin(\pi \frac{a}{\lambda} \sin\beta)} \right]^2$$

Graphs $I(\beta)$ in the case $a = 10\lambda$ and for different numbers of slits N are show on figure bottom. In the case $a \sin\beta = M\lambda$ (M is integer) the denominator for I is zero. This is the known condition for amplification (here we have used M instead of N). Find intensity for these maxima! We encounter the typical problem of division 0/0. So we use L'Hospital rule: in the case of division 0/0 we can separately differentiate nominator and denominator, etc. We prefer to work with $x = a \sin \beta/\lambda$:

$$\lim_{x\to M} \left[\frac{\sin(N\pi x)}{\sin(\pi x)} \right] = \lim_{x\to M} \left[\frac{N\pi\cos(N\pi x)}{\pi\cos(\pi x)} \right] = \frac{N \cdot (-1)^{NM}}{(-1)^{M}}$$

The final result for intensity in maxima is simple: $I = N^2 I_0$. All maxima have equal intensity, but in reality also the width of the slits (neglected here) influences them; in general, the maxima are getting lower for higher M. For very narrow slits, Fig. R10 shows something else: all maxima are increased for larger number of slits N ant they get narrower at the same time; additional small local maxima appear.

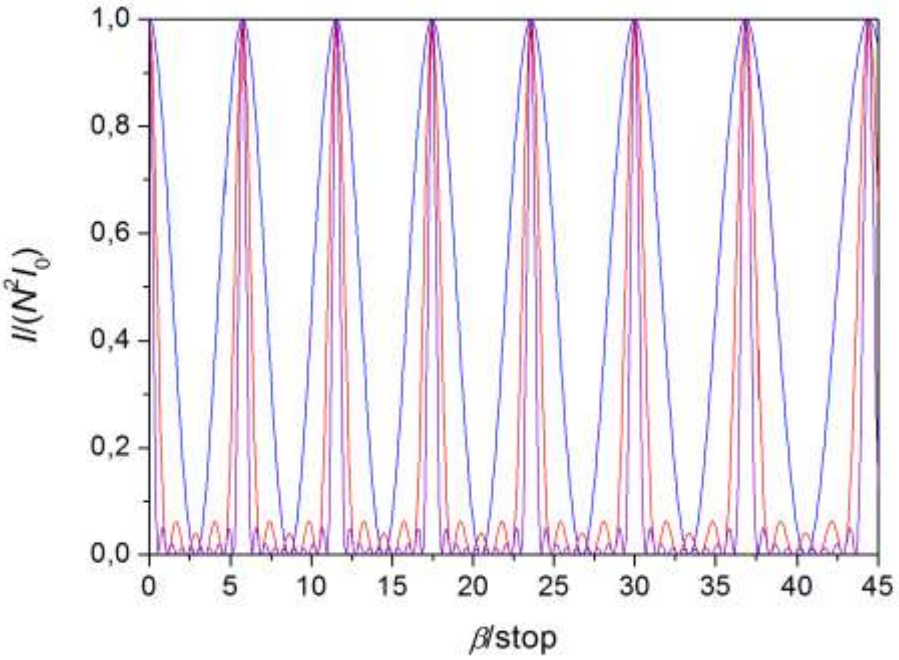


Fig. R10: Graphs of normalized intensity as a function of the angle for three numbers of slits: N = 2 (blue curve), N = 5 (red) and N = 10 (violet). For better comparison all values of intensity were divided by N^2. Comment: “stop” at horizontal axes for the angle β is meant as degrees. ♠

♥ EX. 23

The wave packet can be represented as a sum of several partial waves with slightly different wavelengths and frequencies. Let’s take normalized values of all parameters, so that we write the wave packet with $2n + 1$ partial waves as:

$$\psi = \sum_{i=-n}^{n} \sin[k_i(x - ct)]$$

We also simply take: $k_i = 1 + i\Delta k$, $\Delta k \ll 1$. Suppose there is no dispersion, $c = 1$ independent of k).

Graphs are drawn numerically, with the use of Mathematica or something else. The bottom figure represents the cases with n = 2 (5 partial waves) and n = 5 (11 partial waves); Δk = 0,05. The packets are moving to the right; it is enough to show them at the moment $t = 0$.

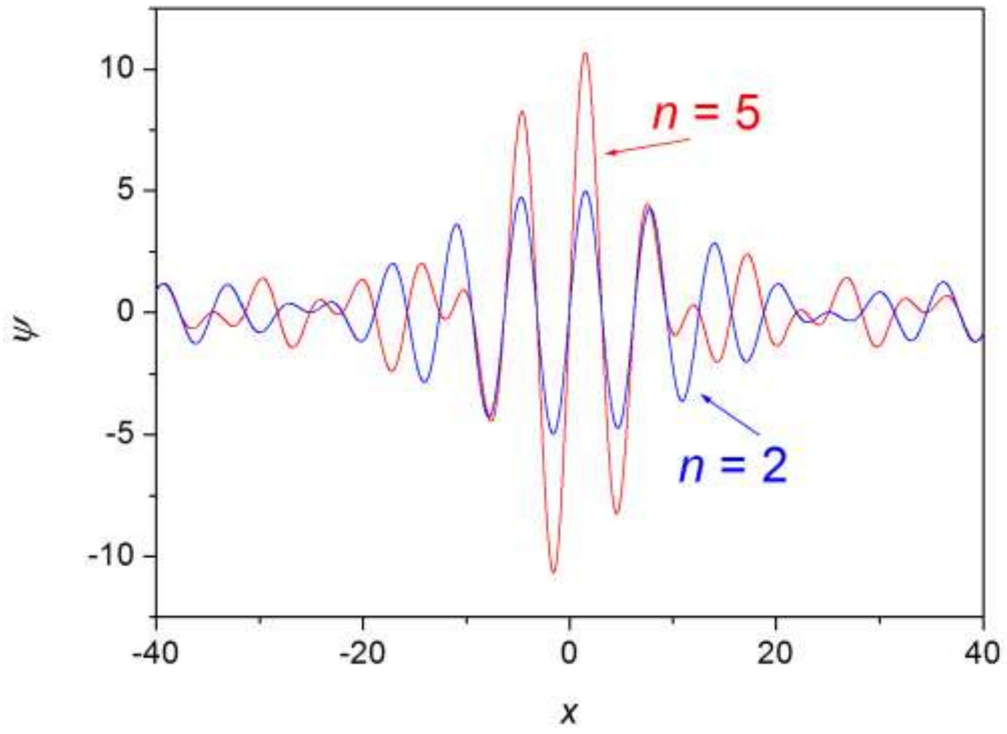


Fig. R11: Two wave packets without dispersion at $t = 0$ ♠

2 PARTICLES, LIGHT, RADIATION AND INTERACTIONS

♥ EX. 2.1

The distribution of some random physical quantity x is described by exponential probability density (Fig. R12): $p(x) = C\exp(-x/x_0)$. Here, x_0 is a characteristic (scale) parameter (with the same physical unit as x), C normalization constant, and the allowed values of x fall in the interval $0 \le x < \infty$. The meaning of the function $p(x)$ is the following: $p(x)\mathrm{d}x$ is a (very small) probability that the value of the variable x chosen randomly will be in the interval $(x, x + \mathrm{d}x)$, supposing $\mathrm{d}x$ to be very small width of the interval. Normalize the function $p(x)$ with the correct value of the constant C. What's the probability for x to be in the interval $0 \le x \le x_0$? What about the interval $x_0 \le x \le 2x_0$? What's the mean value of x? What's the mean value of x^2? What's the standard deviation of x?

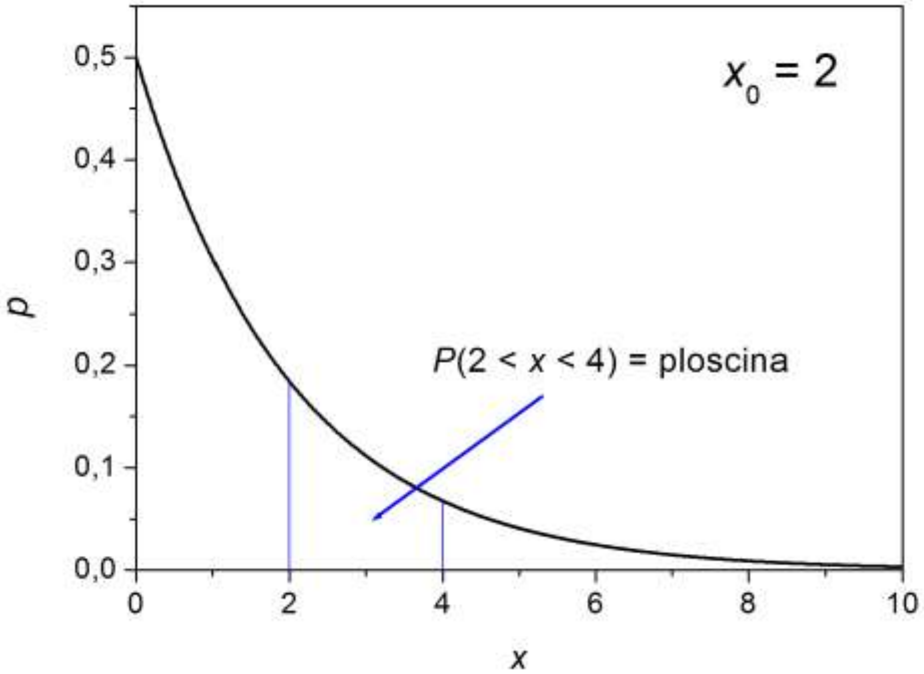


Fig. R12: Exponential distribution function with dimensionless variable x; $x_0 = 2$. Calculation of probability for $x_0 \le x \le 2x_0$ is illuminated. Comment: “ploscina” = area.

Geometrical meaning of given distribution function is sketched on figure. If $p(x)\mathrm{d}x$ is the probability to find x in the small interval, we obtain the probability for broader interval with the integral. For instance, the probability for $a \le x \le b$ is equal to:

$$P(a \le x \le b) = \int_a^b p(x)\mathrm{d}x$$

The probability to find *x* anywhere in the allowed region is equal to 1, thus we normalize integral accordingly. In our case:

$$\int_0^\infty C\exp(-x/x_0)\mathrm{d}x = 1$$

$$-Cx_0\exp(-x/x_0)\Big|_0^\infty = 1$$

$$Cx_0 = 1 \to C = \frac{1}{x_0}$$

According to given definition we can also write $p(x) = \mathrm{d}P/\mathrm{d}x$. Let's calculate the probabilities for the given intervals:

$$P(0 \le x \le x_0) = \frac{1}{x_0}\int_0^{x_0}\exp(-x/x_0)\mathrm{d}x = -\exp(-x/x_0)\Big|_0^{x_0} = 1 - \frac{1}{\mathrm{e}}$$

$$P(x_0 \le x \le 2x_0) = \frac{1}{x_0}\int_{x_0}^{2x_0}\exp(-x/x_0)\mathrm{d}x = -\exp(-x/x_0)\Big|_{x_0}^{2x_0} = \frac{1}{\mathrm{e}} - \frac{1}{\mathrm{e}^2}$$

$$P(x_0 \le x \le 2x_0) = \frac{1}{\mathrm{e}} \cdot P(0 \le x \le x_0)$$

We would obtain similar results for next intervals of width x_0. Average (mean, expected) value of any function $f(x)$ can be calculated with given probability density $p(x)$ by the following integral:

$$< f(x) > = \int_{x_{\mathrm{min}}}^{x_{\mathrm{max}}} f(x)p(x)\mathrm{d}x$$

where x_{min} and x_{max} are the smallest and the biggest allowed value of *x*, respectively. In our case, we are going to express the mean value $<x^n>$ for any natural exponent *n*.

$$< x^n > = \frac{1}{x_0}\int_0^\infty x^n \exp(-\frac{x}{x_0})\mathrm{d}x$$

We use integration per partes: $u = x^n$, $\mathrm{d}v = \exp(-x/x_0)$ → $\mathrm{d}u = nx^{n-1}$, $v = -x_0\exp(-x/x_0)$. So we obtain:

$$< x^n > = \frac{1}{x_0}\left[-x_0 x^n \exp(-\frac{x}{x_0}) \Big|_0^\infty + n x_0 \int_0^\infty x^{n-1} \exp(-\frac{x}{x_0}) \mathrm{d}x \right]$$

The first part is zero at both limits, thus:

$$< x^n > = n x_0 < x^{n-1} >$$

This is a useful recursive relation, so we can proceed in steps: $<x^0> = 1$; $<x> = x_0 \cdot <x^0> = x_0$, $<x^2> = 2x_0 \cdot <x> = 2x_0^2$; $<x^3> = 3x_0 \cdot <x^2> = 6x_0^3$ etc. Standard deviation can be calculated as:

$$\delta x = \sqrt{< x^2 > - < x >^2} = \sqrt{2x_0^{\ 2} - x_0^{\ 2}} = x_0$$

Therefore, here the standard deviation is just equal to the mean value of the variable. ♠

♥ EX. 2.2

The following equation holds for the spectral density of the black-body radiation at temperature T:

$$\frac{\mathrm{d}j}{\mathrm{d}\lambda} = \frac{2\pi h c^2}{\lambda^5 \left(\exp(\frac{hc}{kT\lambda}) - 1 \right)}$$

The meaning of the symbols: j is the light intensity, $j = P/S$, λ is the wavelength, h Planck constant, c speed of light, k Boltzmann constant. The temperature of the star surface is 8000 K. At which wavelength has $\mathrm{d}j/\mathrm{d}\lambda$ maximum? What's the light intensity only in the relatively narrow interval $\lambda_\mathrm{m} \pm 50$ nm around maximum λ_m? What part of the whole spectrum is this?

A warning before solving the problem. The function $\mathrm{d}j/\mathrm{d}\lambda$ has an analogous meaning to the probability density $p(x)$ in previous example, but not quite the same. Integration of $p(x)$ over some interval gives true probability, while the integration of spectral density $\mathrm{d}j/\mathrm{d}\lambda$ over the interval of wavelengths gives the physical quantity j. Thus the unit for spectral density is W/m^3. Of course, appropriate normalization can make some kind of probability density from spectral density, as we will show.

Maximum of spectral density is given by Wien law: $\lambda_\mathrm{m} = k_\mathrm{W}/T = 2{,}9 \cdot 10^{-3}$ m K/(8000 K) = 362 nm. Let's make denotation $\Delta\lambda$ = 50 nm. Intensity j in the area $\lambda_\mathrm{m} \pm 50$ nm can be formally calculated by integral:

$$j = \int_{\lambda_{\mathrm{m}}-\Delta\lambda}^{\lambda_{\mathrm{m}}+\Delta\lambda} (\frac{\mathrm{d}j}{\mathrm{d}\lambda})\mathrm{d}\lambda$$

This must be done numerically since the analytical solution exists only for the entire area (0, ∞), from which also the Boltzmann-Stefan law originates. However, for small interval we can use approximation: $j \approx (\mathrm{d}j/\mathrm{d}\lambda)(\lambda = \lambda_{\mathrm{m}}) \cdot 2\Delta\lambda$. Compare first $\mathrm{d}j/\mathrm{d}\lambda$ for the three key values of wavelength: 312 nm, 362 nm in 412 nm. Let's make a convenient denotation:

$$\frac{\mathrm{d}j}{\mathrm{d}\lambda} = \frac{2\pi(kT)^5}{h^4c^3} \cdot \frac{x^5}{\mathrm{e}^x - 1} \equiv A \cdot \frac{x^5}{\mathrm{e}^x - 1}$$

where $x = hc/(kT\lambda)$. It suffices to observe relative differences in spectral density, i. e., to compare only the expression $x^5/(\mathrm{e}^x - 1)$. This has the values 20,07, 21,20 (at maximum) and 20,37. Just take the average of the three values: 20,55. So, our approximation is justified: $j = 20{,}55 \cdot A \cdot 100\ \mathrm{nm} = 4{,}13 \cdot 10^7\ \mathrm{W/m^2}$. The whole intensity is: $j_{\mathrm{tot}} = \sigma T^4 = 2{,}32 \cdot 10^{10}\ \mathrm{W/m^2}$. The corresponding ratio is $j/j_{\mathrm{tot}} = 1{,}78 \cdot 10^{-3}$. If the spectral density is divided by j_{tot}, we really obtain the probability distribution:

$$p_\lambda(\lambda) = \frac{2\pi hc^2}{\sigma T^4\lambda^5\left(\exp(\frac{hc}{kT\lambda}) - 1\right)}$$

so that it also holds:

$$\int_0^\infty p_\lambda(\lambda)\mathrm{d}\lambda = 1$$

Finally, we mention that the distribution function over frequencies (instead over wavelengths) are not correctly obtained simply by substitution $\lambda = c/\nu$ in the function $p_\lambda(\lambda)$. Instead, we make transformation $p_\lambda(\lambda) \rightarrow p_\nu(\nu)$ with the following trick:

$$p_\nu(\nu) = \frac{dP}{d\nu} = \frac{dP}{d\lambda} \cdot \left|\frac{d\lambda}{d\nu}\right| = p_\lambda(\lambda) \cdot \left|\frac{d(c/\nu)}{d\nu}\right| = p_\lambda(\lambda) \cdot \frac{c}{\nu^2} = p_\lambda(\frac{c}{\nu}) \cdot \frac{c}{\nu^2}$$

Thus the substitution $\lambda = c/\nu$ must be accompanied by multiplication of p_λ with the factor c/ν^2. The result is:

$$p_\nu(\nu) = \frac{2\pi h\nu^3}{\sigma T^4c^2\left(\exp(\frac{h\nu}{kT}) - 1\right)}$$

so that it holds:

$$\int_0^\infty p_\nu(\nu)\mathrm{d}\nu = 1$$ ♠

♥ EX. 2.3

Energy of the photon with wavelength λ is $E_\mathrm{f} = hc/\lambda$, and the energy flux of the monochromatic light of wavelength 500 nm is 500 W/m^2. How many photons strike in time 1 min the screen with area 1 cm^2, which is perpendicular to the light beam? What amplitude of the electric field and magnetic field corresponds to this electromagnetic wave?

Data:

$\lambda = 500$ nm

$j = 500$ W/m^2

$S = 1$ cm^2

$t = 60$ s

$N = ?$

$E_0 = ?$

$B_0 = ?$

Number of photons is the ratio between the whole incident energy within time t and the energy of a single photon:

$$N = \frac{E}{E_\mathrm{f}} = \frac{jSt}{hc/\lambda} = \frac{jSt\lambda}{hc} = 7{,}6 \cdot 10^{18}$$

Amplitude of electric field is denoted by E_0; we must not confuse it with energy. We have: $j = \varepsilon_0 E_0^2 c/2$, with $\varepsilon_0 = 8{,}85 \cdot 10^{-12}$ A s/V m. So:

$$E_0 = \sqrt{\frac{2j}{\varepsilon_0 c}} = 614 \text{ V/m}$$

For magnetic field we use:

$$B_0 = \frac{E_0}{c} = 2{,}05 \cdot 10^{-6} \text{ Vs/m}^2 = 2{,}05 \ \mu\text{T}$$ ♠

♥ EX. 2.4

Use dimensional analysis to derive the relation between light speed c and constants $\varepsilon_0 = 8{,}85 \cdot 10^{-12}$ A s/(V m) and $\mu_0 = 4\pi \cdot 10^{-7}$ V s/(A m). Dimensional analysis in general does not provide also additional dimensionless numerical factor, but this turns out to be just 1 in our case. Calculate light speed numerically.

Use the typical setting: $c = \varepsilon_0^{\,x} \cdot \mu_0^{\,y}$, where x and y are still unknown exponents. We insert in the equation the physical units for these quantities:

$$\frac{\mathrm{m}}{\mathrm{s}} = \left(\frac{\mathrm{As}}{\mathrm{Vm}}\right)^{x} \cdot \left(\frac{\mathrm{Vs}}{\mathrm{Am}}\right)^{y}$$

From this it is easily evident that both exponents are equal, so that the units A and V on the right side of equation cancel. Comparison of units m and s in both sides of equation then shows: $x = y = -1/2$. Thus we obtain:

$$c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} = 3 \cdot 10^{8}\ \mathrm{m/s}$$

We mention that today the constants c and μ_0 are defined mathematically exact (the unit meter was redefined), while ε_0 can be calculated from them optionally accurately.♠

♥ EX. 2.5

“Knockout work” for electrons in some metal is 2 eV (eV = $1{,}6 \cdot 10^{-19}$ J). What is the corresponding limiting wavelength λ_m of photons? This metal is illuminated with the light of wavelength tri times smaller than the limiting value. What’s the speed of the fastest knocked electrons? What’s the ration between energy of photons and kinetic energy of electrons? What’s the ratio of their linear momenta? What stopping voltage prevents the electrons from reaching opposite electrode?

Data:

$\Phi = 2\ \mathrm{eV} = 3{,}2 \cdot 10^{-19}\ \mathrm{J}$

$\lambda = \lambda_\mathrm{m}/3$

$m = 9{,}1 \cdot 10^{-31}\ \mathrm{kg}$

$\lambda_\mathrm{m} = ?$

$v = ?$

$E_{\text{f}}/E_{\text{kin}} = ?$

$p_{\text{f}}/p_{\text{e}} = ?$

$U_{\text{zap}} = ?$

Limiting wavelength of photons corresponds to zero kinetic energy of knocked electrons. Thus it holds: $hc/\lambda_{\text{m}} = \Phi$, so that $\lambda_{\text{m}} = hc/\Phi = 620$ nm. Photons with 3–times smaller wavelength have triple energy: $E_{\text{f}} = 6$ eV. So, there remains kinetic energy $E_{\text{kin}} = 4$ eV for electrons. Therefore, the ratio of corresponding energies is $E_{\text{f}}/E_{\text{kin}} = 1{,}5$. Electrons with kinetic energy 4 eV are stopped with the voltage $U_{\text{zap}} = 4$ V (there's no need to transform energy units!). But to calculate the speed we must of course take kinetic energy in joules:

$$E_{\text{kin}} = \frac{mv^2}{2} \rightarrow v = \sqrt{\frac{2E_{\text{kin}}}{m}} = 1{,}2 \cdot 10^6 \text{ m/s}$$

Finally the momenta:

$$\frac{p_{\text{f}}}{p_{\text{e}}} = \frac{E_{\text{f}}/c}{mv} = 3 \cdot 10^{-3}$$

Although the photon has larger energy than the kinetic energy of electron, its momentum is much smaller. These are very different particles. The story is more educative if it's connected with special theory of relativity. The rest energy of particle with mass m is $E_0 = mc^2$. The electron momentum can be expressed so: $p_{\text{e}} = mv$ in $E_{\text{k}} = mv^2/2 \rightarrow p_{\text{e}} = (2mE_{\text{k}})^{1/2}$.

The ration of momenta will be now expressed slightly differently from above:

$$\frac{p_{\text{f}}}{p_{\text{e}}} = \frac{E_{\text{f}}}{c\sqrt{2mE_{\text{kin}}}} = \sqrt{\frac{E_{\text{f}}^{\ 2}}{2mc^2 E_{\text{kin}}}} = \sqrt{\frac{1}{2}\left(\frac{E_{\text{f}}}{E_{\text{kin}}}\right)\left(\frac{E_{\text{f}}}{E_0}\right)}$$

If the energies E_{f} and E_{kin} are of the same order, as it holds in our case, then the ratio of momenta is given mainly by the ratio of photon energy and electron rest energy, E_{f}/E_0. Electron rest energy is $E_0 \sim 0{,}5$ MeV, much more than $E_{\text{f}} = 6$ eV. ♠

♥ EX. 2.6

The total (kinetic and rest) energy of relativistic particle is twice its rest energy. What's its momentum and speed?

Einstein equation holds :

$$E^2 = (2mc^2)^2 = (mc^2)^2 + p^2c^2$$

Momentum is thus:

$$p = \sqrt{3}mc$$

The speed can be calculated from equation for energy, $E = \gamma mc^2$, or from equation for momentum, $p = \gamma mv$, with relativistic factor:

$$\gamma = \frac{1}{\sqrt{1-(v/c)^2}}$$

It's a little easier to use energy equation:

$$E = \frac{mc^2}{\sqrt{1-(v/c)^2}} \rightarrow v = c\sqrt{1-(\frac{mc^2}{E})^2} = \frac{\sqrt{3}}{2}c \approx 86{,}6\ \%\ c$$ ♠

♥ EX. 2.7

In Compton scattering of the photon of X rays with wavelength 0,1 nm on practically still electron the wavelength of the photon is increased by $\Delta\lambda = \lambda_C(1 - \cos\theta)$, depending on the angle. Compton wavelength in upper equation is λ_C = 2,43 pm. What's the change of the wavelength for the angles θ = 45°, 90° and 180°? Calculate also the speed of electron after collision (you can use non-relativistic kinetic energy). Use differential in calculation of the change of the energy of the photon since the relative change of its wavelength is small.

We express separately the change of the wavelength for the angle θ = 90°: $\Delta\lambda = \lambda_C$ = 2,43 pm. For 180° the change is twice as large, but for 45° it is smaller: $\Delta\lambda \approx 0{,}293\ \lambda_C$ = 0,71 pm. Kinetic energy of electron after collision is:

$$E_{\mathrm{kin}} = |\Delta E_{\mathrm{f}}| \approx \left|\frac{\mathrm{d}E_{\mathrm{f}}}{\mathrm{d}\lambda}\right| \cdot \Delta\lambda = \left|\frac{\mathrm{d}(hc/\lambda)}{\mathrm{d}\lambda}\right| \cdot \Delta\lambda = \frac{hc\Delta\lambda}{\lambda^2}$$

The corresponding speed is:

$$v = \sqrt{\frac{2E_{\mathrm{kin}}}{m_{\mathrm{e}}}} = \sqrt{\frac{2hc\Delta\lambda}{m_{\mathrm{e}}\lambda^2}} = \sqrt{\frac{2hc\lambda_C(1-\cos\theta)}{m_{\mathrm{e}}\lambda^2}}$$

Use also $\lambda_C = h/(m_e c)$:

$$v = \frac{h}{m_\mathrm{e}\lambda} \cdot \sqrt{2(1 - \cos\theta)}$$

This speed has maximum for central collision, $\theta = 180°$:

$$v_\mathrm{max} = \frac{2h}{m_\mathrm{e}\lambda} = 1{,}46 \cdot 10^{7}\ \mathrm{m/s}$$

This is about $c/20$, still in the non-relativistic domain. For 90° the electron speed is $1{,}03 \cdot 10^{7}$ m/s, for 45° it is $5{,}57 \cdot 10^{6}$ m/s. ♠

3 BASIC IDEAS OF QUANTUM MECHANICS

♥ EX. 3.1

The vector in Hilbert space is $\boldsymbol{x} = (1 + \mathrm{i}, 1 - \mathrm{i}, 1, \mathrm{i})$. Calculate its magnitude. The second vector is $\boldsymbol{y} = (1 - \mathrm{i}, \mathrm{i}, \mathrm{i}, y_4)$. What should be its component y_4, in order for the vectors to be orthogonal?

The square of vector magnitude is written in formal mathematical form:

$$< x|x > = [1-\mathrm{i} \quad 1+\mathrm{i} \quad 1 \quad -\mathrm{i}] \cdot \begin{bmatrix} 1+\mathrm{i} \\ 1-\mathrm{i} \\ 1 \\ \mathrm{i} \end{bmatrix} = 2+2+1+1=6$$

Thus $x = 6^{1/2}$. Vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ are orthogonal when:

$$< x|y > = [1-\mathrm{i} \quad 1+\mathrm{i} \quad 1 \quad -\mathrm{i}] \cdot \begin{bmatrix} 1-\mathrm{i} \\ \mathrm{i} \\ \mathrm{i} \\ y_4 \end{bmatrix} = (1-\mathrm{i})^2 + (1+\mathrm{i})\mathrm{i} + \mathrm{i} - \mathrm{i}y_4 = 0$$

This holds when $y_4 = \mathrm{i}$. ♠

♥ EX. 3.2

Find all 5 complex solutions of equation $z^5 = 1$. Write the program for numerical solving of this equation with Newton method, if we start with optional complex starting point $z_0 = x_0 + \mathrm{i}y_0$. Iteration for the next complex approximation z_{n+1} from previous one, z_n, is calculated as:

$$z_{n+1} = \frac{4z_n^{\;5} + 1}{5z_n^{\;4}} = \frac{1}{5}(4z_n + \frac{1}{z_n^{\;4}})$$

Write this separately for real and imaginary component. Check towards which of the 5 solutions the iterative procedure converges for chosen initial point z_0.

Eq. $z^5 = 1$ can be written in polar form, and we also know that the absolute value of the solution is equal to 1. So $z = \exp(\mathrm{i}\varphi)$, and the polar equation is: $\exp(5\mathrm{i}\varphi) = 1 = \exp(2\pi)$. For one of the solutions we just take $\varphi_1 = 2\pi/5$, while for others (including trivial solution $z = 1$) we take the integer multiple of this angle. Solutions ξ_j ($j = 1 – 5$) are therefore:

$$\xi_j = \exp(j \cdot \frac{2\pi}{5} \mathrm{i}) = \cos(j \cdot \frac{2\pi}{5}) + \mathrm{i} \cdot \sin(j \cdot \frac{2\pi}{5})$$

If the approximation is written as $z_n = a_n + \mathrm{i}b_n$, then the upper iteration equation gives:

$$a_{n+1} = \frac{1}{5}(4a_n + \frac{\cos(4\varphi_n)}{(a_n{}^2 + b_n{}^2)^2})$$

$$b_{n+1} = \frac{1}{5}(4b_n - \frac{\sin(4\varphi_n)}{(a_n{}^2 + b_n{}^2)^2})$$

with

$$\varphi_n = \arctan \frac{b_n}{a_n}$$

But we must take care that the »phase« φ_n really corresponds to right quadrant of the number z_n in complex plane, according to signs of components a_n and b_n.

We mention as an interesting point that by using the upper method a beautiful fractal sample (with 5 extensions in our case) can be drawn. The trick is simple: according to the final solution ξ_j to which the iteration converges for given initial z_0, we paint the point that corresponds to z_0 in complex plane with one of the 5 colors. The fractal is shown on Fig. R13.

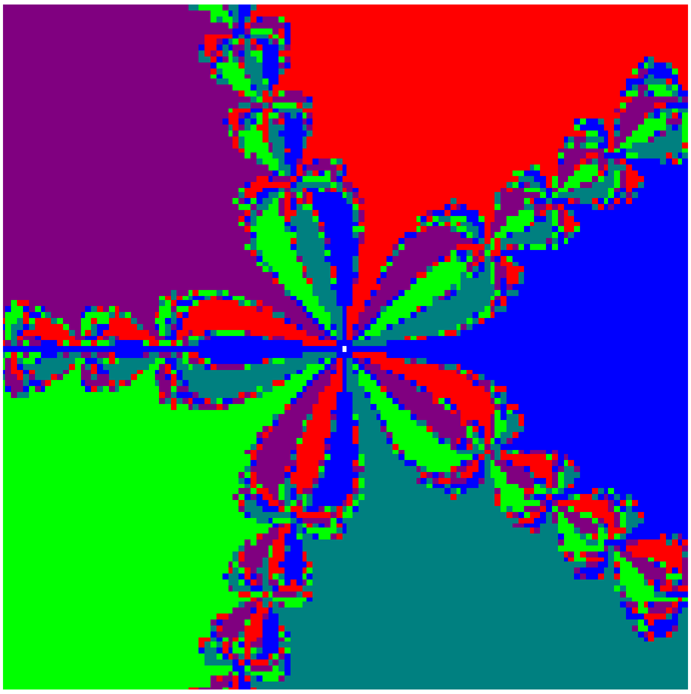


Fig. R13: 5-fold fractal ♠

♥ EX. 3.3

What are the eigenvalues, determinant and trace of rotational matrix and the matrix of mirroring across the plane? Use concrete examples.

Since it is known that the eigenvalues of the true tensor of second rank are independent of the choice of coordinate system, we can take the simplest case for both cases. Let the rotational matrix rotate around *z*-axis by angle φ:

$$R = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

All the three complex eigenvalues are found by setting to zero the determinant of “shifted” matrix, $\det(R - \lambda \mathrm{I}) = 0$:

$$\begin{vmatrix} \cos\varphi - \lambda & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi - \lambda & 0 \\ 0 & 0 & 1-\lambda \end{vmatrix} = 0$$

This results in simple cubic equation:

$$(1-\lambda)\left[(\cos\varphi-\lambda)^2+\sin^2\varphi\right]=0$$

or:

$$(1-\lambda)\left[\lambda^2-2\cos\varphi\cdot\lambda+1\right]=0$$

Its solutions are:

$$\lambda_1=1$$

$$\lambda_{2,3}=\cos\varphi\pm i\sin\varphi$$

The first eigenvalue, $\lambda_1 = 1$, has obvious meaning: vectors that are on rotational axis (in our case z), are left unchanged. Second and third eigenvalues are complex, except for $\varphi = 0$ (trivial unit matrix) and $\varphi = \pi$ (rotation by angle 180°).

The determinant is the product of eigenvalues: $\det R = \lambda_1\lambda_2\lambda_3 = 1$. The trace can be calculated either as the sum of diagonal elements or as the sum of eigenvalues (what always comes out the same): $\mathrm{sl}\, R = 1 + 2\cos\varphi$.

Simple mirror matrix reflects over the plane (x, y), so only the coordinate z of any vector changes sign:

$$Z=\begin{bmatrix}1&0&0\\0&1&0\\0&0&-1\end{bmatrix}$$

The matrix is diagonal and eigenvalues are just diagonal elements: $\lambda_1 = \lambda_2 = 1$, $\lambda_3 = -1$. Determinant is –1 and so is the trace. ♠

♥ EX. 3.4

What do we get if there act on some 3D vector one after one two matrices: R from previous example and matrix A below? Is the order of operating of both matrices on the vector relevant? For additional evidence use some simple vector.

$$A=\begin{bmatrix}-2&0&0\\0&-2&0\\0&0&-2\end{bmatrix}$$

If two matrices commute, i.e., if it holds *AR* = *RA*, then the order of operating of them is not relevant. Our matrix *A* is not only diagonal, but also all its diagonal elements are equal; thus we call it scalar matrix. This means: if the vector is multiplied by it, it is the same as if the vector is multiplied by the scalar (in our case −2). Matrix *A* thus increases the magnitude of any vector by factor 2, but it also turns its direction to opposite side due to minus sign. We can easily check by matrix multiplication that scalar matrices like A commute with all matrices. Therefor the order of acting both matrices is in our case not relevant. Matrices *R* and *A* work so that they rotate it by angle φ around axis *z*, then elongate it by factor 2, and at last turn it to opposite direction (order of these three operations doesn't matter).

Let's take the vector: $\vec{a} = (1,0,0)$. Make operations on it:

$$R\vec{a} = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos\varphi\cdot 1 + (-\sin\varphi)\cdot 0 + 0\cdot 0 \\ \sin\varphi\cdot 1 + \cos\varphi\cdot 0 + 0\cdot 0 \\ 0\cdot 1 + 0\cdot 0 + 0\cdot 0 \end{bmatrix} = \begin{bmatrix} \cos\varphi \\ \sin\varphi \\ 0 \end{bmatrix}$$

$$A(R\vec{a}) = \begin{bmatrix} -2 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -2 \end{bmatrix} \cdot \begin{bmatrix} \cos\varphi \\ \sin\varphi \\ 0 \end{bmatrix} = \begin{bmatrix} -2\cos\varphi \\ -2\sin\varphi \\ 0 \end{bmatrix}$$

♠

♥ EX. 3.5

Prove that rotational matrix preserves the scalar product of transformed vectors.

Let's choose again the simplest representation of the rotational matrix:

$$R = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Multiply by it both vectors:

$$R\vec{a} = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} a_x \\ a_y \\ a_z \end{bmatrix} = \begin{bmatrix} \cos\varphi\cdot a_x - \sin\varphi\cdot a_y \\ \sin\varphi\cdot a_x + \cos\varphi\cdot a_y \\ a_z \end{bmatrix}$$

$$R\vec{b} = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} b_x \\ b_y \\ b_z \end{bmatrix} = \begin{bmatrix} \cos\varphi \cdot b_x - \sin\varphi \cdot b_y \\ \sin\varphi \cdot b_x + \cos\varphi \cdot b_y \\ b_z \end{bmatrix}$$

The scalar product of them is:

$$R\vec{a} \cdot R\vec{b} = \begin{bmatrix} \cos\varphi \cdot a_x - \sin\varphi \cdot a_y & \sin\varphi \cdot a_x + \cos\varphi \cdot a_y & a_z \end{bmatrix} \cdot \begin{bmatrix} \cos\varphi \cdot b_x - \sin\varphi \cdot b_y \\ \sin\varphi \cdot b_x + \cos\varphi \cdot b_y \\ b_z \end{bmatrix}$$

$$R\vec{a} \cdot R\vec{b} = a_x b_x + a_y b_y + a_z b_z = \vec{a} \cdot \vec{b}$$

The reader is invited to check details. ♠

♥ RAČUNSKI ZGLED 3.6

To which matrix corresponds the sequential operation of rotation first by angle φ_1, and then by angle φ_2, both around axis x?

Let the new matrix be named X. We guess that this is the rotational matrix corresponding to angle $\varphi_1 + \varphi_2$ around x, but let's prove this formally by multiplication of matrices:

$$\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi_1 & -\sin\varphi_1 \\ 0 & \sin\varphi_1 & \cos\varphi_1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi_2 & -\sin\varphi_2 \\ 0 & \sin\varphi_2 & \cos\varphi_2 \end{bmatrix}$$

We quickly see that $x_{11} = 1$, $x_{12} = x_{13} = x_{21} = x_{31} = 0$. Let's check the right bottom 2 × 2 part of X. Because of similarity it suffices to check only 2 components of 4:

$$x_{22} = \cos\varphi_1 \cdot \cos\varphi_2 - \sin\varphi_1 \cdot \sin\varphi_2 = \cos(\varphi_1 + \varphi_2)$$

$$x_{32} = \sin\varphi_1 \cdot \cos\varphi_2 + \cos\varphi_1 \cdot \sin\varphi_2 = \sin(\varphi_1 + \varphi_2)$$

So X is:

$$X = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\varphi_1 + \varphi_2) & -\sin(\varphi_1 + \varphi_2) \\ 0 & \sin(\varphi_1 + \varphi_2) & \cos(\varphi_1 + \varphi_2) \end{bmatrix}$$

and really corresponds to rotation by $\varphi_1 + \varphi_2$ around axis x. ♠

♥ EX. 3.7

Prove in general (also for two different rotational axes in 3D space) that the product of two rotational matrices is again rotational matrix. Next, calculate to which rotation (axis and angle) corresponds the following sequence of operation of two matrices on any vector: first rotation by 30° around axis x and then rotation by 45° around axis z (both rotations are in positive sense).

There are two fundamental characteristics of every rotational matrix: 1) preserves the scalar product of transformed vectors 2) its determinant is 1.From these two properties all other follow, e.g., that one of the eigenvalues is 1. Take two rotational matrices R_1 and R_2 and any two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$. The product of matrices is $R = R_1R_2$. Check the scalar product: $R\boldsymbol{a} \cdot R\boldsymbol{b} \equiv (R\boldsymbol{a}, R\boldsymbol{b})$. Use the fact that R_1 in R_2 do satisfy the required condition:

$$(R\boldsymbol{a}, R\boldsymbol{b}) = (R_1R_2\boldsymbol{a}, R_1R_2\boldsymbol{b}) = (R_1(R_2\boldsymbol{a}), R_1(R_2\boldsymbol{b})) = (R_2\boldsymbol{a}, R_2\boldsymbol{b}) = (\boldsymbol{a}, \boldsymbol{b}).$$

In the intermediate step we took the fact that $R_2\boldsymbol{a}$ and $R_2\boldsymbol{b}$ are just vectors as all other, so that the matrix R_1 must preserve the scalar product.

The proof of the second rule is even simpler: $\det(R) = \det(R_1R_2) = \det(R_1) \cdot \det(R_2) = 1 \cdot 1 = 1$.

Now, let’s take the suggested examples:

$$R_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\frac{\pi}{6} & -\sin\frac{\pi}{6} \\ 0 & \sin\frac{\pi}{6} & \cos\frac{\pi}{6} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \end{bmatrix}$$

$$R_2 = \begin{bmatrix} \cos\frac{\pi}{4} & -\sin\frac{\pi}{4} & 0 \\ \sin\frac{\pi}{4} & \cos\frac{\pi}{4} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

We must take the correct sequence of factors: $R = R_2R_1$; this is, because: $R\boldsymbol{a} = (R_2R_1)\boldsymbol{a} = R_2(R_1\boldsymbol{a})$.

Let’s calculate the product:

$$R = R_2 R_1 = \begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \end{bmatrix} = \begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{6}}{4} & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{6}}{4} & -\frac{\sqrt{2}}{4} \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \end{bmatrix}$$

How can the angel of rotation and the rotational axis be calculated from this? In Ex. 3.3 we have found that the trace of rotational matrix is: sl $R = 1 + 2\cos\varphi$. So we see that the angle can be calculated directly from the trace:

$$\varphi = \arccos\left[\frac{1}{2}(slR - 1)\right] = \arccos\left[\frac{1}{2}\left(\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{3}}{2} - 1\right)\right] = 53{,}65^\circ$$

It’s good to comment different solutions for φ. Because cosine function is even, we could also take the angle with opposite sign, but in 3D space this is the same as turn the axis of rotation to opposite direction. So the angle can always be limited to interval $0 \le \varphi \le \pi$, but we must then take care for correct orientation of the axis of rotation.

This axis corresponds to eigenvectors with eigenvalue $\lambda = 1$. These vectors differ in size and in the possibility of opposite directions. So we’ll choose the vector with magnitude 1. We write $R\mathbf{x} = \lambda\mathbf{x} = \mathbf{x}$ in full matrix form:

$$\begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{6}}{4} & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{6}}{4} & -\frac{\sqrt{2}}{4} \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Write this in a different way:

$$\begin{bmatrix} \frac{\sqrt{2}}{2} - 1 & -\frac{\sqrt{6}}{4} & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{6}}{4} - 1 & -\frac{\sqrt{2}}{4} \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} - 1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

This is homogeneous system of linear equations for unknowns x_1, x_2 and x_3. In order to obtain non-trivial solution the determinant of the matrix should be zero. But we already know that $\det(R - \lambda I) = 0$ really holds. The three equations are then not independent (in practice the two of them are sufficient), and also x_1, x_2 and x_3 are not unique (in practice we can choose one of unknowns). Let’s choose $x_3 = 1$, and consider only the 1st and 3rd equation (the 2nd is ignored):

$$(\frac{\sqrt{2}}{2}-1)x_1-\frac{\sqrt{6}}{4}x_2+\frac{\sqrt{2}}{4}\cdot 1=0$$

$$\frac{1}{2}x_2+(\frac{\sqrt{3}}{2}-1)\cdot 1=0$$

Calculate x_2:

$$x_2=2-\sqrt{3}$$

Then calculate x_1:

$$x_1=\frac{2\sqrt{2}-\sqrt{6}}{2-\sqrt{2}}=\frac{(2\sqrt{2}-\sqrt{6})(2+\sqrt{2})}{(2-\sqrt{2})(2+\sqrt{2})}=2+2\sqrt{2}-\sqrt{3}-\sqrt{6}$$

Our vector at the moment is:

$$\vec{x}=(2+2\sqrt{2}-\sqrt{3}-\sqrt{6},2-\sqrt{3},1)$$

Let’s normalize it to unit magnitude:

$$\vec{x}_N=\frac{(x_1,x_2,x_3)}{\sqrt{x_1{}^2+x_2{}^2+x_3{}^2}}$$

In our case:

$$\vec{x}_N=\frac{1}{\sqrt{29+14\sqrt{2}-16\sqrt{3}-8\sqrt{6}}}\cdot(2+2\sqrt{2}-\sqrt{3}-\sqrt{6},2-\sqrt{3},1)$$

Let’s write it in decimals: $\boldsymbol{x}_{\mathrm{N}} \approx (0{,}53,\ 0{,}22,\ 0{,}82)$.

But we are still not certain if the true vector giving correctly the axis is just the opposite of this (i.e., all the components change sign). Be more explicit: positive direction of rotational axis is the following one: if we look in the direction along the axis form “above”, i.e., form positive half-axis to negative half-axis, we see the rotation of vectors in projection plane in counter-clockwise direction by acute angle 53,65°.

One way of checking is to choose some vector $\boldsymbol{a}$, perpendicular to vector $\boldsymbol{x}_{\mathrm{N}}$, for what we have, of course, infinite number of possibilities. For instance, we choose components $a_x = 1$, $a_y = 0$, then we find a_z to make the scalar product zero. We obtain $\boldsymbol{a} \approx (1,\ 0,\ -0{,}65)$. We don’t need to normalize it. Then we calculate:

$$\vec{b} = R\vec{a} = \begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{6}}{4} & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{6}}{4} & -\frac{\sqrt{2}}{4} \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \\ -0{,}65 \end{bmatrix} = \begin{bmatrix} 0{,}48 \\ 0{,}94 \\ -0{,}56 \end{bmatrix}$$

Then we find the vector product:

$$\vec{c} = \vec{a} \times \vec{b} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ 1 & 0 & -0{,}65 \\ 0{,}48 & 0{,}94 & -0{,}56 \end{vmatrix} = \begin{bmatrix} 0{,}61 \\ 0{,}25 \\ 0{,}94 \end{bmatrix}$$

According to Fig. R14 the vector ***c*** which is perpendicular to both vectors , ***a*** in ***b***, should be parallel to vector $\boldsymbol{x}_\mathrm{N}$ on rotational axis. This means: ***c*** is directed either in the same or in opposite direction as $\boldsymbol{x}_\mathrm{N}$; if the direction is the same, we have written $\boldsymbol{x}_\mathrm{N}$ correctly, in other case we must multiply it by −1. As we see, vectors $\boldsymbol{x}_\mathrm{N}$ and ***c*** really point in the same direction since all the components of both vectors are positive. To be 100 % sure, we show that all components are in the same ratio: $c_x/x_{\mathrm{N}x} \approx 1{,}15$, $c_y/x_{\mathrm{N}y} \approx 1{,}14$, $c_z/x_{\mathrm{N}z} \approx 1{,}15$. Everything matches, the small difference is only due to rounding of real numbers.

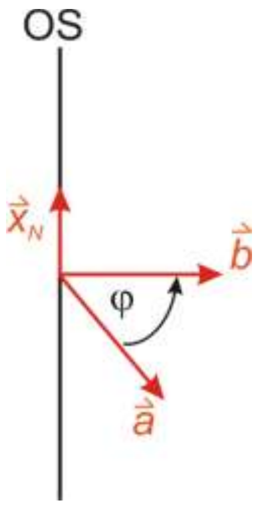


Fig. R14: Vector $\boldsymbol{x}_\mathrm{N}$ in direction of rotational axis and the rotation of perpendicular vector ***a*** to the vector ***b***. It holds: $\boldsymbol{a} \times \boldsymbol{b} \,||\, \boldsymbol{x}_\mathrm{N}$. You must imagine the figure in 3D. ♠

♥ EX. 3.8

Treat the problem of rotation of coordinate axes around *z* axis of »old« Cartesian coordinate system where the physical vectors remain unchanged. But since the axes i *x* and *y* are rotated, both components of the with respect to “new” axes must change. Nothing changes in *z* direction, thus 2D system can be taken. Let the axes *x* and *y* be rotated by $\varphi = \pi/6$ v positive direction, i.e., counter-clockwise. Derive the transformation matrix from beginning, without using the rotation matrices treated before. Check the operation of this matrix on unit vectors ***a*** = (1, 0), ***b*** = (0, 1) and ***c*** = (1/2)($3^{1/2}$, 1). Give the interpretation of mathematical equivalence of matrices corresponding to physical rotation of vectors themselves and rotation of coordinate axes.

Rotation of coordinate axes is shown on Fig. R15. The initial system is denoted by *S*, and the rotated system by *S*'. Unit vectors on old axes are ***i*** and ***j***, and those on new axes ***e*** and ***f***. According to old system *S* these four vectors are written with such components: ***i*** = (1, 0), ***j*** = (0, 1), ***e*** = (cos φ, sin φ), ***f*** = (–sin φ, cos φ). Let's take some vector ***v*** = (*x*, *y*) according to *S*. Transformation of this vector into vector ***v***' = (*x*', *y*') according to *S*' is most easily found if we calculate the new components as orthogonal projections of the vector on new axes:

$$x' = \boldsymbol{e} \cdot \boldsymbol{v} = (\cos\varphi, \sin\varphi) \cdot (x, y) = (\cos\varphi)x + (\sin\varphi)y$$

$$y' = \boldsymbol{f} \cdot \boldsymbol{v} = (-\sin\varphi, \cos\varphi) \cdot (x, y) = (-\sin\varphi)x + (\cos\varphi)y$$

Both relations can be written in the form: ***v***' = *T****v***, where the transformation matrix is:

$$T = \begin{bmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{bmatrix}$$

Matrix *T* is very similar to rotation matrix in 2D space:

$$R = \begin{bmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{bmatrix}$$

This relation is tight – matrices are inverse matrices to each other: $T = R^{-1}$. Geometric meaning of this is evident on Fig. R15: *T* is in fact also rotation matrix (we have used different letter *T* only to stress that it is not about physical rotation of vectors). If, for instance, we rotate *x* axis by angle φ in counter-clockwise direction, the projection of some vector on this axis (what's the same as the component *x*) is the same as if the *x* axis was left intact and the vector itself was rotated instead to opposite direction. That's why the matrices *T* are *R* inverse to each other.

The picture is even clearer if the general vector is written as: ***v*** = (cos α, sin α). Let's see how the matrices change it:

$$T\vec{v} = \begin{bmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{bmatrix} \cdot \begin{bmatrix} \cos\alpha \\ \sin\alpha \end{bmatrix} = \begin{bmatrix} \cos\varphi\cos\alpha + \sin\varphi\sin\alpha \\ -\sin\varphi\cos\alpha + \cos\varphi\sin\alpha \end{bmatrix} = \begin{bmatrix} \cos(\alpha-\varphi) \\ \sin(\alpha-\varphi) \end{bmatrix}$$

$$R\vec{v} = \begin{bmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{bmatrix} \cdot \begin{bmatrix} \cos\alpha \\ \sin\alpha \end{bmatrix} = \begin{bmatrix} \cos\varphi\cos\alpha - \sin\varphi\sin\alpha \\ \sin\varphi\cos\alpha + \cos\varphi\sin\alpha \end{bmatrix} = \begin{bmatrix} \cos(\alpha+\varphi) \\ \sin(\alpha+\varphi) \end{bmatrix}$$

As a test we take the vectors mentioned above and the angle $\varphi = \pi/6$:

$$T\vec{a} = \begin{bmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos\varphi \\ -\sin\varphi \end{bmatrix} = \begin{bmatrix} \sqrt{3}/2 \\ -1/2 \end{bmatrix}$$

$$T\vec{b} = \begin{bmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \sin\varphi \\ \cos\varphi \end{bmatrix} = \begin{bmatrix} 1/2 \\ \sqrt{3}/2 \end{bmatrix}$$

$$T\vec{c} = \begin{bmatrix} \sqrt{3}/2 & 1/2 \\ -1/2 & \sqrt{3}/2 \end{bmatrix} \cdot \begin{bmatrix} \sqrt{3}/2 \\ 1/2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Vectors ***a*** and ***b*** are equal to vectors ***i*** and ***j***. However the transformation *T* doesn't turn them into vectors ***e*** and ***f*** like rotation *R* above, but in opposite direction since now we don't have physical rotation of vectors ***a*** and ***b***. Vector ***c*** makes in system *S* angle 30° with *x* axis and it is in first quadrant. But since also the *x* axis rotates by 30°, the vector ***c*** just coincides with the new *x* axis.

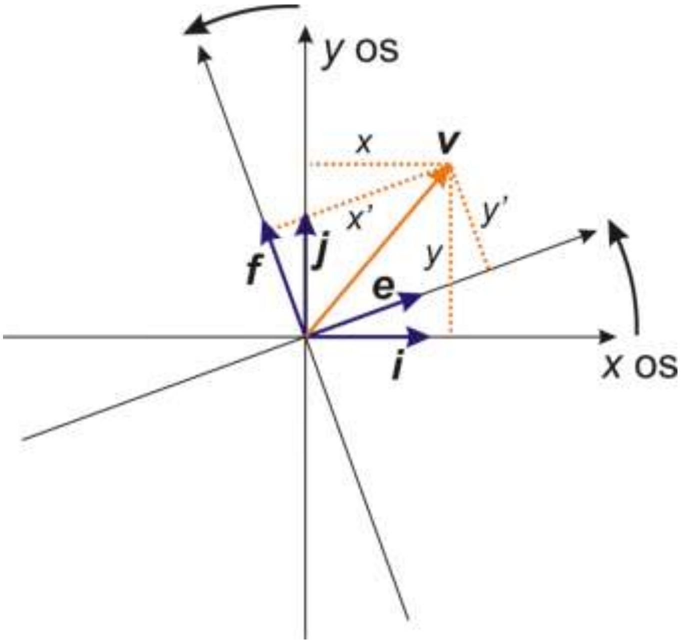


Fig. R15: 2D sketch of rotation if coordinate axes and the transformation of vector components (comment: "os" means axis) ♠

♥ EX. 3.9

3D vectors ***a*** and ***b*** are transformed into vectors ***a***' and ***b***' in the rotation of coordinate system by angle φ around *z* axis. How does transform their vector product ***c*** = ***a*** × ***b***? Consider also a physical example of torque: ***M*** = ***r*** × ***F***.

According to definition $\boldsymbol{c}' = \boldsymbol{a}' \times \boldsymbol{b}'$. If $\boldsymbol{a}' = T\boldsymbol{a}$ and $\boldsymbol{b}' = T\boldsymbol{b}$, it is sensible to expect also $\boldsymbol{c}' = T\boldsymbol{c}$, or written directly $T\boldsymbol{a} \times T\boldsymbol{b} = T(\boldsymbol{a} \times \boldsymbol{b})$. In words: we obtain equal vector according to system S', either if we first transform vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ and then calculate their vector product, or if we first calculate vector product in system S and after that transform it into S'.

Check this. Let's write transformation of vectors in a full form:

$a_x' = a_x \cos \varphi + a_y \sin \varphi$, $\quad a_y' = -a_x \sin \varphi + a_y \cos \varphi$, $\quad a_z' = a_z$

$b_x' = b_x \cos \varphi + b_y \sin \varphi$, $\quad b_y' = -b_x \sin \varphi + b_y \cos \varphi$, $\quad b_z' = b_z$

The components of the corresponding vector product are:

$c_x' = a_y'b_z' - a_z'b_y' = (a_yb_z - a_zb_y)\cos \varphi + (a_zb_x - a_xb_z)\sin \varphi$

$c_y' = a_z'b_x' - a_x'b_z' = -(a_yb_z - a_zb_y)\sin \varphi + (a_zb_x - a_xb_z)\cos \varphi$

$c_z' = a_x'b_y' - a_y'b_x' = a_xb_y - a_yb_x = c_z$

We get the same result for the sequence of operations $\boldsymbol{c} = \mathrm{a} \times \boldsymbol{b} \rightarrow \boldsymbol{c}' = T\boldsymbol{c}$. Prove this:

$c_x = a_yb_z - a_zb_y$

$c_y = a_zb_x - a_xb_z)$

$c_z = a_xb_y - a_yb_x$

$c_x' = c_x \cos \varphi + c_y \sin \varphi = (a_yb_z - a_zb_y)\cos \varphi + (a_zb_x - a_xb_z)\sin \varphi$

$c_y' = -c_x \sin \varphi + c_y \cos \varphi = -(a_yb_z - a_zb_y)\sin \varphi + (a_zb_x - a_xb_z)\cos \varphi$

$c_z' = c_z$

♠

♥ EX. 3.10

If in the rotation of coordinate system vectors transform as $\boldsymbol{x}' = T\boldsymbol{x}$, matrices transform as: $A' = TAT^{-1}$. This is in accordance with the fact that transformation preserves relations between vectors and matrices: $\boldsymbol{y} = A\boldsymbol{x} \rightarrow \boldsymbol{y}' = A'\boldsymbol{x}'$. Prove the written transformation of matrices. Transform diagonal tensor of the moment of inertia in the rotation of coordinate system by angle $\pi/4$ around z axis.

The proof is easy if we use equations: $\mathbf{y} = A\mathbf{x}$, $\mathbf{y}' = A'\mathbf{x}'$, $\mathbf{x}' = T\mathbf{x} \rightarrow \mathbf{x} = T^{-1}\mathbf{x}'$, $\mathbf{y}' = T\mathbf{y} \rightarrow \mathbf{y} = T^{-1}\mathbf{y}'$. Do it:

$$\mathbf{y}' = A'\mathbf{x}' \rightarrow T\mathbf{y} = A'T\mathbf{x} \rightarrow T^{-1}T\mathbf{y} = T^{-1}A'T\mathbf{x} \rightarrow \mathbf{y} = T^{-1}A'T\mathbf{x}$$

But since $\mathbf{y} = A\mathbf{x}$ holds, we have: $A = T^{-1}A'T$. We multiply this equation from left by T, from right by T^{-1} and finally really obtain: $A' = TAT^{-1}$.

Perform transformation on diagonal matrix:

$$J = \begin{bmatrix} J_{11} & 0 & 0 \\ 0 & J_{22} & 0 \\ 0 & 0 & J_{33} \end{bmatrix}$$

where transformation matrix for any angle is:

$$T = \begin{bmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Tensor J' in system S' is then:

$$J' = \begin{bmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} J_{11} & 0 & 0 \\ 0 & J_{22} & 0 \\ 0 & 0 & J_{33} \end{bmatrix} \cdot \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Multiplication gives:

$$J' = \begin{bmatrix} J_{11}\cos^2\varphi + J_{22}\sin^2\varphi & (J_{22} - J_{11})\sin\varphi\cos\varphi & 0 \\ (J_{22} - J_{11})\sin\varphi\cos\varphi & J_{11}\sin^2\varphi + J_{22}\cos^2\varphi & 0 \\ 0 & 0 & J_{33} \end{bmatrix}$$

This is still symmetrical matrix as it should be for most physical tensors of second rank. If we take the angle 45°, we obtain:

$$J' = \begin{bmatrix} (J_{11} + J_{22})/2 & (J_{22} - J_{11})/2 & 0 \\ (J_{22} - J_{11})/2 & (J_{11} + J_{22})/2 & 0 \\ 0 & 0 & J_{33} \end{bmatrix}$$

Eigenvalues of this transformed matrix are J_{11}, J_{22} in J_{33}, just as for original diagonal matrix since it's known that transformation of coordinate system does not alter eigenvalues. ♠

♥ EX. 3.11

When writing vector product $\boldsymbol{c} = \boldsymbol{a} \times \boldsymbol{b}$ we sometimes, e.g., in quantum mechanics, use the antisymmetrical tensor of rank 3: ε_{ijk}. Its elements are different from zero only if all three indices are equal; out of 27 tensor components there are 6 such: $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$, $\varepsilon_{132} = \varepsilon_{321} = \varepsilon_{213} = -1$. Using this tensor we can write the components of $\boldsymbol{c}$ as: $c_i = \varepsilon_{ijk}a_jb_k$ (with Einstein convention of summing over index which appears twice in the expression; thus in our case we must sum over indices j and k). Prove the validity of this equation.

Just take the component c_1. In the sum over indices j and k there appear components of tensor ε which begin with the index 1. There are only two of them different from zero: $\varepsilon_{123} = 1$, $\varepsilon_{132} = -1$. Thus: $c_1 = \varepsilon_{123}a_2b_3 + \varepsilon_{132}a_3b_2 = a_2b_3 - a_3b_2$, which is correct. We check similarly the other two components: $c_2 = \varepsilon_{231}a_3b_1 + \varepsilon_{213}a_1b_{23} = a_3b_1 - a_1b_3$, $c_3 = \varepsilon_{312}a_1b_2 + \varepsilon_{321}a_2b_1 = a_1b_2 - a_2b_1$.

For exercise, we use this notation to write the operator of orbital angular momentum of the particle in quantum mechanics. In classical mechanics the orbital angular momentum with respect to chosen origin of coordinate system equal to vector product of radius vector and linear momentum: $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$, with $\boldsymbol{r} = (x, y, z)$ and $\boldsymbol{p} = (p_x, p_y, p_z)$. In quantum mechanics we use the corresponding operators:

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$$

with operators:

$$\hat{\vec{r}} \equiv \vec{r} = (x, y, z) = (x_1, x_2, x_3)$$

$$\hat{\vec{p}} = -\mathrm{i}\hbar\nabla = -\mathrm{i}\hbar\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) = -\mathrm{i}\hbar\left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right)$$

We have used the practical notation: $x \equiv x_1$, $y \equiv x_2$, $z \equiv x_3$. Now we can write:

$$\hat{L}_j = -\mathrm{i}\hbar\varepsilon_{jmn}x_m\frac{\partial}{\partial x_n}$$

We avoided using index i, since imaginary unit i is present in the expression. ♠

♥ EX. 3.12

In some equations in quantum mechanics in some equations there appears expression $\exp[-2\pi \mathrm{i}Ht/h]$, where i is imaginary unit, H Hamilton (energy) matrix, t time and h Planck constant. What does exponential function of the matrix actually mean? Use Taylor expansion, so that you can generalize usual functions of one scalar variable to functions of matrices. First take for H any diagonal matrix of optional dimension. Next, try to generalize expression to non-diagonal matrix.

Since we can multiply square matrix (with equal number of rows and columns) with itself with no limit, we may just put matrix in Taylor series instead of scalar. Taylor expansion of usual exponential function is:

$\exp(x) = 1 + x + x^2/2 + x^3/6 + \ldots + x^n/n! + \ldots$

So we can write similarly for the matrix A:

$\exp(A) = \mathrm{I} + A + A^2/2 + A^3/6 + \ldots + A^n/n! + \ldots$

The first term is now identity matrix I instead of 1.

Let's take now diagonal matrix D of size $k \times k$, and denote its diagonal elements by λ_i, $i = 1 - k$. Any (m-th) power of diagonal matrix is again diagonal matrix, and its diagonal elements are just λ_i^m, $i = 1 - k$. Therefore, in Taylor expansion for diagonal matrix we obtain individual scalar Taylor series for diagonal elements, but these correspond to initial scalar function. So we conclude: Any function of diagonal matrix which can be expanded in Taylor series, is just equal to new diagonal matrix, the diagonal elements of which are the same function of diagonal elements of original matrix. Be now more explicit and take exponent function of diagonal matrix 4 × 4:

$$D = \begin{bmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 \\ 0 & 0 & 0 & \lambda_4 \end{bmatrix} \rightarrow \exp(D) = \begin{bmatrix} \exp(\lambda_1) & 0 & 0 & 0 \\ 0 & \exp(\lambda_2) & 0 & 0 \\ 0 & 0 & \exp(\lambda_3) & 0 \\ 0 & 0 & 0 & \exp(\lambda_4) \end{bmatrix}$$

Take now diagonal matrix H of size $n \times n$ with diagonal elements corresponding to energies E_i of various stationary quantum states:

$$H = \begin{bmatrix} E_1 & 0 & 0 & 0 \\ 0 & \ldots & 0 & 0 \\ 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & E_n \end{bmatrix} \rightarrow \exp(-2\pi Ht/h) = \begin{bmatrix} \exp(-2\pi E_1 t/h) & 0 & 0 & 0 \\ 0 & \ldots & 0 & 0 \\ 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \exp(-2\pi E_n t/h) \end{bmatrix}$$

In principle we can deal even with matrices $n \times n$, $n \rightarrow \infty$.

However, sometimes we prefer to choose in quantum mechanics such a »coordinate system« (in fact, it is the system of functions with respect to which we calculate matrix elements), where the matrix H is not diagonal. In this case we can make it diagonal by transformation T (see ex. 7.18): $H = T^{-1}H_dT$, where H_d is diagonal matrix with elements E_i. Before we use Taylor expansion, let's check optional power of matrix H:

$$H^m = H \cdot H \cdot \ldots \cdot H = T^{-1}H_dT \cdot T^{-1}H_dT \cdot \ldots T^{-1}H_dT$$

Since $T \cdot T^{-1} = \mathrm{I}$, the expression is simplified:

$$H^m = T^{-1}H_d^{\,m}T$$

So we have also in Taylor series in each term first factor T^{-1}, then powers of diagonal matrix and lastly factor T. We can write the final result:

$$\exp(-2\pi Ht/h) = T^{-1}\cdot\begin{bmatrix}\exp(-2\pi E_1t/h) & 0 & 0 & 0\\ 0 & \ldots & 0 & 0\\ 0 & 0 & \ldots & 0\\ 0 & 0 & 0 & \exp(-2\pi E_nt/h)\end{bmatrix}\cdot T$$ ♠

♥ EX. 3.13

Some 2-level quantum system has in basic level energy E_0, in the higher level energy $E_1 > E_0$ (Fig. R16). Their difference is $\Delta E_{10} = E_1 - E_0 = 5$ eV. Basic (low) level is non-degenerate (only one quantum state), while degeneracy of higher level is $g = 3$: this means that there are three states with the same energy E_1. Let the number of all quantum particles in both levels be N, of this 70 % in low level and 30 % in high level (i.e., 10 % in each of the three quantum states, left side of figure). If quantum particles are not too close together so that their fermionic or bosonic character is nor relevant, their distribution according to energies is given by Boltzmann distribution. The simplest way to present this distribution is with ratio of numbers of particles in different quantum states (e.g., i-th and j-th state with energies E_i and E_j):

$$\frac{N_i}{N_j} = \exp\left(\frac{E_j - E_i}{kT}\right)$$

Here, k is Boltzmann constant, and T absolute temperature of quantum system. Equation indicates that the number of particles in higher energy state is smaller than in state with lower energy. We stress: if the quantum energy levels are degenerate, the equation holds for every state (even within the same energy level). So the equation can be rewritten:

$$\frac{N(E_i)}{N(E_j)} = \frac{g_i}{g_j}\cdot\exp\left(\frac{E_j - E_i}{kT}\right)$$

Here we sum particles for all quantum states at the same energy, so that the numbers g_i and g_j are the corresponding degrees of degeneracy. To avoid ambiguity, we stress that we will count particles with regard to quantum states (not levels) and we'll use first equation. What must be the temperature, so that the upper data for occupation of states hold? What happens with these numbers if the system is disturbed by some external perturbation (e.g., by magnetic field), so that the lower state remains non-degenerate, but the energy of higher states splits into three different values: $E_1 - \Delta E/2$, E_1 in $E_1 + \Delta E/2$ (right part of figure)? Let's take $\Delta E = \Delta E_{10}/10$. Do only the numbers of particles in upper three quantum states rearrange, or do some particles move from higher state to low energy state or in opposite direction?

First, we solve the first part of the problem. We denote the number of particles in the basic level by N_0, and the number in each of the three higher states by N_1. We then have:

$$\frac{N_1}{N_0} = \frac{1}{7} = \exp(-\frac{\Delta E_{10}}{kT}) \rightarrow T = \frac{\Delta E_{10}}{k \ln 7} = 2{,}98 \cdot 10^4 \text{ K}$$

After energy splitting we must treat all four energy levels. Let the new number of particles in basic level be N_0' (we don't know yet whether it is equal to N_0 or not). Sum all 4 (now different!) numbers of particles and use again Boltzmann distribution:

$$N_0' + N_{1a} + N_{1b} + N_{1c} = N$$

$$N_0' \cdot \left[1 + \exp(-\frac{\Delta E_{10} - \Delta E/2}{kT}) + \exp(-\frac{\Delta E_{10}}{kT}) + \exp(-\frac{\Delta E_{10} + \Delta E/2}{kT}) \right] = N$$

$$N_0' \cdot \left[1 + \frac{1}{7} \left\{ 1 + \exp(\frac{\Delta E_{10}/20}{kT}) + \exp(-\frac{\Delta E_{10}/20}{kT}) \right\} \right] = N$$

We have exposed factor $\exp(-\Delta E_{10}/(kT)) = 1/7$ for three terms. Let's go on: $\exp(\Delta E_{10}/(20kT)) = \exp(\Delta E_{10}/(kT))^{1/20} = 7^{1/20}$. So we can write:

$$N_0' \cdot \left[1 + \frac{1}{7} \left\{ 1 + 7^{1/20} + 7^{-1/20} \right\} \right] = N \rightarrow N_0' \approx 69{,}934 \text{ \% } N$$

Before energy splitting of higher level there were 70 % N particles in low energy level, thus 0,066 % N went from basic state to higher levels. Exactly how many (instead of 10 %) there are in each state, is left for exercise for the student. We finally mention that at ordinary temperatures the equilibrium occupations of higher quantum levels are completely negligible in comparison with basic state. For instance, at $T = 300$ K N_1/N_0 at energy difference 5 eV is as small as $1{,}2 \cdot 10^{-84}$. In order to have considerable number of particles at higher energy levels, we have to »pump« them there artificially (e.g., for operation of lasers).

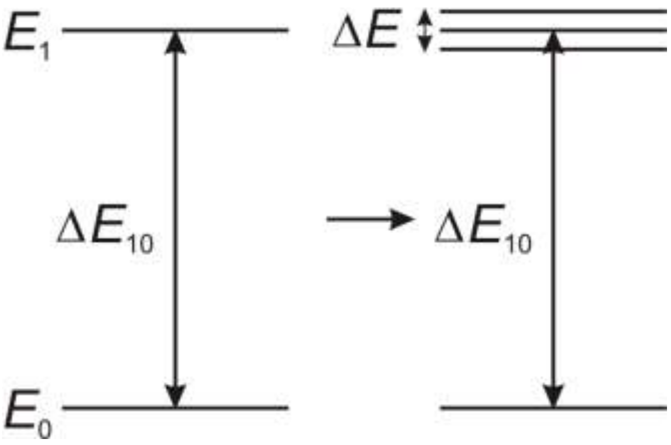


Fig. R16: Splitting of higher energy level ♠

♥ EX. 3.14

1D double potential well is introduced by infinite potential well which has in the middle narrow and high enough potential barrier (Fig. R17). We have chosen suitable coordinate system, so that $x = 0$ in the middle of the well and $V(x)$ is even function. Then the two stationary states with the lowest energies have much lower energy difference than the difference between the first and second level in the well without the barrier. The lower state has symmetrical (even) wave function ψ_S and energy E_S, and the higher state has anti-symmetrical (odd) wave function ψ_A and higher energy E_A. For very high barrier it holds: $\Delta E = E_A - E_S << E_S$, but both functions remind us of sinusoidal stationary solutions of ordinary infinite 1D potential well which will be treated later (these functions are slightly distorted only in the vicinity of the barrier). The sign before the wave function has no physical significance but we optionally choose it for function ψ_A so, that the function is positive in the right half of the well and negative in the left half. It is characteristic for the function of the basic level that it has no zeros inside its definition area (except possibly for edge points $x = \pm a/2$); thus ψ_S has everywhere the same sign and we choose the positive value. Functions ψ_S and ψ_A are normalized and also »orthogonal« on each other. We can use them to compose two new functions:

$$\psi_D = \frac{1}{\sqrt{2}}(\psi_S + \psi_A)$$

$$\psi_L = \frac{1}{\sqrt{2}}(\psi_S - \psi_A)$$

But these do not correspond to stationary states since they we composed of two stationary states with different energies. Do the following in connection with the new functions:

- Prove relation: $\psi_L(-x) = \psi_D(x)$.
- Prove that they are normalized as are ψ_S and ψ_A.

- Calculate their »overlap integral«, which means their scalar product (defined for functions).
- Calculate the mean value of coordinate *x* for each of them and comment the result.
- Calculate 2D Hamilton matrix for this pair of functions.

Use »bra-ket« notation where it's sensible. Let for simplicity all the functions be real, what can be always done for 1D problems.

Let's go on step by step:

$$\psi_{\mathrm{L}}(-x) = \frac{1}{\sqrt{2}}(\psi_{\mathrm{S}}(-x) - \psi_{\mathrm{A}}(-x)) = \frac{1}{\sqrt{2}}(\psi_{\mathrm{S}}(x) + \psi_{\mathrm{A}}(x)) = \psi_{\mathrm{D}}(x)$$

We have used the fact that in changing sign of *x* symmetrical function retains its value, while the sign of anti-symmetrical function is also reversed. Normalization can be checked by the following scalar product:

$$<\psi_{\mathrm{D}}|\psi_{\mathrm{D}}>=\frac{1}{2}<\psi_{\mathrm{S}}+\psi_{\mathrm{A}}|\psi_{\mathrm{S}}+\psi_{\mathrm{A}}>$$

$$<\psi_D|\psi_D>=\frac{1}{2}\left[<\psi_S|\psi_S>+<\psi_S|\psi_A>+<\psi_A|\psi_S>+<\psi_A|\psi_A>\right]$$

Use that fact that original functions are »orthonormal«:

$$<\psi_D|\psi_D>=\frac{1}{2}\left[1+'0+0+1\right]=1$$

In a similar manner the normalization of ψ_{L} can be shown. Their overlap integral is:

$$<\psi_D|\psi_L>=\frac{1}{2}<\psi_S+\psi_A|\psi_S-\psi_A>$$

$$<\psi_D|\psi_L>=\frac{1}{2}\left[<\psi_S|\psi_S>-<\psi_S|\psi_A>+<\psi_A|\psi_S>-<\psi_A|\psi_A>\right]$$

$$<\psi_D|\psi_L>=\frac{1}{2}\left[1-'0+0-1\right]=0$$

The calculation of <*x*> is also first presented with formal »bra-ket« notation, but then we continue with explicit integral to be clear. It suffices to make it for the function ψ_{D}:

$$< x >=<\psi_D|x|\psi_D>\equiv<\psi_D|x\psi_D>=\frac{1}{2}<\psi_S+\psi_A|x(\psi_S+\psi_A)>$$

We use this time the symmetry of the scalar product for real functions:

$$<x>=\frac{1}{2}\left[<\psi_S|x\psi_S>+2<\psi_S|x\psi_A>+<\psi_A|x\psi_A>\right]$$

Scalar product of functions is defined as integral:

$$<\psi_S|x\psi_A>=\int_{-a/2}^{+a/2}x\psi_S\psi_A dx$$

In general, the integration limits are ±∞, but in our case the functions are zero outside interval (–a/2, +a/2), since the potential is infinite there. It holds:

$$<\psi_S|x\psi_S>=\int_{-a/2}^{+a/2}x\psi_S{}^2 dx=0$$

$$<\psi_A|x\psi_A>=\int_{-a/2}^{+a/2}x\psi_A{}^2 dx=0$$

since we integrate odd functions. So:

$$<x>=<\psi_S|x\psi_A>=\int_{-a/2}^{+a/2}x\psi_S\psi_A dx$$

The function under integral is now even, thus:

$$<x>_D=2\int_{0}^{+a/2}x\psi_S\psi_A dx$$

The mean value of x for function ψ_D is positive, what means that the particle is predominantly in the right side of the well (suffix D is from Slovene word “desno” for “right”). Similarly we find for particle with function ψ_L, which is predominantly in the left half of the well: $<x>_L = -<x>_D$.

We are left with calculation of 4 elements of Hamilton matrix:

$$H_{11}=<\psi_D|\hat{H}|\psi_D>\equiv<\psi_D|\hat{H}\psi_D>=\frac{1}{2}<\psi_S+\psi_A|\hat{H}(\psi_S+\psi_A)>$$

We take into account that ψ_S and ψ_A are eigenfunctions of Hamiltonian, as well as their orthogonality:

$$H_{11}=\frac{1}{2}<\psi_S+\psi_A|E_S\psi_S+E_A\psi_A)>=\frac{E_S+E_A}{2}=\overline{E}$$

Similarly:

$$H_{22} = <\psi_L|\hat{H}|\psi_L> = \frac{E_S + E_A}{2} = \bar{E}$$

We know from symmetry of matrix *H*:

$$H_{12} = <\psi_D|\hat{H}|\psi_L> = H_{21} = <\psi_L|\hat{H}|\psi_D>$$

Let’s calculate these elements:

$$H_{12} = \frac{1}{2} < \psi_S - \psi_A|\hat{H}(\psi_S + \psi_A)>$$

$$H_{12} = \frac{1}{2} < \psi_S - \psi_A|E_S\psi_S + E_A\psi_A)> = \frac{E_S - E_A}{2} = \frac{\Delta E}{2}$$

The matrix is:

$$H = \begin{bmatrix} \bar{E} & \frac{\Delta E}{2} \\ \frac{\Delta E}{2} & \bar{E} \end{bmatrix}$$

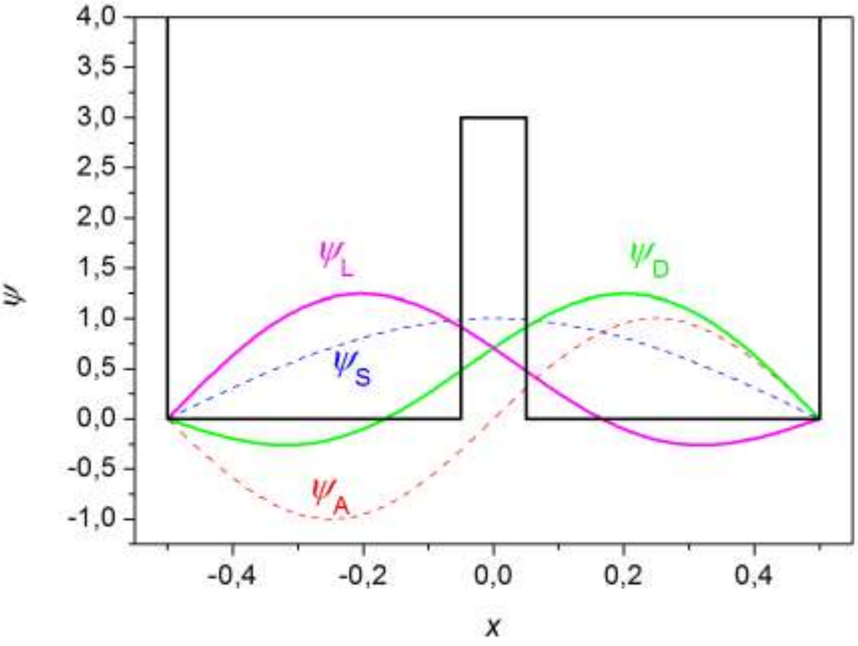


Fig. R17: Schematic sketch of 1D infinite potential well with potential barrier in the middle; the wave functions ψ_S and ψ_A are approximately shown as sinusoidal curves (dashed lines) and also ψ_D and ψ_L (solid lines). Exact calculation shows that the solutions in the area of barrier should have exponential and not sinusoidal form (but at first glance we wouldn’t notice qualitative difference, only the function inside barrier would become lower). ♠

♥ EX. 3.15

Playing dice is ground so that the sides with numbers from 2 to 5 are a little smaller. So, the probability to get in the throw numbers 1 and 6 is rised: $P_1 = P_6 = 20$ %, $P_2 = P_3 = P_4 = P_5 =$ 15 %. We throw dice twice. What's the probability that the sum of numbers for both throws will be 7?

Among all possibilities we obtain the sum 7 only for these double throws: 1 + 6, 6 + 1, 2 + 5, 5 + 2, 3 + 4 in 4 + 3. These are disjunctive events, thus the total probability for sum 7 is equal to the sum: $P = 2\mathrm{P}(1, 6) + 4P(2, 5)$. This is because P(2, 5) = P(3, 4). But two sequential throws are taken as independent and we must multiply corresponding probabilities:

$P(\text{sum } 7) = 2P_1P_6 + 4P_2P_5 = 2P_1^2 + 4P_2^2 = 17$ %. ♠

Ex. 3.16 is omitted since it is not so relevant.

♥ EX. 3.17

Square wire loop with the side $a = 10$ cm and mass $m = 2$ kg is hung on vertical thread, so that the plane of the loop is vertical. The loop is composed of many windings so that a large current $I = 5$ A is flowing through it. The loop is positioned in horizontal homogeneous magnetic field with strength $B = 1$ T. In equilibrium the normal to the loop points in the same direction as the field. If we rotate it by angle φ around vertical axis (torsion due to thread is neglected), the torque $M = -\mu B \sin \varphi$ acts on the loop, tending to return the loop to equilibrium direction. Magnetic dipole moment of the loop is $\mu = IS = Ia^2$. When we calculate its moment of inertia we imagine the loop as composed of 4 equal thin sticks, two horizontal and two vertical. What's the oscillation time of the loop for small deviation φ?

We set »Newton law« for rotation of the rigid body:

$$J\alpha = M$$

$$2(J_1 + J_2)\ddot{\varphi} = -\mu B \sin\varphi$$

The two horizontal sticks rotate around their centers of mass, so each has moment of inertia $J_1 = (m/4)a^2/12 = ma^2/48$. For vertical sticks all their points are (approximately) at equal distance from vertical rotation axis, i.e., $a/2$, so $J_2 = (m/4)(a/2)^2 = ma^2/16$. Continue:

$$2\left(\frac{ma^2}{48}+\frac{ma^2}{16}\right)\ddot{\varphi}=-Ia^2B\sin\varphi$$

$$\ddot{\varphi}=-\frac{6IB}{m}\sin\varphi\approx-\frac{6IB}{m}\varphi$$

Thus, for small angles this is equation for harmonic oscillation with:

$$T=2\pi\sqrt{\frac{m}{6IB}}=1{,}62\text{ s}$$ ♠

♥ EX. 3.18

Find the simplest possible relation between kinetic energy and orbital magnetic moment and between the orbital angular momentum and orbital magnetic moment of the particle with charge *e* and mass *m*, orbiting in homogeneous magnetic field *B* in the circle with radius *R*.

We first find the relation between *B*, *R* and the particle speed *v* by identifying magnetic and centripetal force:

$$F_\mathrm{m}=F_\mathrm{c}$$

$$evB=\frac{mv^2}{R}$$

$$v=\frac{eBR}{m}$$

Next we express kinetic energy E_k, angular momentum *L* and magnetic moment μ with parameters *m* and *e* and variables *B* and *R*:

$$E_\mathrm{k}=\frac{1}{2}mv^2=\frac{e^2B^2R^2}{2m}$$

$$L=mRv=eBR^2$$

$$\mu=IS=\frac{e}{T}\cdot\pi R^2=\frac{e}{2\pi R/v}\cdot\pi R^2=\frac{evR}{2}=\frac{e^2BR^2}{2m}$$

The required relations are:

$$E_\mathrm{k}=B\mu$$

$$L = \frac{2m}{e}\mu$$ ♠

♥ EX. 3.19

In one of the variants of Stern-Gerlach experiment we observe the splitting and vertical displacement of the beam of potassium atoms into two partial beams when the inhomogeneous magnetic field is entered, due to spin angular momentum and the corresponding magnetic moment of the most weakly bound electron in basic state. Gaseous potassium is heated in an oven at the temperature 1000° C, and the atoms exit the oven in horizontal direction and pass the short area (1 cm wide) of inhomogeneous magnetic field. This is directed vertically and is 10 T/cm in the same direction. Both partial beams hit the 1 m distant screen or the system of detectors. What's the distance between the points where the beams hit the screen? Atomic mass of potassium is $A = 39$.

Spin magnetic moment of electron μ is equal to Bohr magneton:

$$\mu = \mu_\mathrm{B} = \frac{e_0\hbar}{2m_\mathrm{e}} = \frac{e_0 h}{4\pi m_\mathrm{e}}$$

where $e_0 = 1{,}6 \cdot 10^{-19}$ A s, $h = 6{,}6 \cdot 10^{-34}$ J, $m_\mathrm{e} = 9{,}1 \cdot 10^{-31}$ kg. We have rounded the factor g_S which appears in the relation between spin orbital momentum and magnetic moment, to the value 2. Quantized component of magnetic moment (because of spin ½) in the z axis direction (direction of magnetic field) is $\mu_z = \pm\mu_\mathrm{B}$. Magnetic force of inhomogeneous field on magnetic moment is $F_z = \mu_z \cdot (\mathrm{d}B_z/\mathrm{d}z)$. Instead of partial derivative with respect to coordinate z we have simply written usual derivative, because the field varies only in the direction z. Thus the acceleration of the whole potassium atom in vertical direction is:

$$a_z = \frac{F_z}{m} = \pm\frac{e_0 h}{4\pi m m_\mathrm{e}} \cdot \frac{\mathrm{d}B_z}{\mathrm{d}z}$$

Here m is the mass of the atom. The atom comes to the area of inhomogeneous magnetic field with the speed v_0, which can be approximated from mean thermal translational kinetic energy:

$$v_0 \approx \sqrt{\frac{3kT}{m}}$$

Boltzmann constant is $k = 1{,}38 \cdot 10^{-23}$ J/K, mass of atom is: $m = Am_1$, with atomic mass unit $m_1 = 1$ kg/N_A, where $N_\mathrm{A} = 6 \cdot 10^{26}$/kmol is Avogadro number. The width of the area with inhomogeneous field is x, and atoms pass it in time $t = x/v_0$. During this time they acquire also vertical component of velocity:

$$v_z = a_z t = \pm \frac{e_0 h}{4\pi m m_e} \cdot \frac{\mathrm{d}B_z}{\mathrm{d}z} \cdot \frac{x}{v_0}$$

When atoms leave small area of inhomogeneous field their paths are declined from horizontal direction by angle $\pm\varphi$, where:

$$\tan|\varphi| = \frac{|v_z|}{v_0} = \frac{e_0 h}{4\pi m m_e} \cdot \frac{\mathrm{d}B_z}{\mathrm{d}z} \cdot \frac{x}{{v_0}^2}$$

It is interesting to note that after inserting the square of initial speed into the expression for the angle the mass of atoms cancel and we don't need this information:

$$\tan|\varphi| = \frac{|v_z|}{v_0} = \frac{e_0 h x}{12\pi m_e kT} \cdot \frac{\mathrm{d}B_z}{\mathrm{d}z}$$

The locations of impact of partial beams on $X = 1$ m distant screen are separated by:

$$Z = 2X \tan|\varphi| = \frac{e_0 h x X}{6\pi m_e kT} \cdot \frac{\mathrm{d}B_z}{\mathrm{d}z} = 4{,}5 \text{ mm}$$

It is necessary to take care that there are no ionized atoms in the beam, or as few as possible (these carry one positive fundamental charge). This is because the displacement of charged particles due to direct magnetic force in characteristic magnetic fields is incomparably larger than the displacement due to magnetic dipole moment. ♠

♥ EX. 3.20

Pauli spins matrices σ_x, σ_y and σ_z below, which are used in quantum mechanics for particles with spin 1/2, are of size 2 × 2. Calculate their eigenvalues, trace, determinant and products.

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \sigma_y = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix} \qquad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

In the second matrix, i is imaginary unit.

All three Pauli matrices have equal pair of eigenvalues: $\lambda_1 = +1$ and $\lambda_2 = -1$. Prove this for one of them:

$$\det(\sigma_x - \lambda I) = \det \begin{bmatrix} -\lambda & 1 \\ 1 & -\lambda \end{bmatrix} = \lambda^2 - 1 = 0 \rightarrow \lambda_{1,2} = \pm 1$$

Find also the corresponding eigenvectors:

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = 1\cdot\begin{bmatrix} x \\ y \end{bmatrix} \to \begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} x \\ y \end{bmatrix} \to x = y$$

Normalized eigenvector belonging to eigenvalue +1 is thus: $\boldsymbol{x}^1 = (x, y) = (1/2^{1/2}, 1/2^{1/2})$. Similarly for the second one:

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = -1\cdot\begin{bmatrix} x \\ y \end{bmatrix} \to \begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} -x \\ -y \end{bmatrix} \to x = -y$$

Normalized eigenvector belonging to eigenvalue –1 is thus: $\boldsymbol{x}^2 = (x, y) = (1/2^{1/2}, -1/2^{1/2})$. Vectors $\boldsymbol{x}^1$ and $\boldsymbol{x}^2$ are mutually perpendicular, as they should since they belong to two different eigenvalues of Hermitian matrix. It holds for such matrix: $A^T = A^*$ or in words: transposed matrix is equal to complex conjugated matrix. The meaning of transposed matrix: $(A^T)_{ij} = A_{ji}$.

Consider now matrix σ_y:

$$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = 1\cdot\begin{bmatrix} x \\ y \end{bmatrix} \to \begin{bmatrix} -iy \\ ix \end{bmatrix} = \begin{bmatrix} x \\ y \end{bmatrix} \to y = ix$$

The eigenvector: $\boldsymbol{x}^1 = (x, y) = (1/2^{1/2}, i/2^{1/2})$.

$$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = -1\cdot\begin{bmatrix} x \\ y \end{bmatrix} \to \begin{bmatrix} -iy \\ ix \end{bmatrix} = \begin{bmatrix} -x \\ -y \end{bmatrix} \to y = -ix$$

The eigenvector: $\boldsymbol{x}^2 = (x, y) = (1/2^{1/2}, -i/2^{1/2})$. Vectors $\boldsymbol{x}^1$ and $\boldsymbol{x}^2$ are mutually perpendicular also in this case. But now we deal with complex numbers and the scalar product is defined as: $\boldsymbol{x}^1 \cdot \boldsymbol{x}^2 = (x^1)_1(x^2)_1^* + (x^1)_2(x^2)_2^* = 1/2^{1/2} \cdot 1/2^{1/2} + i/2^{1/2} \cdot i/2^{1/2} = 1/2 - 1/2 = 0$.

Eigenvectors of the diagonal matrix σ_z are trivial: $\boldsymbol{x}^1 = (1, 0)$, $\boldsymbol{x}^2 = (0, 1)$.

Since all matrices have the same eigenvalues ±1, also their trace and determinant is the same: $\mathrm{sl}(\sigma_i) = \lambda_1 + \lambda_2 = 0$, $\det(\sigma_i) = \lambda_1 \cdot \lambda_2 = -1$, $i = x$ or y or z.

Square of every matrix is unit matrix. For instance:

$$\sigma_x{}^2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\cdot\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Multiply also two different matrices. For instance:

$$\sigma_x \cdot \sigma_y = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\cdot\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} = i\sigma_z$$

Product of these matrices is anti-commutative, which means that it changes sign when the order of factors is reversed:

$$\sigma_y \cdot \sigma_x = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix} = -i\sigma_z$$

We have similarly: $\sigma_y \cdot \sigma_z = -\sigma_z \cdot \sigma_y = i\sigma_x$ in $\sigma_z \cdot \sigma_x = -\sigma_x \cdot \sigma_z = i\sigma_y$. ♠

♥ EX. 3.21

Two different quantum states in two-level system which are related to qubits are described with the following vectors in Hilbert space:

$$|\psi_1\rangle = \cos\frac{\theta_1}{2}|0\rangle + \exp(\mathrm{i}\phi_1)\sin\frac{\theta_1}{2}|1\rangle$$

$$|\psi_2\rangle = \cos\frac{\theta_2}{2}|0\rangle + \exp(\mathrm{i}\phi_2)\sin\frac{\theta_2}{2}|1\rangle$$

Here |0> and |1> are orthonormal stationary states. Express both scalar products of composed vectors. Find condition for their orthogonality.

Since <0|0> = <1|1> = 1 in <0|1> = <1|0> = 0, we find:

$$\langle\psi_1|\psi_2\rangle = \cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2} + \exp(\mathrm{i}\Delta\phi)\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}$$

$$\langle\psi_2|\psi_1\rangle = \cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2} + \exp(-\mathrm{i}\Delta\phi)\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}$$

We denoted the phase difference $\Delta\phi = \phi_2 - \phi_1$. If we want zero scalar product, both real and imaginary components must be zero. The imaginary component is zero only if $\Delta\phi = 0$ or integer multiple of π; choose $\Delta\phi = 0$. Then both scalar products are real; they are zero if:

$$\cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2} + \sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2} \equiv \cos\frac{\theta_1 - \theta_2}{2} = 0 \rightarrow \theta_1 - \theta_2 = (2k+1)\pi$$

Here, k is any integer number, and let's choose $k = 0$. So, for now: $\phi_2 = \phi_1$, $\theta_2 = \theta_1 + \pi$.

But we must stress that we can define ϕ per modulus of 2π because of periodicity of exponential function with imaginary exponent. Since the half angle θ appears in the functions, it can be in principle defined per modulus of 4π. However, when we make transformation θ

$\to 2\pi + \theta$, both sine and cosine change sign. This means that the whole vector (or wave function) just changes sign, which is physically the same state. Therefore, it is sufficient to limit polar angle θ to half interval $(0, 2\pi)$. But if we consider another transformation, $\phi \to \phi + \pi$, $\theta \to 2\pi - \theta$, we find the following: cosine function in the equation of state changes sign, but not the sine function; also the exponential function in sine part changes sign. Again, the whole vector only changes sign. So θ can be even more limited: $0 \leq \theta \leq \pi$. This is a proof that Bloch sphere is enough for representation of qubits. We find also something else: if we take to orthogonal vectors, two diametral points on Bloch sphere correspond to them. If we want to limit θ to interval $(0, \pi)$, we must take for the second vector instead of $\phi_2 = \phi_1$, $\theta_2 = \theta_1 + \pi$ some more suitable pair of angles. Let's be definite and take the acute angles of the first vector: $0 < \phi_1, \theta_1 < \pi/2$. Then, it holds for the pair of angles of second vector: $0 < \phi_2 < \pi/2$, $\pi < \theta_2 < 3\pi/2$. Then we use transformation mentioned above: $\phi_2 \to \phi_2 + \pi$, $\theta_2 \to 2\pi - \theta_2$, so we get: $\pi < \phi_2 < 3\pi/2$, $\pi/2 < \theta_2 < \pi$. Now we have the desired intervals for all angles: $\phi_2 = \phi_1 + \pi$, $\theta_2 = \pi - \theta_1$. ♠

4 QANTUM CALCULATIONS

♥ EX. 4.1

In physics, we often define matrix – the tensor of second rank – as a tensor product of two vectors. If we take vectors $\boldsymbol{a} = (a_1, a_2, a_3)$ and $\boldsymbol{b} = (b_1, b_2, b_3)$, we obtain matrix $C = \boldsymbol{a} \otimes \boldsymbol{b}$, with elements: $C_{ij} = a_i b_j$. In words: the element of i-th row and j-th column of this matrix is the product of i-th component of first vector and the j-th component of second vector. Show that in rotation of coordinate system this matrix transforms correctly: $C' = TCT^{-1}$, if both vectors transform as $\boldsymbol{a}' = T\boldsymbol{a}$ and $\boldsymbol{b}' = T\boldsymbol{b}$. Describe main characteristics of this matrix.

Correct transformation of the matrix means: $T(\boldsymbol{a} \otimes \boldsymbol{b})T^{-1} = (T\boldsymbol{a}) \otimes (T\boldsymbol{b})$. In words: tensor product of already transformed vectors is the same as transformed matrix which has first calculated from original vectors.

The proof will be a fine exercise of calculation and summing terms over some indices, something usual for algebra which deals with vectors and matrices. But before solution of the task just look again at characteristic transformation (rotation) matrix:

$$T = \begin{bmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Matrices like this have some additional property useful for proof of different rules connected with them. If we take some optional row of matrix T and imagine it as a vector, then the scalar product of two different rows is always zero. But the scalar product of the same row with itself is 1. The same holds for the columns of the matrix.

Since any rotation matrix (optional axis and angle) can be obtained as a product of more simple matrices for rotation around coordinate axes the rule mentioned above holds for any rotation. Thus, we have to prove that if the matrices A and B have such property, the same holds for their product $C = AB$.

In this task we'll learn to use Einstein convention for summing over repeated indices: if in some expression some index repeats twice this means that we must sum over this index and we needn't write the symbol for sum. In this way we simplify notation, e.g.:

$$A_{ik} B_{kj} \equiv \sum_{k=1}^{3} A_{ik} B_{kj}$$

Expression that we took as an example corresponds to multiplication of matrices A and B – this is just element C_{ij}. Now we take matrices A and B which have orthonormal rows and columns. We'll prove the same for their product. We'll use Einstein convention. Let's check scalar product of i-th and j-th row of C:

$$s = C_{i1}C_{j1} + C_{i2}C_{j2} + C_{i3}C_{j3} \equiv C_{ik}C_{jk} = (AB)_{ik}(AB)_{jk}$$

$$s = (A_{il}B_{lk})(A_{jm}B_{mk})$$

We obtained triple sum (over k, l and m). We may rearrange the order of in an appropriate way:

$$s = (A_{il}A_{jm})(B_{lk}B_{mk})$$

Now the main trick: since the summation index k only in second parenthesis we first calculate that sum over k. But this is just the scalar product of l-th and m-th row of B, which is zero for different l and m, but for $l = m$ it is equal to 1. So in the whole expression for scalar product s we keep only the first parenthesis with elements of matrix A, putting $l = m$:

$$s = A_{im}A_{jm}$$

But this is just scalar product of i-th and j-th row of A, which is 1 for $i = j$, and zero otherwise. The proof is finished.

The orthonormality of rows and columns of transformation matrix will not be used directly here, but nevertheless this property is related with the requirement that the inverse matrix of matrix T is just equal to its transposed matrix.

Now turn to the proof that $T(\mathbf{a} \otimes \mathbf{b})T^{-1} = (T\mathbf{a}) \otimes (T\mathbf{b})$, if the matrix T has the property of orthonormality of rows and columns. We'll multiply three matrices at the same time: $(ABC)_{ij} = A_{ik}B_{kl}C_{lj}$, which is left for reader to prove. We'll use also this: $(T^{-1})_{ij} = (T^{\mathrm{T}})_{ij} = T_{\mathrm{ji}}$.

Left side:

$$[T(\mathbf{a} \otimes \mathbf{b})T^{-1}]_{ij} = T_{ik}(\mathbf{a}\otimes\mathbf{b})_{kl}(T^{-1})_{lj} = T_{ik}a_kb_lT_{jl} = T_{ik}T_{jl}a_kb_l$$

Right side:

$$[(T\mathbf{a}) \otimes (\mathrm{T}\mathbf{b})]_{ij} = (T\mathbf{a})_i(T\mathbf{b})_j = (T_{ik}a_k)(T_{jl}b_l) = T_{ik}T_{jl}a_kb_l$$

Everything matches. ♠

♥ EX. 4.3

What does the product (***a*** ⊗ ***b***) · (***c*** ⊗ ***d***) mean? Here ***a***, ***b***, ***c*** and ***d*** are 3D physical vectors. Both tensor products are 3 × 3 matrices, while the dot denotes usual product of matrices.

Let's use short denotations: $M = \boldsymbol{a} \otimes \boldsymbol{b}$, $N = \boldsymbol{c} \otimes \boldsymbol{d}$, $P = M \cdot N$. If the vectors in components are $\boldsymbol{a} = (a_1, a_2, a_3)$, $\boldsymbol{b} = (b_1, b_2, b_3)$, $\boldsymbol{c} = (c_1, c_2, c_3)$ and $\boldsymbol{d} = (d_1, d_2, d_3)$, the matrix multiplication is:

$$P = M \cdot N \rightarrow \begin{bmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{bmatrix} = \begin{bmatrix} a_1b_1 & a_1b_2 & a_1b_3 \\ a_2b_1 & a_2b_2 & a_2b_3 \\ a_3b_1 & a_3b_2 & a_3b_3 \end{bmatrix} \cdot \begin{bmatrix} c_1d_1 & c_1d_2 & c_1d_3 \\ c_2d_1 & c_2d_2 & c_2d_3 \\ c_3d_1 & c_3d_2 & c_3d_3 \end{bmatrix}$$

Choose as an example one of the elements of matrix P: $P_{11} = a_1b_1c_1d_1 + a_1b_2c_2d_1 + a_1b_3c_3d_1 = (\boldsymbol{b} \cdot \boldsymbol{c})a_1d_1$. We obtain similar thing for any element of P: $P_{ij} = M_{ik}N_{kj}$ (Einstein convention for index k). Next:

$P_{ij} = a_ib_kc_kd_j = (\boldsymbol{b} \cdot \boldsymbol{c})a_id_j$.

We write finally: $(\boldsymbol{a} \otimes \boldsymbol{b}) \cdot (\boldsymbol{c} \otimes \boldsymbol{d}) = (\boldsymbol{b} \cdot \boldsymbol{c})\boldsymbol{a} \otimes \boldsymbol{d}$. ♠

♥ EX. 4.4

Two normalized states of some spins system with spin ½ are $|\psi_1\rangle = (a_1, b_1)$ and $|\psi_2\rangle = (a_2, b_2)$, where the components are in general complex numbers. Express tensor product of both vectors in two ways, either as a 2 × 2 matrix, or as a vector with 4 components. What's the relation between 2D matrix and 4D vector? What's the magnitude of the vector?

Tensor product as matrix is:

$$|\psi_1 > \otimes |\psi_2 > = \begin{bmatrix} a_1a_2 & a_1b_2 \\ b_1a_2 & b_1b_2 \end{bmatrix}$$

and as vector:

$$|\psi_1 > \otimes |\psi_2 > = \begin{bmatrix} a_1a_2 \\ a_1b_2 \\ b_1a_2 \\ b_1b_2 \end{bmatrix}$$

We obtain it by taking rows of the matrix in right sequence and put them into vector. New vector is denoted by $|\psi\rangle$ and its size is:

$$\left\| \psi > \right|^2 = <\psi|\psi> = \begin{bmatrix} a_1{*}a_2{*} & a_1{*}b_2{*} & b_1{*}a_2{*} & b_1{*}b_2{*} \end{bmatrix} \cdot \begin{bmatrix} a_1a_2 \\ a_1b_2 \\ b_1a_2 \\ b_1b_2 \end{bmatrix}$$

$$\left\| \psi > \right|^2 = |a_1|^2|a_2|^2 + |a_1|^2|b_2|^2 + |b_1|^2|a_2|^2 + |b_1|^2|b_2|^2$$

Collect terms in pairs and use normalization of $|\psi_1>$ and $|\psi_2>$:

$$\left\| \psi > \right|^2 = |a_1|^2 \left\| \psi_2 > \right|^2 + |b_1|^2 \left\| \psi_2 > \right|^2 = |a_1|^2 + |b_1|^2 = \left\| \psi_1 > \right|^2 = 1$$

Thus, also the new vector is normalized. ♠

♥ Ex. 4.7

Write how the operator $\sigma_x \otimes \sigma_x \otimes \sigma_z$ (tensor product of Pauli matrices) acts in all of 8 base tensor products $s_{z1} \otimes s_{z2} \otimes s_{z3}$ of individual spin states (s = ½). What are the eigenvalues and corresponding states of the operator?

Let's write first operations of both matrices on one spin for both states:

$$\sigma_x|\uparrow> = |\downarrow>$$

$$\sigma_x|\downarrow> = |\uparrow>$$

$$\sigma_z|\uparrow> = |\uparrow>$$

$$\sigma_z|\downarrow> = -|\downarrow>$$

For the tensor product we have:

$$(\sigma_x \otimes \sigma_x \otimes \sigma_z)|\uparrow\uparrow\uparrow> = |\downarrow\downarrow\uparrow>$$

$$(\sigma_x \otimes \sigma_x \otimes \sigma_z)|\uparrow\uparrow\downarrow> = -|\downarrow\downarrow\downarrow>$$

$$(\sigma_x \otimes \sigma_x \otimes \sigma_z)|\uparrow\downarrow\uparrow> = |\downarrow\uparrow\uparrow>$$

$$(\sigma_x \otimes \sigma_x \otimes \sigma_z)|\uparrow\downarrow\downarrow> = -|\downarrow\uparrow\downarrow>$$

$$(\sigma_x \otimes \sigma_x \otimes \sigma_z)|\downarrow\uparrow\uparrow> = |\uparrow\downarrow\uparrow>$$

$$(\sigma_x \otimes \sigma_x \otimes \sigma_z)|\downarrow\uparrow\downarrow> = -|\uparrow\downarrow\downarrow>$$

$$(\sigma_x \otimes \sigma_x \otimes \sigma_z)|\downarrow\downarrow\uparrow> = |\uparrow\uparrow\uparrow>$$

$$(\sigma_x \otimes \sigma_x \otimes \sigma_z)|\downarrow\downarrow\downarrow> = -|\uparrow\uparrow\downarrow>$$

None of the base states is also eigenstate since operator σ_x always flips the spin. Eigenstate of the operator σ_x is thus symmetrical or antisymmetrical combination of spins »up« and »down«:

$$\sigma_x\left[\frac{1}{\sqrt{2}}(|\uparrow>)+|\downarrow>)\right] = +1\cdot\left[\frac{1}{\sqrt{2}}(|\uparrow>)+|\downarrow>)\right]$$

$$\sigma_x\left[\frac{1}{\sqrt{2}}(|\uparrow>)-|\downarrow>)\right] = -1\cdot\left[\frac{1}{\sqrt{2}}(|\uparrow>)-|\downarrow>)\right]$$

Eigenvalues are ±1, what we have already found in ex. 3.19. Also for the tensor product of Pauli operators the eigenvalues are ±1. Let's write just one of possible states and the corresponding equation:

$$|\psi> = \left[\frac{1}{\sqrt{2}}(|\uparrow>)-|\downarrow>)\right] \otimes \left[\frac{1}{\sqrt{2}}(|\uparrow>)+|\downarrow>)\right] \otimes |\uparrow>$$

$$(\sigma_x \otimes \sigma_x \otimes \sigma_z)|\psi> = (-1)\cdot(+1)\cdot(+1)|\psi> = -|\psi>$$ ♠

♥ EX. 4.8

The state of how many qubits simultaneously can be described with 10^{12} complex amplitudes?

Since the following equation holds for the number of necessary amplitudes for n qubits holds: $N = 2^n$, we obtain after taking logarithm of it: $\ln N = n \ln 2 \rightarrow n = \ln N/\ln 2 = \ln(10^{12})/\ln 2 = 12 \cdot (\ln 10/\ln 2) = 39{,}86$. This must be always truncated down: the maximum number of qubits is 39.

♥ RAČUNSKI ZGLED 4.9

State of the system of 4 qubits is described with the vector:

$$|\psi> = a_{1111}|1111> + a_{1110}|1110> + \ldots + a_{0000}|0000>$$

which is given by 16 complex amplitudes a_{ijkl}. During simultaneous measurement of the first two qubits we find states $|0>$ and $|1>$. Into what does the original state collapse?

Vector after measurement of first two qubits is (we keep only the amplitudes with first indices 0 and 1):

$$|\varphi> = C(a_{0111}|0111> + a_{0110}|0110> + a_{0101}|0101> + a_{0100}|0100>)$$

where additional normalization constant is:

$$C = 1/\sqrt{a_{0111}{}^2 + a_{0110}{}^2 + a_{0101}{}^2 + a_{0100}{}^2}$$

This is because before measurement the function was normalized with respect to all 16 amplitudes, but now only four remain and the function must be normalized again. ♠

♥ EX. 4.10

Operator (matrix) A is hermitian: $A^+ = A$. We define a new operator: $B = \exp(\mathrm{i}A)$, where i is imaginary unit. Using Taylor expansion prove that operator B is unitary, i.e.: $B^+B = BB+ = \mathrm{I}$.

Operator $B = \exp(\mathrm{i}A)$ can be formally expanded into Taylor series similarly as usual exponential function:

$$B = \sum_{j=0}^{\infty} \frac{1}{j!} (\mathrm{i}A)^j$$

We find to this operator B^+. Operation of such conjugation goes term by term, and it is also half homogeneous: $(\alpha A + \beta B)^+ = \alpha^* A^+ + \beta^* B^+$, where α and β are scalars, and A and B operators. This rule can be slightly generalized with respet to scalar factors: $(\alpha^m A + \beta^n B)^+ = (\alpha^*)^m A^+ + (\beta^*)^n B^+$, where m and n are optional integer exponents. It holds for the product: $(AB)^+ = B^+A^+$. But if $B = A$, we needn't worry about the order of operators, so: $(A^2)^+ = (A^+)^2$. Using induction reasoning we obtain: $(A^j)^+ = (A^+)^j$. But since A is hermitian, we have $A^+ = A$. Finally:

$$B^+ = \sum_{j=0}^{\infty} \frac{1}{j!} (-\mathrm{i}A)^j$$

This is the same as: $B = \exp(-\mathrm{i}A)$. We conclude:

$B^+B = \exp(-\mathrm{i}A)\exp(\mathrm{i}A) = \exp(-\mathrm{i}A + \mathrm{i}A) = \exp(0) = \mathrm{I}$ ♠

5 DYNAMICS OF QUANTUM PARTICLES

♥ EX. 5.1

How does the operator of linear momentum in 1D quantum problem act on wave function $\psi = A\sin(kx)$, limited to interval $0 \le x \le a$, so that boundary condition $\psi(0) = \psi(a) = 0$ is fulfilled? Normalize wave function. What's the mean value of linear momentum in this state? How does the operator of kinetic energy act in this function?

Condition $\psi(0) = 0$ is automatically fulfilled for sine function. In order $\psi(a) = 0$ to hold, we must have $\sin(ka) = 0$, that is, $ka = n\pi$. For the values of n we need only natural (positive integer) numbers. Thus: $\psi = A\sin(n\pi x/a)$. Constant A is calculated with normalization of wave function:

$$\int_0^a \psi^2 \mathrm{d}x = A^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right)\mathrm{d}x = A^2 \cdot \frac{a}{2} = 1 \rightarrow A = \sqrt{\frac{2}{a}}$$

Operator of momentum acts in this way:

$$\hat{p}\psi = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\left[A\sin(kx)\right] = -\mathrm{i}\hbar kA\cos(kx) = \mathrm{i}\hbar kA\sin\left(kx + \frac{3}{2}\pi\right)$$

Function ψ isn't eigenfunction of this operator. The mean value of linear momentum is zero. This can be checked in a few ways. The first way is the simplest: mean value of some operator which corresponds to true physical quantity must be real. But if the wave function is real we obtain in calculation because of the factor i purely imaginary quantity. So, the mean value of momentum for any real function must be automatically zero. The second way is the direct calculation:

$$<p> = <\psi|\hat{p}\psi> = -\mathrm{i}\hbar A^2 \int_0^a \sin(kx)\frac{\mathrm{d}}{\mathrm{d}x}\left[\sin(kx)\right]\mathrm{d}x = -\mathrm{i}\hbar A^2 k\int_0^a \sin(kx)\cos(kx)\mathrm{d}x = 0$$

Third proof is such, that we use Euler formula to split sine function into two exponential parts: $\sin(kx) = (\mathrm{e}^{\mathrm{i}kx} - \mathrm{e}^{-\mathrm{i}kx})/(2\mathrm{i})$. Exponential functions are eigenfunctions of the operator of momentum with the opposite eigenvalues which then cancel.

Operator of kinetic energy acts as:

$$\hat{E}_{\mathrm{kin}}\psi = -\frac{\hbar^2}{2m}\cdot\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left[A\sin(kx)\right] = \frac{\hbar^2 k^2}{2m}\cdot A\sin(kx)$$

Function ψ is the eigenfunction of this operator. ♠

♥ EX. 5.2

The lowest energy of the proton in 1D infinite potential well is 1 MeV. What's the width of the well?

What's the probability to find at some moment the particle in the middle third of the well?

Data:

E_1 = 1 MeV = $1{,}6 \cdot 10^{-13}$ J

$m = 1{,}67 \cdot 10^{-27}$ kg

----

a = ?

The width of the well a is expressed from Eq. (2.12 b):

$$E_1 == \frac{h^2 1^2}{8ma^2} \to a = \sqrt{\frac{h^2}{8mE_1}} = 1{,}43 \cdot 10^{-14} \text{ m} = 14{,}3 \text{ fm}$$

We use integral to calculate probability:

$$P = \int_{a/3}^{2a/3} \psi^2 \mathrm{d}x = \frac{2}{a} \int_{a/3}^{2a/3} \sin^2(kx) \mathrm{d}x = \frac{2}{a} \int_{a/3}^{2a/3} \frac{1}{2}(1 - \cos(2kx)) \mathrm{d}x$$

$$P = \frac{1}{a}\left(x - \frac{1}{2k}\sin(2kx)\right)\Bigg|_{a/3}^{2a/3} = \frac{1}{3} - \frac{1}{2n\pi}\left[\sin\left(\frac{4n\pi}{3}\right) - \sin\left(\frac{2n\pi}{3}\right)\right]$$

We have also used $k = n\pi/a$. First few values of quantum number n:

$$n = 1 \Rightarrow P = \frac{1}{3} + \frac{\sqrt{3}}{2\pi} = 0{,}609$$

$$n = 2 \Rightarrow P = \frac{1}{3} - \frac{\sqrt{3}}{4\pi} = 0{,}196$$

$$n = 3 \Rightarrow P = \frac{1}{3} = 0{,}333$$

$$n=4 \Rightarrow P=\frac{1}{3}+\frac{\sqrt{3}}{8\pi}=0{,}402$$

$$n=5 \Rightarrow P=\frac{1}{3}-\frac{\sqrt{3}}{10\pi}=0{,}278$$

$$n=6 \Rightarrow P=\frac{1}{3}=0{,}333$$

$$n=7 \Rightarrow P=\frac{1}{3}+\frac{\sqrt{3}}{14\pi}=0{,}373$$

$$n=8 \Rightarrow P=\frac{1}{3}-\frac{\sqrt{3}}{16\pi}=0{,}299$$

$$n=9 \Rightarrow P=\frac{1}{3}=0{,}333$$

$$n=10 \Rightarrow P=\frac{1}{3}+\frac{\sqrt{3}}{20\pi}=0{,}361$$

$$n=11 \Rightarrow P=\frac{1}{3}-\frac{\sqrt{3}}{24\pi}=0{,}310$$

$$n=12 \Rightarrow P=\frac{1}{3}=0{,}333$$ ♠

♥ EX. 5.3

How do we write the linear combination of two wave functions with different quantum numbers 1 and 2, for 1D infinite potential well, if the first energy is 3–times more probable than the second? Take real coefficients.

We write the sum in the form:

$$|\psi> = c_1|\psi_1> + c_2|\psi_2> \equiv c_1\sqrt{\frac{2}{a}}\sin(\frac{\pi}{a}x) + c_2\sqrt{\frac{2}{a}}\sin(\frac{2\pi}{a}x)$$

Since the probability for one of the stationary functions is the square of the corresponding coefficient, it holds: $c_1^2 = 3c_2^2$. At the same time the whole function must be normalized:

$$<\psi|\psi> = <c_1\psi_1 + c_2\psi_2|c_1\psi_1 + c_2\psi_2> = 1$$

$$<c_1\psi_1|c_1\psi_1> + <c_1\psi_1|c_2\psi_2> + <c_2\psi_2|c_1\psi_1> + <c_2\psi_2|c_2\psi_2> = 1$$

The second and the third term are zero due to orthogonality of the functions. But the functions ψ_1 and ψ_2 are already normalized. So, the simple equation remains: $c_1^2 + c_2^2 = 1$. Finally, we obtain: $c_1 = 3^{1/2}/2$, $c_2 = ½$. ♠

♥ EX. 5.4

Consider energy levels and their degeneracy in 3D infinite potential well. This is a cube with side a and with captured quantum particle with mass m. Generalize 1D case to 3D.

In 3D we have one energy term for each of the three degrees of freedom:

$$E = \frac{\hbar^2}{2m}\cdot(k_x^2 + k_y^2 + k_z^2) = \frac{h^2}{8ma^2}(n_1^2 + n_2^2 + n_3^2)$$

If quantum numbers n_1, n_2 and n_3 interchange values, also the wave function changes, but the energy remains the same. If n_1, n_2 and n_3 are all different, such as 1, 2 and 3, there are 6 permutations of them; this is also the degeneracy d of the energy level. Table shows some lowest stationary states, where energy is normalized to $E_0 = h^2/(8ma^2)$.

n_1	n_2	n_3	E/E_0	d
1	1	1	3	1
1	1	2		

1	2	1	6	3
2	1	1		
1	2	2	9	3
2	1	2		
2	2	1		
1	1	3	11	3
1	3	1		
3	1	1		
2	2	2	12	1
1	2	3	14	6
1	3	2		
2	1	3		
2	3	1		
3	1	2		
3	2	1		

♠

♥ EX. 5.5

Consider the splitting of energy levels in 2D infinite potential well. This is at first square with size *a* and with captured quantum particle with mass *m*, but then the square deforms into rectangle with edges *a* and $b = a + \Delta a$. Let it hold $\Delta a << a$.

Energy levels in a square are degenerate except for two equal quantum numbers. Let's take then two different quantum numbers n_1 and n_2:

$$E_{\mathrm{kv}} = \frac{h^2}{8ma^2}({n_1}^2 + {n_2}^2)$$

Replace the square with rectangle:

$$E_{\mathrm{pr}} = \frac{h^2}{8m}(\frac{{n_1}^2}{a^2} + \frac{{n_2}^2}{(a+\Delta a)^2}) = \frac{h^2}{8ma^2}({n_1}^2 + \frac{{n_2}^2}{(1+\Delta a/a)^2})$$

We can use a small part of Taylor series for the second term, $(1 + \Delta a/a)^{-2} \approx 1 - 2\Delta a/a$, thus:

$$E_{\mathrm{pr}}(n_1, n_2) \approx \frac{h^2}{8ma^2}({n_1}^2 + {n_2}^2(1 - 2\Delta a/a))$$

Change quantum numbers:

$$E_{\mathrm{pr}}(n_2, n_1) \approx \frac{h^2}{8ma^2}({n_2}^2 + {n_1}^2(1 - 2\Delta a/a))$$

and calculate the absolute value of energy difference:

$$\Delta E = \left|E_{\mathrm{pr}}(n_2, n_1) - E_{\mathrm{pr}}(n_1, n_2)\right| = \frac{h^2}{8ma^2}\left|n_2^{\ 2} - n_1^{\ 2}\right| \cdot \frac{2|\Delta a|}{a}$$

The relative energy difference with respect to the energy of original square is of interest:

$$\frac{\Delta E}{E_{\mathrm{kv}}} = \frac{\left|n_2^{\ 2} - n_1^{\ 2}\right|}{n_2^{\ 2} + n_1^{\ 2}} \cdot \frac{2|\Delta a|}{a}$$

To every energy level of original square there corresponds a pair of nearby levels for rectangle if $n_1 \neq n_2$. Treat very different cases, first $n_1 = 1$, $n_2 = 2$:

$$\frac{\Delta E}{E_{\mathrm{kv}}} = \frac{3}{5} \cdot \frac{2|\Delta a|}{a}$$

Next, the numbers differ by 1 again, but they are both much larger than 1. We can then use a new approximation:

$$\frac{\Delta E}{E_{\mathrm{kv}}} = \frac{(n_1+1)^2 - n_1^{\ 2}}{(n_1+1)^2 + n_1^{\ 2}} \cdot \frac{2|\Delta a|}{a} \approx \frac{2n_1}{2n_1^{\ 2}} \cdot \frac{2|\Delta a|}{a} = \frac{1}{n_1} \cdot \frac{2|\Delta a|}{a}$$

And, lastly, let one quantum number be much larger than the other:

$$\frac{\Delta E}{E_{\mathrm{kv}}} \approx \frac{2|\Delta a|}{a}$$

This is the largest possible energy splitting of pairs of states in rectangle. ♠

♥ EX. 5.6

We observe oscillations of atoms in all possible directions and this is a 3D problem. The elastic energy is generalized: $V = (k_1x^2 + k_2y^2 + k_3z^2)/2$. We'll also use the corresponding angular frequency $\omega = 2\pi\nu$, characteristic for spring pendulum with constant k and with weight of mass m: $\omega_1 = (k_1/m)^{1/2}$, $\omega_2 = (k_2/m)^{1/2}$, $\omega_3 = (k_3/m)^{1/2}$. Energy of quantum stationary state is:

$$E_{n_1,n_2,n_3} = \hbar\left[\omega_1(n_1 + \frac{1}{2}) + \omega_2(n_2 + \frac{1}{2}) + \omega_3(n_3 + \frac{1}{2})\right]$$

There are 3 quantum numbers due to 3D problem: n_1, n_2, n_3.

We consider only symmetric case:

$$E_{n_1,n_2,n_3} = \hbar\omega(n_1 + n_2 + n_3 + \frac{3}{2})$$

Treat the degeneracy of energy levels.

This is shown in the table.

Table 1: Quantum states and energy levels for symmetrical 3D harmonic oscillator; energies are given in units $E_0 = (h/2\pi)\omega = h\nu$.

n_1	n_2	n_3	E/E_0	d
0	0	0	3/2	1
1	0	0	5/2	3
0	1	0		
0	0	1		
1	1	0	7/2	6
1	0	1		
0	1	1		
2	0	0		
0	2	0		
0	0	2		
1	1	1	9/2	10
2	1	0		
2	0	1		
1	2	0		
1	0	2		
0	1	2		
0	2	1		
3	0	0		
0	3	0		
0	0	3		
…				

♠

♥ EX. 5.7

Finite potential step (jump) is shown in Fig. R19. It holds: $V(x) = 0$ for $x < 0$ and $V(x) = V_0$ for $x > 0$. Treat the coefficient of reflectivity R in transition of the wave from left to right subject to the condition $E \geq V_0$.

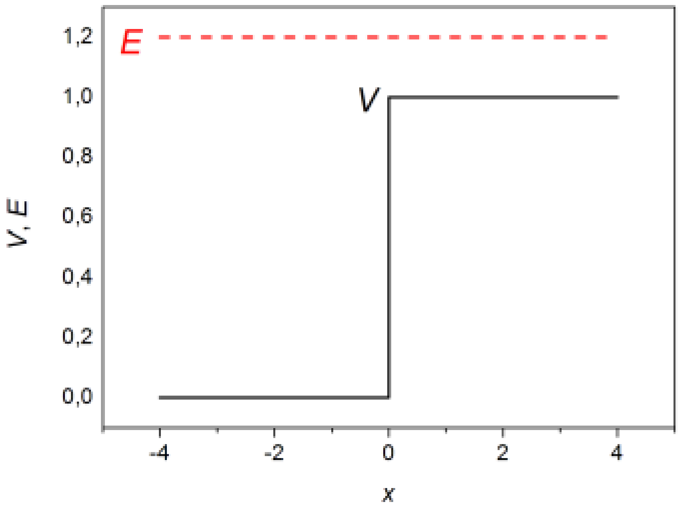


Fig. R19: Potential and full energy for potential step in the case $E > V_0$. Units in graph are without physical dimension, so that $V_0 = 1$.

The reflectivity coefficient is:

$$R = \left(\frac{k - k_1}{k + k_1}\right)^2$$

Here we have two wave vectors: $k = [2mE/(h/2\pi)^2]^{1/2}$ on the left and $k_1 = [2m(E - V_0)/(h/2\pi)^2]^{1/2}$ on the right side.

Write the condition, so that $R = 25\ \%$.

From equation for R it follows $k = 3k_1 \rightarrow k^2 = 9k_1^2$, or:

$$\frac{2mE}{\hbar^2} = 9 \cdot \frac{2m(E - V_0)}{\hbar^2} \rightarrow E = \frac{9}{8} V_0$$

Fig. R20 shows dependence of coefficients R and $T = 1 - R$ on the ratio E/V_0.

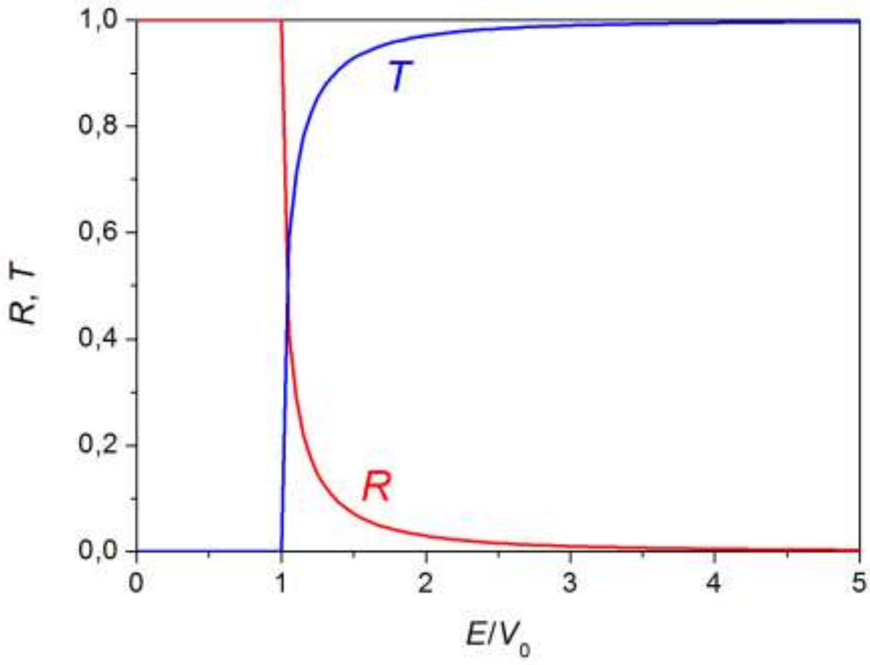


Fig. R20: Graphs $R(E/V_0)$ and $T(E/V_0)$ for finite potential step. In classical mechanics we would have instead of smooth curves just jump at $E = V_0$: 0 → 1 for T and 1 → 0 for R. But we see that this difference is not so significant since T approaches the value 1 quickly, and also R the value 0, when $E > V_0$. ♠

♥ EX. 5.8

In quantum mechanics we often deal with problems where we compare the wave function of some particle in classically allowed ($E > V$) and prohibited ($E < V$) area. In the case of constant potential $V(x)$ in one dimension the wave functions are combinations of imaginary ($E > V$) and real exponential functions ($E < V$). Instead of this, we can take the linear combination of sine and cosine functions or hyperbolic functions. We can avoid unnecessary repeating of calculations with the appropriate substitution of functions and parameters when the particle comes from classically allowed to prohibited area. So, sometimes the direct relation $\sin z \rightarrow \sinh z$ and $\cos z \rightarrow \cosh z$ is useful, where z is complec number. Generalize the Euler formula $\exp(\mathrm{i}x) = \cos x + \mathrm{i} \sin x$ to complex numbers to express sin(iz) and cos(iz) with hyperbolic functions.

We first express Euler formula for two equally large arguments with opposite signs, ±x: $\exp(\mathrm{i}x) = \cos x + \mathrm{i} \sin x$, $\exp(-\mathrm{i}x) = \cos x - \mathrm{i} \sin x$. Once, we sum both equations, and next we subtract them, so that we obtain:

$$\cos x = \frac{1}{2}(e^{\mathrm{i}x} + e^{-\mathrm{i}x})$$

$$\sin x = \frac{1}{2\mathrm{i}}(e^{\mathrm{i}x} - e^{-\mathrm{i}x})$$

Then we substitute $x \rightarrow \mathrm{i}z$:

$$\cos(\mathrm{i}z) = \frac{1}{2}(e^{\mathrm{i}(\mathrm{i}z)} + e^{-\mathrm{i}(\mathrm{i}z)}) = \frac{1}{2}(e^{-z} + e^{+z}) = \cosh z$$

$$\sin(\mathrm{i}z) = \frac{1}{2\mathrm{i}}(e^{\mathrm{i}(\mathrm{i}z)} - e^{-\mathrm{i}(\mathrm{i}z)}) = \frac{1}{2\mathrm{i}}(e^{-z} - e^{+z}) = -\frac{1}{\mathrm{i}}\sinh z = \mathrm{i}\cdot\sinh z$$

♠

♥ EX. 5.9

Derive general equation for the probability that the free quantum particle with energy E in the wave form the left »goes through« rectangular potential barrier with height $V > 0$ and width a for both cases: $V < E$ (Fig. R22) and $V > E$ (Fig. R21).

The detailed investigation of the first case is sufficient. Schroedinger equation for the stationary state with energy E and constant potential $V < E$ is:

$$-\frac{\hbar^2}{2m}\psi'' + V\psi = E\psi \rightarrow \psi'' = -k_1{}^2\psi$$

with the wave vector

$$k_1 = \sqrt{\frac{2m}{\hbar^2}(E - V)}$$

We have already used this vector in Ex. 5.7. The general solution of the above ordinary linear differential equation of second order is simple: $\psi = A\exp(\mathrm{i}kx) + B\exp(-\mathrm{i}kx)$. We could have used sine and cosine functions instead of imaginary exponential functions. However, exponential functions are more appropriate in this case since we observe travelling waves. The same holds in both areas with zero potential. Let's write the whole wave function for the three areas in Fig. R21:

1. $\psi_1 = A\exp(\mathrm{i}kx) + B\exp(-\mathrm{i}kx)$, to the left ($x < 0$), $k = [2mE/(h/2\pi)^2]^{1/2}$;
2. $\psi_2 = C\exp(\mathrm{i}k_1x) + D\exp(-\mathrm{i}k_1x)$, area of barrier ($0 < x < a$), $k_1 = [2m(E - V)/(h/2\pi)^2]^{1/2}$;
3. $\psi_3 = E\exp(\mathrm{i}kx) + F\exp(-\mathrm{i}kx)$, to the right ($x > a$), the same k as for ψ_1.

In all the three functions the first term means the wave which moves to the right while the second terms corresponds to the wave moving to the left. In general, all 6 coefficients are complex. But we can immediately simplify the first and third wave function. Here, we needn't normalize the wave function, but we need only the ratios of the coefficients. So we may put $A = 1$. Next, since the wave comes from the left, the third function cannot contain the wave moving to the left, so $F = 0$. We are mainly interested in the coefficient *E,* which will be used to calculate the transmission coefficient.

We must thus find 4 unknowns: *B*, *C*, *D* and *E*. We need 4 equations; we obtain them with 4 »boundary conditions«: the wave function as well as its first derivative with respect to *x* must be continuous at $x = 0$ and $x = a$. We obtain:

$\psi_1(0) = \psi_2(0) \rightarrow 1 + B = C + D$

$\psi_1'(0) = \psi_2'(0) \rightarrow (\mathrm{i}k) + B(-\mathrm{i}k) = C(\mathrm{i}k_1) + D(-\mathrm{i}k_1)$

$\psi_2(a) = \psi_3(a) \rightarrow C\exp(\mathrm{i}k_1a) + D\exp(-\mathrm{i}k_1a) = E\exp(\mathrm{i}ka)$

$\psi_2'(a) = \psi_3'(a) \rightarrow C(\mathrm{i}k_1)\exp(\mathrm{i}k_1a) + D(-\mathrm{i}k_1)\exp(-\mathrm{i}k_1a) = E(\mathrm{i}k)\exp(\mathrm{i}ka)$

This is the system of 4 linear equations for 4 unknowns; the system is inhomogeneous (nonzero right side) and uniquely solvable (determinant of the matrix is different from zero). We solve it easily, but with a lot of writing. Just write the final expression for *T*:

$$T = |E|^2 = \frac{4k^2k_1^{\,2}}{(k^2 - k_1^{\,2})^2\sin^2(k_1a) + 4k^2k_1^{\,2}} = \frac{1}{(1/4)(k/k_1 - k_1/k)^2\sin^2(k_1a) + 1}$$

$$k = \frac{\sqrt{2mE}}{\hbar} = \frac{2\pi\cdot\sqrt{2mE}}{h}$$

$$k_1 = \frac{\sqrt{2m(E - V_0)}}{\hbar} = \frac{2\pi\cdot\sqrt{2m(E - V_0)}}{h}$$

In the case $V > E_0$ the wave vector k_1 becomes imaginary and can be written as $k_1 = \mathrm{i}\kappa_1$, and the corresponding equations change:

$$T = \frac{4k^2\kappa_1^{\,2}}{(k^2 + \kappa_1^{\,2})^2\sinh^2(\kappa_1a) + 4k^2\kappa_1^{\,2}} = \frac{1}{(1/4)(k/\kappa_1 + \kappa_1/k)^2\sinh^2(\kappa_1a) + 1}$$

$$k = \frac{\sqrt{2mE}}{\hbar} = \frac{2\pi\cdot\sqrt{2mE}}{h}$$

$$\kappa_1 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} = \frac{2\pi\cdot\sqrt{2m(V_0 - E)}}{h}$$

According to Ex. 5.8 we have substituted sin(*ix*) → sinh *x*. ♠

♥ EX. 5.10

What’s the probability that the quantum particle in travelling wave from the left tunnels through the rectangular potential barrier if its potential is twice as large as kinetic energy of the particle: $V_0 = 2E$? The barrier width is *a* (Fig. R21).

We use the equations from previous example in the case $E < V_0$.

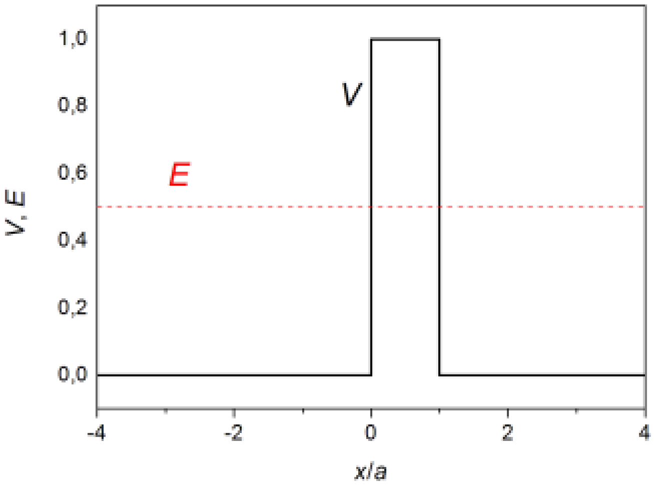


Fig. R21: Potential barrier and energy of particle incoming from left, $E = (1/2)V_0$. Units are set so that je $V_0 = 1$.

We insert in equation for *T* expressions for both wave vectors:

$$T = \frac{1}{\left(\frac{k^2+\kappa_1^2}{2k\kappa_1}\right)^2 \sinh^2(\kappa_1 a) + 1}$$

$$T = \frac{1}{\frac{V_0^2}{2E(V_0-E)}\sinh^2(\kappa_1 a) + 1}$$

In the case $V_0 = 2E$ the coefficient still depends on the width *a*:

$$T = \frac{1}{2\sinh^2(\kappa_1 a) + 1} = \frac{1}{2\sinh^2(\sqrt{2mE}\cdot a/\hbar) + 1}$$

We used $V_0 - E = 2E - E = E$; so k and κ_1 are equal. In the case of very small width a we have $T \approx 1$. Look at the opposite limit, large a. We make simplification $\sinh x = (e^x + e^{-x})/2 \approx e^x/2$, and we also neglect 1 in the denominator. Thus:

$$T \approx 2\exp(-\frac{2\sqrt{2mE}\cdot a}{\hbar})$$

For some feeling, let's find a to obtain $T = 1$ % if we have electron with mass $m = 9{,}1 \cdot 10^{-31}$ kg and kinetic energy $E = 1$ eV, so that $V_0 = 2$ eV:

$$a = \frac{\hbar \cdot \ln(2/T)}{2\sqrt{2mE}} = 0{,}52 \text{ nm}$$

Let's mention one more limiting case: $E \to V_0$. Then the parameter κ_1 is small and we substitute $\sinh(\kappa_1 a) \approx \kappa_1 a$:

$$T(E = V_0) = \frac{1}{(ka/2)^2 + 1}$$ ♠

♥ EX. 5.11

What's the probability that the quantum particle in the wave from left goes through the barrier if the potential is half the kinetic energy: $V_0 = E/2$ (Fig. R22)?

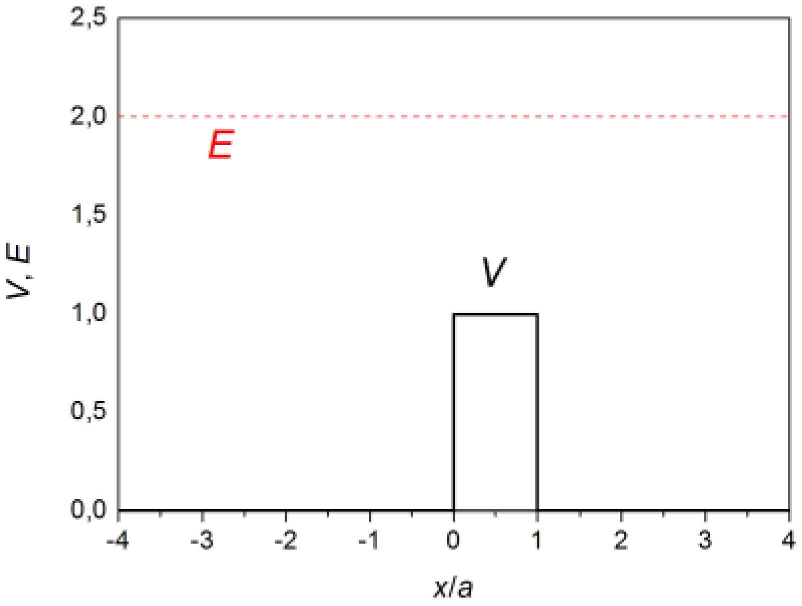


Fig. R22: Potential barrier end particle energy, $E = 2V_0$. Units in figure are set so that $V_0 = 1$.

We use equations for $E > V_0$. For $V_0 = E/2$ we have $k/k_1 = 2^{1/2}$, so:

$$T = \frac{1}{\sin^2(k_1 a)/8+1} = \frac{1}{\sin^2(\sqrt{mE}\cdot a/\hbar)/8+1}$$

It still depends on relation between E and a. In classical picture the transmission coefficient would be always 1, if the particle's energy exceeds potential barrier, but not so in quantum mechanics. But something else is also unusual: if we have definite barrier (fixed values of V_0 and a) and we gradually vary energy $E > V_0$, it happens that for some exact values of energy sine function in denominator is zero and so transmission coefficient is 1.

Let's draw graph $T(E/V_0)$ for $E \geq 0$, both for $E < V_0$ and $E > V_0$ (Figs. R23 in R24). We vary energy E, but we choose such barrier that the following relation holds between V_0 and a:

$$\kappa_{10} a \equiv \kappa_1(E=0)a = \frac{2\pi\cdot\sqrt{2mV_0}}{h}\cdot a = \frac{\pi}{2}$$

So $\sin(\kappa_{10}a) = 1$ and $\sinh(\kappa_{10}a) \approx 2{,}30$.

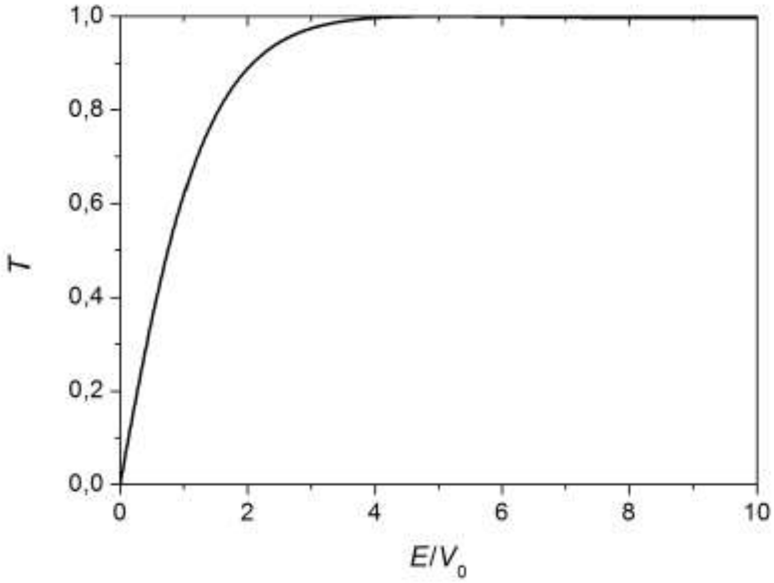


Fig. R23: Graph $T(E/V_0)$ for rectangular barrier corresponding to Figs. R21 and R22. Function for $E > V_0$ isn't strictly monotonically increasing, but has slight oscillations for high energies (which are quite little pronounced, see next figure). First maximum (T = 1 exactly) for our parameters is at $E = 5V_0$.

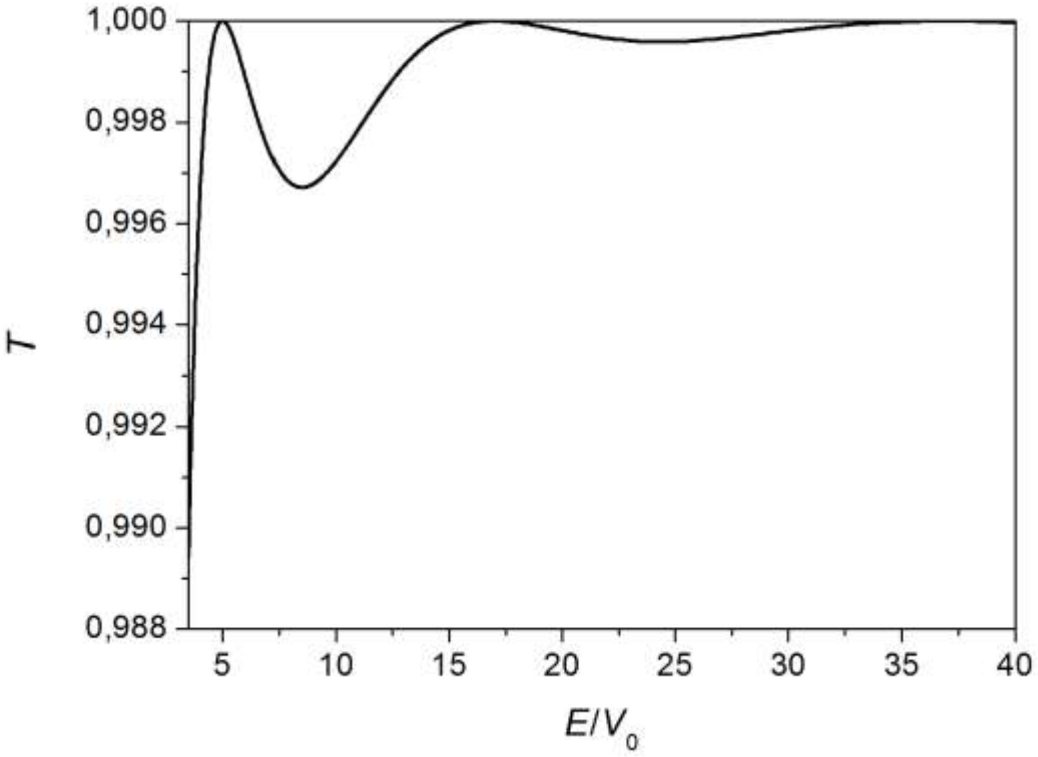


Fig. R24: As previous figure, but from some energy on, so that oscillations are more pronounced ♠

♥ EX. 5.12

What's the probability that the quantum particle in wave from left goes through the barrier in the shape of negative parabolic potential $V(x) = -kx^2/2$ (Fig. R25)? Equation for the probability T for any energy E (positive or negative) of the particle is:

$$T = \frac{1}{1 + \exp(-2\pi\varepsilon)}$$

$$\varepsilon = \frac{E}{\hbar} \cdot \sqrt{\frac{m}{k}}$$

Calculate T for three different values of dimensionless energy: $\varepsilon = 0, \pm 1/(2\pi)$, then find asymptotic behavior for $\varepsilon \rightarrow \pm\infty$. Draw graph $T(\varepsilon)$.

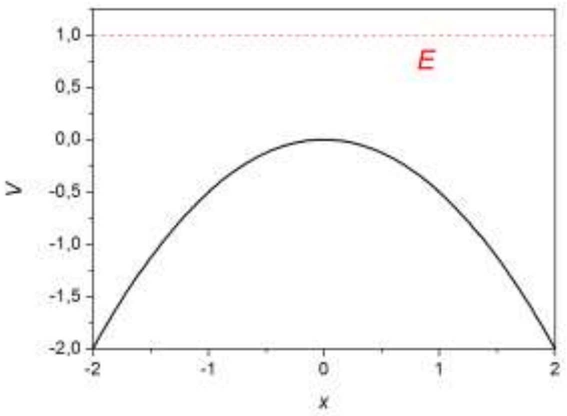


Fig. R25: Parabolic potential barrier and particle's energy; particle approaches from the left.

In the case $\varepsilon = 0$ we have $T = 0{,}5$. Function $T(\varepsilon)$ is increasing: for positive energies it holds $T > 0{,}5$, for negative energies $T < 0{,}5$. For $\varepsilon = 1/(2\pi)$ we have $T \approx 0{,}731$, for $\varepsilon = -1/(2\pi)$ we have $T \approx 0{,}269$. When $\varepsilon \to +\infty$, the exponential term in denominator is much smaller than 1, so approximately $T \approx 1 - \exp(-2\pi\varepsilon)$. But when $\varepsilon \to -\infty$ we have $T \approx \exp(2\pi\varepsilon)$. Graph is shown in Fig. R26. If the origin is moved to the point (0, ½), we get odd function hyperbolic tangens since:

$$T - \frac{1}{2} = \frac{1}{2}\tanh(\pi\varepsilon)$$

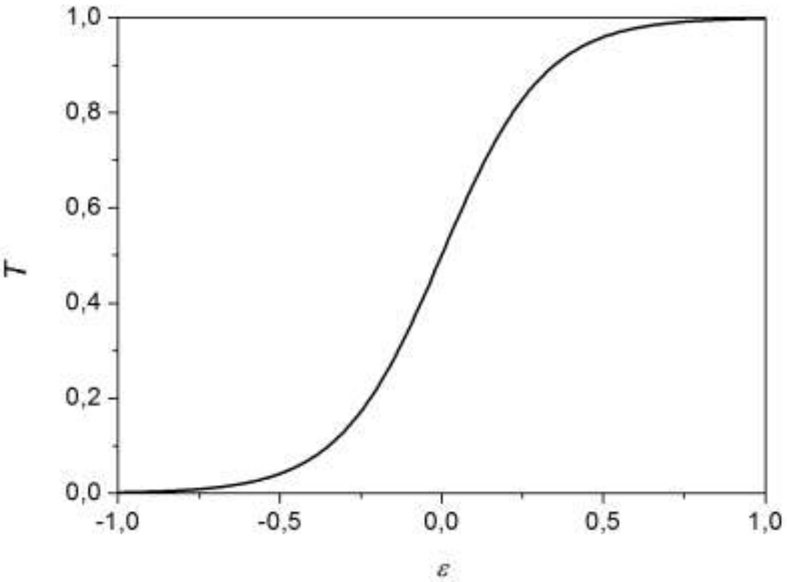


Fig. R26: Graph $T(\varepsilon)$ for parabolic barrier ♠

6 QUANTUM UNCERTAINTY

♥ EX. 6.1

We measure the coordinate x of the electron to 10 nm exactly. What's in principle the best exactness of the simultaneous measurement of its velocity component v_x? We measure the coordinate x of the runner on 100 m to 1 mm exactly (some definite point of its body). What's in principle the best exactness of the simultaneous measurement of its velocity component v_x if his mass is 80 kg?

We use equation:

$$\delta x \cdot \delta p_x = \delta x \cdot m \delta v_x = \frac{\hbar}{2} \rightarrow \delta v_x = \frac{\hbar}{2m\delta x} = \frac{h}{4\pi m \delta x}$$

We calculate for electron with mass $9{,}1 \cdot 10^{-31}$ kg $\delta v_x = 5{,}8 \cdot 10^3$ m/s. This seems a lot, but it's still much less than the light speed. We calculate for the 100 m runner: $6{,}6 \cdot 10^{-34}$ m/s! ♠

♥ EX. 6.2

The energy of the hydrogen atom in basic state can be estimated in the following way. The energy is the sum of kinetic and electrostatic parts: $E = mv^2/2 - e_0^2/(4\pi\varepsilon_0 r)$, with $m = 9{,}11 \cdot 10^{-31}$ kg (for more exact calculation we should use the reduced mass instead of the electron mass, but it's almost the same), $e_0 = 1{,}60 \cdot 10^{-19}$ As, $\varepsilon_0 = 8{,}85 \cdot 10^{-12}$ As/(Vm), r is some effective distance between electron and nucleus, and v the speed of circulating electron in the Bohr planet interpretation. According to Heisenberg principle, we estimate the relation between radius r and speed v so: $v \sim h/(4\pi \cdot mr)$, where $h = 6{,}63 \cdot 10^{-34}$ Js is Planck constant. This relation is obtained so that we rewrite inequality $\delta x \cdot \delta p_x \geq h/(4\pi)$ as equation and substitute $\delta x \rightarrow r$, $\delta p_x \rightarrow mv$. Calculate energy with its minimization over radius r, and also estimate r and v.

Energy expressed with independent variable r is:

$$E = \frac{h^2}{32\pi^2 \cdot mr^2} - \frac{e_0^{\ 2}}{4\pi\varepsilon_0 r}$$

We minimize it:

$$\frac{\mathrm{d}E}{\mathrm{d}r}=\frac{-h^2}{16\pi^2 mr^3}+\frac{e_0{}^2}{4\pi\varepsilon_0 r^2}=0\rightarrow r=\frac{\varepsilon_0 h^2}{4\pi m e_0{}^2}\rightarrow E=-\frac{me_0{}^4}{2\varepsilon_0{}^2 h^2}$$

We obtain rough estimations: $r \sim 0{,}2$ nm, $E \sim -54$ eV. ♠

♥ EX. 6.3

What's the product of the standard deviations of coordinate and linear momentum of the particle in 1D infinite potential well in basic state? Compare the exact result with the smallest possible product according to Heisenberg equation.

We already know the mean values of coordinate and momentum due to symmetry: $<x> = a/2$ (we take the interval $0 \le x \le$ a), $<p> = 0$. So we must still calculate the corresponding mean values of the squares of both quantities. First $<x^2>$:

$$<x^2>=\int_0^a x^2\psi^2 \mathrm{d}x=\frac{2}{a}\int_0^a x^2\sin^2(\frac{\pi}{a}x)\mathrm{d}x$$

We use the equation $\sin^2(kx) = (1 - \cos(2kx))/2$, and then the per partes method twice. We get:

$$<x^2>=a^2\cdot(\frac{1}{3}-\frac{1}{2\pi^2})$$

But the mean value of the square of momentum follows directly from the relation between the momentum and kinetic energy since ψ is eigenfunction of the operator of kinetic energy:

$$<p^2>=2mE_{\mathrm{kin}}=2mE=2m\cdot\frac{\hbar^2\pi^2}{2ma^2}=\frac{\hbar^2\pi^2}{a^2}$$

So:

$$\delta x=\sqrt{<x^2>-<x>^2}=a\cdot\sqrt{(\frac{1}{3}-\frac{1}{2\pi^2})-\frac{1}{4}}=a\cdot\sqrt{\frac{1}{12}-\frac{1}{2\pi^2}}\approx 0{,}18\ a$$

$$\delta p=\sqrt{<p^2>-<p>^2}=\sqrt{<p^2>}=\frac{\hbar\pi}{a}$$

The corresponding product is:

$$\delta x\cdot\delta p=0{,}18\pi\hbar=0{,}57\hbar>\frac{\hbar}{2}$$

This product is thus larger as the Heisenberg limit, as it should be. ♠

♥ EX. 6.4

Use the relation for the minimum product of the uncertainty for coordinate and momentum component to obtain similar relation for energy and time. Take kinetic energy of free particle: $E = p^2/(2m)$; use also $x = vt$.

Deviation of energy from deviation of momentum is estimated in the same way as differential: $\delta E = (\mathrm{d}E/\mathrm{d}p)\delta p = (p/m)\delta p = v\delta p$. To express the deviation of x we take only the deviation for time, but not so for velocity: $\delta x = v\delta t \rightarrow \delta t = \delta x/v$. The product is then:

$$\delta E \cdot \delta t = (v\delta p)\cdot(\delta x / v) = \delta p \cdot \delta x = \frac{\hbar}{2}$$

This derivation was not physically exact, but the final result is nevertheless correct. But the physical meaning of the last equation is quite different from the corresponding equation for coordinate and momentum. While the uncertainty of coordinate and momentum is connected with measurement of both quantities at the same time, we can in principle measure and compare the energy of the system at two different moments. ♠

♥ EX. 6.5

Relations for the uncertainty of the components of orbital (and also spin) angular momentum are different from ones for coordinates and components of linear momentum. This is because we calculate orbital angular momentum as a vector product of radius vector and linear momentum. While the uncertainty principle doesn’t prohibit exact simultaneous measurement of all three components of linear momentum, this in principle cannot be done in the case of angular momentum. Let’s consider the characteristic example, where quantum numbers l and m are given, and with them also:

$$\Gamma = \sqrt{l(l+1)}\cdot\hbar$$

$$\Gamma_z = m\cdot\hbar$$

Here, we must have $-l \le m \le l$. In this case the other two components of angular momentum are continuously distributed according to simple geometrical construction (at least, until they are measured). We imagine that the vector $\boldsymbol{\Gamma} = (\Gamma_x, \Gamma_y, \Gamma_z)$ rotates over the cone so that its magnitude and z–component (in the direction of the symmetry axis of the cone) are constant. Evaluate the uncertainty of both components of angular momentum for optional values of l and m and show some examples. When is the uncertainty of both components the smallest/largest?

Take any possible values of *l* and *m*. Then the component Γ_x has extremal values when $\Gamma_y = 0$:

$$\Gamma_x = \pm\sqrt{\Gamma^2 - \Gamma_z{}^2} = \pm\sqrt{l(l+1) - m^2} \cdot \hbar$$

The same is true for Γ_y, thus we can take estimation:

$$\delta\Gamma_x = \delta\Gamma_y = \sqrt{l(l+1) - m^2} \cdot \hbar$$

For given value of *l* this uncertainty is the smallest for $m = l$:

$$\delta\Gamma_{x\min} = \delta\Gamma_{y\min} = \sqrt{l} \cdot \hbar$$

and the largest for $m = 0$, i.e., when the vector of angular momentum rotates in the plane (x, y):

$$\delta\Gamma_{x\max} = \delta\Gamma_{y\max} = \sqrt{l(l+1)} \cdot \hbar = \Gamma$$

Some examples:

$$l = 1, m = 0 \to \delta\Gamma_x = \delta\Gamma_y = \sqrt{2} \cdot \hbar$$

$$l = 1, m = 1 \to \delta\Gamma_x = \delta\Gamma_y = \hbar$$

$$l = 2, m = 0 \to \delta\Gamma_x = \delta\Gamma_y = \sqrt{6} \cdot \hbar$$

$$l = 2, m = 1 \to \delta\Gamma_x = \delta\Gamma_y = \sqrt{5} \cdot \hbar$$

$$l = 2, m = 2 \to \delta\Gamma_x = \delta\Gamma_y = \sqrt{2} \cdot \hbar$$

The only exception in regard to uncertainty of the components of angular momentum is the case $l = m = 0$, where all three components are exactly zero.

♥ EX. 6.6

This example is connected to the previous, but now we are interested in spin angular momentum. Some elementary particle has spin $s = ½$, which means that it can have in some chosen direction (usually denoted as axis *z*) the eigenvalue $\Gamma_z = \pm(1/2)(h/(2\pi))$. Let the electron be in the eigenstate with $\Gamma_z = +(1/2)(h/(2\pi))$. What's the mean value of the component of the spin angular momentum in the direction of axis *z*' which makes an angle $\theta < 90°$ with the axis *z*?

As in the previous case with orbital angular momentum we may think that the vector $\boldsymbol{\Gamma}$ = (Γ_x, Γ_y, Γ_z) rotates over the cone. Now we write:

$$\Gamma_z = s\hbar$$

$$\Gamma = \sqrt{s(s+1)}\hbar > \Gamma_z$$

So the z axis and the vector of angular momentum make all the time the same angle:

$$\alpha = \arccos\frac{\Gamma_z}{\Gamma} = \arccos\frac{s}{\sqrt{s(s+1)}}$$

But the vector also depends on the angle φ:

$$\vec{\Gamma} = \Gamma(\sin\alpha\cos\varphi, \sin\alpha\sin\varphi, \cos\alpha)$$

In order to make calculation simpler we choose the unit direction vector of the new axis z' in the plane (x, z), but the final result does not depend on this choice:

$$\vec{e}_{z'} = (\sin\theta, 0, \cos\theta)$$

The component of angular momentum in the direction of the new axis is calculated with the following scalar product:

$$\Gamma_{z'} = \vec{\Gamma}\cdot\vec{e}_{z'} = \Gamma(\sin\alpha\cos\varphi\cdot\sin\theta + \cos\alpha\cdot\cos\theta)$$

Its average value is obtained with integration over azimuthal angle:

$$<\Gamma_{z'}> = \frac{1}{2\pi}\int_0^{2\pi}\vec{\Gamma}\cdot\vec{e}_{z'}d\varphi = \frac{\Gamma}{2\pi}\int_0^{2\pi}(\sin\alpha\cos\varphi\cdot\sin\theta + \cos\alpha\cdot\cos\theta)d\varphi$$

Integral of the first term is zero and the result is simple:

$$<\Gamma_{z'}> = \Gamma\cos\alpha\cdot\cos\theta = \Gamma_z\cdot\cos\theta = \frac{\hbar}{2}\cdot\cos\theta$$

In the limiting case $\theta \rightarrow \pi/2$ this gives zero since the z' axis becomes x axis and the negative values of Γ_x are equally probable as positive ones. We stress that the old axis z has no preference in comparison with z'. Therefore, the eigenvalues of the component of angular momentum with respect to z' are of course equal as for z. If we have the eigenstate with the component $\Gamma_z = +(1/2)(h/(2\pi))$, it can still be thought as a linear combination of the states, where for the new axis $\Gamma_{z'} = \pm(1/2)(h/(2\pi))$.

In regard to Stern-Gerlach experiment we can ask the following question. Say, we have measured the component in the direction of chosen z axis and we found the value Γ_z = +(1/2)(h/(2π)). Now, we repeat the measurement according to the new axis z'. Again, we expect on of the two possibilities $\Gamma_{z'}$ = ±(1/2)(h/(2π)) and we are interested in the probability for both of them. For acute angle between the axes these probabilities are different. Denote them by P_+ (for positive value) and P_-; it is sensible to expect $P_- < P_+$. They are calculated from:

$$< \Gamma_{z'} >= \frac{\hbar}{2} \cdot \cos\theta = \frac{\hbar}{2} \cdot P_+ + (-\frac{\hbar}{2})P_-$$

$$P_+ + P_- = 1$$

We obtain:

$$P_+ = \cos^2\frac{\theta}{2}$$

$$P_- = \sin^2\frac{\theta}{2}$$

As expected, only for $\theta = \pi/2$ are they the same: $P+ = P- = ½$. ♠

7 ELECTRON MICROSCOPY

♥ EX. 7.1

Although the resolution of the electron microscope nowadays is more limited with the size of the spot of the electron beam on the sample surface, the Broglie wavelength of the electron is still a crucial factor. If we estimate the threshold of resolution as $d \approx \lambda/2$, what should be the acceleration voltage of electrons in order to achieve the resolution $d = 1$ nm?

It holds:

$$d = \frac{\lambda}{2} = \frac{h}{2p} = \frac{h}{2\sqrt{2mE_\mathrm{k}}}$$

Here m is the electron mass, while kinetic energy is equal to electric work: $E_\mathrm{k} = eU$. So we have:

$$d = \frac{h}{2\sqrt{2me_0U}} \rightarrow U = \frac{h^2}{8me_0d^2} = 0{,}37\ \mathrm{V}$$

In fact, the typical voltages for scanning electron microscope are of the order of 10 kV. We find that the true limitation to the resolution is due to the size of the spot of electron beam as mentioned above. ♠

♥ EX. 7.3

SEM of polished surface of polycrystalline matter, such as engineering ceramics, where the boundaries between crystal grains are clearly visible (Fig. R28), is an appropriate tool for measurement and calculation of the size distribution of crystal grains and correspondingly their mean size. 2D image can be statistically treated, either manually (what is time demanding) or with the use of some program package. Since the grains have irregular shapes (we see them on SEM image as objects with several sides), we must choose the appropriate criterion for their size. Thus, the grain size is usually defined as the diameter of the circle with the same area as the area of the object on image. However, the simple reasoning tells us that this size estimation (for real 3D grains from their 2D projections) gives systematically too low values of grain sizes. This is because by polishing we cut the grains at different locations and not with the largest 2D cross-section, since there is no space ordering of the positions of crystal grains. Statistical calculation with grains of non-real ideal spherical shape shows that in this way we measure by factor $4/\pi \approx 1{,}27$ too small value of mean size of grains. So, we often take this factor as a correction to the calculation of the size of 3D grains. Derive this factor if you take that all grains have the shape of sphere with the same radius *R*, but in 2D image we cut such spheres at different heights with equal probability.

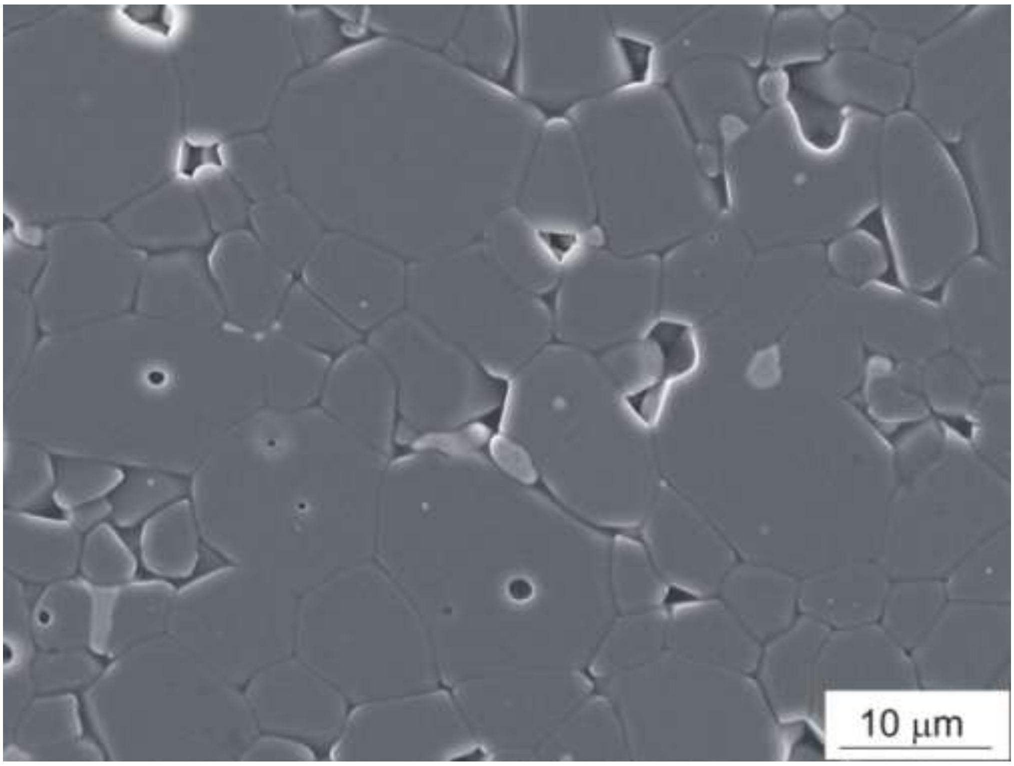


Fig. R28: SEM image of polished surface of Al_2O_3. Dark holes are pores.

We consider a sphere with radius *R* and with the center at the origin of coordinate system, so that the following equation holds: $x^2 + y^2 + z^2 = R^2$. The sphere can be intersected with the horizontal plane parallel to (x, y) plane at different coordinates *z*. Because of symmetry it suffices to consider only positive *z*: $0 \leq z \leq R$. We suppose the uniform distribution of *z* on this interval: $p(z) = 1/R$. For given *z* the projection of sphere on the plane is a circle with smaller radius $r = (R^2 - z^2)^{1/2}$. Average radius is then:

$$\bar{r} = \frac{1}{R}\int_0^R r\mathrm{d}z = \frac{1}{R}\int_0^R \sqrt{R^2 - z^2} \cdot \mathrm{d}z$$

We next introduce the new integration variable φ: $z = R \sin \varphi$, $\mathrm{d}z = R \cos \varphi \cdot \mathrm{d}\varphi$, use relation $\cos^2\varphi = (1 + \cos(2\varphi))/2$, finish integration in we indeed obtain the result $(\pi/4)R$. ♠

♥ EX. 7.4

In the tunneling electron microscope the distance between the tip and the surface of the sample is so small that the electrons tunnel through the classically forbidden area (vacuum between the tip and sample surface) with measurable probability:

$$T = \exp\left[-2\cdot\frac{\sqrt{2m_{\mathrm{e}}V}}{\hbar}\cdot d\right]$$

Here, m_{e} is the electron mass, V potential energy of prohibited area, kinetic energy may be neglected, d is the distance between microscope tip and sample surface. Potential energy V is estimated as the knock-out work for electrons and we take the value V = 1 eV, next, the characteristic distance is d = 1 nm, while the depth resolution is Δd = 0,01 nm. Calculate the transmission coefficient T for d = 1 nm and its relative change for Δd = 0,01 nm.

For d = 1 nm we get $T = 3{,}6\cdot 10^{-5}$. Relative change is:

$$\frac{\Delta T}{T}\approx\left|\frac{\mathrm{d}T}{\mathrm{d}d}\right|\cdot\frac{\Delta d}{T}=\frac{2\sqrt{2m_{\mathrm{e}}V}}{\hbar}\cdot\Delta d\ = 10{,}2\ \% \ \spadesuit$$

♥ Ex. 7.5

We use for scanning tunneling electron microscope very high vacuum where we can achieve very low value of pressure, around 10^{-8} Pa (ultra high vacuum) and even significantly lower values. Estimate the mean free path $<l>$ of residual gas molecules at this pressure if you take the fact that a single molecule occupies effective volume (before collision with another molecule) $V_1 = \pi d^2 <l>$, where $d \approx 0{,}1$ nm is the effective diameter of the molecule (the size of the molecule has no direct classical meaning, but its value is given by interaction with other molecules). We take in this estimation for effective volume diameter instead of radius because the centers of both molecules which move along two nearby parallel trajectories at least one diameter apart. Use the gas equation $p = nkT$, where p is pressure, n number of molecules per unit volume, k Boltzmann constant, and T pa absolute temperature. Take T = 4 K, which is typical for systems cooled with liquid helium.

If we take in definition $n = N/V$ only one molecule, N = 1, to which the volume V_1 belongs, we derive the following equation:

$$n=\frac{1}{V_1}=\frac{1}{\pi d^2<l>}\rightarrow<l>=\frac{1}{\pi d^2 n}=\frac{kT}{\pi d^2 p}\ = 1{,}8\cdot 10^5\ \mathrm{m}$$

In physical sense this means that the mean free path of the molecules is entirely determined with the size of vacuum system, i.e., the frequency of collisions between the molecules is negligible in comparison with the collisions from the walls of vacuum chamber. We mention that in more exact calculation we should also add the correction factor $2^{1/2}$ in the denominator in the expression for $<l>$ which takes into account the relative movement of the colliding molecules. But this factor is not significant for the estimation of the order of magnitude of $<l>$.

Source: https://cas.web.cern.ch/cas/Spain-2006/PDFs/Dylla-4.pdf

◆

8 ELECTRONS IN MATTER

♥ EX. 8.1

The difference between the neighboring energy levels in hydrogen atom is 0,306 eV. Which quantum states (n and $n + 1$) does this difference correspond to?

Energy difference between the two levels is:

$$\Delta E = E_{n+1} - E_n = E_0 \cdot (\frac{1}{n^2} - \frac{1}{(n+1)^2})$$

Here $E_0 = 13{,}6$ eV. Since we obtain after rearrangement the equation of the fourth level for n (which otherwise has analytical solution), its direct solving is too long. Thus we prefer to try with small values of n from 1 on. The right value is $n = 4$.

♥ EX. 8.2

Electron in hydrogen atom goes from quantum state $n = 4$ to lower state so that it emits photon with wavelength 485,3 nm. Which is this lower state?

Instead of using direct relation between the wavelength and both quantum numbers, we will use energy equation for exercise. The photon energy is:

$$E_{\mathrm{f}} = h\upsilon = \frac{hc}{\lambda} = 2{,}55 \text{ eV}$$

The energy difference between the levels with quantum numbers n and $m < n$ is:

$$\Delta E = E_{\mathrm{f}} = E_0 \cdot (\frac{1}{m^2} - \frac{1}{n^2}) \rightarrow m = 1/\sqrt{1/n^2 + E_{\mathrm{f}} / E_0} = 2 \spadesuit$$

♥ EX. 8.3

The wave function for the electron in hydrogen atom is composed of radial and angular factors. Radial part tells how the function varies with distance r form the nucleus, and it depends on quantum numbers n (principal quantum number) and l (connected with orbital angular momentum of electron). We give the radial function for three states with the lowest quantum numbers (the first index means n, the second l):

$$R_{10}(x) = 2\exp(-x)$$

$$R_{20}(x) = \frac{1}{\sqrt{2}}\exp(-x/2)\cdot(1-x/2)$$

$$R_{21}(x) = \frac{1}{2\sqrt{6}}\exp(-x/2)\cdot x$$

Here $x = r/r_0$, and r_0 Bohr radius. All radial functions are normalized:

$$\int_0^\infty R_{nl}{}^2 x^2 \mathrm{d}x = 1$$

Additional factor x^2 in the integral is present because the volume element after integration over angles (this element corresponds to the thin spherical shell with radius r and thickness dr) os $\mathrm{d}V = 4\pi r^2 \mathrm{d}r$. But additional factor 4π is already included in correct normalization of the angular part of the wave function. Calculate the most probable radius r for each of the given functions; this corresponds to x, where the function $x^2 R_{nl}{}^2$ has maximum.

Let's present calculation only for R_{10}:

$$y = x^2 R_{10}{}^2 = 4x^2\exp(-2x)$$

$$\frac{\mathrm{d}y}{\mathrm{d}x} = 8\left[x - x^2\right]\exp(-2x) = 0$$

The solution $x = 0$ corresponds to minimum; this is logical: the probability density (with respect to r) to find the electron in the nucleus is zero. We are interested in maximum here: $x = 1$ or $r = r_0$. Similarly we find that to function R_{20} there corresponds the most probable radius $r = 2r_0$. To function R_{21} there corresponds $r = 4r_0$. The increase of the most probable radius in comparison with the function R_{20} is related to the positive orbital angular momentum for $l = 1$.

♠

♥ EX. 8.4

The angular part of the wave function for electron in hydrogen atom (and also more generally for centrally symmetrical potential) consists for definite quantum numbers l and m from two factors: $Y_{lm}(\theta, \varphi) = C\exp(im\varphi)\,f_{lm}(\theta)$. C is the normalization constant. We are interested here only in the function of the angle θ according to chosen axis in space. We consider just the case with $m = 0$; in this case $f_{l0}(\theta) = P_l(\cos\theta)$, and $P_l(x)$ is the Legendre polynomial of degree l. Let's write some of them:

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = \frac{1}{2}(3x^2 - 1)$$

Treat zeros of the corresponding functions $Y_{l0}(\theta, \varphi)$.

The factor, which is a function of φ, has no zeros. Therefore, the zeros of Y_{l0} are determined by zeros of Legendre polynomials. Function Y_{00} has no zeros. Function Y_{10} is due to polynomial $P_1(x)$ equal to zero for $x = 0$, i.e., $\theta = \pi/2$. Function Y_{20} is zero for $x^2 = 1/3$, resulting in angles 54,74° and 125,26°. The entire wave function for hydrogen atom, including radial part, is thus equal tom zero for some definite values of radius r and polar angle θ; the higher the quantum numbers, more zeros exist. ♠

♥ EX. 8.5

Potential for weak chemical bonds in the simple Lennard-Jones model is described by the function:

$$V(r) = \varepsilon \cdot \left[(\frac{a}{r})^{12} - (\frac{a}{r})^{6} \right]$$

Here ε is the characteristic energy, and a characteristic distance. Find minimum of the potential. Where is the potential equal to zero? Write asymptotic behavior of potential for $r \rightarrow 0$ and $r \rightarrow \infty$.

Minimum is calculated with condition dV/dr = 0. The corresponding distance is

$$r_0 = a \cdot \sqrt[6]{2}$$

and potential

$$V_0 = -\frac{\varepsilon}{4}$$

Potential is zero at $r = a$. For small r we may neglect the second term in expression for $V(r)$, but for large r we may neglect the first term. Asymptotic behavior of $V(r)$ is then:

$$r \rightarrow 0 \Rightarrow V(r) \approx \varepsilon \cdot (\frac{a}{r})^{12}$$

$$r \to \infty \Rightarrow V(r) \approx -\varepsilon \cdot (\frac{a}{r})^6$$ ♠

♥ EX. 8.6

Carbon (as diamond) and two key semiconductor elements, silicon and germanium, have diamond crystal structure. Relative positions of the nearest atoms (take C) are presented with tetrahedron, so that four C atoms are in the corners and one is in the mass center (T), this is on the quarter of the body height (as seen from base surface towards the top point V). Calculate the angle between neighboring C–C covalent bonds. Use the three vectors to define tetrahedron (Fig. R29).

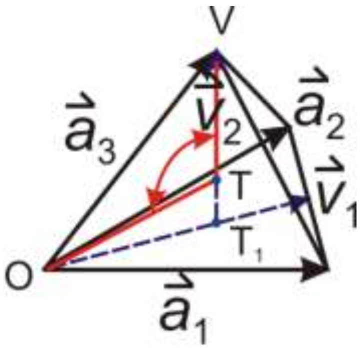


Fig. R29: Tetrahedron with C–C bonds; red curved double arrow denotes the angle we seek.

All three vectors in figure, $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ in $\boldsymbol{a}_3$, have the length a, and the angle between any two of them is 60°. We will also use vectors $\boldsymbol{v}_1$ in $\boldsymbol{v}_2$: the former goes along the height of the triangle – base face and it is equal to $\boldsymbol{v}_1 = (\boldsymbol{a}_1 + \boldsymbol{a}_2)/2$. Vector $\boldsymbol{v}_2$ goes along the body height of tetrahedron. Since the body height goes up from mass-center T_1 of bottom triangle, and this point is in turn on the 2/3 of area height of bottom triangle (starting from point O towards opposite line of triangle), we calculate vector $\boldsymbol{v}_2$ so: $\boldsymbol{v}_2 = \boldsymbol{a}_3 - (2/3)\boldsymbol{v}_1 = \boldsymbol{a}_3 - (\boldsymbol{a}_1 + \boldsymbol{a}_2)/3$. The angle between the C–C bonds is calculated as an angle between vectors $\boldsymbol{x} = \mathrm{TV} = 3\boldsymbol{v}_2/4$ and $\boldsymbol{y} = \mathrm{TO} = -(2\boldsymbol{v}_1/3 + \boldsymbol{v}_2/4)$; in order not to make the figure too full, we have not signed vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ separately, but the red lines correspond to them. Let's express $\boldsymbol{x}$ and $\boldsymbol{y}$ with vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{a}_3$: $\boldsymbol{x} = (3\boldsymbol{a}_3 - (\boldsymbol{a}_1 + \boldsymbol{a}_2))/4$, $\boldsymbol{y} = -(\boldsymbol{a}_1 + \boldsymbol{a}_2 + \boldsymbol{a}_3)/4$. Next, we calculate their size, so that we take $\boldsymbol{a}_1 \cdot \boldsymbol{a}_1 = a^2$ in $\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 = a^2 \cos 60° = a^2/2$, etc., and we obtain:

$$x = \sqrt{\vec{x} \cdot \vec{x}} = a \cdot \frac{\sqrt{6}}{4}$$

$$y = \sqrt{\vec{y} \cdot \vec{y}} = a \cdot \frac{\sqrt{6}}{4}$$

Of course, sizes of both vectors must be equal since this means the distance between the nearest C atoms. This was a test that the central atom in fact lies on the quarter of body height. At last we find the angle:

$$\varphi = \arccos\frac{\vec{x}\cdot\vec{y}}{xy} = \arccos(-\frac{1}{3}) = 109{,}5^\circ$$ ♠

♥ EX. 8.7

Body centered cubic crystal structure (*bcc*) for many elementary metals (e.g., barium, chromium, sodium, tungsten and iron) is represented by unit cell – cube which has atoms in its corners, and one additional atom in the center of cube. The cube has 8 atoms in corners, but at the same time each atom in the corner is shared by 8 sticking cubes, which gives effectively 1 corner atom per cell. The central atom is added to this, so that each unit cell contains 2 equal atoms. We speak about unit crystal cell with the base since it has more than one atom. So, effective volume $a^3/2$ belongs to one atom. Instead of this, we can find 3 such lattice vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{a}_3$ (which are not orthogonal), that the unit cell (spanned on these vectors) contains just one atom. At the same time, if we move along the crystal lattice spanned on these three vectors, we much reach every atom in the crystal. The choice of appropriate vectors is not unique. It turns out that the suitable choice is: $\boldsymbol{a}_1 = (a/2)(-1, 1, 1)$, $\boldsymbol{a}_2 = (a/2)(1, -1, 1)$, $\boldsymbol{a}_3 = (a/2)(1, 1, -1)$. In this way we can come from a chosen corner atom, to which we assign coordinates (0, 0, 0) directly to the center atoms in the three neighboring cubes. Prove that such choice of lattice vectors really gives primitive cell, i.e., the cell to which only one atom belongs.

The proof is to show that the volume of parallelepipede, spanned on these three vectors, is indeed equal to the value $a^3/3$. The volume is calculated by mixed (pseudoscalar) product:

$$V = (\vec{a}_1, \vec{a}_2, \vec{a}_3) \equiv \vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) = \begin{vmatrix} a_{1x} & a_{1y} & a_{1z} \\ a_{2x} & a_{2y} & a_{2z} \\ a_{3x} & a_{3y} & a_{3z} \end{vmatrix}$$

So, we use the determinant of the 3 × 3 matrix, but we take absolute value of it if it is negative. Proceed:

$$V = \frac{a^3}{8}\cdot\begin{vmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} = \frac{a^3}{2}$$ ♠

♥ EX. 8.8

Face centered cubic crystal structure (*fcc*) for many elementary metals (e.g., aluminum, copper, calcium, silver and gold) is represented by unit cell – cube which has atoms in its corners, and 6 additional atoms in the centers of the faces of cube. As for *bcc* structure there is 1 corner atom per cell. We add to this 6 atoms on faces, but each such atom is shared by two cubes, so only 3 face atoms come effectively per cube. Thus one cell contains 4 atoms and there belongs the effective volume $a^3/4$ to one atom. Instead of this, we can find 3 such lattice vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{a}_3$, that the unit cell (spanned on these vectors) contains just one atom. One suitable choice is: $\boldsymbol{a}_1 = (\boldsymbol{a}/2)(0, 1, 1)$, $\boldsymbol{a}_2 = (\boldsymbol{a}/2)(1, 0, 1)$, $\boldsymbol{a}_3 = (\boldsymbol{a}/2)(1, 1, -0)$. Prove that with such a choice we get a primitive cell.

$$V = \frac{a^3}{8} \cdot \begin{vmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \frac{a^3}{4} \quad \spadesuit$$

♥ EX. 8.9

Prove that the reciprocal lattice of reciprocal lattice is again direct (original) Bravais lattice. We first construct from lattice vectors $\boldsymbol{a}_i$, $i = 1 - 3$, the vectors of reciprocal lattice, $\boldsymbol{b}_i = 2\pi\, \boldsymbol{a}_j \times \boldsymbol{a}_k/(\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3)$, where the triple of indices is $ijk = 123$ or both cyclic permutations of this. We use $(\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3)$ to denote shortly the mixed product $\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$. If we now use vectors $\boldsymbol{b}_i$ to construct new reciprocal vectors $\boldsymbol{c}_i$, it turns out that $\boldsymbol{c}_i = \boldsymbol{a}_i$. This is to be proved.

Let’s write the definition of vectors $\boldsymbol{b}_i$:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{(\vec{a}_1, \vec{a}_2, \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{(\vec{a}_1, \vec{a}_2, \vec{a}_3)}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{(\vec{a}_1, \vec{a}_2, \vec{a}_3)}$$

We prepare the relation to be used later:

$$(\vec{a}_3 \times \vec{a}_1) \times (\vec{a}_1 \times \vec{a}_2) = (\vec{a}_1, \vec{a}_2, \vec{a}_3)\vec{a}_1 \qquad (*)$$

This can be shown directly by components. But the fact that the vector on the right side of equation is indeed in the direction of $\boldsymbol{a}_1$, is evident by geometrical inspection, because we seek for vector product (middle ×) of two vectors which are perpendicular to $\boldsymbol{a}_1$ (because of vector products with $\boldsymbol{a}_1$ in both parentheses).

Next step:

$$(\vec{b}_1,\vec{b}_2,\vec{b}_3)=\left[\frac{2\pi}{(\vec{a}_1,\vec{a}_2,\vec{a}_3)}\right]^3\cdot(\vec{a}_2\times\vec{a}_3)\cdot\left[(\vec{a}_3\times\vec{a}_1)\times(\vec{a}_1\times\vec{a}_2)\right]$$

$$(\vec{b}_1,\vec{b}_2,\vec{b}_3)=\left[\frac{2\pi}{(\vec{a}_1,\vec{a}_2,\vec{a}_3)}\right]^3\cdot(\vec{a}_2\times\vec{a}_3)\cdot\left[(\vec{a}_1,\vec{a}_2,\vec{a}_3)\vec{a}_1\right]$$

$$(\vec{b}_1,\vec{b}_2,\vec{b}_3)=\left[\frac{2\pi}{(\vec{a}_1,\vec{a}_2,\vec{a}_3)}\right]^3\cdot(\vec{a}_1,\vec{a}_2,\vec{a}_3)(\vec{a}_2\times\vec{a}_3)\cdot\vec{a}_1$$

Last factor, $(\boldsymbol{a}_2 \times \boldsymbol{a}_3) \cdot \boldsymbol{a}_1$ is again $(\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3)$, thus we obtain:

$$(\vec{b}_1,\vec{b}_2,\vec{b}_3)=\frac{(2\pi)^3}{(\vec{a}_1,\vec{a}_2,\vec{a}_3)} \qquad (**)$$

It suffices to calculate $\boldsymbol{c}_1$:

$$\vec{c}_1=2\pi\frac{\vec{b}_2\times\vec{b}_3}{(\vec{b}_1,\vec{b}_2,\vec{b}_3)}$$

$$\vec{c}_1=\frac{2\pi}{(\vec{b}_1,\vec{b}_2,\vec{b}_3)}\cdot\left[2\pi\frac{\vec{a}_3\times\vec{a}_1}{(\vec{a}_1,\vec{a}_2,\vec{a}_3)}\right]\times\left[2\pi\frac{\vec{a}_3\times\vec{a}_1}{(\vec{a}_1,\vec{a}_2,\vec{a}_3)}\right]$$

Use (*) and (**), and we really find $\boldsymbol{c}_1 = \boldsymbol{a}_1$. Similarly $\boldsymbol{c}_2 = \boldsymbol{a}_2$ and $\boldsymbol{c}_3 = \boldsymbol{a}_3$. ♠

♥ EX. 8.10

In aluminum one of the distances between nearest lattice plane is d = 0,405 nm. We illuminate aluminum crystal with X-rays of wavelength 0,3 nm. What must be the angle of the incident beam with respect to lattice plane in order to obtain the enforcement of the first (second, third …) order?

Bragg equation $2d \sin \theta = \lambda$ gives: $\theta = \arcsin(\lambda/(2d)) = 21{,}74°$. In the case of second order (N = 2): $2d \sin \theta = 2\lambda \rightarrow \theta = \arcsin(\lambda/d) = 47{,}79°$. There are no higher orders. ♠

9 METALS, SEMICONDUCTORS AND INSULATORS

♥ EX. 9.1

Copper has the Fermi energy 7,00 eV. Calculate the number of conducting electrons per unit volume. Check the result in a different way, with the following data: valence is 1, density is 8,96 kg/dm^3, atomic mass number is A = 63,55.

We first calculate the Fermi wave vector:

$$E_\mathrm{F} = \frac{\hbar^2 k_\mathrm{F}^{\;2}}{2m_\mathrm{e}} \rightarrow k_\mathrm{F} = \frac{\sqrt{2m_\mathrm{e}E_\mathrm{F}}}{\hbar} = 1{,}36 \cdot 10^{10}/\mathrm{m}$$

Here m_e is the electron mass. The density of conducting electrons is:

$$n = \frac{k_\mathrm{F}^{\;3}}{3\pi^2} = 8{,}5 \cdot 10^{28}/\mathrm{m}^3$$

Check:

$$n = \frac{ZN_\mathrm{A}\rho}{M} = 8{,}5 \cdot 10^{28}/\mathrm{m}^3$$

Here N_A is Avogadro number, kilomole mass M is in number equal to atomic mass number A, just the unit is kg/kmol. ♠

♥ EX. 9.2

What’s the mean kinetic energy of conducting electrons in the metal in comparison with the Fermi energy according to the Sommerfeld model? On the basis of this write more exact measure for the effective (average) speed of electrons instead of the Fermi speed. What error would me make if instead of this speed according to quantum mechanical laws we used the thermal speed from classical thermodynamics?

First we remember how we have calculated the number of conducting electrons in the metal by taking all quantum states up to Fermi wave vector:

$$N = \frac{V}{4\pi^3}\iiint \mathrm{d}k_x \mathrm{d}k_y \mathrm{d}k_z = \frac{V}{4\pi^3}\cdot 4\pi \cdot \int_0^{k_\mathrm{F}} k^2 \mathrm{d}k = \frac{Vk_\mathrm{F}^{\;3}}{3\pi^2}$$

We calculate the total kinetic energy of all conducting electrons similarly, so that we add as a factor kinetic energy in the previous integral:

$$E_{\mathrm{kin}} = \frac{V}{4\pi^3} \cdot 4\pi \cdot \int_0^{k_{\mathrm{F}}} \frac{\hbar^2 k^2}{2m_{\mathrm{e}}} \cdot k^2 \mathrm{d}k = \frac{V\hbar^2 k_{\mathrm{F}}{}^5}{10\pi^2 m_{\mathrm{e}}}$$

Kinetic energy calculated per electron is:

$$< E_{\mathrm{kin}} > \equiv \frac{E_{\mathrm{kin}}}{N} = \frac{3\hbar^2 k_{\mathrm{F}}{}^2}{10 m_{\mathrm{e}}}$$

Compare it with the Fermi energy

$$E_{\mathrm{F}} = \frac{\hbar^2 k_{\mathrm{F}}{}^2}{2m_{\mathrm{e}}}$$

We find:

$$< E_{\mathrm{kin}} > = \frac{3}{5} E_{\mathrm{F}}$$

Since the kinetic energy is proportional with the square of velocity we can define the mean speed of conducting electrons in the following way:

$$v_{\mathrm{RMS}} = \sqrt{\frac{3}{5}} v_{\mathrm{F}} \approx 0{,}77 v_{\mathrm{F}}$$

The denotation RMS means »root mean square«. The mean speed in the usual sense means something else, but it is no so different and we needn’t consider such details here. Similarly, we can define classical thermal speed v_{T}, but this depends on temperature. Using equipartition theorem we have:

$$\frac{1}{2} m_{\mathrm{e}} v_{\mathrm{T}}{}^2 = \frac{3}{2} kT \rightarrow v_{\mathrm{T}} = \sqrt{\frac{3kT}{m_{\mathrm{e}}}}$$

Let’s take copper again, for which we have already calculated Fermi velocity. Compare both velocities at the temperature 300 K: $v_{\mathrm{RMS}} = 1{,}22 \cdot 10^6$ m/s, $v_{\mathrm{T}} = 1{,}17 \cdot 10^5$ m/s; the error is one order of magnitude. ♠

♥ EX. 9.3

The density of levels, i.e., the number of conducting electrons in the metal per unit energy, is given by function:

$$g=\frac{V}{2\pi^2}\cdot\frac{(2m_\mathrm{e})^{3/2}}{\hbar^3}\cdot\sqrt{E}$$

How many conducting electrons are there in 1 cm^3 of aluminum at the Fermi energy 11,7 eV in the energy interval 0,025 eV, which corresponds to thermal energy at room temperature?

The number of conducting electrons in the given interval is:

$$N=g\cdot\Delta E=\frac{V}{2\pi^2}\cdot\frac{(2m_\mathrm{e})^{3/2}}{\hbar^3}\cdot\sqrt{E}\cdot\Delta E\ =5{,}9\cdot 10^{20}$$ ♠

♥ EX. 9.4

Fermi distribution function which holds for protons, electrons, neutrons and other fermions, is written as $f(x) = 1/(\mathrm{e}^x+1)$, where we usually take as dimensionless variable $x = (E-\mu)/(kT)$. Here E is energy, μ chemical potential, k Boltzmann constant and T absolute temperature. Function $f(x)$ is decreasing monotonically. First develop $f(x)$ into Taylor series around $x = 0$, then to the third order x^3 exactly calculate f in four cases: $E = \mu \pm kT$, $E = \mu \pm 2kT$.

Take first $f(0) = 1/2$. Next we prepare a few derivatives of the function. Instead of bothering with higher derivatives directly we write the function in a different way:

$$f=\frac{1}{\mathrm{e}^x+1}=\frac{1}{2}+(\frac{1}{\mathrm{e}^x+1}-\frac{1}{2})=\frac{1}{2}+\frac{1-\mathrm{e}^x}{2(\mathrm{e}^x+1)}$$

We multiply the numerator and denominator of the second term with the factor $\exp(-x/2)$, and we obtain hyperbolic tangens:

$$f=\frac{1}{2}(1-\tanh\frac{x}{2})=\frac{1}{2}\left[1-\frac{\exp(x/2)-\exp(-x/2)}{\exp(x/2)-\exp(-x/2)}\right]$$

We write next: $\tanh(x) = \sinh(x)/\cosh(x)$. We have: $(\mathrm{d}/\mathrm{d}x)(\sinh(x)) = \cosh(x)$, $(\mathrm{d}/\mathrm{d}x)(\cosh(x)) = \sinh(x)$. We also note that tanh is an odd function, thus only odd powers of x are present in Taylor expansion. Use also $\cosh^2 x - \sinh^2 x = 1$, $\cosh 0 = 1$, $\sinh 0 = 0$, and we get finally:

$$\frac{\mathrm{d}y}{\mathrm{d}x}=\frac{1}{\cosh^2 x}\rightarrow\frac{\mathrm{d}y}{\mathrm{d}x}(0)=1$$

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2}=-2\frac{\sinh x}{\cosh^3 x}\rightarrow\frac{\mathrm{d}^2y}{\mathrm{d}x^2}(0)=0$$

$$\frac{\mathrm{d}^3 y}{\mathrm{d}x^3} = \frac{4}{\cosh^2 x} - \frac{6}{\cosh^4 x} \rightarrow \frac{\mathrm{d}^3 y}{\mathrm{d}x^3}(0) = -2$$

Then we can write down the expansion: $f(x) = (1/2)[1 - (x/2) + (x/2)^3/3 + \ldots]$. If we move the origin of coordinate system by $y = 1/2$ up, we find $f(x)$ to be odd function with respect to the point (0, 1/2). We obtain: $f(\pm 1) = [1 -$

$(\pm 11/24)]/2 = 0{,}27$ in 0,73; $f(\pm 2) = [1 - (\pm 2/3)]/2 = 1/6$ in 5/6. For $x = \pm 1$ the approximate value agrees well with the exact value, but for $x = \pm 2$ more terms would be useful. The graph is shown in Fig. R30.

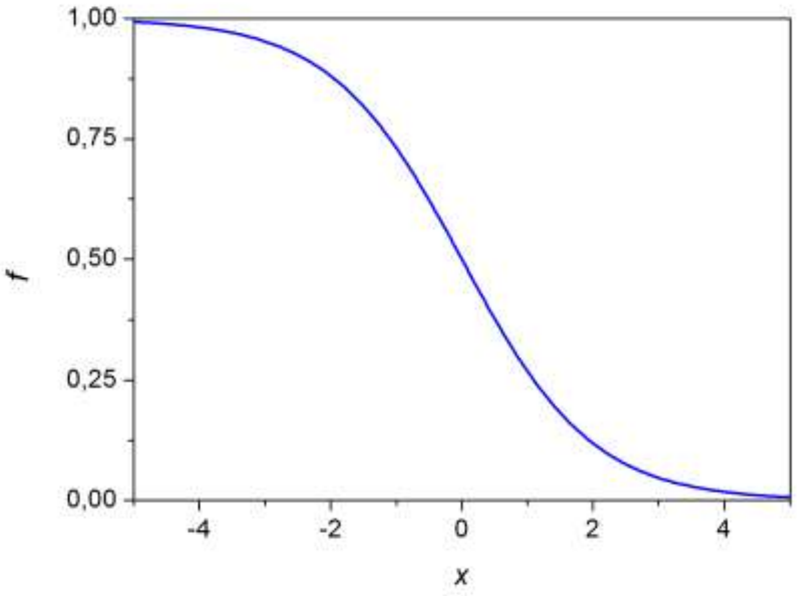


Fig. R30: Graph of Fermi function ♠

♥ EX. 9.5

The density of conducting electrons in copper is $n = 8{,}5 \cdot 10^{28}/\mathrm{m}^3$, specific resistivity is 1,56 μΩ · cm. What's relaxation time? What's the mean free path of the electron between two sequential collisions with the ions in the crystal lattice if we take Fermi speed for moving electrons?

Relaxation time τ is:

$$\tau = \frac{m}{\rho_\mathrm{R} n e_0^{\,2}}$$

Specific resistivity is denoted by ρ_R, to distinguish it from the density ρ; m is the electron mass, e_0 fundamental charge. We obtain $\tau = 2{,}7 \cdot 10^{-14}$ s. To calculate the Fermi speed we use the Fermi wave vector from previous example. We write the momentum in two ways:

$$p = \hbar k_\mathrm{F} = m v_\mathrm{F} \rightarrow v_\mathrm{F} = \frac{\hbar k_\mathrm{F}}{m} = 1{,}57 \cdot 10^6 \text{ m/s}$$

The characteristic free path of the electron is then $\langle l \rangle = v_\mathrm{F}\tau = 42$ nm, and it is two orders of magnitude larger than the distance between the nearest atoms in the lattice. This piece of data tells that electrons don't move as classical particles from atom to atom; in this case the mean free path would be of the order of inter-atomic distance. ♠

♥ EX. 9.6

Copper wire with cross-section 2 mm^2 and length 4 m is connected to voltage 60 V. What directed velocity opposite to electric current direction do conducting electrons travel along the wire with? Specific resistivity of copper is 17,5 nΩ m, the number of conducting electrons per unit volume is $8{,}5 \cdot 10^{28}/\mathrm{m}^3$. How long does it take for electron to arrive from one end of wire to the opposite end? But how long does it take for the control bulb to light after the switch is closed?

Podatki:

$L = 4$ m

$S = 2$ mm^2

$U = 60$ V

$\zeta = 17{,}5$ nΩ m

$n = 8{,}5 \cdot 10^{28}/\mathrm{m}^3$

$v = ?$

Combine equations, $j = I/S = ne_0 v$, $I = U/R$ in $R = \zeta L/S$, and calculate velocity in one step:

$$v = \frac{j}{ne_0} = \frac{I}{Sne_0} = \frac{U}{RSne_0} = \frac{SU}{\xi LSne_0} = \frac{U}{\xi Lne_0} = 63\ \mathrm{mm/s}$$

The corresponding time is: $t = L/v = 63{,}5$ s. But the time for the bulb to light on isn't related to the speed of electrons, but rather to the setup of electric field along the wire. Since the electromagnetic disturbance spreads at most with the light speed in vacuum, we estimate the corresponding time as: $t = L/c = 13{,}3$ ns (nanoseconds!). ♠

♥ EX. 9.7

Measurement of cyclotrone frequency in magnetic field shows that the effective mass of electron in sodium is: $m^* = 1{,}2\ m_e$. What's the cyclotrone frequency in magnetic field 1 T? What's the orbiting time of electrons? What's the radius if we take the Fermi speed? Fermi wave vector for sodium is $9{,}2 \cdot 10^9\ \mathrm{m}^{-1}$.

Frequency is usually denoted by symbol ν, but also with f.

$$f = \frac{e_0 B}{2\pi m^*} = 23{,}3\ \mathrm{MHz}$$

Orbiting time is $t_0 = 1/f = 43$ ns. Given Fermi wave vector was calculated from the density of conducting electrons, so it's independent of effective electron mass. We identify centripetal and magnetic force for orbiting electron: $m^* v^2/r = e_0 B v \rightarrow m^* v = e_0 B r$. So we have:

$$p_\mathrm{F} = \hbar k_\mathrm{F} = m^* v_\mathrm{F} = e_0 B r \rightarrow r = \frac{\hbar k_\mathrm{F}}{e_0 B} = 38\ \mu\mathrm{m}$$ ♠

♥ EX. 9.10

According to Drude model of electrical conductivity of metals the probability to find randomly chosen electron from random moment (which is denoted by initial time $t = 0$) on scatters from ion in a very short period dt, equal to $dP = dt/\tau$, where τ is relaxation time. This probability is independent of the history, i.e., what happened to this electron before. First we ask for probability that from some moment on ($t = 0$) electron is **first scattered** from an ion just between the moments t and $t + dt$. Also the time interval $(0, t)$, within which the electron does not suffer collision yet, is conveniently divided into short time intervals dt. Their number should be natural: $N = t/dt$, what can be achieved with appropriate choice of dt. From the aspect of events and probability theory the event of suffering collision just within $(t, t + dt)$ may be thought as a composed from $N + 1$ **sequential independent events**: that the electron doesn't collide in any of the N intervals dt, and that it collides in the last, $(N+1)$-th interval. Maybe first a question: why can we claim that these $N + 1$ events are really independent of each other? This is not just evident, quite opposite: we are used to the fact that some event depends on previous events. So, the claim about independent events is predominantly a mathematical model, which should be confirmed by experiment (or more sophisticated microscopic theories). Since the probability for the negation of the event is $1 – dP = 1 – dt/\tau$, we finally have:

$$P(t,t+dt) = (1-\frac{dt}{\tau})^N \cdot \frac{dt}{\tau}$$

$$P(t,t+dt) = \left[(1-\frac{t}{N\tau})^{N\tau/t}\right]^{t/\tau} \cdot \frac{dt}{\tau}$$

The expression in square parenthesis in the limit $N \rightarrow \infty$ is 1/e. Thus:

$$P(t,t+dt) = e^{-t/\tau} \cdot \frac{dt}{\tau} \qquad (*1)$$

We introduce the probability density function for the time of next collision:

$$\rho(t) = \frac{e^{-t/\tau}}{\tau} \qquad (*2)$$

Expressions (*1) and (*2) are important for the following derivations.

Let's calculate first the mean time for collision from chosen moment on:

$$< t >= \int_0^\infty t\rho(t)dt = \tau \qquad (*3)$$

This time is just the relaxation time τ.

We can do similar for the past: the mean time (taken positive) from some randomly chosen event to the last collision before this moment is just τ.

Next we take again some random moment $t = 0$, look into future for the first collision (t_1) and into past for last collision (t_2), sum the times and average it:

$$< t_1 + t_2 >= \int_0^\infty \int_0^\infty (t_1 + t_2) e^{-t_1/\tau} e^{-t_2/\tau} \frac{dt_1}{\tau} \frac{dt_2}{\tau} = 2\tau \qquad (*4)$$

This result was somehow expected. But it would be wrong to conclude that this means the mean time $<\Delta t>$ between two successive collisions! We will show that this is again τ and not 2τ! Why does (*4) not give correct value for $<\Delta t>$? Because it doesn't take into account the correctly movable bottom integration limit for t_1: if time t_2 (taken positive) assigns past, the time t_1 should start from negative values, otherwise we lose some part of time between two collisions.

Do now the correct derivation of $<\Delta t>$, but for the sake of clarity let's put both collisions to future. Times of the first and second collision are t_1 and t_2. So, $t_1 \leq t_2$, thus the bottom integration limit for t_2 is equal to time t_1 instead of 0. Next, we seek for the probability for the second collision in the manner of relative time, so we must insert in the second exponent $t_2 - t_1$ and not t_2:

$$< \Delta t >= \frac{1}{\tau^2} \int_0^\infty dt_1 \int_{t_1}^\infty dt_2 (t_2 - t_1) e^{-t_1/\tau} e^{-(t_2 - t_1)/\tau} = \tau \qquad (*5)$$

Lastly, we resolve »the secret«, why in the presence of electric field the mean directed velocity of electrons (in opposite direction to ***E***) is: $<v_E> = a\tau$ and not $a\tau/2$, where a is acceleration and the initial directed velocity is zero.

We must not seek for the statistical mean velocity in the sense:

$$< v_E >= \int_0^\infty v_p(t) \rho(t) dt = \int_0^\infty (\frac{1}{2} at) e^{-t/\tau} dt / \tau = \frac{1}{2} a\tau$$

Instead, we must take the basic definition $<v> = s/t$ and average over several collisions of the same electron (take N colliions):

$$< v_E > = \frac{s}{t} = \frac{\sum_{i=1}^{N} s_i}{\sum_{i=1}^{N} t_i} = \frac{N < s >}{N < t >} = \frac{< s >}{\tau} \tag{*6}$$

$$< s > = \int_0^\infty (\frac{1}{2}at^2) e^{-t/\tau} dt / \tau = a\tau^2$$

Put this into (*6) and we really obtain $<v_E> = a\tau$.

♥ EX. 9.11

The relation between electric current and voltage in a very small electronic element is described by Landauer equation: $I = (2e_0^2 T/h)U$, where the transmission coefficient is T = 80 %. What's the current through the element at 1 V? For comparison calculate the current for copper, where you take as a characteristic size a = 0,1 nm comparable with the size of atoms. The resistor is then in the shape of cube with side a. Specific resistivity of copper is ρ = 1,56 μΩ cm.

Electric current is $6{,}2 \cdot 10^{-5}$ A. Classical calculation gives: $I = U/R = U/(\rho a/a^2) = Ua/\rho = 6{,}4 \cdot 10^{-3}$ A, much too much. ♠

♥ EX. 9.12

Germanium has energy gap E_g = 0,67 eV. What's the density of conduction electrons in it at 300 K? What's the increase of the electron density for temperature increase of 1 K?

For 300 K:

$$n = \frac{1}{\sqrt{2}} \cdot (\frac{m_e k_B T}{\pi \hbar^2})^{3/2} \exp\left[-\frac{E_g}{2k_B T}\right] = 6{,}04 \cdot 10^{19}/\mathrm{m}^3$$

This is much less than for metals where n is of the order $10^{28}/\mathrm{m}^3$. For small temperature increase we use differential: $\Delta n/n \approx (\mathrm{d}n/\mathrm{d}T) \cdot \Delta T/n$. We then have:

$$\frac{\Delta n}{n} \approx (\frac{3}{2} + \frac{E_g}{2k_B T}) \cdot \frac{\Delta T}{T}$$

As expected, the first term in parenthesis is smaller than the second, but we take both:

$$\Delta n \approx n(\frac{3}{2} + \frac{E_{\mathrm{g}}}{2k_{\mathrm{B}}T}) \cdot \frac{\Delta T}{T} = 2{,}9 \cdot 10^{18}/\mathrm{m}^3$$

This is slightly less than 5 %; such large increasing of *n* with temperature is mostly due to exponential factor. ♠

♥ EX. 9.13

Some semiconductor has at 300 K the electron density $10^{10}/\mathrm{m}^3$. What's the energy gap?

From

$$n = \frac{1}{\sqrt{2}} \cdot (\frac{m_{\mathrm{e}} k_{\mathrm{B}} T}{\pi \hbar^2})^{3/2} \exp\left[-\frac{E_{\mathrm{g}}}{2k_{\mathrm{B}}T} \right]$$

we obtain:

$$E_{\mathrm{g}} = 2k_{\mathrm{B}}T \cdot \ln\left[(\frac{m_{\mathrm{e}} k_{\mathrm{B}} T}{\pi \hbar^2})^{3/2} /(\sqrt{2}n) \right] = 1{,}83 \text{ eV}$$ ♠

♥ EX. 9.14

At room temperature the density of charge carriers (for each: electrons and holes) in pure silicon is $1{,}1 \cdot 10^{10}/\mathrm{cm}^3$, the movability of electrons is 1400 $\mathrm{cm}^2/(\mathrm{V\ s})$ and the movability of holes is 450 $\mathrm{cm}^2/(\mathrm{V\ s})$. What's the electric conductivity? What electric field yields the current density 1 $\mathrm{mA/cm}^2$?

Conductivity: $\sigma = e_0(\beta_{\mathrm{e}} + \beta_{\mathrm{v}})n = 3{,}26 \cdot 10^{-4}\ \Omega^{-1}\mathrm{m}^{-1}$. From $j = \sigma E$ we have $E = j/\sigma = 3{,}07 \cdot 10^4$ V/m. ♠

♥ EX. 9.15

Silicon is doped with arsenic atoms, so that the concentration (number of added atoms per unit volume) of impurities is $10^{15}/\mathrm{cm}^3$. What's the conductivity of such semiconductor of type n? What about if we dope silicon with boron instead?

The conductivity of silicon of type n, when the contribution of holes can be neglected, is $\sigma = e_0\beta_e n = 22{,}4\ \Omega^{-1}\mathrm{m}^{-1}$. We take for n just the concentration of arsenic atoms. For semiconductor doped with boron (type p) we have: $\sigma = e_0\beta_v n = 7{,}2\ \Omega^{-1}\mathrm{m}^{-1}$. ♠

10 PROPERTIES AND USE OF SEMICONDUCTORS

♥ Ex. 10.1

Silicon is doped with arsenic atoms. If we don’t know the concentration of dopant, we can use Hall effect to measure the volume density of majority charge carriers. A narrow stripe of doped silicon with thickness t = 0,1 mm is in the perpendicular magnetic field with magnitude 1 T. If the electric current 0,1 mA flows through the stripe, the Hall voltage 3,125 mV appears in transverse direction (across the stripe width). What’s the concentration of dopant and how many silicon atoms come on average per one arsenic atom?

Equation for Hall voltage is:

$$U_{\mathrm{H}} = \frac{IB}{e_0 nt}$$

so that

$$n = \frac{IB}{e_0 U_{\mathrm{H}} t} = 2 \cdot 10^{15}/\mathrm{cm}^3$$

This is also the volume density of As atoms in silicon. But the density of Si atoms is:

$$n_{\mathrm{Si}} = \frac{N_{\mathrm{Si}}}{V} = \frac{N_{\mathrm{A}} \rho_{\mathrm{Si}}}{M_{\mathrm{Si}}} = 5 \cdot 10^{22}/\mathrm{cm}^3$$

The corresponding ratio is $n_{\mathrm{Si}}/n = 2{,}5 \cdot 10^7$, thus to every $2{,}5 \cdot 10^7$ silicon atoms there comes one arsenic atom. ♠

♥ EX. 10.2

Energy gap in pure semiconductor PbS is 2,4 eV and corresponds to green light. We use monochromatic light source with the same energy of photons and with intensity j = 1 mW/cm^2 to illuminate the plate from this material with area 0,5 cm^2. What’s the electric current through this photovoltaic device if the »efficiency« is η = 1 %, i.e., every hundredth photon shifts one electron from the valence to conducting band?

Electric current is:

$$I = \frac{e}{t} = \frac{N_e e_0}{t} = \frac{\eta N_f e_0}{t} = \frac{\eta E e_0}{E_g t}$$

The symbols mean: N_e is the number of passing electrons, N_f the number of incoming photons; E is the total energy of photons, E_g is energy gap and the energy of one photon. Since the light intensity is defined as $j = E/(St)$, we have $E = jSt$ and we finally calculate the electric current:

$$I == \frac{\eta j S e_0}{E_g} = 2{,}08\ \mu\text{A}.$$ ♠

♥ EX. 10.3

Electric current through semiconductor diode is given by exponential function of voltage:

$$I = I_0 \cdot \left[\exp(\frac{e_0 U}{k_B T}) - 1\right]$$

Write the approximation for current in three limiting cases: 1) for negative voltage with very large absolute value, 2) for voltage with very small absolute value (both positive or negative voltage) and 3) for very high positive voltage. Write also the quantitative criterion when we can take these approximations.

For “very high negative” voltage we may neglect exponential term and obtain: $I \approx -I_0$. On the contrary, for “very high positive” voltage we keep only exponential term: $I \approx I_0 \cdot \exp(e_0U/(k_BT))$. For small absolute value of voltage we expand exponential function into Taylor series till linear term: $\exp x - 1 \approx 1 + x - 1 = x$, where $x = e_0U/(k_BT)$. So we obtain: $I \approx I_0e_0U/(k_BT)$. Criterion is the magnitude of dimensionless parameter x:

1) $x << -1 \rightarrow I \approx -I_0$,

2) $|x| << 1 \rightarrow I \approx I_0e_0U/(k_BT)$,

3) $x >> 1 \rightarrow I \approx I_0 \cdot \exp(e_0U/(k_BT))$. ♠

♥ EX. 10.4

Reverse current of diode is I_0 = 100 nA, and the temperature is 300 K. At what voltage is the current equal to 500 nA?

$$I = I_0 \cdot \left[\exp(\frac{e_0 U}{k_\mathrm{B} T}) - 1 \right]$$

$$\exp(\frac{e_0 U}{k_\mathrm{B} T}) = I / I_0 + 1$$

$$U = \frac{k_\mathrm{B} T}{e_0} \cdot \ln(I / I_0 + 1) = 46{,}4\ \mathrm{mV}$$ ♠

♥ EX. 10.5

LED diode has large light efficiency, even 300 lm/W. What part of electric work is transformed into energy of visible light? Physical meaning of the unit lumen is: lm = cd · sr; cd = candela = (1/638) W/sr at light frequency 540 THz, sr = steradian (3D space angle that is 4π-times smaller than full angle).

Both lumen and candela are physiological units related to light sensitivity of human eye, thus the corresponding physical power depends also on wavelength. But we won't make any differences here: we have from above definition lm = (1/638) W. Therefore:

$$\frac{P_\mathrm{sv}}{P_\mathrm{el}} = \frac{300 \cdot \mathrm{W} / 638}{\mathrm{W}} = 47\ \%$$

As an interesting fact we mention that in order to achieve appropriate functioning of LED to imitate white light it was necessary to find suitable semiconductor with satisfactory energy gap (galium nitride, GaN), which gives the blue light component. The problem was difficult enough to require thirty years of research, so that the Nobel prize for this achievement was awarded in 2014 by Isamu Akasaki, Hiroshi Amano and Shuji Nakamura. ♠

♥ EX. 10.6

Diode is successively with Ohm resistor to the source of constant voltage U. What electric current flows through the circuit? Treat in particular the limiting cases where the equations are simplified. How are these conditions related to the parameters for diode and resistor? Finally consider the source with sinusoidal voltage.

The voltage on diode is denoted by U_d, on resistor by U_u (we take both as positive quantities). So it holds: $U = U_\mathrm{d} + U_\mathrm{u}$. Since the same current flows through resistor and diode, we can write the following transcendental equation for U_d:

$$\frac{U - U_\mathrm{d}}{R} = I_0 \cdot \left[\exp(\frac{e_0 U_\mathrm{d}}{k_\mathrm{B} T}) - 1 \right]$$

In order to solve it numerically it is sensible to introduce the following dimensionless variables/parameters: $x = e_0U_\mathrm{d}/(kT)$, $a = U/(RI_0)$, $b = kT/(e_0RI_0)$. In our problem a and b are known parameters. We thus have instead of the above equation: $a - bx = \mathrm{e}^x - 1$.

We first solve the equation approximately for small absolute value of the unknown x, but we must then check for various values of parameters a and b, if the value of x is indeed small. We expand exponential function, $\mathrm{e}^x \approx 1 + x$, and the solution becomes:

$$x \approx \frac{a}{b+1}$$

Take first positive U and thus positive parameter a. When is then $x << 1$? We have two possibilities in regard to how large is the parameter b in comparison with 1. In the case $b >> 1$ (in practice this means that the resistance R is small) we must have $a << b$ or $U << kT/e_0$. This requirement is equivalent to the requirement for the area of linear dependence $I(U)$ for diode alone. For typical reverse current of diode 100 nA and temperature 300 K the condition $b >> 1$ means $R << kT/(e_0I_0) = 2{,}6 \cdot 10^5\ \Omega$, what holds practically always in microelectronics. So we won't consider the other possibility, $b << 1$. The above simple solution can be further simplified if 1 is neglected in denominator: $x \approx a/b$. The current through circuit for $x << 1$ is $I \approx I_0x = I_0a/b = I_0e_0U/(kT)$. The same approximation for small negative voltage holds, just the direction of current is reversed.

Also for larger and very large absolute values of negative voltage where $a << -1$ is the solution simple. In equation $\mathrm{e}^x \approx 1 + x$ we just neglect very small exponential term and find:

$$x \approx \frac{a+1}{b} \approx \frac{a}{b}$$

So, we can expand the simplified solution $x \approx a/b$ to the entire interval $-\infty < U < \sim 0{,}1\ kT/e_0$. This equation means in accordance with definitions for x, a in b that $U_\mathrm{d} \approx U$, that is, in the entire mentioned interval the effective resistance of the diode is so much larger that the Ohm resistance of resistor that practically all the voltage is on diode, and the electric current through the circuit is at most of the order of reverse current.

Also for large positive voltage the behavior of this circuit is simple. In this case the effective resistance of diode is negligible in comparison with the resistor. So the current through the circuit is approximately U/R, as if there were no diode.

If now we take sinusoidal voltage, $U = U_0 \sin(\omega t)$, the influence of the diode is the following. For intervals of negative voltage the current through the resistor is practically equal to negative reverse current of diode, which is very small value; for positive voltage the situation is as if there was no diode. For a little more exact calculation we must solve the above equation only in the relatively small interval of voltage $-kT/e_0 < U < kT/e_0$. Even more exactly: for $-kT/e_0 < U < 0{,}1kT/e_0$ we just take equation for the current through the diode, without resistor, but for $0{,}1kT/e_0 < U < kT/e_0$ the equation must be solved numerically. ♠

11 HETEROSTRUCTURES, OPTICAL ELEMENTS AND NANODEVICES

♥ EX. 11.1

In 2D quantum well the characteristic thickness of the layer is d = 10 nm, and the areal density of electrons is n_S = 10^{11}/cm^2. What's the effective volume density of electrons? What's the characteristic distance between the nearest electrons? Estimate the uncertainty of the component of their velocity in direction perpendicular to the plane of layer.

The volume electron density is:

$$n = \frac{N}{V} = \frac{N}{Sd} = \frac{n_S}{d} = 10^{17}/\mathrm{cm}^3$$

For comparison: the density of charge carriers, both electrons and holes, in pure silicon is about 10^{10}/cm^3, but in doped silicon 10^{15}/cm^3, still much less than in 2D quantum well.

If we imagine a little square with size l per electron, we calculate the distances between nearest neighbors as:

$$n_S = \frac{N}{S} = \frac{1}{l^2} \rightarrow l = \frac{1}{\sqrt{n_S}} = 32\ \mathrm{nm}$$

This is three times as much as the layer thickness, so the estimation of the distance with 2D geometry is valid. The uncertainty of the velocity component is estimated with Heisenberg relation:

$$\delta v_z = \frac{\delta p_z}{m_\mathrm{e}} \approx \frac{h}{\delta z \cdot m_\mathrm{e}} \approx \frac{h}{d \cdot m_\mathrm{e}} = 7{,}3 \cdot 10^5\ \mathrm{m/s}$$ ♠

♥ EX. 11.2

Imagine that using the very thin layer of copper, d = 1 nm, we would force the effective 2D directional distribution of wave vectors of conducting electrons. How can we estimate the Fermi wave vector if we take as a piece of data the known real volume density of conducting electrons n for usual 3D geometry, while the component k_z of the wave vector is estimated with the uncertainty principle? Compare this value of Fermi wave vector with that for 3D system.

As in previous case we relate area and volume densities of conducting electrons: $n_S = dn$. The magnitude of the Fermi wave vector in the (x, y) plane for thin layer is:

$$k_{\mathrm{F}xy} = \sqrt{2\pi n_S} = \sqrt{2\pi dn}$$

The third component is approximately $k_{\mathrm{Fz}} = p/(h/2\pi) \approx 2\pi/d$. The whole wave vector is:

$$k_{\mathrm{F}} = \sqrt{k_{\mathrm{F}xy}{}^2 + k_{\mathrm{Fz}}{}^2} = \sqrt{2\pi(dn + 1/d^2)}$$

With data for copper, $n = 8{,}5 \cdot 10^{28}/\mathrm{m}^3$ we compare both terms in parenthesis: $dn = 8{,}5 \cdot 10^{19}/\mathrm{m}^2$, $1/d^2 = 10^{18}/\mathrm{m}^2$. The second term can be neglected, so: $k_{\mathrm{F}} \approx k_{\mathrm{F}xy} = 2{,}3 \cdot 10^{10}/\mathrm{m}$, what is more than in example 9.1 for copper in 3D ($1{,}4 \cdot 10^{10}/\mathrm{m}$). ♠

♥ EX. 11.3

How many carbon atoms does nanotube of diameter 1 nm and million times larger length contain? Carbon atoms are arranged in regular hexagons of size $a = 0{,}14$ nm.

The regular hexagon is composed of six equal regular, thus its area is:

$$S_6 = 6 \cdot \frac{a^2\sqrt{3}}{4} = \frac{3a^2\sqrt{3}}{2}$$

We must consider that the hexagon has 6 atoms, but at the same time one atom is shared by three neighboring hexagons, so effectively there are only 2 atoms per hexagon. The area of cylinder of diameter d and height h is (without two basic circles) $S_\mathrm{v} = \pi dh$, so the numer of carbon atoms in nanotube is:

$$N = \frac{2S_\mathrm{v}}{S_6} = \frac{2\pi dh}{(3/2)a^2\sqrt{3}} = \frac{4\pi}{3\sqrt{3}} \cdot 10^6 \cdot \left(\frac{d}{a}\right)^2 = 1{,}23 \cdot 10^8$$ ♠