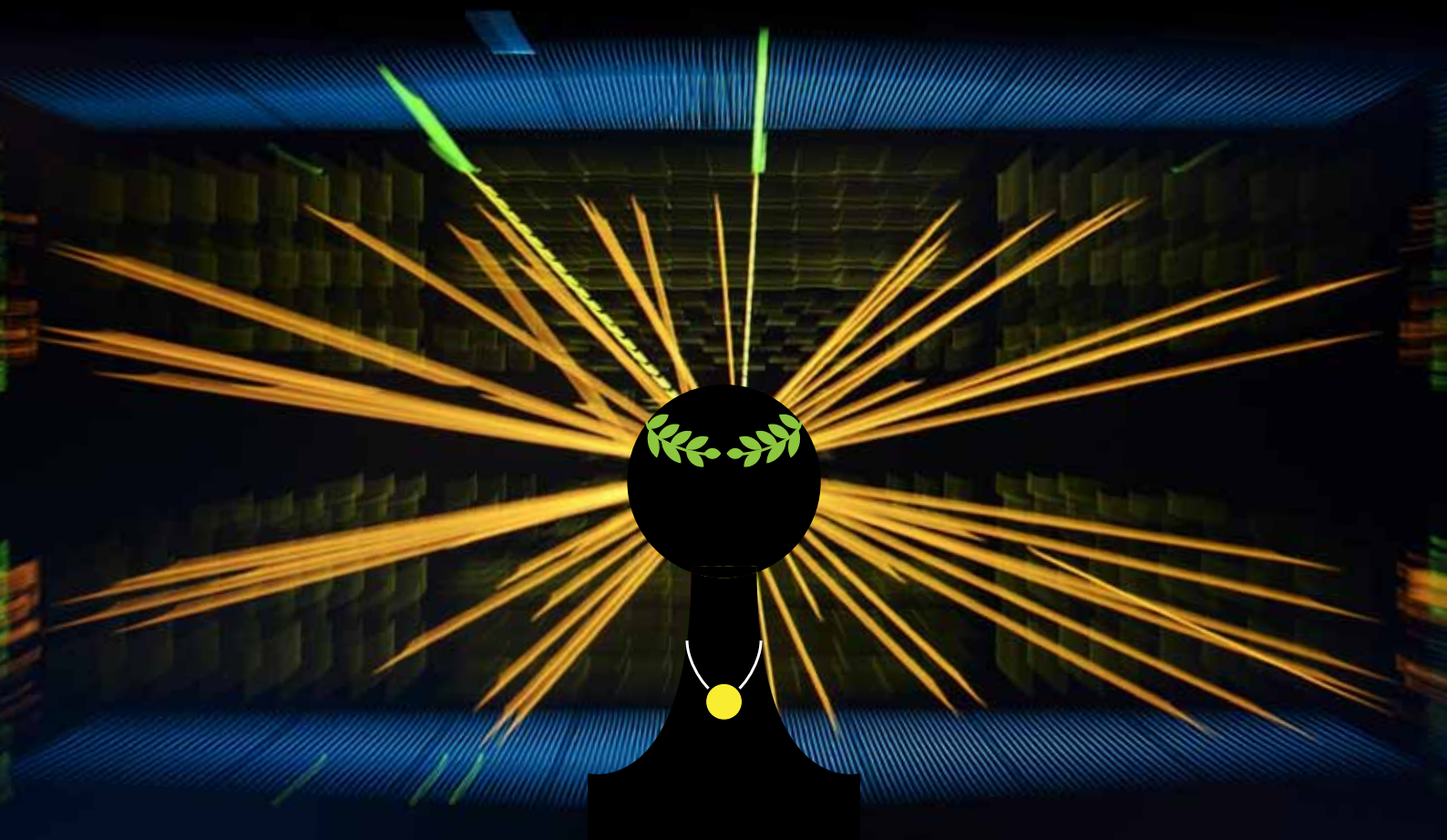


# Opgaven PION 2014



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ASML

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## ChamPIONS in physics



Stichting Physica



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# PION 2014 - Delft

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## Introduction

Dear PION-competitor,

After a good cup of coffee or tea, an informative lecture and a filling lunch, it is time for the reason why you are here; the exercises. We would like to present the problems of PION 2014! With thanks to a lot of professors we have made a set of problems which combine many parts of the physical world surrounding you. These exercises will be more challenging than any exam you have ever made. Before you start with the olympiad we would like to wish you all the luck and we hope you have a great day! Show us why your team consists of ChamPIONS in Physics and should participate in PLANCKS this year!

Good luck!

*Martijn Nagtegaal, Emma Gründeman, Tjeerd van Aalst, Matthijs Doelman, Thijs van de Mortel en Jordi Wassenburg*

Pioncommissie 2014

## Content

- There will be 11 problems
- Not every problem is worth the same number of points. The maximum of points that you can get per problem can be seen on the next page.
- A total of 110 points can be earned, 20 extra points for master parts
- You have 3 hours to work on the problems
- Every problem should be made on a separate sheet
- Write your team name and the name of the problem on each sheet

## Rules

- Only BINAS is allowed to use as a reference
- It is forbidden to communicate with any one but your teammates and the PION committee
- It is forbidden to use a graphic calculator with more features than a TI-84 or equivalent calculator

## On the cover

The picture on the cover shows an artist impression of a collision in the particle detectors used by CERN.

Source: AFP/Getty Images.

# PION 2014 - Delft

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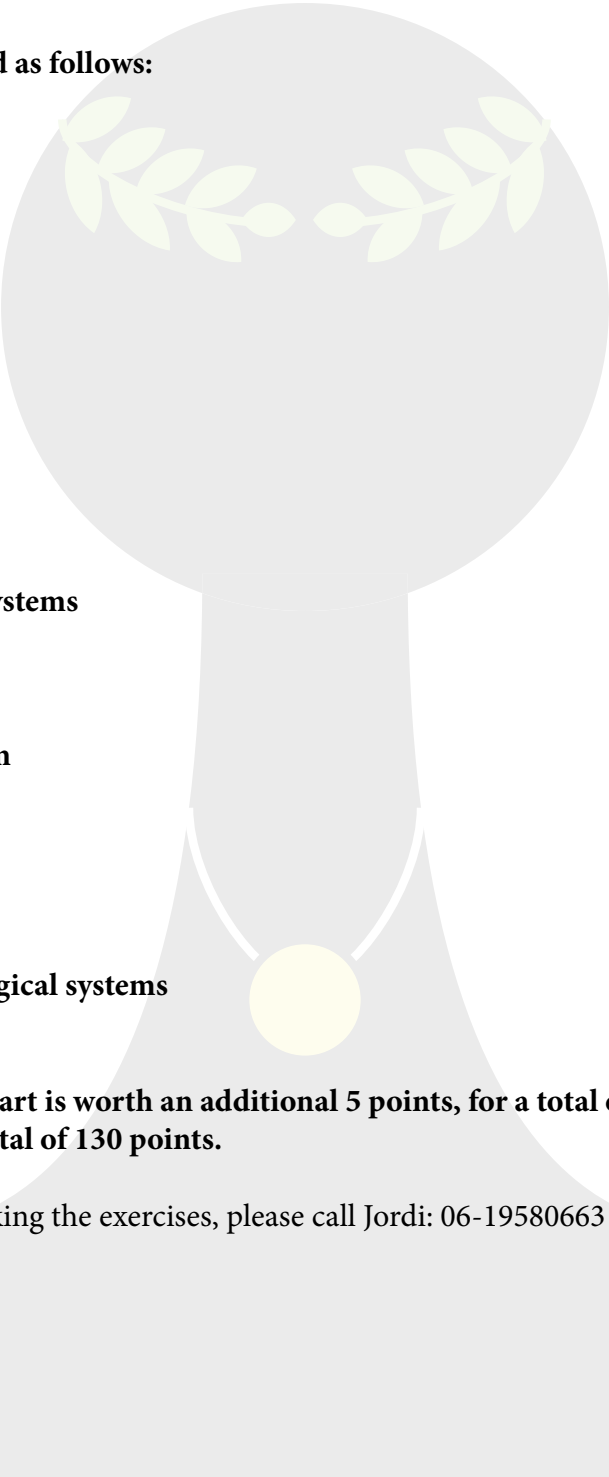
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## Distribution of points

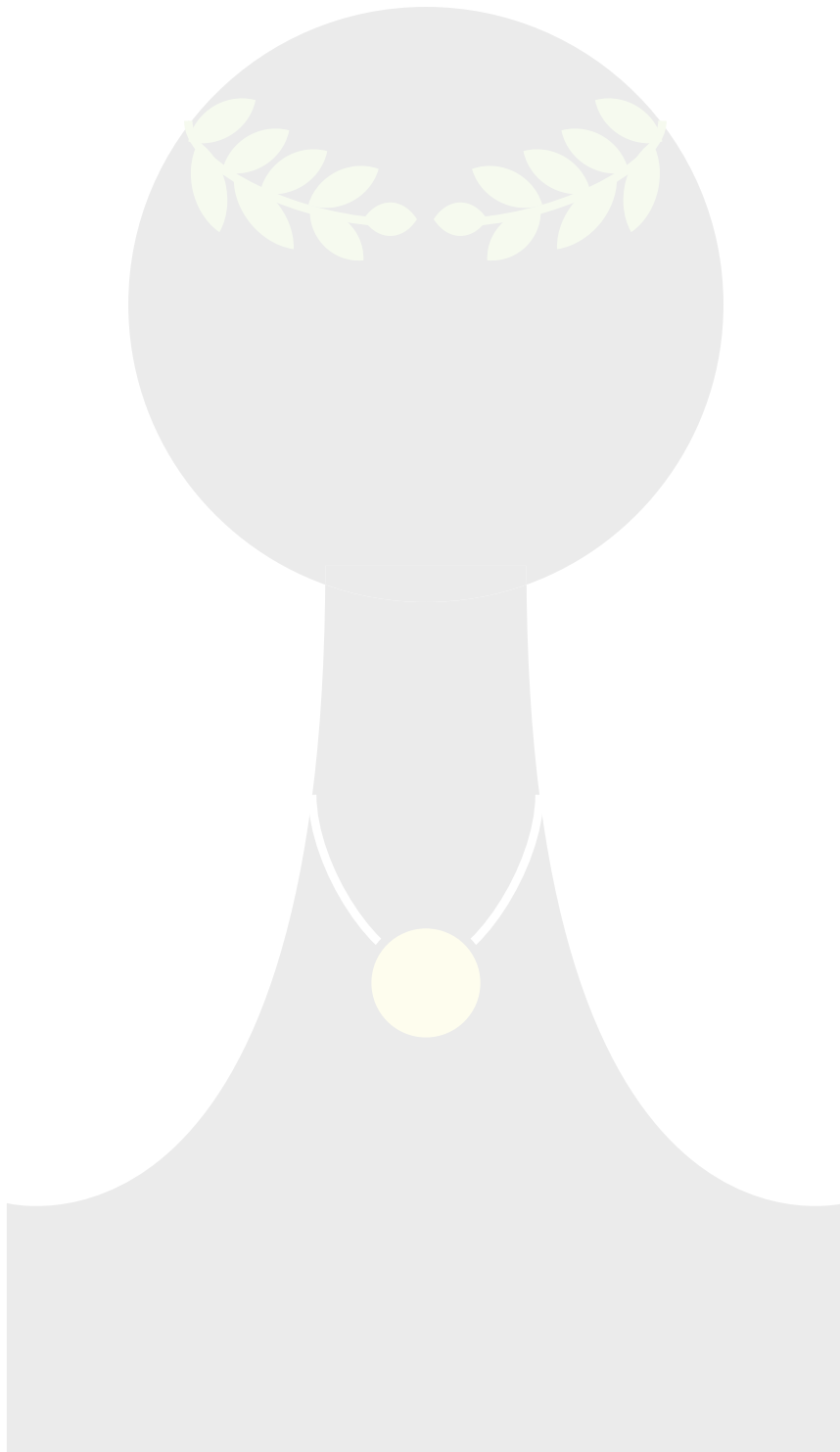
The 110 points are distributed as follows:



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**IMPORTANT: Each master part is worth an additional 5 points, for a total of 20 extra points. The master teams can get a total of 130 points.**

For direct questions while making the exercises, please call Jordi: 06-19580663



## *Bicycle Physics*

The back rear wheel of a bike is driven by a chain and a gearbox. In this problem, we will take a look at the physics behind the movement of a bicycle. A person riding a bike has to provide a certain amount of muscular power to retain a steady frequency of the circulation of the pedals. We will consider two situations. One is a biker riding uphill with speed:  $v = 15$  km/h, the other is a biker riding on a flat road with speed:  $v = 40$  km/h. Both bikers supply the same power:  $P = 400$  W. They also have the same frequency of circulation of the pedals:  $f = 60$  rev/min.

- a) Using a calculation, explain why a biker will notice the difference between these situations immediately.
- b) Can you think of a mechanism to power the bike that would reduce this difference?

Imagine you are accelerating on a bike in a frictionless environment. Obviously, a force is needed to cause this acceleration. We call the force that the road exercises on the rear wheel of the bike  $F$ .

- c) Which of the following statements about  $F$  is correct?  
 $F < ma$ ,  $F = ma$ ,  $F > ma$ , in which  $m$  is the total combined mass of the bike and the cyclist and  $a$  is the resulting acceleration. Give an explanation for your answer.
- d) Suppose a cyclist falls when his/her speed drops below 0.1m/s. Consider the following two situations:
  1. A cyclist (total mass 80kg) is biking up a hill (angle with the horizontal 0.25 rad = 14.4 deg) with a speed  $v=2$ m/s along the slope. Assume gravity is the dominant force. Determine how far the cyclist will ride on before falling after he/she stops pedalling.
  2. The same cyclist is now biking on a flat road, still providing the same power only at a speed of 43.2 km/h. Assume the dominant force is the wind resistance, proportional to the speed squared. How far will the cyclist travel after he/she stops pedalling this time?

*Prof. dr. W. J. van der Zande (RU Nijmegen)*

## Magnetic monopole

Up to today real magnetic monopoles have not been found. However, a theoretical magnetic monopole can be constructed by considering a thin long, current carrying, solenoid with one of its ends at the origin and the other end stretching to infinity, in this limit only the (mono)pole at the origin contributes to the magnetic field that can be described by:

$$\vec{B} = \frac{\mu_0 q_m}{4\pi r^2} \hat{r}$$

with  $q_m$  is the magnetic charge of the monopole, and  $\hat{r} = \frac{\vec{r}}{r}$  the unit vector in the  $\vec{r}$  direction.

In this problem we consider the motion of an electron (mass  $m$ , electric charge  $q_e$ ) moving in the field of a magnetic monopole (of which the magnetic field is given by the equation above) that is stationary at the origin.

- Give an expression for the acceleration  $\vec{a}$  of the electron in terms of  $q_e$ ,  $q_m$ ,  $m$  and the position and velocity of the electron ( $\vec{r}$  and  $\vec{v}$ , respectively).
- Show that the kinetic energy of the electron,  $T = \frac{1}{2}m|\vec{v}|^2$  is a constant of motion.
- The angular momentum of the electron is given  $\vec{L} = m(\vec{r} \times \vec{v})$  by . Show that  $|\vec{L}|^2$  is also a constant of motion.
- Now consider the vector  $\vec{P}$  first introduced by Henri Poincaré in 1896,

$$\vec{P} = \vec{L} - \frac{\mu_0 q_e q_m}{4\pi} \hat{r}$$

and show that this vector is a third constant of motion.

Choose a new coordinate system such that the Poincaré vector points in the positive z-direction and the origin is at the position of the monopole. Work in spherical coordinates.

- Proof that in this coordinate system  $\theta = \theta_p$  (the angle with the positive z-axis) is a constant of motion (Hint: Calculate  $\vec{P} \cdot \hat{\varphi}$  ). Show that this constant angle  $\theta_p$  is given by (Hint: Calculate  $\vec{P} \cdot \hat{r}$  ).

$$\cos \theta_p = -\frac{\mu_0 q_e q_m}{4\pi |\vec{P}|}$$

What does this result imply for the motion of the electron?



-- Master Part --

- f) Show that for the radial coordinate of the trajectory of the electron in the field of the monopole the following inequality holds.

$$r \geq r_m = \frac{|\vec{L}|}{\sqrt{2mT}}$$

Derive and solve the equation of motion of  $r$  ( $r$  as a function of  $t$ ) and speculate on the trajectories followed by electrons in the field of a magnetic monopole.

*dr. E.R. van der Graaf (RUG)*

## Formation of a rainbow

The formation of a rainbow in the sky can be understood as a reflection of the sun rays within a water droplet. A ray of monochromatic light, part of a white light beam, enters into a spherical drop of refractive index  $n$  and undergoes inside the droplet multiple refraction/reflection (see figure 1).

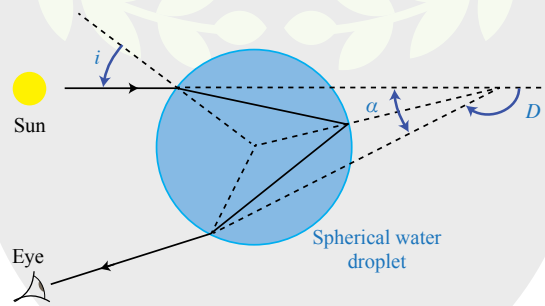


Figure 1: Schematic gure of the trajectory of a sun ray in a spherical water droplet

- What is the deviation  $D$  of the incident beam as a function of the angle of incidence  $i$  and of the first refracted angle  $r$ ?
- Find the value of  $\sin i$ , as a function of  $n$ , for which the deviation of the incident beam is minimal.
- Calculate numerically  $\alpha = \pi - D$  for a droplet of water ( $n = 1.33$ ) and for a glass droplet ( $n=1.31$ ).
- We assumed that the variation of the refractive index  $n$  of water to the wavelength  $\lambda_0$  in vacuum satisfies the Cauchy's law, i.e.:

$$n = n_0 + \frac{C}{\lambda_0^2}$$

$n_0$  and  $C$  two positive constants. What is this phenomenon named?

- We know that the intensity out of the drop is maximum for the minimum deviation; acknowledging Cauchy's Law, explain the formation of the rainbow in the sky when the light is white and the position of the colours.
- Why does the rainbow look like a bow?
- Let's suppose the sun to be setting (i.e. at the West, where are on Earth), with a  $10^\circ$  inclination above the horizon. A curtain of rain far away is pouring. Where should you be standing to see a rainbow.

# PION 2014 - Delft

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- h) According to the Irish folk's tradition, a Leprechaun (kind of fairy) has hidden his pot of gold at the end of the rainbow. Can you reach it and become rich (by stealing it if you have no morality)? Why?

-- Master Part --

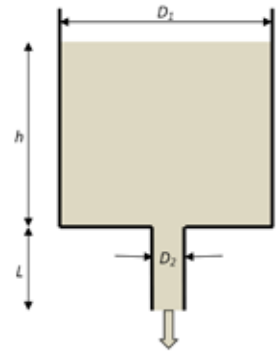
It happens sometimes that a second rainbow is visible at the same time along with the one described in the first part.

- i) Explain the origin of this second rainbow. Where will it be compared to the original one? How does it look? Why do we say "sometimes"?
- j) Calculate  $\beta = \pi - D_2$  with  $D_2$  the new deviation angle for this second rainbow. [Hint: make a second drawing]

*dr. A.J.L. Adam (TU Delft)*

## Draining a barrel

A cylindrical barrel (diameter  $D_1$ ) is filled up to a height  $h_0$  with a Newtonian fluid. A small circular hole (diameter  $D_2$ ) is drilled in the bottom of the barrel and sealed with a small faucet. A rigid vertical hose (also diameter  $D_2$ ) of length  $L$  is attached to this faucet. At  $t=0$  the faucet is opened and the force of gravity  $g$  starts to drain the barrel in a quasi-stationary fashion. The fluid is subject to forces of friction during the draining process, resulting in an energy loss of  $e_{\text{fr}} = cLv^2$  per kg of fluid (where  $v$  is the speed of the fluid in the hose and  $c$  is a constant with dimension  $\text{m}^{-1}$ ). The barrel is completely empty at  $t=\tau$ .



- Find an expression for  $\tau$  in terms of the quantities  $D_1$ ,  $D_2$ ,  $h$ ,  $L$ ,  $g$  and  $c$ .
- Determine  $\tau$  for  $L = 0$  and  $L \rightarrow \infty$ .

-- Master Part --

- For which hose length  $L$  is the drain time  $\tau$  minimal?
- And what is this minimal drain time  $\tau$ ?

prof. dr. ir. C. Kleijn (TU Delft)

## *A precarious equilibrium*

Suppose we want to balance a long needle with its tip on a flat, hard surface. Of course the surface must not be slippery and the experiment will have to be carried out in a vibration-free room and at a very low temperature. It should be possible - we have thought of everything. Or have we?

*Well not everything, one branch of physics holds out against the physicists... quantum mechanics!*

Assume the needle is a very thin (one-dimensional) rod with a homogenous mass distribution, length  $l$  and total mass  $m$ . Ideally, you would set the needle down at  $t=0$  in a perfectly vertical position in such a way that both the initial angle with the vertical  $\theta_0$  and the initial angular velocity  $\omega_0$  are zero. Unfortunately, Heisenberg's uncertainty principle prohibits this. Perform the following steps to estimate how well this equilibrium can be maintained:

- Determine the moment of inertia for the falling motion of the needle. Note: this falling motion is a rotation about the tip of the needle, described by the angle  $\theta$  between the needle and the vertical.
- Consider the falling motion of the needle from a classical perspective. Give the equations of motion that describe the fall, and determine the solution  $\theta(t)$  for small angles where  $\sin(\theta) \approx \theta$ . Use  $\theta(0) = \theta_0 \geq 0$  and  $\dot{\theta}(0) = \omega_{(0)}$ .

Now the Heisenberg uncertainty principle dictates  $\Delta q \Delta p_q \geq \hbar/2$ , where  $\Delta q$  is the quantummechanical uncertainty in the generalized coordinate  $q$  and  $\Delta p$  is the uncertainty in the corresponding momentum  $p_q$ . How we should apply this quantum mechanical limit in this case isn't easy to say, but for now let's assume we can simply apply the principle to the initial situation by imposing  $\theta(0)p_\theta(0) \geq \hbar/2$ .

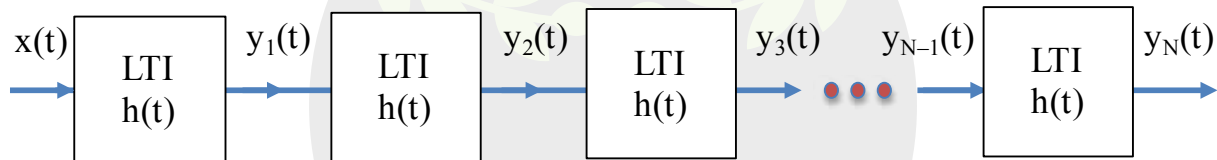
- Give, using this assumption, an estimate for the maximal time  $\tau_{max}$  it takes the needle to reach an angle  $\theta_M=0.1$  assuming the initial situation is as close the perfect classical equilibrium (i.e.  $\theta_0 = \omega_0 = 0$ ) as possible. Use the data given below.
- The lowest temperature ever reached in laboratories is in the order of 0.1nK. Suppose we could cool the needle to such a temperature. Is this enough to be able to observe the quantum effect from part (c)? Use the classical principle of equipartition of energy and apply this to the rotational degrees of freedom of the needle.

*Prof. dr. W.J.P. Beenakker (RU Nijmegen)*

|  |
|--|
| $m = 0.01 \text{ kg}, \ell = 0.1 \text{ m}, g = \text{gravitationele valversnelling} = 9.81 \text{ m s}^{-2},$<br>$\hbar = 1.055 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1} \text{ en } k = 1.381 \times 10^{-23} \text{ kg m}^2 \text{ s}^{-2} \text{ K}^{-1}$ |
|--|

## Filtering by many identical systems

A linear, time-invariant system has impulse response  $h(t)$ , that is, when the input is  $x(t) = \delta(t)$ , the output is  $y(t) = h(t)$ . The output of this system can then be used as the input for one or more *identical* systems as shown below.



The impulse response is given by:

$$h(t) = \begin{cases} \frac{1}{2\sqrt{3}} & |t| \leq \sqrt{3} \\ 0 & |t| > \sqrt{3} \end{cases}$$

The following Fourier Transform pair  $\{x(t), X(\omega)\}$  may (or may not) be useful:

$$X(\omega) = \int_{-\infty}^{+\infty} x(t)e^{-i\omega t} dt$$

$$x(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} X(\omega)e^{i\omega t} d\omega$$

where  $i^2 = -1$ .

- Determine and sketch  $H(\omega)$ , the Fourier Transform of  $h(t)$ . Your sketch should include labels and numerical values where possible.
- Determine and sketch  $y_1(t)$  and  $y_2(t)$  when  $x(t) = \delta(t)$ . Again, your sketch should include labels and numerical values.
- Sketch  $y_3(t)$  and  $y_{100}(t)$ . You do not have to work out the analytical forms (unless you want to). And, yes, that is  $N = 100$ .
- Describe in words your result for  $N = 100$ . Be as precise as possible in your reasoning.

If we consider the class of signals that are everywhere non-negative, the center of a signal,  $y_c$ , can be defined in the same way as the “center-of-gravity”. That is:

$$y_c = \frac{\int_{-\infty}^{\infty} ty(t)dt}{\int_{-\infty}^{\infty} y(t)dt}$$

The root-mean-square width of a signal,  $y_{rms}$ , can be similarly defined as:

$$y_{rms} = \sqrt{\frac{\int_{-\infty}^{\infty} (t - y_c)^2 y(t) dt}{\int_{-\infty}^{\infty} y(t) dt}}$$

- e) Determine  $y_c$  and  $y_{rms}$  for  $y_1(t)$ ,  $y_2(t)$  and the general case  $y_N(t)$ . Reduce your answers to the simplest possible form.

The impulse response is now replaced by a new impulse response:

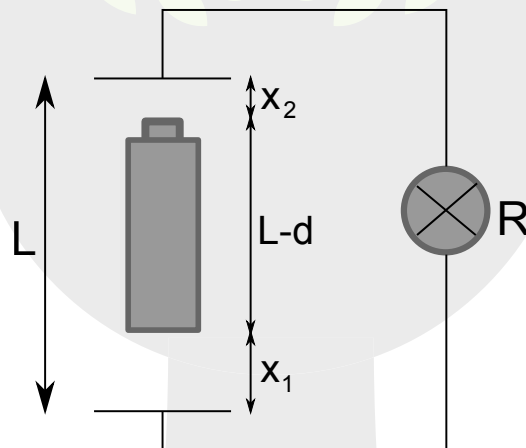
$$h(t) = \begin{cases} \cos(5\pi t) & |t| \leq \sqrt{3} \\ 0 & |t| > \sqrt{3} \end{cases}$$

- f) Determine and sketch the new  $H(\omega)$ , the Fourier Transform of the new  $h(t)$ . Your sketch should include labels and numerical values where possible.
- g) Sketch  $y_1(t)$  and  $y_2(t)$  when  $x(t) = \delta(t)$ . Again, your sketch should include labels and numerical values. You do not have to give the analytical form for either signal.
- h) Sketch  $y_{100}(t)$ . Again, you do not have to work out the analytical form (unless you want to). And, once again, that is  $N = 100$ .

*Prof. I.T. Young (TU Delft)*

## *Bouncing Battery*

While cycling homewards my bicycle light broke off and landed so hard on the ground that the clip that holds the battery in place was completely crushed. The battery could now slide back and forth and make electrical contact on one side only. This led to the following question: Is it (theoretically) possible to make a light bulb glow by bouncing a battery between two contacts?



- a) Argue whether this is possible and give an expression for the current in terms of  $x_1(t)$ . You may assume that the battery contacts resemble parallel plate capacitors. Distinguish between two cases.
- b) Estimate the maximum power dissipated in a light bulb with resistance  $R = 5\Omega$  when a cylindrical battery with 1cm diameter is bounced back and forth 10 times a second across a 1mm gap. Assume that the battery is a 1.5V type with a protruding positive contact which covers a quarter of the top surface of the battery and a negative contact covering half of the bottom surface.

*Prof. dr. ir. T.H. Oosterkamp (LU)*



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## *Temperature in a finite system*

In statistical physics, we usually deal with systems in the thermodynamic limit, i.e. where the particle number and volume are infinitely large. However, in some relevant situations, researchers would like to generalize concepts such as temperature and (thermodynamic) energy to finite systems. This is useful for simulations or in mesoscopic systems, where the number of degrees is large but does not tend to infinity. In this problem we carefully analyze how temperature and energy can be evaluated for such systems.

In the microcanonical ensemble, the number of particles, volume and energy of a large system are kept fixed. In this problem we analyze the temperature of such a system. A quick (and commonly used) estimate for the temperature is based on the equipartition theorem: the kinetic energy of the system is determined as the  $Mk_B T/2$ , where  $M$  is the number of degrees of freedom of the system.

Let's consider a gas of point particles in a cubic volume  $L \times L \times L$  with periodic boundary conditions. The latter imply that a particle leaving the system through the right wall, enters again through the left wall.

- Argue whether in that case the total momentum is conserved.
- Suppose that in a computer simulation of this system, you can calculate the kinetic energy at all times. What would be your estimate for the temperature at any time in terms of the kinetic energy  $K$  of the system, using the equipartition theorem?
- Now we want to check whether the simple argument given above is indeed correct. The proper way to calculate the temperature is

$$\frac{1}{T} = \left( \frac{\partial S}{\partial E} \right)$$

at constant volume and particle number. Here,  $S(E) = k_B \ln \Omega(E)$ , where  $\Omega(E)$  is the number of states with energy  $E$  accessible to the system. This number is given by

$$\Omega = \sum_{all\ states} \delta [E - H(p, q)]$$

where  $p$  and  $q$  denote all momenta and positions of the particles in the system. Taking into account the fact that the total momentum is conserved, this leads to

$$\Omega = \frac{1}{h^{3N-3} N!} \int \delta [E - H(p, q)] d^{3N-3} p d^{3N} q$$

Here,  $h$  is Planck's constant; it occurs with exponent  $3N-3$  as a result of momentum conservation. The factor  $N!$  accounts for the indistinguishability of the particles. Show that can be written as

$$\Omega = \frac{(2m)^{(3N-3)/2} \omega(3N-3)}{2h^{3N-3} N!} \int [E - V(q)]^{(3N-5)/2} d^{3N} q$$

where  $\omega(D)$  is the surface of a unit sphere in  $D$  dimensions. Show that from this it follows that

$$\frac{1}{k_B T} = \frac{3N-5}{2} \left\langle \frac{1}{K} \right\rangle$$

How does the difference between this expression and that found in (b) scale as a function of the particle number  $N$ ?

- d) Now suppose we can also perform (numerical or analytic) calculations for the *total* energy of a many-particle system in the canonical ensemble. In this ensemble, the expectation value for the total energy is given as
- where the sum over  $i$  denotes a sum over all states, and the  $\beta = 1/(k_B T)$  is fixed. The sum over

$$\langle E \rangle = \frac{\sum_i E_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}}$$

all states can be replaced by an integral over the energy:

$$\sum_i \rightarrow \int g(E) dE$$

where  $g(E)$  is the density of states, given as

$$g(E) = e^{S(E)/k_B}$$

Expand the quantity  $-\beta + S(E)$  around the  $E^*$ , which is the energy at which this function attains its maximum. Note that  $E^*$  is the energy of the microcanonical ensemble. We shall see that in the canonical ensemble, the energy deviates from this value, even if the temperature is the same as for the microcanonical version. The expansion up to third order in the deviation  $\Delta E$  from  $E^*$  reads:

$$-\beta E + S(E)/k_B = -\beta E^* + S(E^*)/k_B - \alpha \Delta E^2 - \gamma \Delta E^3 + \dots$$

Show that

$$\langle E \rangle = E^* - \frac{3\gamma}{4\alpha^2}$$

Hint: expand the integrand to first order in  $\Delta E$  to keep only Gaussians and powers of  $\Delta E$  in the integrals.

e) Show that

$$-2k_B\alpha = \frac{3N-5}{4} \left[ (3N-7) \left\langle \frac{1}{K^2} \right\rangle - (3N-5) \left\langle \frac{1}{K} \right\rangle^2 \right],$$

and

$$-6k_B\gamma = \frac{(3N-5)(3N-7)(3N-9)}{8} \left\langle \frac{1}{K^3} \right\rangle - 3 \frac{(3N-5)^2(3N-7)}{8} \left\langle \frac{1}{K^2} \right\rangle \left\langle \frac{1}{K} \right\rangle + \frac{(3N-5)^3}{4} \left\langle \frac{1}{K} \right\rangle^3.$$

*dr. J. Thijssen (TU Delft)*

## *Space Mirrors*

During one of the missions of the USS Enterprise in deep space, far away from any massive objects, captain Kirk asks his crew to conduct an experiment. At time  $t=0$ , two identical mirrors are sent into space. One of the mirrors, mirror A, is sent in the positive  $x$ -direction, the other one, mirror B, is sent in the negative  $x$ -direction. Both mirrors have the same velocity  $V/c = 4/5$ .

After a certain amount of time  $T$ , the crew in the ship fires a laser pulse towards mirror A. The frequency of the light is, according to the crew,  $f_0$ . At mirror A, the pulse is reflected and propagates back into the direction of mirror B. After some time, the pulse will reflect from mirror B and find its way back to the USS Enterprise, where it is detected. Captain Kirk would like to know at what time the USS Enterprise will detect the pulse and what frequency the pulse then has.

- a) Calculate the time of the detection and the frequency of the pulse for captain Kirk.

Moreover, captain Kirk has sent a part of his crew with each mirror. He wants them to measure the time of arrival and the frequency of the light that hits their respective mirrors.

- b) For both mirrors, calculate the time of arrival of the pulse and the frequencies of the light.

*Prof. dr. R.F. Mudde (TU Delft)*

## Shapiro spikes

When two superconductors (S) are separated by a thin insulating (I) layer (a so-called SIS junction) a “supercurrent” can tunnel from one superconductor to the other in the absence of an applied bias voltage. This supercurrent  $I_s$  consists of pairs of electrons, the Cooper pairs, which are described by a common macroscopic wavefunction  $\psi(\vec{r}) = |\psi(\vec{r})| e^{i\theta(\vec{r})}$ . The current  $I_s$  is a periodic function of the phase difference  $\phi \equiv \theta_1 - \theta_2$  of the wavefunctions in the two superconducting layers:

$$I_s = I_c \sin(\phi)$$

This equation represents the dc Josephson effect, named after its discoverer B.D. Josephson. When a dc voltage  $V$  is applied across the junction the phase difference becomes time-dependent and changes as

$$\frac{d\phi}{dt} = \frac{2eV}{\hbar}$$

In this problem we consider the situation in which a voltage  $V(t)$  is applied across the junction that contains both a dc and an ac component:

$$V(t) = V_0 + V_1 \cos(\omega t)$$

- a) Show that the (time-dependent) supercurrent for the applied voltage  $V(t)$  is given by

$$I_s(t) = I_c \operatorname{Im} \left[ \exp \left( i \left( \phi_0 + \frac{2e}{\hbar} V_0 t + \frac{2eV_1}{\hbar\omega} \sin(\omega t) \right) \right) \right]$$

- b) Use the substitutions:

$$\omega_j \equiv \frac{2e}{\hbar} V_0$$

$$z \equiv \frac{2eV_1}{\hbar\omega}$$

$$\alpha \equiv \omega t$$

and the expansion into Bessel functions  $J_k(z)$ :

$$e^{iz \sin(\alpha)} = \sum_{k=-\infty}^{\infty} J_k(z) \cos(k\alpha) + i \sum_{k=-\infty}^{\infty} J_k(z) \sin(k\alpha)$$

to rewrite the supercurrent  $I_s(t)$  in the form:

$$I_s(t) = I_c \sum_{k=-\infty}^{\infty} f(k) \sin(\phi_0 + \omega_j t + x)$$

Give expressions for  $f(k)$  and  $x$ .

Hint: Bessel functions obey the parity relation  $J_k(z) = (-1)^k J_{-k}(z)$ .

c) We now add the shunt current  $V_0/R$  so that the total current  $I$  through the junction becomes

$$I(t) = I_s(t) + \frac{V_0}{R}$$

with  $I_s(t)$  given in b). Use reverse substitution to express  $I_s(t)$  again in terms of  $V_0$ ,  $V_1$  and  $\omega$ . What is the dc part of the current? What do you think is meant by “Shapiro spikes”? Motivate your answer. Also make a (qualitative) sketch of the dc component of the current  $I(t)$  as a function of voltage  $V_0$ .

-- Master Part --

We now consider small deviations of the voltages around the Shapiro spikes found under (c). Derive an expression for the resulting supercurrent  $I_s(t)$  for  $\phi_0 = \pi/2$  and describe how it behaves.

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## Cooperative binding in biological systems



Figure 1: A four-protein complex (green) can bind up to four small ligand molecules (red)

In biology, many proteins are designed to bind a small molecule called a ligand. We can think of these proteins as existing in one of two states, bound or unbound. Furthermore, identical proteins are sometimes found assembled into larger complexes that exhibit what is called *cooperative binding*. In cooperative binding, the proteins in a complex prefer to be either all bound or all unbound. Here we will develop a simple model of this phenomenon.

- a) Consider a protein complex made of  $N=4$  individual proteins arranged in a ring, as shown in the figure above. Let  $b_i = 1,0$  represent whether the  $i$ th protein is bound or unbound to a ligand, respectively. The change in energy associated with binding of one additional ligand is  $-\mu$ . Additionally, there is an interaction energy between neighboring proteins denoted by  $\epsilon$  where  $\epsilon > 0$ . Two neighboring proteins in the same state contribute an energy  $-\epsilon$ , while two neighboring proteins in opposite states contribute an energy  $\epsilon$ . Because of the ring configuration, proteins 1 and 4 are neighboring each other. As an example, the energy of the five configurations shown in the figure above would be (from left to right):

$$-4\epsilon, -\mu, -2\mu, -3\mu, \text{ and } -4\epsilon - 4\mu$$

Write the partition function of this system, in terms of  $\epsilon$ ,  $\mu$ , and the Boltzmann factor  $\beta$

$$\beta = \frac{1}{k_B T}$$

- b) Let's first set  $\mu = 0$ . What is the average number of ligands bound to the protein complex? What is the probability that exactly this average number of ligands is bound to the complex? What is the asymptotic value of this probability as the interaction energy  $\epsilon$  becomes large? Write all answers in terms of in terms of  $\epsilon$ ,  $\mu$ , and  $\beta$ .
- c) Now consider the limit that,  $\mu\beta \ll 0$  which occurs when the ligand becomes dilute. What is the average energy of the complex? What is the probability that any ligands are bound to the complex? What is the asymptotic value of this probability as the interaction energy  $\epsilon$  becomes large? Write all answers in terms of in terms of  $\epsilon$ ,  $\mu$ , and  $\beta$ .



- d) Returning again to the case where  $\mu=0$ , write a generalized partition function for  $N$  proteins in a ring complex where  $N$  is even. Write the partition function of this system in terms of  $\varepsilon, \beta$ , and the hyperbolic functions (cosh, tanh, etc.). Write your answer in a compact form, i.e. do not leave your answer expressed as a summation.

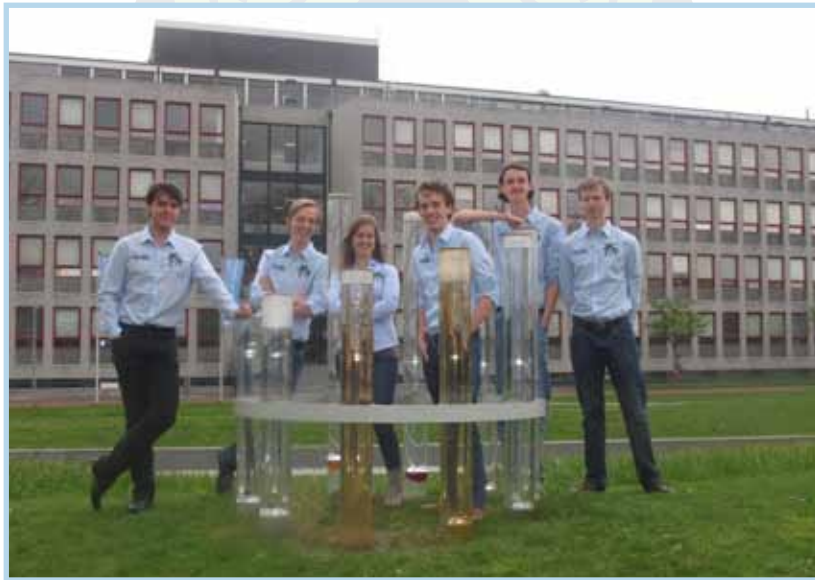
*dr. E. Abbondanzieri (TU Delft)*

*The end*

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