Ferromagnetic domain wall dynamics

In this problem you will calculate physical quantities using the Ferromagnetic Similator program. The detailed program description is provided at the end of the problem.

Record the obtained numerical values in Excel files, specifying the number of the corresponding problem section in the title of each file. In each column indicate which physical quantity it contains. Graphs can be plotted in the same files. Include the necessary formulas for calculations and figures explaining your solution in the answer sheets. Save all the files generated during the solution to the "**report"** folder.

Warning! The program may run calculations for several minutes. To speed up your work, you can launch multiple instances of the program. You can analyze graphs obtained from one instance while another performs calculations. Remember to save your results so you can use them later.

Ferromagnets are materials that can have a nonzero magnetic moment even in the absence of an external magnetic field. The state of a ferromagnetic material is characterized by magnetic moment density $\vec{M}$, called magnetization. In equillibrium magnetic moment distribution corresponds to a local energy minimum. The ferromagnet is divided into regions with different magnetic moment orientations -- domains. These domains are separated by domain walls -- transition regions where the magnetization changes direction.

If the energy is not minimal, or if an external magnetic field is applied, the magnetization changes with time. The magnetization evolution is governed by the Landau-Lifshitz-Gilbert (LLG) equation:

$$\frac{\partial \vec{M}}{\partial t} = -\gamma \vec{M} \times \vec{B}_{\text{eff}} + \alpha \frac{\vec{M}}{M_0} \times \frac{\partial \vec{M}}{\partial t}.$$

The first term describes magnetization precession in magnetic field and the second term describes energy dissipation. Here $\vec{B}_{\text{eff}}$ is effective magnetic field acting at a given point. The effective field depends on magnetization at a given point and magnetization in its neighbourhood. Here γ is gyromagnetic ratio, (the ratio of the electron's magnetic moment to its angular momentum), α is dimensionless Gilbert damping constant, M_0 is magnetization magnitude.

Suppose that the ferromagnet energy density (i.e. energy per unit volume) is known as a function of magnetization $w(\vec{M})$. The effective magnetic field can be calculated as derivative

$$\vec{B}_{\text{eff}} = -\frac{\partial w}{\partial \vec{M}},$$

where derivative over a vector is a vector made of derivatives with respect to magnetization components

$$B_{\text{eff},x} = -\frac{\partial w}{\partial M_x}, \quad B_{\text{eff},y} = -\frac{\partial w}{\partial M_y}, \quad B_{\text{eff},z} = -\frac{\partial w}{\partial M_z}.$$

For instance, if material is placed into an external magnetic field $\vec{B}_0$, corresponding contribution to energy density is

$$\Delta w_B = -\vec{M} \cdot \vec{B}_0,$$

and corresponding effective magnetic field change is $\Delta \vec{B}_{\text{eff}} = \vec{B}_0$.

In this problem you may use the following formulas for vector product in Cartesian coordinates

$$(\vec{a} \times \vec{b})_x = a_y b_z - a_z b_y,$$

$$(\vec{a} \times \vec{b})_y = a_z b_x - a_x b_z,$$

$$(\vec{a} \times \vec{b})_z = a_x b_y - a_y b_x.$$

Unit vectors along coordinate axes x, y и z are $\vec{e}_x$, $\vec{e}_y$, $\vec{e}_z$ respectively.

Parts A, B and C can be solved independently.

Part A. Single magnetic moment (2.0 points)

A.1	Show that if magnetization $\vec{M}$ evolves according to LLG equation, vector $\vec{M}$ magnitude is constant over time.	0.3 pt

Suppose that magnetization is homogeneous (does not depend on coordinates). Define unit vector $\vec{m} = \vec{M}/M_0$, where $M_0 = |\vec{M}|$. The LLG equation can be written in the form

$$\frac{d\vec{m}}{dt} = -\gamma \vec{m} \times \vec{B}_{\text{eff}} + \alpha \vec{m} \times \frac{d\vec{m}}{dt}.$$

Magnetization depends only on time so we can write full derivative instead of partial derivative. For calculations it is useful to have an explicit formula for time derivative

$$\frac{d\vec{m}}{dt} = -\frac{\gamma}{1+\alpha^2}\vec{m} \times \vec{B}_{\text{eff}} - \frac{\alpha\gamma}{1+\alpha^2}\left((\vec{m}\cdot\vec{B}_{\text{eff}})\,\vec{m} - \vec{B}_{\text{eff}}\right).$$

A.2	Suppose that ferromagnet is placed into homogeneous constant magnetic field B_0 directed along z axis. Then $\vec{B}_{\text{eff}} = B_0\vec{e}_z$. Find the time dependence of the component $m_z(t)$. At the initial time moment $m_y = m_z = 0$, $m_x = 1$. You may use the following integral $$\int \frac{dx}{1-x^2} = \frac{1}{2}\ln\left|\frac{1+x}{1-x}\right| + C.$$	0.9 pt

A.3	Consider the system described in the previous task. Show that magnetic moment $\vec{m}$ projection onto the xy plane rotates around z axis with constant angular velocity. Find this angular velosity Ω, express answer in terms of γ, α, B_0.	0.8 pt

Therefore magnetic moment precesses around the effective magnetic field $\vec{B}_{\text{eff}}$, and magnetic moment gradually gets aligned with magnetic field.

Part B. Static domain wall (3.5 points)

In this part we consider thin ferromagnetic wire with square section (square side size is a), wire length is L. Let us divide the wire into $N = L/a$ cubic cells with side length a. We will assume that within each cell, the magnetization $\vec{M}_i$ is uniform. Since the magnitude of the magnetization M_0 is constant, it is sufficient to specify the unit vector $\vec{m}_i = \vec{M}_i/M_0$. Let the x axis be directed along the wire and y, z axis are along the section sides.

Each cubic cell (with side a) energy consists of the following terms:

1. Anizotropy energy, which depends on magnetization direction. For the considered wire

$$W_{an} = -\frac{Ka^3M_z^2}{2M_0^2} + \frac{K_1a^3M_y^2}{2M_0^2}.$$

where $K, K_1 > 0$ are constants. This energy is minimal when magnetization is directed along z axis.

2. Exchange energy, which depends on relative orientation of neighbouring pair of cell magnetic moments. For one pair of cells the energy is

$$W_{ex,i} = -\frac{A}{M_0^2}\vec{M}_i\vec{M}_{i+1}a,$$

where $A > 0$ is constant, therefore configuration with magnetic moments aligned in the same direction is preferred. There is such contribution for each pair of neighbouring cells.

3. Energy in external magnetic field

$$W_B = -a^3\vec{B}\vec{M}.$$

Note that the expressions above are for energy, not energy density. Thus for **calculating effective magnetic field** $\vec{B}_{\text{eff}}$ projections one should differentiate the energy with respect to magnetization and **divide by** a^3.

Consider the material with following parameters:

1. $A = 4.5 \times 10^{-10}\ J/m$;
2. $K = 5.0 \cdot 10^5\ J/m^3$;
3. $\gamma = 1.76 \cdot 10^{11}\ s^{-1} \cdot T^{-1}$;
4. $M_0 = 6.0 \cdot 10^5\ A/m$.

Cubic cell side size is $a = 3.0\ nm$.

B.1 Effective magnetic field corresponding to the energy above can be written as 0.5 pt

$$\vec{B}_{\text{eff},i} = B_{\text{an}}m_{i,z}\vec{e}_z + B_{\text{ex}}(\vec{m}_{i-1} + \vec{m}_{i+1}) - k_1 B_{\text{an}}m_{i,y}\vec{e}_y + \vec{B}_0.$$

Here $k_1 = K_1/K$ is a dimensionless coeffisient. In all calculation we use $k_1 = 1$. Find formulas and numerical values for fields B_{ex} и B_{an}. Calculate characteristic frequency of magnetic moment precession $\omega = \gamma B_{\text{an}}$.

Below all magnetic fields are measured in units of B_{an}, time is measured in units of $1/\omega$, $\tau = \omega t$. Thus dimensionless effective field is

$$\vec{b}_{\text{eff},i} = m_{i,z}\vec{e}_z + \beta(\vec{m}_{i-1} + \vec{m}_{i+1}) - k_1 m_{i,y}\vec{e}_y + \vec{b},$$

and LLG equation is

$$\frac{d\vec{m}_i}{d\tau} = -\vec{m}_i \times \vec{b}_{\text{eff}} + \alpha\vec{m}_i \times \frac{d\vec{m}_i}{d\tau}.$$

Anizotropy energy is minimal when magnetic moments are collinear with z axis, $m_{i,z} = \pm 1$. Domain wall between regions with $m_{i,z} = +1$ and $m_{i,z} = -1$ is a transitional region, where magnetization direction changes from positive z axis direction to negative z axis direction. You will use **Ferromagnetic Simulator** program to study magnetization dependence on coordinate x inside the domain wall.

At the initial moment of time in the left part of the wire magnetization is $m_{i,z} = +1$, while in the right part $m_{i,z} = -1$. Abrupt change in magnetization direction leads to large exchange energy, therefore this configuration is not optimal. Let us set a large dissipation constant α and consider how system changes over time. After relatively short time period the system energy becomes close to minimal and the system almost stops changing.

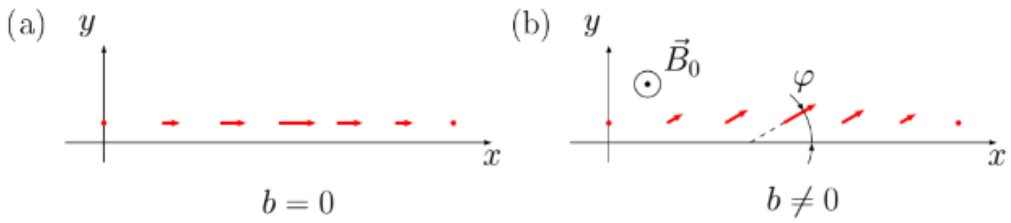
In parts B2-B4 external magnetic field is zero, $b = 0$!

B.2	In the program set parameters $\beta = 100$, $b = 0$. Choose time of evolution T and damping constant in such a way that after time T system change speed is negligible. Indicate used values of α, T in the answer sheets. In "report" folder save the program output for the chosen values of parameters α and T, choose file name "B2". Domain wall width d is distance between points with $m_z = \pm 0.5$. Find the value of d in the a units.	1.0 pt

B.3	Study the dependence of domain wall width on the exchange energy (proportional to value of β) in the interval from $\beta = 20$ to $\beta = 400$. Obtain at least 5 points. Write the values of β you used and corresponding values of d into an Excel file "B3". Remember to write the physical quantities' names for the colomns you used. Save to "report" folder the program output with file name "B3_j", where j is a measurement number. Provide necessary calculations and explanation in working sheets.	1.5 pt

B.4	If $d(\beta) \sim \beta^c$, calculate value of c using results from the previous part. If you need to plot a graph, save it to Excel file "B3".	0.5 pt

Part C. Domain wall motion in external field (4.5 points)



Magnetic moment projection on xy plane dependence on x coordinate: (a) without external magnetic field, (b) in external field

Switch on external magnetic field along z axis, $b_{0,z} = b > 0$. Domain wall starts moving. If $b < b_{\text{cr}}$, domain wall settles into uniform motion, and for $b > b_{\text{cr}}$ the motion stays non-uniform. Critical magnetic field value b_{cr} is called Walker limit.

Magnetic moment distribution in moving domain wall can be related to that of static domain wall. Without magnetic field $m_x(x) = f(x - x_0)$, $m_y = 0$, where x_0 is domain wall center coordinate. Then after magnetic field is turned on $m_x(x) = f(x - x_0)\cos\varphi$, $m_y = f(x - x_0)\sin\varphi$, where angle φ does not depend on coordinate and x_0 is domain wall center coordinate at a given time. During uniform motion angle φ does not depend on time.

In part C all the lengths are measured in units of a, and all the times in units of $1/\omega$, always use values $\beta = 100$, $\alpha = 0.2$.

C.1	In which direction the wall starts moving (to the right or to the left)?	0.2 pt

C.2 In program set the values $\alpha = 0.2$, $\beta = 100$. Obtain the dependence of domain wall velocity v and angle φ on external field b. Study the magnetic fields in range from $b = 0$ to $b = b_{\text{cr}}$. Write used values b and corresponding values of v and φ in Excel file "C2". Remember to write the physical quantities' names for the colomns you used. Save to "report" folder the program output with file name "C2_j", where j is a measurement number. Provide necessary calculations and explanation in working sheets. It is known that $b_{\text{cr}} < 0.15$. You should obtain at least 5 points in the range $b < b_{\text{cr}}$. Note that if during the domain wall motion distance from its center to the wire edge becomes less than 40, the edge effects modify the solution significantly and you will not be able to obtain correct results form it. Thus for field values close to critial you may need to use the maximum available length $L = 200$. For smaller field values you may use shorter length to speed up calculations. — 2.0 pt

C.3 Plot the dependence $v(b)$, calculate the slope $\dfrac{dv}{db}$ for the linear part. For plotting use Excel file "C2". — 0.4 pt

C.4 It follows from theoretical calculations that for $b < b_{\text{cr}}$ the velosity is equal to — 0.6 pt

$$v = v_c \sin 2\varphi.$$

Using data from part C2, plot a linearized graph and find values of v_c and b_{cr}. For plotting use Excel file "C2".

C.5 Using numerical values form part B, calculate v_c in m/s, and $B_{\text{cr}} = B_{\text{an}} b_{\text{cr}}$ in T. — 0.3 pt

C.6 Let us study domain wall motion for $b > b_{\text{cr}}$. For $b = 0.2$ measure the depencence of domain wall coordinate on time. Write domain wall coordinates and corresponding time values in Excel file "C6", remember to write names of physical quantities in corresponding colomns. Plot this dependence. Save the program output you used to "report" folder in file "C6". — 1.0 pt

Instructions for Ferromagnetic Simulator program

The Ferromagnetic Simulator program numerically solves the Landau-Lifshitz-Gilbert (LLG) equation for a system of magnetic moments described in Part B. By toggling the radio buttons at the top, you may select the problem section (B or C). It affects the number of cubes (N) and the initial magnetic moment values.

10Specifying parameters

For both problem sections the following parameters can be specified :

1. Gilbert damping coefficient α (input field: *alpha*), the input value must satisfy $\alpha \in [0; 1]$.
2. Parameter β (input field: *beta*), the input value must satisfy $\beta \in [0; 500]$.
3. External magnetic field b (input field: *b*), the input value must satisfy $b \in [0, 1]$.
4. Simulation time T (input field:*T*, in dimensionless units, as defined in Part B), the input value must satisfy $T \in [0, 100]$. The program computes the solution over the interval $t \in [0, T]$.

In Part C, you may also specify the distance L from the initial position of the domain wall center to the right edge of the wire, measured in units of the cubic cell size a. The input value must satisfy $L \in [50, 200]$.

Increasing L improves the observation of domain wall motion but increases computation time. The domain wall is always positioned at a fixed distance $L_1 = 50$ from the left edge, so the total system length is $L_1 + L$.

Running the Simulation

Set the desired parameters and click **Solve**. The program will numerically integrate the LLG equation. For some initial conditions, computation may take several minutes. Once the solution is computed, the **Plot** button becomes active.

Plotting the Results

Specify a time $t \in [0, T]$ and click **Plot**. The program will display smoothed curves of $m_x(x)$, $m_y(x)$ and $m_z(x)$ at time t.

Note that the actual computed values are only at integer positions $x = i$. The program yelds solutions at **200 time points**, equally spaced at intervals of $T/200$. **If a requested time does not match, it is rounded to the nearest available value.**

Save/Load Functionality

Use **Save** to store solutions in the "report" folder. Use **Load** to retrieve previously saved solutions. Once loaded, you can plot $m_x(x)$, $m_y(x)$, and $m_z(x)$ for any of the 200 saved time points without recomputing.

Note: save all the solutions you use.

Initial conditions

In Part B the program assumes $N = 201$ and the following initial conditions

1. $m_{i,z} = +1$ for $i = 0, \ldots, 97$,
2. $m_{i,x} = 1$ for $i = 98, \ldots, 102$,
3. $m_{i,z} = -1$ for $i = 103, \ldots, 200$.

All other components of $\vec{m}_i$ are zero.

As an initial state for part C the program precomputes static solution for $\beta = 100$ with $N = 401$ cubic cells. To match the specified system length (determined by parameter L), excess values beyond the required domain are truncated.

Vibrational structure of polyynes

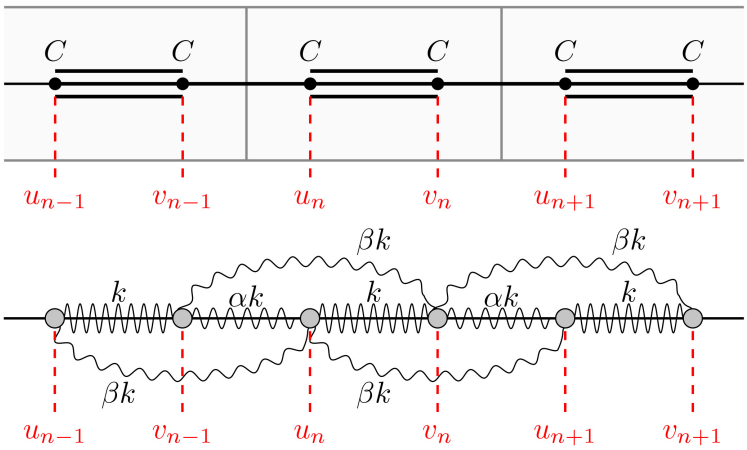
In this problem, you will explore *polyynes* — organic compounds that contain several alternating single and triple bonds between carbon atoms in their structure. You may use the following constants:

- $N_A = 6.02 \cdot 10^{23}\ \text{mol}^{-1}$ — Avogadro's number,
- $M_C = 12.0\ \text{g/mol}$ — the molar mass of a carbon atom,
- $\hbar = \dfrac{h}{2\pi} = 1.055 \cdot 10^{-34}\ \text{J} \cdot \text{s}$ — the reduced Planck constant.

Part A. An infinite chain of carbon atoms (6.5 points)

First, examine an infinite one-dimensional chain of carbon atoms with alternating single and triple bonds, as shown in the figure. We will describe the system using the ball-and-spring model. Assume that all carbon atoms (balls) have identical masses equal to m, the triple bond corresponds to a spring with spring constant k, the single bond to a spring with constant αk, and additionally, every other atom (ball) is connected by a spring with constant βk (for visualization convenience, such springs are shown in a curved shape itn he figure; in reality, all springs are horizontal).

Use the following notation: u_n, v_n — the displacements from equilibrium positions for the left and right atoms (balls), connected by a triple bond, respectively. We will say that two such atoms form a unit cell. Note that index n ranges over all **integer** values.



A.1	Write the expression for the total energy of the system. Express your answer in terms of all coordinates u_n, v_n, their first-order time derivatives, as well as the parameters m, k, α, β.	0.8 pt

The time derivative of the system's total energy can be expressed as $\dot{E} = \sum_n (A\dot{u}_n + B\dot{v}_n)$, where A and B are expressions containing u_n, v_n, and their second-order time derivatives. The equations $A = 0$ and $B = 0$ describe the system's motion and turn out to be equivalent to Newton's second law.

Note that an infinite sum of the form $\sum_n a_n b_{n-1}$ can be transformed by «shifting» indices

$$\sum_n a_n b_{n-1} = \sum_n a_{n+1} b_n.$$

A.2 Derive the system of differential equations describing the motion of all atoms. Express your answer in terms of coordinates u_n, v_n and their second time derivatives, along with the parameters m, k, α, β. 0.8 pt

To solve such systems of linear differential equations, the method of complex amplitudes is used. This involves seeking solutions in the form of complex functions, while the true solution corresponds to their real (or imaginary) part. In this problem we are interested in solutions that are plane waves

$$u_n(t) = U \cdot \exp(-i\omega t + iqn), \quad v_n(t) = V \cdot \exp(-i\omega t + iqn).$$

A.3 Derive a system of linear equations for the coefficients U and V of the form 0.9 pt

$$\begin{cases} a \cdot U + b \cdot V = 0, \\ c \cdot U + d \cdot V = 0. \end{cases}$$

Express the coefficients a, b, c, and d in terms of m, k, α, β, ω, and q. You may need Euler's formula

$$\exp(ix) = \cos x + i \sin x.$$

The resulting system of equations necessarily admits the trivial solution $U = V = 0$. However, we are interested in the alternative case when the carbon chain undergoes oscillations. The following fact will be useful: **a system of linear equations of this form has a non-trivial solution if and only if the relation $ad - bc = 0$ is satisfied**. Importantly, in this case there are infinitely many solutions: they correspond to oscillations of the same form but with different amplitudes.

The collective oscillatory motion of the chain's atoms is called a phonon. We say that a phonon «runs» along the chain. The quantity ω is called the frequency, while q is the phonon's quasimomentum.

The phonon dispersion relation (spectrum) refers to the dependence of the phonon frequency ω on its quasimomentum q.

A.4 Derive the dispersion relations for the two possible phonons that can propagate in the considered carbon chain. As your answer, specify the ratio ω/ω_0, where $\omega_0 = \sqrt{k/m}$. The answer (the specified ratio) may only include the parameters α, β and q. 1.0 pt

A.5 Simplify the dispersion relations found in the previous part for the case $q \to 0$ by expanding them in a Taylor series about $q = 0$. Your answer should include the first non-zero, non-constant term in the expansion.
Use the following approximation formulas: $1 - \cos x \simeq x^2/2$ and $(1+x)^\gamma \simeq 1 + \gamma x$ for $x \to 0$. 1.0 pt

Phonons for which $\omega(q) \propto q$ as $q \to 0$ are called **acoustic**; all other phonons are **optical**.

A.6 Simplify the dispersion relations obtained in the previous part for the case $q \to \pi$ by expanding them in a Taylor series with respect to $(q - \pi)$ about 0. Assume that $\alpha < 1$ is known. Your answer should include the first non-zero, non-constant term in the expansion. 1.0 pt

A.7 Sketch the graph of dispersion curves $\omega(q)$ for $q \in [-\pi, \pi]$ for the following cases: 1.0 pt
- $\alpha = 0.5$, $\beta = 0.1$;
- $\alpha = 0.5$, $\beta = 3.0$.

Pay attention to the relative arrangement of the curves, their behavior near the points $q = 0$ and $q = \pi$ and possible extremums.

Part B. Spectroscopy of polyynes (3.5 points)

The model discussed in Part A of the problem provides a reasonably accurate description of **polyynes** — the organic compounds that will be discussed further. It is important to note that, unlike the model in Part A, real molecules have a finite length, which affects their phonon spectrum.

Let us consider the same chain as in Part A, but of finite length. Suppose it consists of $N+1$ unit cells. In other words, the index n takes all integer values from 0 to N. Assume both ends of the chain are fixed, i. e., the displacements $u_0 = u_N = v_0 = v_N = 0$ at any moment in time.

In the infinite chain model, solutions were found in the form of traveling plane waves. Since the dynamics of such a system is described by a system of linear equations, any linear combination of solutions is also its solution. In other words, if the sets of functions u_n, v_n and $\tilde{u}_n, \tilde{v}_n$ are solutions, then the set of functions $\mu u_n + \eta \tilde{u}_n, \mu v_n + \eta \tilde{v}_n$ (μ, η are arbitrary complex numbers) also satisfies the system of equations describing the system's dynamics.

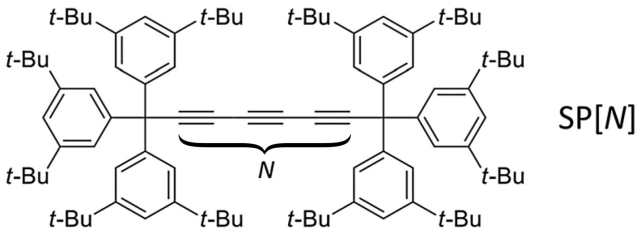
Consider a linear combination with coefficients μ and η of two plane waves propagating in opposite directions in the chain (i. e., with quasimomenta q and $-q$).

B.1 Apply the boundary conditions for the finite chain with $N+1$ unit cells and obtain a system of two linear equations for μ and η. The coefficients in the equation may depend only on the quantities q and N. 0.8 pt

The linear combination with coefficients μ and η satisfying the derived system represents a solution to the dynamics equations describing the finite chain with the specified boundary conditions.

B.2 For what values q_l of quasimomentum the system has a nontrivial solution? Express the answer in terms of N and integer number l. 0.7 pt

In the early 2010s, Canadian scientists from the University of Alberta, Wesley A. Chalifoux and Rik R. Tykwinski, developed a method to synthesize symmetric endcapped polyynes $SP[N]$, where N denotes the number of triple bonds in the carbon chain. The molecular structure is shown in the figure.



SP[*N*]

The physical meaning of the end groups is that they determine the boundary conditions. The specified end groups allow us to consider both ends of the chain (atoms bonded to four neighbors) as fixed. As you saw in questions B1–B2, the finite size of the chain and the introduction of boundary conditions result in only discrete resonances being observed in the phonon spectrum.

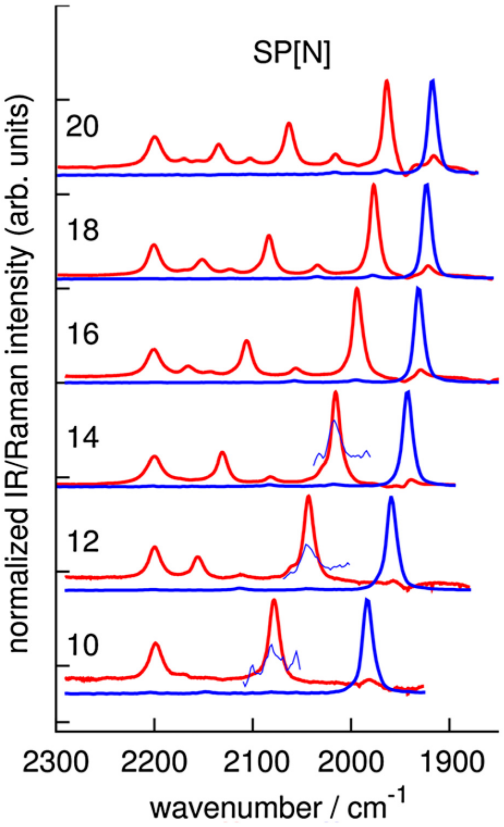
The positions of resonances could be determined experimentally using IR and Raman spectroscopy —

methods based on light-matter interaction. For $SP[N]$ polyynes with different numbers N of triple bonds, the energies of phonons that can arise in the molecule are measured. The figure shows the phonon spectrum: red color indicates results obtained by IR spectroscopy, while blue represents Raman spectroscopy data. The excitation of the low-energy optical phonon corresponds to the far-right intensity peak (in all cases shown in the figure, it appears as "blue"). The phonon energy E is related to its frequency ω by the formula $E = \hbar\omega$. Note: the horizontal axis shows energy in inverse centimeters. Use the following conversion formula to obtain energy in Joules

$$1\ \mathrm{cm}^{-1} = 1.99 \cdot 10^{-23}\ \mathrm{J}.$$

Since only one atom is fixed rather than an entire unit cell as in questions B1–B2, we need to use the following approach to describe the system. We imaginarily add one carbon atom to each end of the chain, bonded to the terminal atoms via triple bonds, and fix the terminal unit cells. This results in a chain consisting of $N + 2$ unit cells with fixed ends.

Since the number N in the experimentally studied chains is sufficiently large, the distant coupling (βk) at the very edge, which appeared after the described approach, has practically no effect on the phonon spectrum. In further analysis of experimental data, use only the rightmost blue intensity peak; ignore all others.



B.3	Using the value $\beta = 3.0$ and the experimental results (only the rightmost peak), determine the spring constants of the single and triple bonds.Assume it is known that for the parameters α and β realized in the experiment, the dispersion relation $\omega(q)$ is an increasing function on the interval $(0; \pi)$.	2.0 pt

The carbon chains you were asked to investigate are of scientific interest as they can be used in molecular electronics. The problem incorporates experimental results published in the article: Agarwal, N.R., Lucotti, A., Fazzi, D., Tommasini, M., Castiglioni, C., Chalifoux, W.A. and Tykwinski, R.R. (2013), Structure

and chain polarization of long polyynes investigated with infrared and Raman spectroscopy. J. Raman Spectrosc., 44: 1398-1410.

Single-electron transistor

In all parts of this problem, the elementary charge $e = 1.6 \times 10^{-19}\ C$ may appear in the answer.

The single-electron transistor is an electronic component whose operation is based on the *Coulomb blockade* phenomenon observed at low temperatures (on the order of several kelvin). In this problem, we will investigate this effect and explain the operating principle of a single-electron transistor at zero temperature.

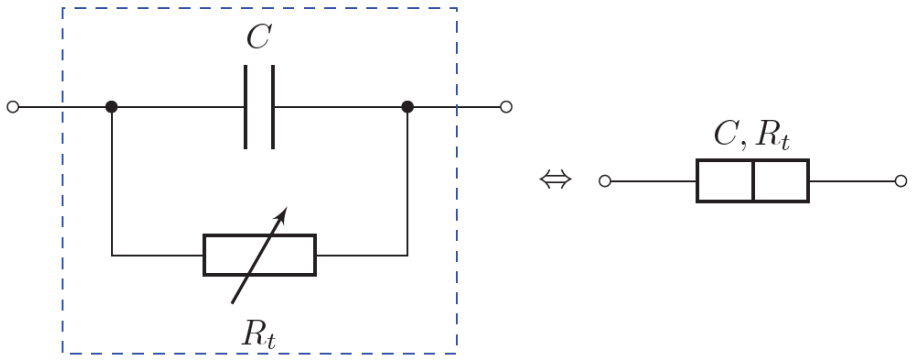
Note: In electrical circuits, the "ground" refers to the point where the potential is defined as zero. The "ground" symbol is shown in the figure.

Part A. Tunneling effect (3.0 points)

The Coulomb blockade phenomenon is fundamentally based on *tunneling*, or *the tunnel effect*. Its essence lies in the fact that, under certain conditions, a system can overcome potential energy barriers. Tunneling is possible if the final energy does not exceed the initial energy. The excess energy releases as heat.

Tunneling constitutes the sequential transfer of individual elementary charges between the plates of a tunnel junction. In the "classical" model of this system, electron transport occurs through a resistor R_t connected in parallel with a capacitor. Energy dissipates on the resistor. The resistance remains finite when tunneling is energetically permissible, and becomes infinite otherwise.

Further, the charge or energy of the tunnel junction shall imply the charge or energy of the capacitor.



Tunnel junction circuit (left) and its symbol in electrical circuit diagrams (right)

Let us consider a tunnel junction disconnected from the power supply.

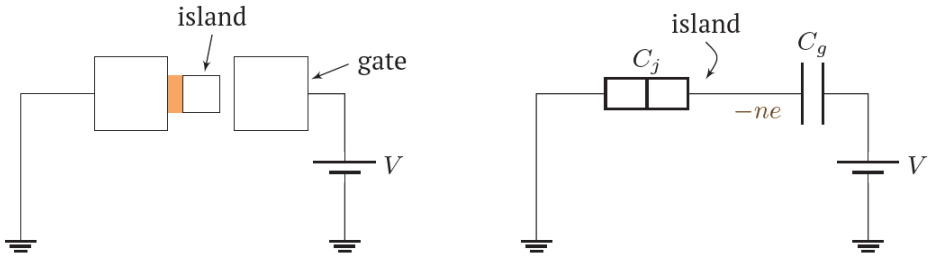
A.1	Write the expression for the energy of a capacitor with capacitance C (in the equivalent circuit of a tunnel junction) when its plates hold a charge equal to n electron charges. Now let the value n increase by one. What is the change in the capacitor's energy ΔW?	0.1 pt

Hereafter, we consider tunnel junctions connected in an electrical circuit with other elements. In circuit diagrams, a tunnel junction is represented as two touching rectangles.

Single-electron box

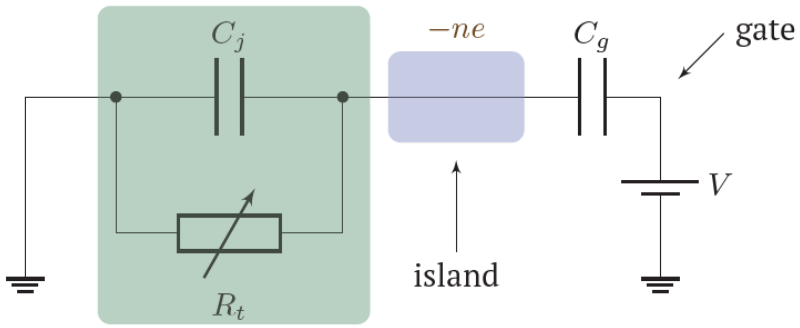
The single-electron box is a system comprising three aligned electrodes. The central electrode is called the island, while the lateral electrodes are called the banks. The island contains n electrons — a quantity that may vary through tunneling events. Note that n can be **either positive or negative** (indicating an excess or deficiency of electrons on the island).

Between the island and the left bank lies a tunnel junction with capacitance C_j, while the island and right bank form a conventional capacitor with capacitance C_g. In this configuration, the right bank is designated as the *gate*. A constant potential difference V is maintained between the banks. The corresponding electrical circuit diagram, specifying all component parameters, is shown in the figure.



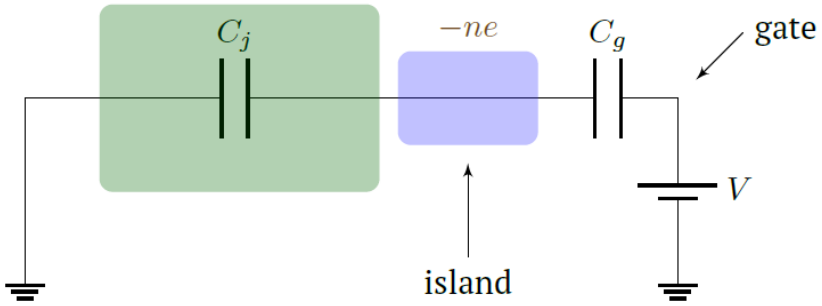
Single-electron box

The "classical" model of tunneling when it is energetically permissible.



Tunneling is permissible

The "classical" model of tunneling when it is energetically forbidden.



Forbidden tunneling

A.2	Derive expressions for the charges on the capacitor and tunnel junction q_g and q_j. The capacitances of the capacitor and tunnel junction are C_g and C_j, respectively, the source voltage is V, and the number of electrons on the island is n.	0.3 pt

A.3	Derive the expression for the change in energy of the system consisting of the capacitor and tunnel junction when the number n of electrons on the island increases by one. Express the answer in terms of n, C_g, $C = C_j + C_g$.	0.3 pt

A.4	Derive expressions for the work done by the voltage source A and the heat dissipation Q in the circuit during the tunneling of one electron onto the island (corresponding to an increase by one in the number n of island electrons). Express the answers in terms of n, C_g, C, V.	0.5 pt

Hereafter, we will consider tunneling to be allowed when the amount of heat Q dissipated in the circuit is greater than zero.

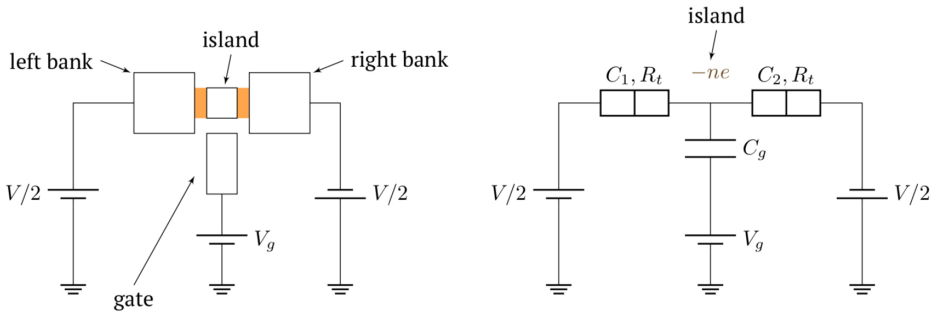
A.5	Assume that the heat Q is dissipated during current flow through the tunnel resistance R_t. Derive the expression for the current I_t through R_t during tunneling of one electron onto the island. Also, specify the constraint on n for which this expression is valid (i.e., when tunneling is energetically permissible). Express the answers in terms of n, C_g, C, V, R_t.	0.5 pt

A.6	Assuming tunneling is energetically permissible, express the current I flowing through the source in terms of the tunnel current I_t. The positive current direction is toward the negative terminal of the source. The expression may also include the quantities C_g, C, V. Consider processes corresponding to both an increase and a decrease in the number of electrons on the island.	0.3 pt

A.7	Plot the $I(V)$ characteristics for $n = 0$ and $n = 1$ on the single graph. Display the dependencies over a sufficiently wide voltage range to capture all distinctive features.	1.0 pt

Part B. Single-electron transistor (4.5 points)

The single-electron transistor consists of an island connected to two banks via tunnel junctions and a gate that forms a capacitor with the island. The gate is purely capacitively coupled (its resistance is infinite). A voltage $+V/2$ is applied to the left bank, and a voltage $-V/2$ is applied to the right bank. The transistor's circuit diagram and equivalent circuit, with specified parameters of the electronic components, are shown in the figure.



Single-electron transistor.

B.1	Let the island contain n electrons. Express the island's potential φ in terms of n, V, V_g, C_1, C_2, C_g.	0.2 pt

B.2	Derive the expression for the total work done by the voltage sources during the tunneling of one electron onto the island from the left (first) bank. Express your answer in terms of V, V_g, C_1, C_2, C_g.	1.0 pt

B.3	Let the island contain n electrons. Express the total heat dissipated in the circuit during the tunneling of one electron onto the island from the left (first) bank. Express the answer in terms of n, V, V_g, C_1, C_2, C_g.	1.0 pt

B.4	Derive the condition (inequality) for V corresponding to heat dissipation positivity during the tunneling from the left bank **onto** the island. Express the answer in terms of n, V, V_g, C_g, C_2.	0.3 pt

B.5	Derive conditions for V analogous to those in question B4 in cases of tunneling **onto** the island from the right bank and tunneling **from** the island onto the both banks. Sketch a diagram of regions corresponding to the existence of n electrons on the island after sufficient time has elapsed. The diagram should be plotted in axes V vs V_g. For each region specify the values of n on the diagram.	1.5 pt

Consider regions on the (V, V_g) diagram where, after sufficient time, only two transitions are energetically permissible: $n \to n+1$ through one junction and $n+1 \to n$ through the other junction. In this case, a steady current flows through the island from one bank to the other. We now determine its magnitude.

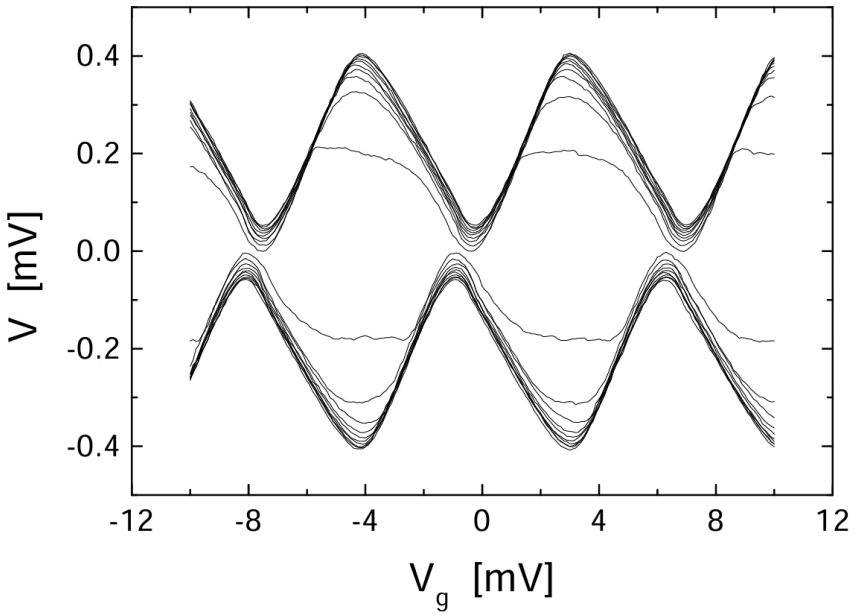
Since the island's charge remains unchanged after a pair of tunneling events, the charges on the capaci-

tors also remain constant. Consequently, the resulting current is determined by the sum of the tunneling times through the first and second junctions.

B.6	Assume the tunnel junctions are identical: each has a capacitance C_1 and tunnel resistance R_t. Consider voltage pairs (V_g, V) for which, after sufficient time, only states with $n = 0$ and $n = 1$ electrons on the island are possible. Determine the magnitude of the tunnel current $I(V_g, V)$ in the circuit. The positive current direction is from the left bank to the right bank.	0.5 pt

Part C. Tunneling at finite temperature (2.5 points)

C.1	The graph shows the experimental $V(V_g)$ dependence at low temperature $T = 10\ \mathrm{mK}$, measured for fixed current values $I \approx 1\ \mathrm{pA}$. Based on the results obtained in Part B, determine the capacitances $C_1 = C_2$ and C_g.	0.5 pt



V. A. Krupenin et al., 2001

Consider a fixed positive temperature T. Let $\Gamma^{(i)}_{n\to n\pm1}$ denote the probability **per unit time** (rate) of tunneling to/from the island through the i-th junction, and let $p(n)$ be the probability of finding n electrons on the island.

Note: If a process has a rate Γ, then during time dt it occurs with probability $dp = \Gamma dt$.

C.2	Let $\Gamma_{n\to n\pm1} = \Gamma^{(1)}_{n\to n\pm1} + \Gamma^{(2)}_{n\to n\pm1}$. An electron can tunnel to/from either bank. Express the time derivative $dp(n)/dt$ of the probability of having n electrons on the island in terms of the probabilities $p(n)$, $p(n \pm 1)$ and the rates $\Gamma_{n\to n\pm1}$, $\Gamma_{n\pm1\to n}$.	0.3 pt

We will examine the steady-state current flow through the transistor (meaning all probabilities $p(n)$ are constant). We also assume there exists a critical number n_0 of electrons on the island, beyond which tunneling ceases: $p(n) = 0$ and $\Gamma_{n-1\to n} = 0$ for $n > n_0$.

C.3	From the stated assumptions and established boundary condition, derive a relation connecting $p(n)$ and $p(n+1)$ in the form $p(n+1) = A \cdot p(n)$, where A is an expression containing only the rates $\Gamma_{m \to m \pm 1}$ for various m.	0.5 pt

We will consider low temperatures ($kT \ll e^2/C$) and small voltages: $|V| \ll e/C$, $|V_g - e/2C_g| \ll e/C_g$. According to quantum mechanics, the general form for the tunneling rate per unit time to/from the island through the i-th junction is:

$$\Gamma^{(i)}_{n \to n \pm 1} = \frac{1}{e^2 R_t} \frac{Q^{(i)}_{\pm}(n)}{1 - \exp\left[-\dfrac{Q^{(i)}_{\pm}(n)}{kT}\right]}$$

where $Q^{(i)}_{\pm}(n)$ is the heat dissipated during the tunneling process.

C.4	Using the expression derived in question B3 and analogous relations, show that $\Gamma_{n \to n+1}$ for $n > 0$ and $\Gamma_{n \to n-1}$ for $n < 1$ **decay** exponentially with changing n. Assume that $T \to 0$.	0.3 pt

Hereafter, all $p(n)$ except $p(0)$ and $p(1)$ will be treated as zero.

C.5	Express the probabilities $p(0)$ and $p(1)$ in terms of the rates $\Gamma_{0 \to 1}$ and $\Gamma_{1 \to 0}$. Take into account that $p(0) + p(1) = 1$.	0.5 pt

C.6	Write the expression for the current through the transistor. Express the answer in terms of $\Gamma^{(i)}_{0 \to 1}$, $\Gamma^{(i)}_{1 \to 0}$.	0.4 pt

Substituting the expressions for heat into the formula for the tunneling rates $\Gamma^{(i)}_{n \to n \pm 1}$ yields, after extensive calculations, the current's dependence on voltage and temperature. This pronounced dependence enables the use of a single-electron transistor as a low-temperature measurement device, as explored in the science festival problem.