Solution

A1. The length of $\vec{M}$ squared is equal to

$$M^2 = \vec{M} \cdot \vec{M},$$

thus, its time derivative is

$$\frac{\partial}{\partial t} M^2 = 2\vec{M} \cdot \frac{\partial \vec{M}}{\partial t}.$$

For any vectors $\vec{a}, \vec{b}$, their vector product $\vec{a} \times \vec{b}$ is orthogonal to the vectors. In particular, vectors $\vec{M} \times \vec{B}_{\text{eff}}$ and $\vec{M} \times \frac{\partial \vec{M}}{\partial t}$ are orthogonal to $\vec{M}$, so according to LLG equation $\vec{M}$ and $\frac{\partial \vec{M}}{\partial t}$ are perpendicular, therefore

$$\vec{M} \cdot \frac{\partial \vec{M}}{\partial t} = 0, \quad \frac{\partial}{\partial t} M^2 = 0,$$

and the magnitude of $\vec{M}$ is constant.

$$\boxed{\frac{\partial}{\partial t} M^2 = 2\vec{M} \cdot \frac{\partial \vec{M}}{\partial t} = 0}$$

A2. Consider the z-component of the equation

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

The vector product $(\vec{m} \times \vec{B}_{\text{eff}})$ is perpendicular to z axis, so only the second term contributes to the equation. Taking into account $\vec{m} \cdot \vec{B}_{\text{eff}} = m_z B_0$ we get

$$\dot{m}_z = \frac{\alpha\gamma}{1+\alpha^2} B_0 (1 - m_z^2).$$

Separating variables

$$\frac{\mathrm{d}m_z}{1 - m_z^2} = \frac{\alpha\gamma}{1+\alpha^2} B_0 \, \mathrm{d}t$$

and integrating the resulting expression from 0 to t we obtain

$$\frac{1}{2} \ln \left(\frac{1 + m_z(t)}{1 - m_z(t)} \right) \Bigg|_0^t = \frac{\alpha\gamma}{1+\alpha^2} B_0 t.$$

Substituting initial condition $m_z(0) = 0$,

$$\frac{1}{2} \ln \left(\frac{1 + m_z(t)}{1 - m_z(t)} \right) = \frac{\alpha\gamma}{1+\alpha^2} B_0 t,$$

we find the answer

$$\boxed{m_z(t) = \frac{\exp\left(\frac{\alpha\gamma B_0 t}{1+\alpha^2}\right) - \exp\left(-\frac{\alpha\gamma B_0 t}{1+\alpha^2}\right)}{\exp\left(\frac{\alpha\gamma B_0 t}{1+\alpha^2}\right) + \exp\left(-\frac{\alpha\gamma B_0 t}{1+\alpha^2}\right)} = \tanh\left(\frac{\alpha\gamma B_0 t}{1+\alpha^2}\right)}$$

A3. The first solution

Denote by $\vec{m}_{xy}$ the projection of the vector $\vec{m}$ onto the xy-plane. The vector $\vec{B}_{\text{eff}}$ is directed along the z axis, so that its projection onto the xy-plane is zero. Next, $\vec{m} \cdot \vec{B}_{\text{eff}} = m_z B_0$ and

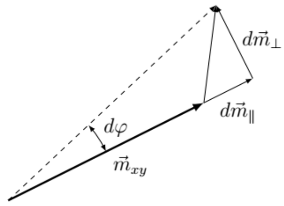
$$\vec{m} \times \vec{B}_{\text{eff}} = (\vec{m}_{xy} + m_z \vec{e}_z) \times \vec{B}_{\text{eff}} = \vec{m}_{xy} \times \vec{B}_{\text{eff}}, \quad (\vec{e}_z \times \vec{B}_{\text{eff}} = 0),$$

so that the projection of the LLG equation onto the xy-plane takes the form

$$\frac{\mathrm{d}\vec{m}_{xy}}{\mathrm{d}t} = -\frac{\gamma}{1+\alpha^2}\vec{m}_{xy} \times \vec{B}_{\text{eff}} - \frac{\alpha\gamma}{1+\alpha^2} m_z B_0 \, \vec{m}_{xy}.$$

Here the first term (with magnitude $\gamma B_0 m_{xy}/(1+\alpha^2)$) is orthogonal to $\vec{m}_{xy}$ and hence leads to the rotation of $\vec{m}_{xy}$. The second term is parallel to $\vec{m}_{xy}$ and leads to the length change.

During the time period $\mathrm{d}t$, a perpendicular change component is



$$\mathrm{d}m_\perp = \frac{\gamma B_0 m_{xy}}{1+\alpha^2}\mathrm{d}t,$$

so that the rotation angle is $\mathrm{d}\varphi = \mathrm{d}m_\perp / m_{xy}$, and the angular velocity is

$$\Omega = \frac{\mathrm{d}\varphi}{\mathrm{d}t} = \frac{\gamma B_0}{1+\alpha^2}.$$

Another way to obtain Ω is to notice that if some vector rotates with an angular velocity $\vec{\Omega}$, then its time derivative is equal to

$$\frac{\mathrm{d}\vec{m}_{xy}}{\mathrm{d}t} = \vec{\Omega} \times \vec{m}_{xy}.$$

Comparing with the first term in the LLG equation, we immediately get

$$\vec{\Omega} = \frac{\gamma \vec{B}_{\text{eff}}}{1+\alpha^2} = \frac{\gamma B_0}{1+\alpha^2}\vec{e}_z.$$

So the answer is

$$\boxed{\Omega = \frac{\gamma B_0}{1+\alpha^2}}$$

A3. The second solution

Project the LLG equation onto the x and y axis:

$$\begin{cases} \dot{m}_x = -\dfrac{\gamma B_0}{1+\alpha^2} m_y - \dfrac{\alpha\gamma B_0 m_z}{1+\alpha^2} m_x, \\[2ex] \dot{m}_y = \dfrac{\gamma B_0}{1+\alpha^2} m_x - \dfrac{\alpha\gamma B_0 m_z}{1+\alpha^2} m_y. \end{cases}$$

Introduce a new complex variable $\hat{m} = m_x + i m_y$ and take a sum of two equations above, where the second equation is multiplied by i firstly:

$$\frac{\mathrm{d}}{\mathrm{d}t}(m_x + i m_y) = -\frac{\gamma B_0}{1+\alpha^2}(-m_y + i m_x) - \frac{\alpha\gamma m_z B_0}{1+\alpha^2}(m_x + i m_y).$$

The resulting equation can be rewritten as

$$\frac{\mathrm{d}\hat{m}}{\mathrm{d}t} = i\frac{\gamma B_0}{1+\alpha^2}\hat{m} - \frac{\alpha\gamma B_0 m_z}{1+\alpha^2}\hat{m}.$$

Separate variables and get

$$\int \frac{\mathrm{d}\hat{m}}{\hat{m}} = \int \mathrm{d}t \left(\frac{i\gamma B_0}{1+\alpha^2} - \frac{\alpha\gamma B_0}{1+\alpha^2} m_z \right).$$

Due to the initial condition $\hat{m}(0) = m_x(0) + i m_y(0) = 1$ we have

$$\ln \hat{m} = \frac{i\gamma B_0 t}{1+\alpha^2} - \frac{\alpha\gamma B_0}{1+\alpha^2} \int\limits_0^t \mathrm{d}t\, m_z(t), \quad \hat{m} = A(t) e^{i\varphi(t)},$$

where the expression

$$A(t) = \exp\left(-\frac{\alpha\gamma B_0}{1+\alpha^2} \int\limits_0^t m_z(t)\,\mathrm{d}t \right)$$

is the magnitude of $\vec{m}_{xy}$, and the expression

$$\varphi = \frac{\gamma B_0 t}{1+\alpha^2}$$

corresponds to an angle of rotation of $\vec{m}_{xy}$ since

$$m_x(t) = A(t)\cos\varphi(t), \quad m_y(t) = A(t)\sin\varphi(t).$$

The angle φ is a linear function in t, so that the angular velocity is constant, and its value coincides with the one obtained earlier. Using the explicit formula for $m_z(t)$ one can find the magnitude $A(t)$. Indeed,

$$\ln A(t) = -\frac{\alpha\gamma B_0}{1+\alpha^2} \int\limits_0^t m_z(t)\,\mathrm{d}t = -\int\limits_0^t \frac{\alpha\gamma B_0 \mathrm{d}t}{1+\alpha^2} \tanh \frac{\alpha\gamma B_0 t}{1+\alpha^2} = -\ln\cosh\frac{\alpha\gamma B_0 t}{1+\alpha^2},$$

what implies

$$A(t) = \frac{1}{\cosh \dfrac{\alpha\gamma B_0 t}{1+\alpha^2}},$$

so that $m_z^2 + m_{xy}^2 = 1$, i.e. the magnitude of $\vec{m}$ is constant and equals 1.

Here we use the formula

$$\int \tanh x\,\mathrm{d}x = \int \frac{\sinh x}{\cosh x}\mathrm{d}x = \int \frac{\mathrm{d}(\cosh x)}{\cosh x} = \ln\cosh x + C,$$

and the relation

$$\tanh^2 x + \frac{1}{\cosh^2 x} = 1.$$

One can avoid the use of complex numbers and find the solution in the form

$$m_x = A(t)\cos\varphi(t), \quad m_y(t) = A(t)\sin\varphi(t).$$

Substitute these expressions to the equations for $\dot{m}_x, \dot{m}_y$ and get

$$\frac{\mathrm{d}A}{\mathrm{d}t}\cos\varphi - A\sin\varphi\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -\frac{\gamma B_0}{1+\alpha^2} A\sin\varphi - \frac{\alpha\gamma B_0 m_z}{1+\alpha^2} A\cos\varphi;$$

$$\frac{\mathrm{d}A}{\mathrm{d}t}\sin\varphi + A\cos\varphi\frac{\mathrm{d}\varphi}{\mathrm{d}t} = \frac{\gamma B_0}{1+\alpha^2} A\cos\varphi - \frac{\alpha\gamma B_0 m_z}{1+\alpha^2} A\sin\varphi.$$

From these equations one can get the time derivatives of the magnitude and the angle:

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = \frac{\gamma B_0}{1+\alpha^2}, \quad \frac{\mathrm{d}A}{\mathrm{d}t} = -\frac{\alpha\gamma B_0 m_z}{1+\alpha^2}A.$$

Note that these relations are nothing but the equalities of the coefficients at $\cos\varphi$ and $\sin\varphi$ in the initial system of equations. The first equation gives a former expression for an angular velocity, and the second one — for the magnitude derivative.

$$\boxed{\Omega = \frac{\gamma B_0}{1+\alpha^2}}$$

B1. By definition

$$\vec{B}_{\text{eff},i} = -\frac{1}{a^3}\frac{\partial W(\vec{M}_i)}{\partial \vec{M}_i},$$

where W is the energy of the system. It consists of contributions given in the task:

$$W = \sum_i a^3\left(-\frac{KM_{i,z}^2}{2M_0^2} + \frac{K_1 M_{i,y}^2}{2M_0^2}\right) - \sum_i A\vec{M}_i\vec{M}_{i+1}\frac{a}{M_0^2} - \sum_i a^3\vec{B}_0\vec{M}_i.$$

Here the first term represents anisotropy energy, only one term in it depends on a magnetization of every cell, so the corresponding magnetic field has the form

$$\vec{B}_{an,i} = \frac{\partial}{\partial M_{z,i}}\left(\frac{KM_{i,z}^2}{2M_0^2}\right)\vec{e}_z - \frac{\partial}{\partial M_{y,i}}\left(\frac{K_1 M_{i,y}^2}{2M_0^2}\right)\vec{e}_y = \frac{KM_{i,z}}{M_0^2}\vec{e}_z - \frac{k_1 K M_{i,y}}{M_0^2}\vec{e}_y = \frac{K}{M_0}\left(m_{i,z}\vec{e}_z - k_1 m_{i,y}\vec{e}_y\right).$$

Comparing with the formula from the task we can find

$$B_{\text{an}} = \frac{K}{M_0}.$$

The second term in W represents the exchange energy, two terms in it depend on $\vec{M}_i$

$$-\frac{Aa}{M_0^2}\vec{M}_i(\vec{M}_{i-1} + \vec{M}_{i+1}),$$

so the effective magnetic field is

$$\vec{B}_{\text{ex}} = -\frac{1}{a^3}\frac{\partial}{\partial\vec{M}_i}\left(-\frac{Aa}{M_0^2}\vec{M}_i(\vec{M}_{i-1} + \vec{M}_{i+1})\right) = \frac{A}{a^2M_0^2}(\vec{M}_{i-1} + \vec{M}_{i+1}) = \frac{A}{a^2M_0}(\vec{m}_{i-1} + \vec{m}_{i+1}).$$

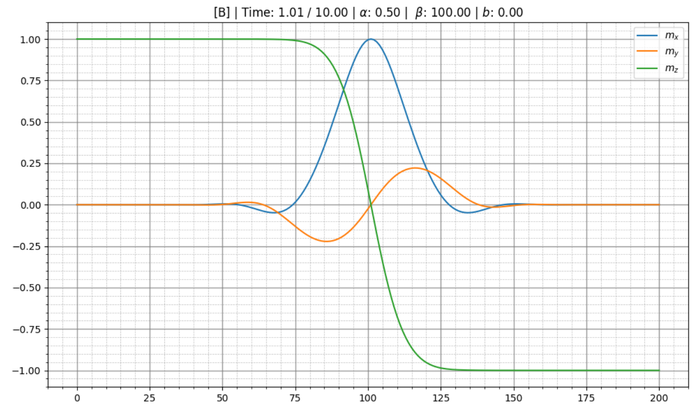
Therefore

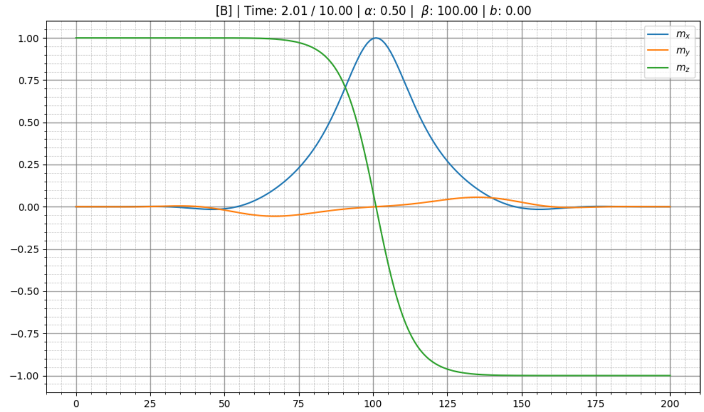
$$B_{\text{ex}} = \frac{A}{a^2M_0}.$$

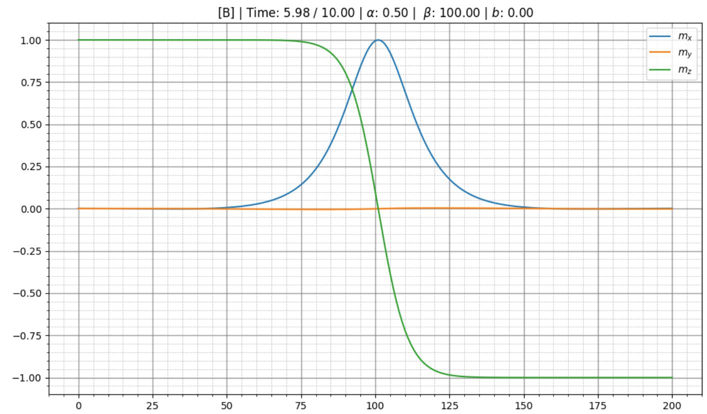
Differentiating the last term, we get a contribution to the effective magnetic field from the external magnetic field $\vec{B}_0$ as it is stated in the task.

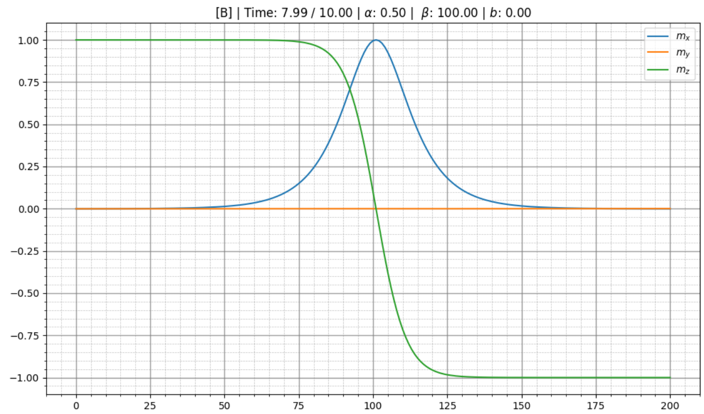
$$\boxed{B_{\text{an}} = \frac{K}{M_0} \approx 0.83\ \text{T}; \qquad B_{\text{ex}} = \frac{A}{M_0a^2} \approx 83.33\ \text{T}; \qquad \omega \approx 1.47\cdot 10^{11}\ \text{s}^{-1}.}$$

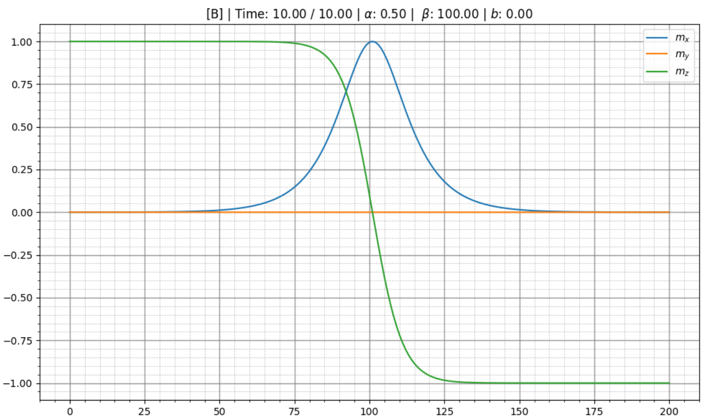
B2. Let us run the program for $\alpha = 0.5$, $\beta = 100$, $b = 0$, $T = 10$. The pictures show graphs of m_x, m_y, m_z for different t in range $[0, 10]$. Note that the magnetization distribution on the last two pictures is approximately the same, so we can consider it stationary. In particular, one of the features of the stationary state regime is that $m_y(x) = 0$ for all x.



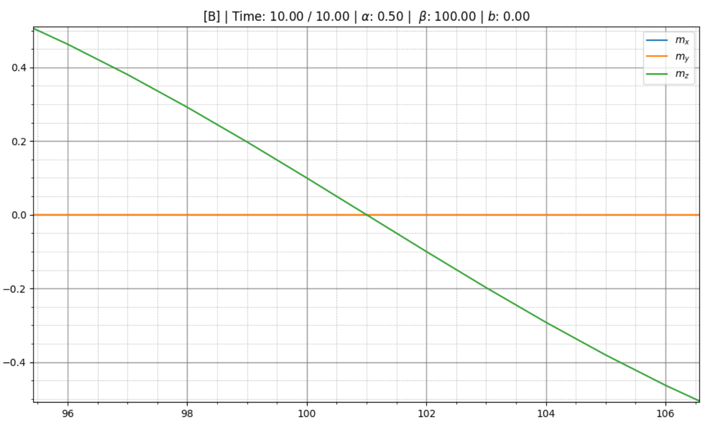








To increase an accuracy of d measurement let us zoom in the part of the plot $m_z(x)$ for $t = 10$ in such a way that the side points correspond to $m_z = \pm 0.5$. The x-coordinates of the points with $m_z = 0.5$ and $m_z = -0.5$ are equal to $x_{\text{left}} = 95.5$ and $x_{\text{right}} = 106.5$ respectively, so that $d = x_{\text{right}} - x_{\text{left}} = 11.0$.



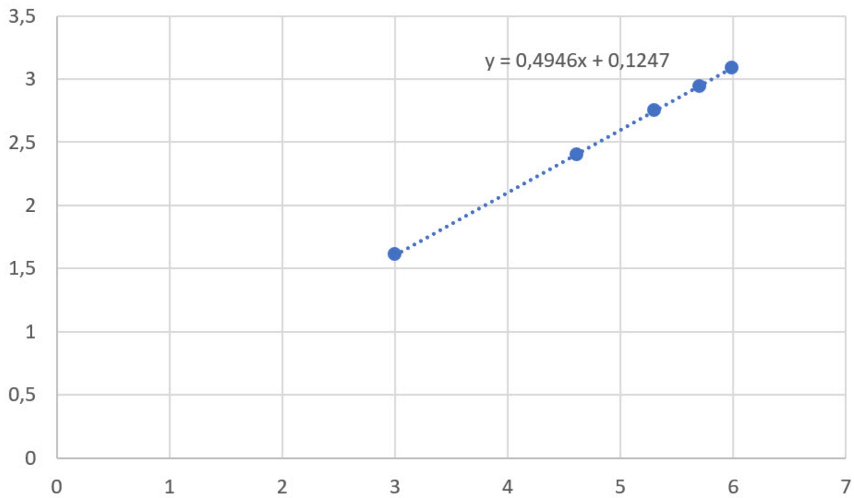
$$\boxed{d = 11.0}$$

B3. In part B2 we have seen that for $\alpha = 0.5$, $\beta = 100$, $b = 0$ and $T = 10$, the steady state regime occurs in the end. Thus, in the present part we will use the same values of the parameters α and T, and different $\beta \in [20, 400]$. We will find the width d in the way described in the solution of B2, for $t = 10$. To ensure that the system is indeed in stationary state, we check that $m_y \equiv 0$ at $t = 10$ on the graph. Denote by x_{left}, (resp. x_{right}) the coordinates of the left (resp. right) borders of the domain wall. The width of the wall can be computed using the formula $d = x_{\text{right}} - x_{\text{left}}$.

β	x_{left}	x_{right}	d
20	98.5	103.5	5.0
100	95.5	106.5	11.0
200	93.2	108.8	15.6
300	91.5	110.5	19.0
400	90.0	112.0	22.0

B4. Let $d(\beta) = \gamma\beta^c$, where γ is a constant coefficient. Then $\ln d(\beta) = \ln\gamma + c\ln\beta$, so that the dependence $\ln d\,(\ln\beta)$ is linear, and the slope is equal to c. Calculate $\log d$ and $\log\beta$ for the points obtained in B3, and then draw a graph in Excel using the resulting data.

$\ln\beta$	$\ln d$
3.00	1.61
4.61	2.40
5.30	2.75
5.70	2.94
5.99	3.09



The plot $\ln d\,(\ln\beta)$.

$$\boxed{c = 0.495}$$

C1. Set some $b \neq 0$ and run the program. We see that the domain wall moves to the right.

$$\boxed{\text{To the right.}}$$

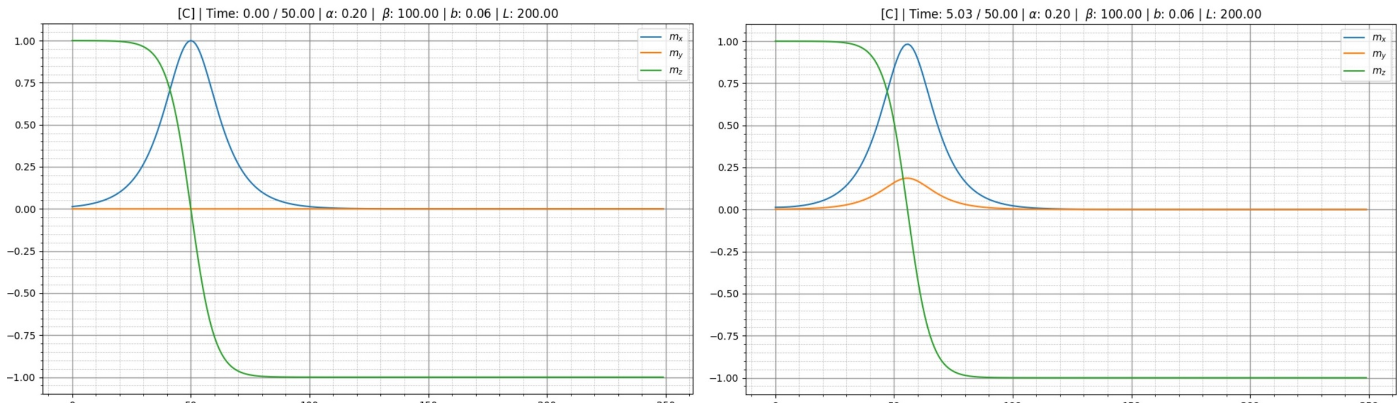
C2. After the start of the program, the transient process begins. For small enough values of b the system settles into uniform motion, and the angle of magnetic fields rotation φ stops changing. The evolution time should be large enough so that the motion becomes uniform. The length L should be such that the domain wall does not reach the right side during the evolution time. On the other hand, with the growth of T and L, the runtime increases, so that one should find optimal parameters.

Since just after the start of the program the uniform motion is not established yet, the velocity can not be computed using the formula $v = \frac{x - x_0}{t}$, where x_0 is the initial position of the center of the domain wall. The measurements should be taken in a steady state regime, so that one needs to determine the duration of the transient process. To do this one need to measure the dependence $x(t)$ for some b, and estimate the typical transient time. Another way to get correct measurements is to take them only when the shape of m_y stops changing over time (one can see the change of m_y only after zooming the plot). In a steady state regime, due to a high accuracy of measurements, it is enough to compute the velocity of the center of the wall by the formula $v = \frac{x_2 - x_1}{t_2 - t_1}$, i.e. using only two points.

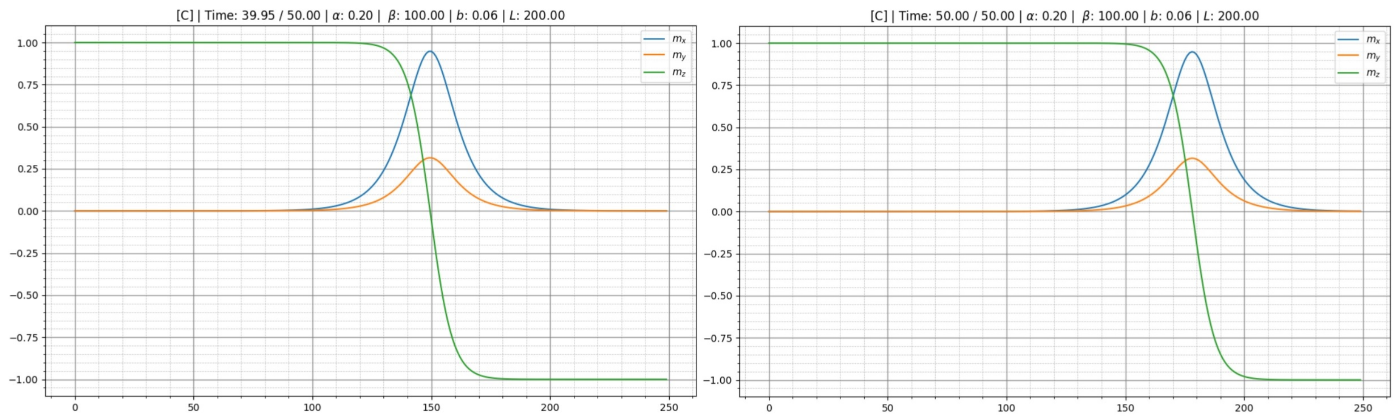
In the center of the domain wall we have $m_z = 0$, and both $m_x = m_{x0}$, $m_y = m_{y0}$ are maximal. (One can see from the plots that the coordinates of the maxima of m_x and m_y and the coordinate x such that $m_z(x) = 0$, almost coincide). Therefore, we can find the angle φ using either of the equivalent relations $m_{x0} = \cos\varphi,\ m_{y0} = \sin\varphi$, but only when the uniform motion is already established. Thus,

$$\varphi = \arcsin m_{y0} = \arccos m_{x0} = \arctan \frac{m_{y0}}{m_{x0}}.$$

If one constructs the graph of m_y/m_x, it can be seen that φ indeed does not depend on the coordinate (participants are not required to do such a verification).



Transient process: m_y increases.



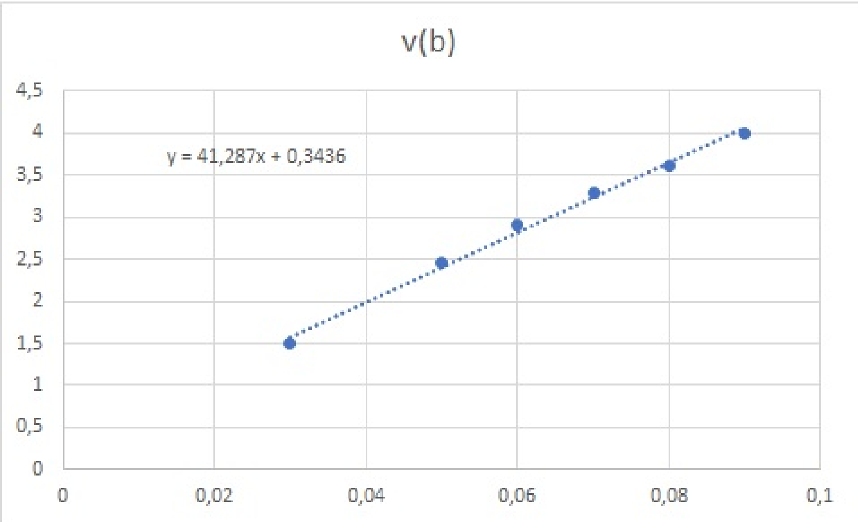
Steady state regime: m_y shape is constant.

If $b > 0.1$, the domain wall behavior changes. Magnetization angle φ increases, magnetic moment rotates around z axis. The domain wall motion is accompanied by its center oscillations. Unlike the case $b < 0.1$, m_y is sometimes greater than m_x (orange and blue graphs swap). Hence $b_{\text{cr}} \approx 0.1$.

Let us measure $v(b)$ and $\varphi(b)$ for $b < 0.1$.

b	m_y	t_1	x_1	t_2	x_2	v	φ
0.03	0.152	40	101,5	50	116,5	1,50	0,152
0.05	0.258	40	134,0	50	158,5	2,45	0,261
0.06	0.316	40	149,0	50	178,0	2,90	0,322
0.07	0.378	40	164,0	50	197,0	3,30	0,387
0.08	0.446	35	159,0	45	195,0	3,60	0,462
0.09	0.525	37	176,0	43	200,0	4,00	0,893

C3. Plot the graph $v(b)$.

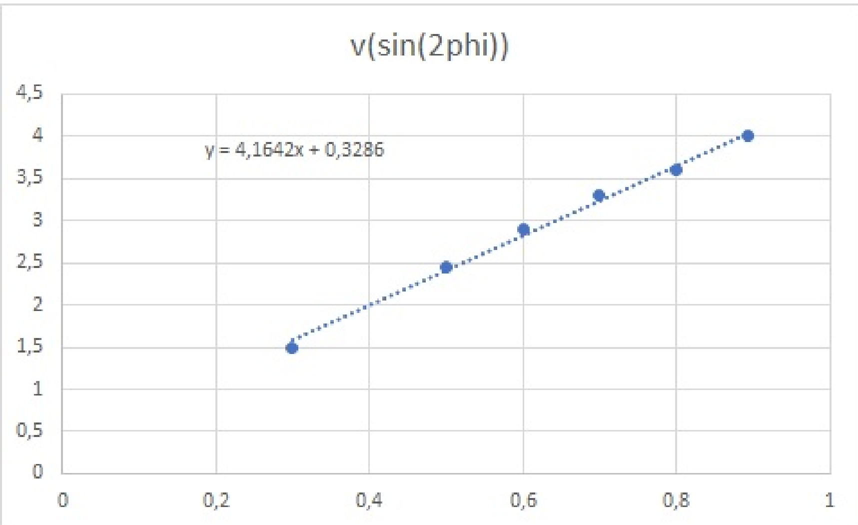


Its slope is

$$\boxed{\frac{\mathrm{d}v}{\mathrm{d}b} = 42}$$

C4. Plot the graph $v(\sin 2\varphi)$. Its slope is $v_c = 4.2$. At $b = b_{\text{cr}}$ the domain wall velocity becomes critical, so that

$$b_{\text{cr}} = \frac{v_c}{\mathrm{d}v/\mathrm{d}b} = 0.10.$$



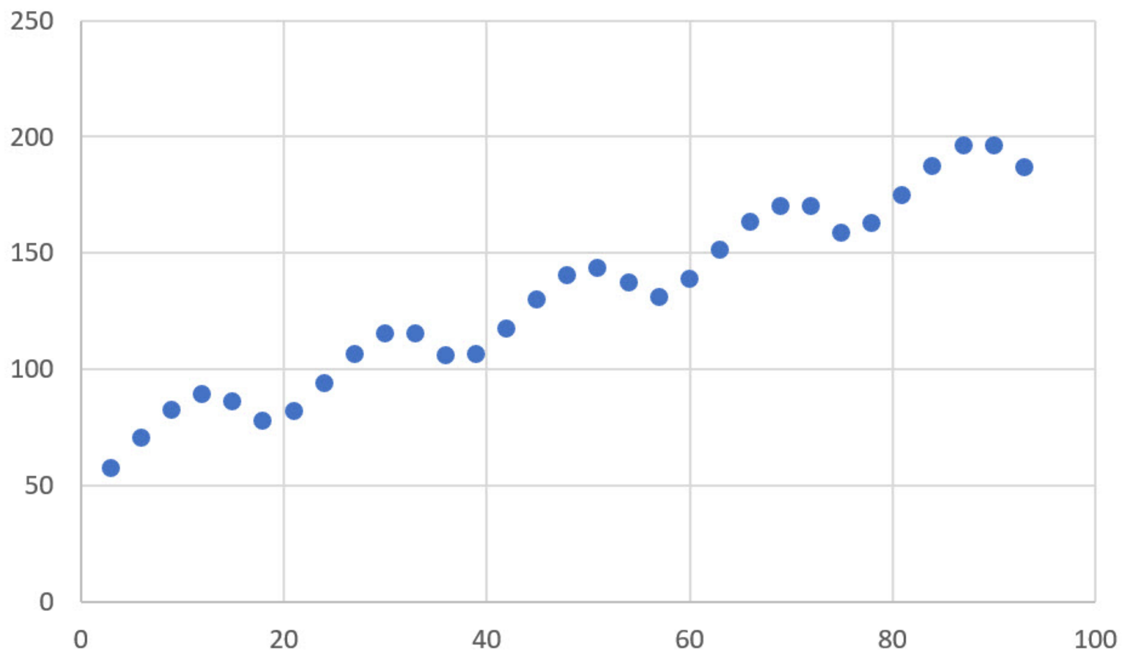
$$\boxed{v_c = 4.2, \qquad b_{\text{cr}} = 0.10}$$

C5. Answer

$$\boxed{v_c = 4.2\, a\omega = 1850\ \text{m/s}; \qquad B_{\text{cr}} = b_{\text{cr}} B_{\text{an}} = 0.083\ \text{T}.}$$

C6. Run the program for $\alpha = 0.2$, $\beta = 100$, $b = 0.2$, $T = 100$, $L = 200$. Plot $m_z(x)$ for $t = 3, 6, 9, 12, \ldots, 90$ and determine x_{center} as an x-coordinate of the intersection of the graph with the x-axis.

t	x_{center}	t	x_{center}	t	x_{center}
3	57.4	33	115.2	63	151.4
6	70.1	36	105.9	66	163.3
9	82.0	39	106.2	69	170.2
12	89.2	42	117.1	72	170.0
15	86.1	45	129.9	75	158.3
18	77.3	48	140.2	78	162.8
21	81.5	51	143.6	81	174.9
24	93.6	54	137.2	84	187.4
27	106.1	57	131.0	87	196.2
30	115.0	60	138.7	90	196.1



The plot $x_{center}(t)$.

Solution

A1. The full energy consists of the potential energy of deformed springs and the kinetic energy of atomic motion, so

$$\boxed{E=\sum_n\left(\frac{k(u_n-v_n)^2}{2}+\frac{\alpha k(u_{n+1}-v_n)^2}{2}+\frac{\beta k(u_{n+1}-u_n)^2}{2}+\frac{\beta k(v_{n+1}-v_n)^2}{2}+\frac{m\dot u_n^2}{2}+\frac{m\dot v_n^2}{2}\right)}$$

A2. Differentiating the energy expression, we obtain

$$\dot E=\sum_n\Big(k(u_n-v_n)(\dot u_n-\dot v_n)+\alpha k(u_{n+1}-v_n)(\dot u_{n+1}-\dot v_n)+\beta k(u_{n+1}-u_n)(\dot u_{n+1}-\dot u_n)$$
$$+\beta k(v_{n+1}-v_n)(\dot v_{n+1}-\dot v_n)+m\dot u_n\ddot u_n+m\dot v_n\ddot v_n\Big).$$

Grouping the terms containing $\dot v_n$ and $\dot u_n$

$$\dot E=\sum_n\Big(\dot v_n(m\ddot v_n+kv_n(\alpha+1+2\beta)-ku_n-\alpha ku_{n+1}-\beta k(v_{n-1}+v_{n+1}))$$
$$+\dot u_n(m\ddot u_n+ku_n(\alpha+1+2\beta)-kv_n-\alpha kv_{n-1}-\beta k(u_{n-1}+u_{n+1}))\Big).$$

Here we used that

$$\sum_n\dot v_{n+1}(v_{n+1}-v_n)=\sum_n\dot v_n(v_n-v_{n-1}),\qquad\sum_n\dot u_{n+1}(u_{n+1}-v_n)=\sum_n\dot u_n(u_n-v_{n-1}),$$

and

$$\sum_n\dot u_{n+1}(u_{n+1}-u_n)=\sum_n\dot u_n(u_n-u_{n-1}).$$

Setting the coefficients A and B to zero leads to the system of differential equations.

$$\boxed{\begin{cases}m\ddot v_n+kv_n(\alpha+1+2\beta)-ku_n-\alpha ku_{n+1}-\beta k(v_{n-1}+v_{n+1})=0,\\ m\ddot u_n+ku_n(\alpha+1+2\beta)-kv_n-\alpha kv_{n-1}-\beta k(u_{n-1}+u_{n+1})=0.\end{cases}}$$

We recognize that the derived equations describe Newtonian dynamics of the two atoms in the unit cell.

A3. Using $u_n(t)=U\cdot\exp\left(-i\omega t+iqn\right),v_n(t)=V\cdot\exp\left(-i\omega t+iqn\right)$ we obtain expressions for the second time derivatives of the displacements

$$\ddot u_n(t)=-\omega^2U\cdot\exp\left(-i\omega t+iqn\right),\quad\ddot v_n(t)=-\omega^2V\cdot\exp\left(-i\omega t+iqn\right).$$

Substituting these expressions into system from A2 and dividing by $\exp\left(-i\omega t+iqn\right)$. We obtain

$$\begin{cases}-\omega^2mV+kV(\alpha+1+2\beta)-kU-\alpha kU\exp(iq)-\beta kV(\exp(-iq)+\exp(iq))=0,\\ -\omega^2mU+kU(\alpha+1+2\beta)-kV-\alpha kV\exp(-iq)-\beta kU(\exp(-iq)+\exp(iq))=0.\end{cases}$$

After regrouping the terms, the system takes the required form

$$\begin{cases}k(1+\alpha\exp(iq))\cdot U+(\omega^2m-k(\alpha+1+2\beta)+\beta k(\exp(-iq)+\exp(iq)))\cdot V=0,\\ (\omega^2m-k(\alpha+1+2\beta)+\beta k(\exp(-iq)+\exp(iq)))\cdot U+k(1+\alpha\exp(iq))\cdot V=0.\end{cases}$$

Using Euler's formula, we find that $\exp(-iq) + \exp(iq) = 2\cos q$. The system transforms to

$$\boxed{\begin{cases} k(1+\alpha\exp(iq))\cdot U + (\omega^2 m - k(\alpha+1+2\beta) + 2\beta k\cos q)\cdot V = 0, \\ (\omega^2 m - k(\alpha+1+2\beta) + 2\beta k\cos q)\cdot U + k(1+\alpha\exp(-iq))\cdot V = 0. \end{cases}}$$

A4. If a phonon can propagate in the chain, then non-trivial solutions to system $A3$ exist which implies the condition $ad - bc = 0$. Therefore

$$k^2(1+\alpha\exp(iq))(1+\alpha\exp(-iq)) = (\omega^2 m - k(\alpha+1+2\beta) + 2\beta k\cos q)^2.$$

The direct consequence of Euler's formula is

$$(1+\alpha\exp(iq))(1+\alpha\exp(-iq)) = 1+\alpha^2+\alpha(\exp(iq)+\exp(-iq)) = 1+2\alpha\cos q+\alpha^2.$$

Substitute this into the original equation and divide by k^2, hence we obtain

$$1+2\alpha\cos q+\alpha^2 = \left(\frac{\omega^2}{\omega_0^2} - (\alpha+1+2\beta) + 2\beta\cos q\right)^2.$$

Therefore

$$\pm\sqrt{1+2\alpha\cos q+\alpha^2} = \frac{\omega^2}{\omega_0^2} - (\alpha+1+2\beta) + 2\beta\cos q,$$

and the dispersion relation takes the form

$$\boxed{\frac{\omega}{\omega_0} = \sqrt{\pm\sqrt{1+2\alpha\cos q+\alpha^2} - 2\beta\cos q + \alpha + 1 + 2\beta}}$$

A5. For $q \to 0$ the approximation $\cos q \simeq 1 - \frac{q^2}{2}$ holds. The dispersion relation takes the form

$$\frac{\omega}{\omega_0} \simeq \sqrt{\pm\sqrt{1+2\alpha-\alpha q^2+\alpha^2} + \beta q^2 + \alpha + 1} = \sqrt{(1+\alpha)\left(\pm\sqrt{1-\frac{\alpha q^2}{(1+\alpha)^2}} + \frac{\beta q^2}{1+\alpha} + 1\right)}.$$

Expanding the square root in a Taylor series

$$\frac{\omega}{\omega_0} \simeq \sqrt{(1+\alpha)\left(\pm\left(1-\frac{\alpha q^2}{2(1+\alpha)^2}\right) + \frac{\beta q^2}{1+\alpha} + 1\right)}.$$

Next, we examine the first phonon solution

$$\left(\frac{\omega}{\omega_0}\right)_1 \simeq \sqrt{\frac{\alpha q^2}{2(1+\alpha)} + \beta q^2}.$$

$$\boxed{\left(\frac{\omega}{\omega_0}\right)_1 \simeq |q|\sqrt{\frac{\alpha}{2(1+\alpha)} + \beta}}$$

For the second phonon

$$\frac{\omega}{\omega_0} \simeq \sqrt{2(1+\alpha)\left(1-\frac{\alpha q^2}{4(1+\alpha)^2} + \frac{\beta q^2}{2(1+\alpha)}\right)}.$$

Again, we expand the square root in a Taylor series

$$\boxed{\left(\frac{\omega}{\omega_0}\right)_2 \simeq \sqrt{2(1+\alpha)}\left(1+\frac{1}{4}\left(\frac{\beta}{1+\alpha}-\frac{\alpha}{2(1+\alpha)^2}\right)q^2\right)}$$

A6. Using the variable $p = q - \pi$. The dispersion relation takes the form

$$\frac{\omega}{\omega_0} \simeq \sqrt{\alpha+1+4\beta-\beta p^2 \pm \sqrt{1-2\alpha+\alpha p^2+\alpha^2}} = \sqrt{\alpha+1+4\beta-\beta p^2 \pm (1-\alpha)\sqrt{1+\frac{\alpha p^2}{(1-\alpha)^2}}}.$$

Therefore, for the acoustic phonon

$$\frac{\omega}{\omega_0} \simeq \sqrt{2\alpha+4\beta-\left(\beta+\frac{\alpha}{2(1-\alpha)}\right)p^2} = \sqrt{2\alpha+4\beta}\sqrt{1-\frac{1}{2(\alpha+2\beta)}\left(\beta+\frac{\alpha}{2(1-\alpha)}\right)p^2}.$$

Again, we expand the square root in a Taylor series

$$\boxed{\left(\frac{\omega}{\omega_0}\right)_1 \simeq \sqrt{2\alpha+4\beta}\left(1-\frac{1}{4(\alpha+2\beta)}\left(\beta+\frac{\alpha}{2(1-\alpha)}\right)p^2\right)}$$

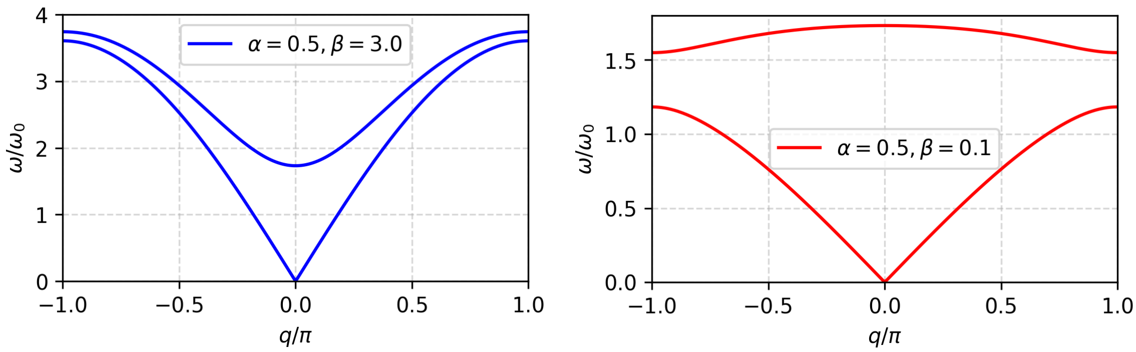
For the optical phonon:

$$\frac{\omega}{\omega_0} \simeq \sqrt{2+4\beta-\left(\beta-\frac{\alpha}{2(1-\alpha)}\right)p^2} \simeq \sqrt{2+4\beta}\sqrt{1-\frac{1}{2(1+2\beta)}\left(\beta-\frac{\alpha}{2(1-\alpha)}\right)p^2}.$$

Again, we expand the square root in a Taylor series

$$\boxed{\left(\frac{\omega}{\omega_0}\right)_2 \simeq \sqrt{2+4\beta}\left(1-\frac{1}{4(1+2\beta)}\left(\beta-\frac{\alpha}{2(1-\alpha)}\right)p^2\right)}$$

A7.



B1. Substituting the solutions in the form of plane waves, we obtain

$$u_n^{\Sigma} = \mu u_n + \eta \tilde{u}_n = U\exp(-i\omega t)\left(\mu\exp(iqn)+\eta\exp(-iqn)\right),$$

and similarly

$$v_n^{\Sigma} = \mu v_n + \eta \tilde{v}_n = V\exp(-i\omega t)\left(\mu\exp(iqn)+\eta\exp(-iqn)\right).$$

The conditions $u_0^{\Sigma}=0$ and $v_0^{\Sigma}=0$ turn out to be equivalent to each other, just as the conditions $u_N^{\Sigma}=0$ and $v_N^{\Sigma}=0$ are. Thus,

$$\boxed{\begin{cases}\mu+\eta=0,\\ \mu\exp(iqN)+\eta\exp(-iqN)=0.\end{cases}}$$

B2. To answer this question, one can use the technique described in part A of this problem. However, it is simpler to substitute $\eta = -\mu$ from the first equation into the second and divide by μ, taking into account the existence of a nontrivial solution. We obtain $\exp(iqN) = \exp(-iqN)$, which is equivalent to $\exp(2iqN) = 1$, i.e., $2qN = 2\pi l$, $l \in \mathbb{Z}$. Note that at $q = 0$ the phonon amplitude becomes zero, so $l = 0$ must be excluded from the answer.

$$\boxed{q = \frac{\pi l}{N}, \quad l \in \mathbb{Z}, l \neq 0}$$

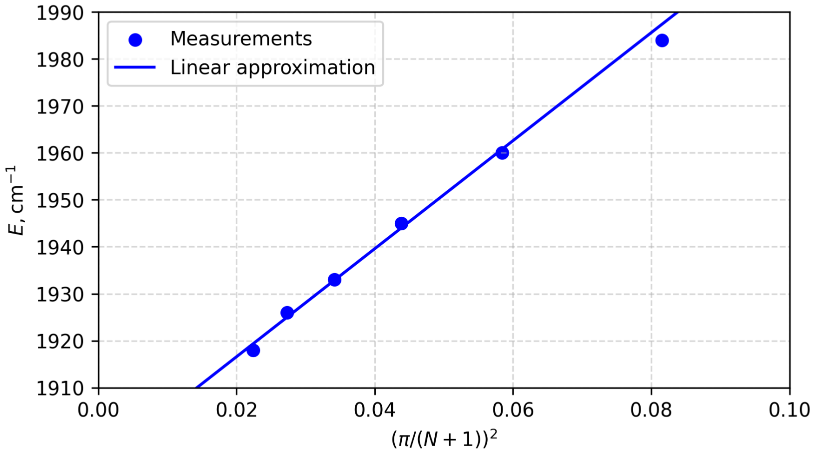
B3. From the condition, it follows that the quasimomentum q can be expressed as $q = \frac{\pi l}{N+1}$, $l \in \mathbb{Z}$ (since after applying the described technique, the chain contains $N + 2$ unit cells). The low-energy phonon corresponds to the minimum absolute value of quasimomentum, i.e., $q = \frac{\pi}{N+1}$.

Using the provided experimental plot, we extract the dependence of the low-energy phonon's energy on N. We employ the Taylor series expansion of ω/ω_0 near the point $q = 0$. Thus,

$$\frac{\omega}{\omega_0} \simeq \sqrt{2(1+\alpha)} \left(1 + \left(\frac{\beta}{4(1+\alpha)} - \frac{\alpha}{8(\alpha+1)^2}\right)\left(\frac{\pi}{N+1}\right)^2\right).$$

N	E, cm^{-1}	$\pi^2/(N+1)^2$
20	1918	0.0224
18	1926	0.0273
16	1933	0.0341
14	1945	0.0439
12	1960	0.0584
10	1984	0.0816

Let's plot the dependence $E\,(x = (\pi/(N+1))^2)$. As theoretically expected, it turned out to be linear. From the plot, we find the equation of the approximating line $E = (1150x + 1900)\,(\text{cm}^{-1})$.



From the above, we obtain the system of equations

$$\begin{cases} 1150\ \text{cm}^{-1} = \hbar\omega_0\sqrt{2(1+\alpha)}\left(\dfrac{\beta}{4(1+\alpha)} - \dfrac{\alpha}{8(\alpha+1)^2}\right), \\ 1900\ \text{cm}^{-1} = \hbar\omega_0\sqrt{2(1+\alpha)}. \end{cases}$$

Solving this system yields

$$\alpha = 0.204, \quad \omega_0 = 2.31 \cdot 10^{14}\ \text{s}^{-1}.$$

Given that $\omega_0 = \sqrt{\dfrac{k}{m}}$, we find

$$k = \omega_0^2 m = 1.06 \cdot 10^3\ \text{N/m}.$$

$$\boxed{\alpha k = 216\ \text{N/m}, \quad k = 1.06 \cdot 10^3\ \text{N/m}}$$

Solution

A1. According to the capacitor energy formula

$$W = \frac{(ne)^2}{2C} \quad \Rightarrow \quad \Delta W = \frac{e^2}{2C} \cdot \left((n+1)^2 - n^2\right).$$

$$\boxed{\Delta W = \frac{e^2}{C}(n + 1/2)}$$

A2. The sum of charges on the capacitor plates is determined by the number n of electrons on the island. The sum of voltages across the capacitors is determined by the voltage source.

By writing the charge conservation law and the sum of voltage drops, we obtain:

$$\begin{cases} q_j - q_g = -ne, \\ V = \dfrac{q_j}{C_j} + \dfrac{q_g}{C_g}. \end{cases}$$

If $C = C_j + C_g$, then after transformations the required expressions are obtained.

$$\boxed{\begin{cases} q_g = \dfrac{C_g}{C} \cdot (VC_j + ne) \\ q_j = \dfrac{C_j}{C} \cdot (VC_g - ne) \end{cases}}$$

A3. The total energy of the system:

$$W_n = \frac{q_g^2}{2C_g} + \frac{q_j^2}{2C_j} = \frac{VC_jC_g + n^2e^2}{2C}.$$

When the number of electrons on the island changes $n \to n + 1$:

$$W_{n+1} = \frac{q_g^2}{2C_g} + \frac{q_j^2}{2C_j} = \frac{VC_jC_g + (n+1)^2e^2}{2C}.$$

The energy increment is $\Delta W = W_{n+1} - W_n = \frac{e^2}{C}(n + 1/2)$.

$$\boxed{\Delta W = \frac{e^2}{C}(n + 1/2)}$$

A4. The work done by the source equals the product of its voltage and the amount of charge that has flowed through it. The amount of charge that has flowed through the source equals the change in the gate charge Δq_g, therefore the source work is:

$$A = V\Delta q_g.$$

According to task A2 $\Delta q_g = eC_g/C$, which gives the answer for the source work.

$$\boxed{A = \frac{C_g}{C}eV}$$

The heat losses are determined by the energy conservation law:

$$Q = A - \Delta W,$$

from which, according to task A2, we obtain the answer.

$$\boxed{Q = \frac{e}{C}\left[VC_g - e(n+1/2)\right]}$$

A5. The amount of heat released by the resistor equals the product of the resistor voltage and the charge that has passed through it:

$$Q = I_t R_t e$$

Using the expression for Q from point A4, we obtain

$$I_t = \frac{VC_g - e(n+1/2)}{CR_t}$$

Tunneling is possible when $Q = I_t R_t e > 0$, i.e. when $V > \frac{e}{C_g}(n+1/2)$, which gives the condition for n.

$$\boxed{I_t = \frac{VC_g - e(n+1/2)}{CR_t}}$$

$$\boxed{n < \frac{C_g V}{e} - \frac{1}{2}}$$

A6. Differentiating the expression for the gate charge obtained in point A2 with respect to time gives:

$$\dot{q}_g = \frac{C_g}{C}\frac{\Delta n}{\Delta t}e.$$

Taking into account $I = \dot{q}_g$, $I_t = \frac{\Delta n}{\Delta t}e$ we obtain the answer.

$$\boxed{I = \frac{C_g}{C}I_t}$$

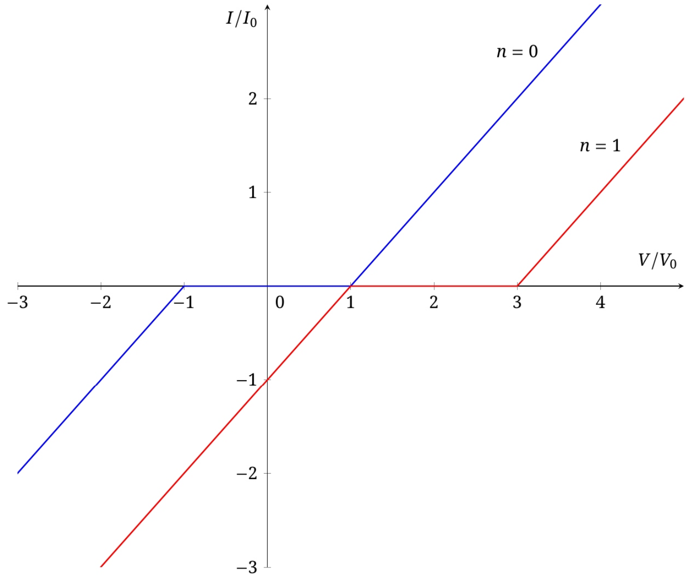
A7. From the two previous tasks:

$$I = \frac{C_g^2}{C^2 R_t}\left[V - \frac{e}{C_g}(n+1/2)\right] \quad \text{if} \quad V > \frac{e}{C_g}(n+1/2).$$

Performing similar calculations for the case of decreasing the number n of electrons on the island leads to the possibility of negative current flow:

$$I = \frac{C_g^2}{C^2 R_t}\left[V - \frac{e}{C_g}(n-1/2)\right] \quad \text{if} \quad V < \frac{e}{C_g}(n-1/2).$$

Outside the specified intervals, tunneling is impossible, meaning $I(V) = 0$. The required graphs are shown in the figure below.



The current-voltage characteristic of the single-electron box: $V_0 = \frac{e}{2C_g}$, $I_0 = \frac{eC_g}{2C^2R_t}$

B1. The sum of charges on the capacitors equals the charge on the island:

$$C_1(\varphi - V_1) + C_2(\varphi - V_2) + C_g(\varphi - V_g) = -ne.$$

Substituting the expressions for V_1, V_2, we obtain the answer.

$$\boxed{\varphi = \frac{(C_1 - C_2)V/2 + C_gV_g - ne}{C_1 + C_2 + C_g}}$$

B2. First, we express the changes in charges on the capacitor plates when the number of electrons on the island changes:

$$q_1 = C_1(\varphi - V_1) = \frac{C_1}{C}\left[(C_1 - C)V_1 + C_2V_2 + C_gV_g - ne\right]$$

$$\Delta q_1 = -\frac{eC_1}{C}\Delta n.$$

Here and hereafter in part B $C = C_1 + C_2 + C_g$. Similarly

$$\Delta q_2 = -\frac{eC_2}{C}\Delta n, \qquad \Delta q_g = -\frac{eC_g}{C}\Delta n.$$

The work done by the sources is determined by the charge flowing through them. For the branch where tunneling occurs, one must account for the transfer of the tunneling charge itself $q_t = -\Delta ne$. Thus, the total work done by the sources in our case takes the form

$$A = -V_1\Delta q_1 - V_2\Delta q_2 - V_g\Delta q_g + V_1 q_t.$$

Substituting the expressions for the charges, we obtain:

$$A = \frac{e\Delta n}{C}\left[V_1(C_1 - C) + V_2C_2 + V_gC_g\right].$$

Taking into account $\Delta n = 1$ and the expressions for V_1, V_2, we write the result.

$$\boxed{A = \frac{e}{C}\left[V_gC_g - V/2\,(C_g + 2C_2)\right]}$$

B3. The total energy of the system

$$W_n = \frac{C_1}{2}(\varphi - V_1)^2 + \frac{C_2}{2}(\varphi - V_2)^2 + \frac{C_g}{2}(\varphi - V_g)^2$$

after substituting the expression for the island potential φ and simplification takes the form

$$W_n = \frac{(ne)^2}{2C} + W_0,$$

where W_0 is a term independent of the number n of electrons on the island.

Then the energy increment resulting from tunneling of one electron

$$\Delta W_n = \frac{e^2}{2C}((\Delta n)^2 + 2n\Delta n) = \frac{e^2}{C}\left(\frac{1}{2} \pm n\right),$$

where the $+$ sign corresponds to an increase in the number of electrons on the island.

The amount of heat released is determined from the energy conservation law:

$$Q = A - \Delta W_n = \pm\frac{e}{C}\left[V_1(C_1 - C) + V_2C_2 + V_gC_g - e(n \pm 1/2)\right].$$

Considering the case of increasing the number of electrons, we obtain the answer.

$$\boxed{Q = \frac{e}{C}\left[V_gC_g - V/2\,(C_g + 2C_2) - e(n + 1/2)\right]}$$

B4. Taking into account the expressions for V_1, V_2, we obtain the following for the heat released in the circuit:

$$Q = \pm\frac{e}{C}\left[V_gC_g - V/2\,(C_g + 2C_2) - e(n \pm 1/2)\right],$$

where the $+$ sign still corresponds to an increase in the number of electrons on the island.

From the inequality $Q > 0$ for the upper signs we obtain:

$$\boxed{V < \frac{V_gC_g - e(n + 1/2)}{C_2 + C_g/2}}$$

B5. For electron tunneling from the island through the first junction we obtain:

$$V > \frac{V_gC_g - e(n - 1/2)}{C_2 + C_g/2}.$$

In the case of tunneling through the second junction, we replace $V \to -V, C_1 \to C_2$ in the expression for the released heat and obtain the condition:

$$Q = \pm\frac{e}{C}\left[V_gC_g + V/2\,(C_g + 2C_2) - e(n \pm 1/2)\right] > 0.$$

From this, for tunneling onto the island we obtain the inequality

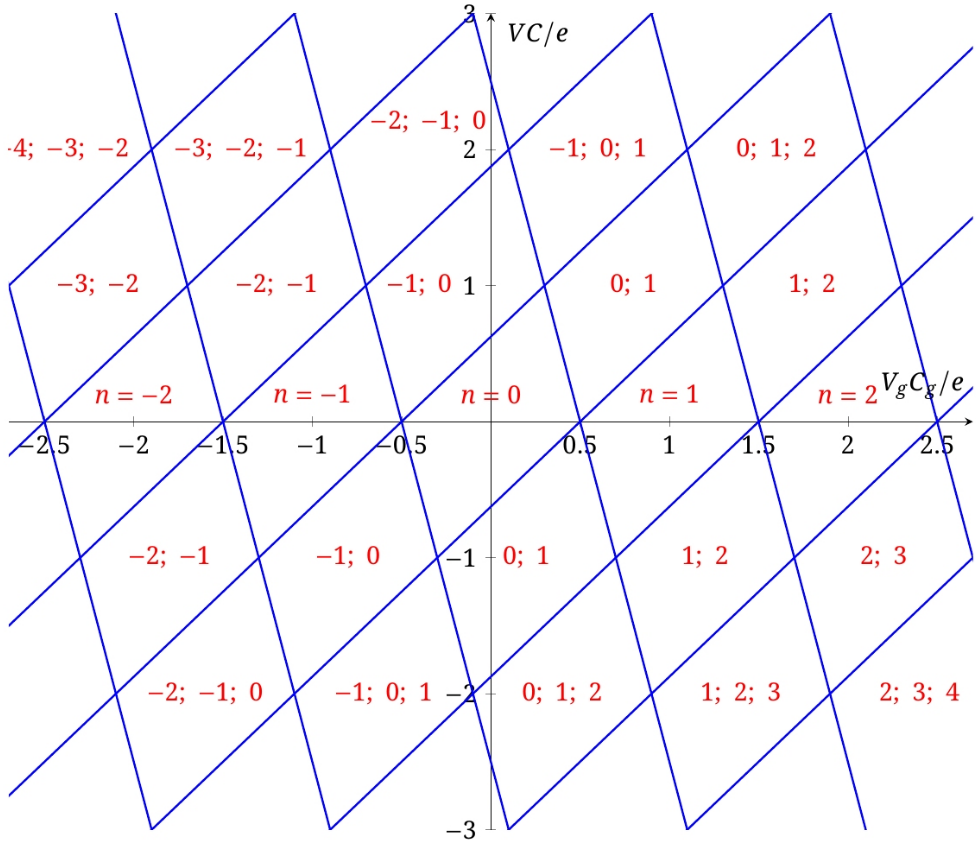
$$V > -\frac{V_gC_g - e(n + 1/2)}{C_1 + C_g/2}.$$

For tunneling from the island:

$$V < -\frac{V_gC_g - e(n - 1/2)}{C_1 + C_g/2}.$$

Thus, in the coordinates V, V_g the regions of possible tunneling are separated by two families of straight lines: with slope coefficients $k_1 = \frac{C_g}{C_2+C_g/2}$ and $k_2 = -\frac{C_g}{C_1+C_g/2}$.

Each region forms a parallelogram. The parallelograms containing the abscissa axis correspond to a single equilibrium number n. These regions represent Coulomb blockade — the impossibility of current flow through the transistor. In other regions, the resistance becomes finite, and current can flow.



The V, V_g voltage diagram of the transistor

B6. Positive current corresponds to tunneling from the second bank to the island, and then from the island to the first bank. Let us consider both these processes and use the equality $Q_\alpha = I_\alpha R_t e;\ \alpha = 1, 2$ — the tunneling process number:

$$\begin{cases} I_1 R_t e = \dfrac{e}{C}\left[V(C_1 + C_g/2) + V_g C_g - e(n + 1/2)\right], \\ I_2 R_t e = -\dfrac{e}{C}\left[-V(C_2 + C_g/2) + V_g C_g - e(n + 1 - 1/2)\right]. \end{cases}$$

For the total current flowing through the transistor, determined by the total tunneling time across both junctions, we obtain $I = (I_1^{-1} + I_2^{-1})^{-1}$. Introducing the quantity $Q_g = V_g C_g - e\bar{n}$, where $\bar{n} = (n + (n+1))/2$ is the average number of electrons on the island, then after simplification the dependence takes the form:

$$I(V, Q_g) = \frac{C^2 V^2/4 - Q_g^2}{V C^2 R_t}.$$

Particularly for $n = 0, \bar{n} = 1/2$, we obtain the required dependence.

$$\boxed{I(V, V_g) = \frac{1}{4R_t}\left[V - \frac{4}{VC^2}\left(C_g V_g - e/2\right)^2\right]}$$

C1. The graph clearly shows the "Coulomb diamonds" obtained in the task B5. The measurement of period ΔV_g allows determination of the gate capacitance, while the maximum voltage $V_{\max}$ gives the total capacitance. From the graph $\Delta V_g = 7$ mV, $V_{\max} = 0.4$ mV. Hence $C_g = e/\Delta V_g = 23$ aF, $C = e/V_{\max} = 400$ aF, $C_1 = C_2 = (C - C_g)/2 = 190$ aF.

$$\boxed{C_1 = C_2 = 190 \text{ aF}}$$

$$\boxed{C_g = 23 \text{ aF}}$$

C2. The change in probability of having n electrons on the island is related to possible processes $n+1 \to n$ and $n-1 \to n$ that increase this probability, as well as reverse processes that decrease it:

$$\boxed{\mathrm{d}p(n)/\mathrm{d}t = p(n-1)\cdot\Gamma_{n-1\to n} + p(n+1)\cdot\Gamma_{n+1\to n} - p(n)\cdot(\Gamma_{n\to n-1} + \Gamma_{n\to n+1})}$$

C3. From the previous point it is known that for arbitrary n the following holds:

$$p(n-1)\cdot\Gamma_{n-1\to n} - p(n)\cdot\Gamma_{n\to n-1} = p(n)\cdot\Gamma_{n\to n+1} - p(n+1)\cdot\Gamma_{n+1\to n}.$$

Taking into account the definition of n_0:

$$p(n_0-1)\cdot\Gamma_{n_0-1\to n_0} = p(n_0)\cdot\Gamma_{n_0\to n_0-1}.$$

From this it follows that for all n less than n_0, the following holds:

$$p(n-1)\cdot\Gamma_{n-1\to n} = p(n)\cdot\Gamma_{n\to n-1}.$$

Indeed, relations of this type imply vanishing of the left-hand side of the original equality for arbitrary n. Consequently, the right-hand side, corresponding to n differing by unity, also vanishes. This leads to the answer.

$$\boxed{A = \frac{\Gamma_{n\to n+1}}{\Gamma_{n+1\to n}}}$$

C4. The expressions for the released heat were obtained in part B and take the form:

$$Q^{(i)}_{n\to n\pm1} = \pm\frac{e}{C}\left[(-1)^i\, VC/2 + (V_g C_g - e/2) - e(n - 1/2 \pm 1/2)\right].$$

Considering $|V| \ll e/C, |V_g - e/2C_g| \ll e/C_g$, for both tunneling junctions, increasing the number n of electrons when $n > 0$ leads to a negative value of the released heat $|Q_{n\to n\pm1}| > e^2/C \gg kT$. The same inequality occurs when decreasing n for $n < 1$.

Thus, under the specified conditions, a large positive value appears in the exponent, and the unity in the denominator can be neglected. This leads to the required result.

C5. Using the result from point C3:

$$p(0)\cdot\Gamma_{0\to1} = p(1)\cdot\Gamma_{1\to0}$$

Taking into account the normalization condition $p(0) + p(1) = 1$, we express the probabilities $p(0)$ and $p(1)$.

$$\boxed{\begin{cases} p(0) = \dfrac{\Gamma_{1\to0}}{\Gamma_{0\to1} + \Gamma_{1\to0}} \\[2ex] p(1) = \dfrac{\Gamma_{0\to1}}{\Gamma_{0\to1} + \Gamma_{1\to0}} \end{cases}}$$

C6. The current through the transistor is determined by the number of tunnelings through one of the junctions (tunnelings through the other occur such that the number of electrons on the island remains unchanged):

$$I = e\left(p(1)\cdot\Gamma^{(1)}_{1\to 0} - p(0)\cdot\Gamma^{(1)}_{0\to 1}\right) = -e\left(p(1)\cdot\Gamma^{(2)}_{1\to 0} - p(0)\cdot\Gamma^{(2)}_{0\to 1}\right).$$

Note that the transition from one expression to another is easily accomplished using

$$p(0)\cdot\Gamma_{0\to 1} = p(1)\cdot\Gamma_{1\to 0}.$$

Substitution of the expressions for probabilities $p(0), p(1)$ leads to the required result.

$$\boxed{I = e\frac{\Gamma^{(2)}_{0\to 1}\Gamma^{(1)}_{1\to 0} - \Gamma^{(1)}_{0\to 1}\Gamma^{(2)}_{1\to 0}}{\Gamma^{(1)}_{0\to 1} + \Gamma^{(2)}_{0\to 1} + \Gamma^{(1)}_{1\to 0} + \Gamma^{(2)}_{1\to 0}}}$$