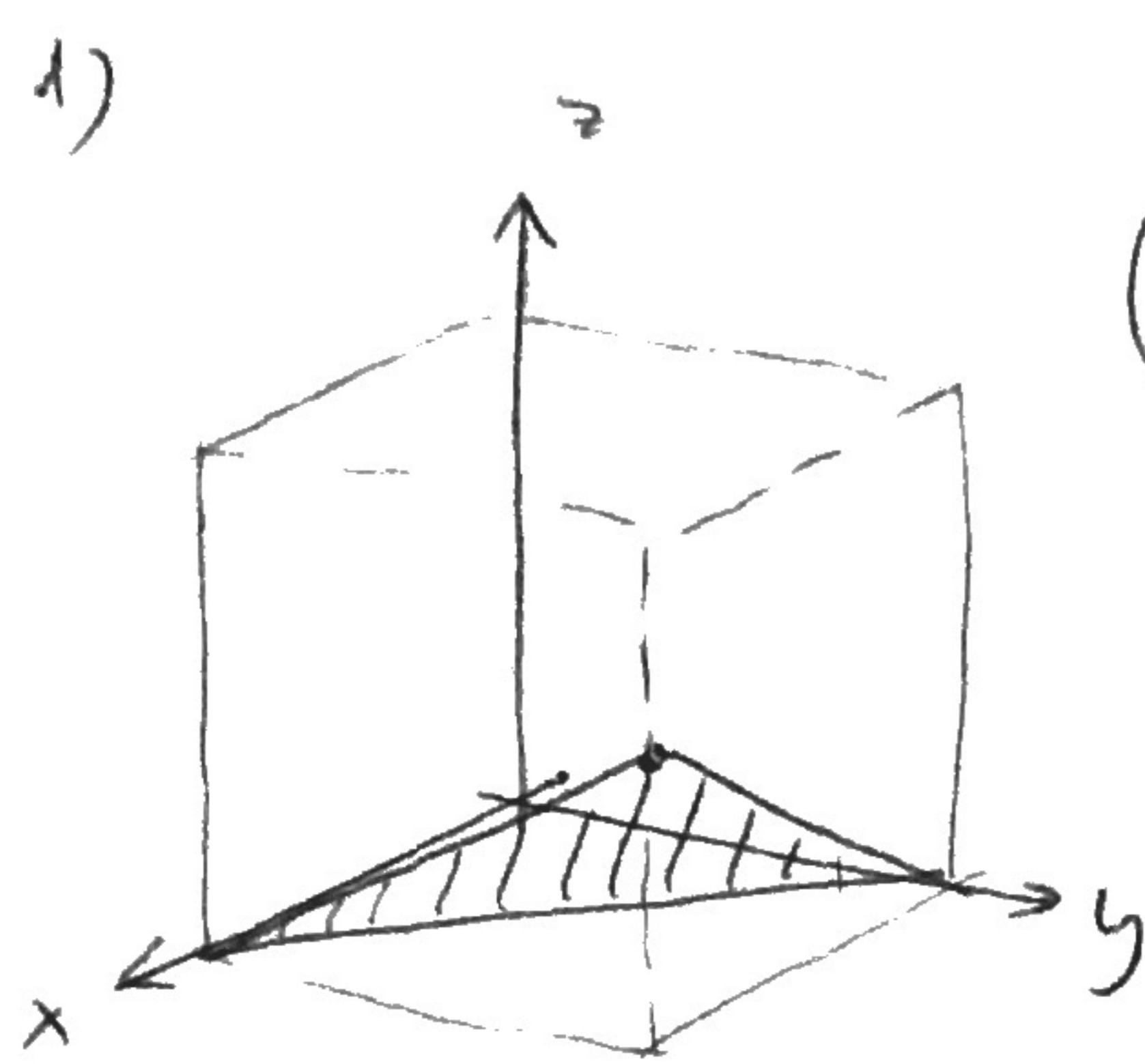
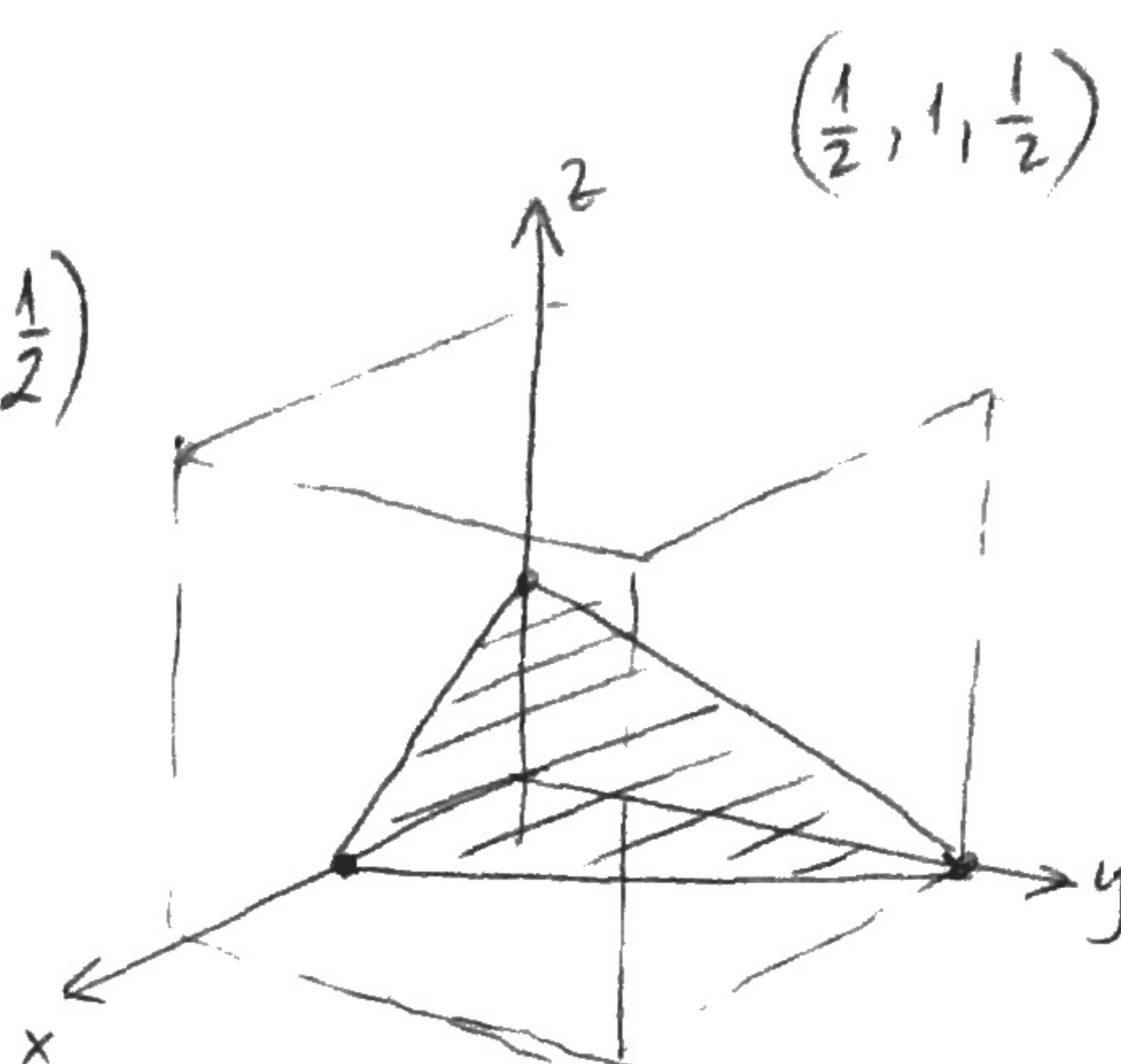


I. pot zárt helyi dologzat.



$$hkl = 1\bar{1}\bar{2}$$

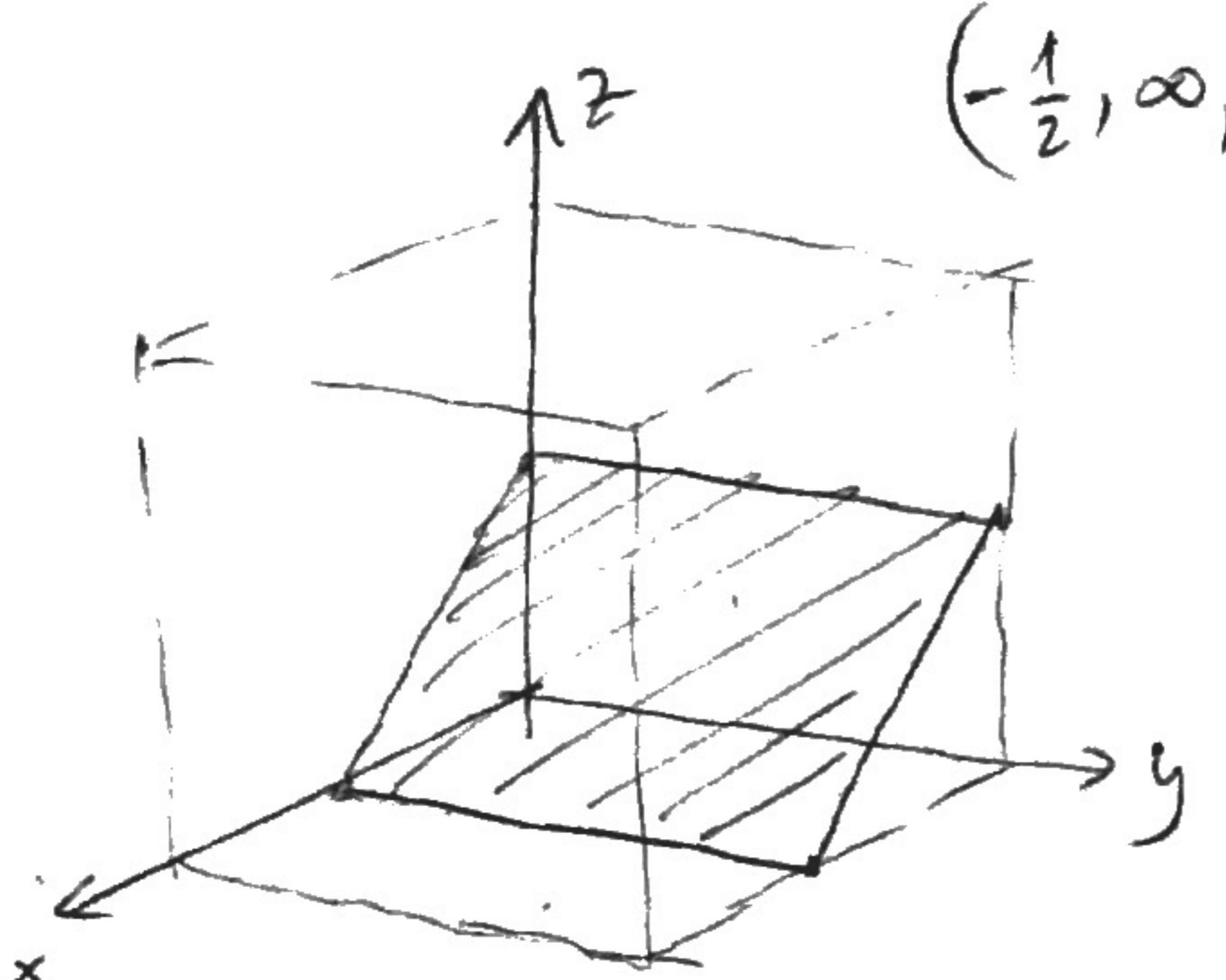
$$\left(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right)$$



$$hkl = 212$$

$$\left(\frac{1}{2}, 1, \frac{1}{2}\right)$$

$$3 \times 6 = 18$$



$$hkl = \bar{2}0\bar{2}$$

$$\left(-\frac{1}{2}, \infty, -\frac{1}{2}\right)$$

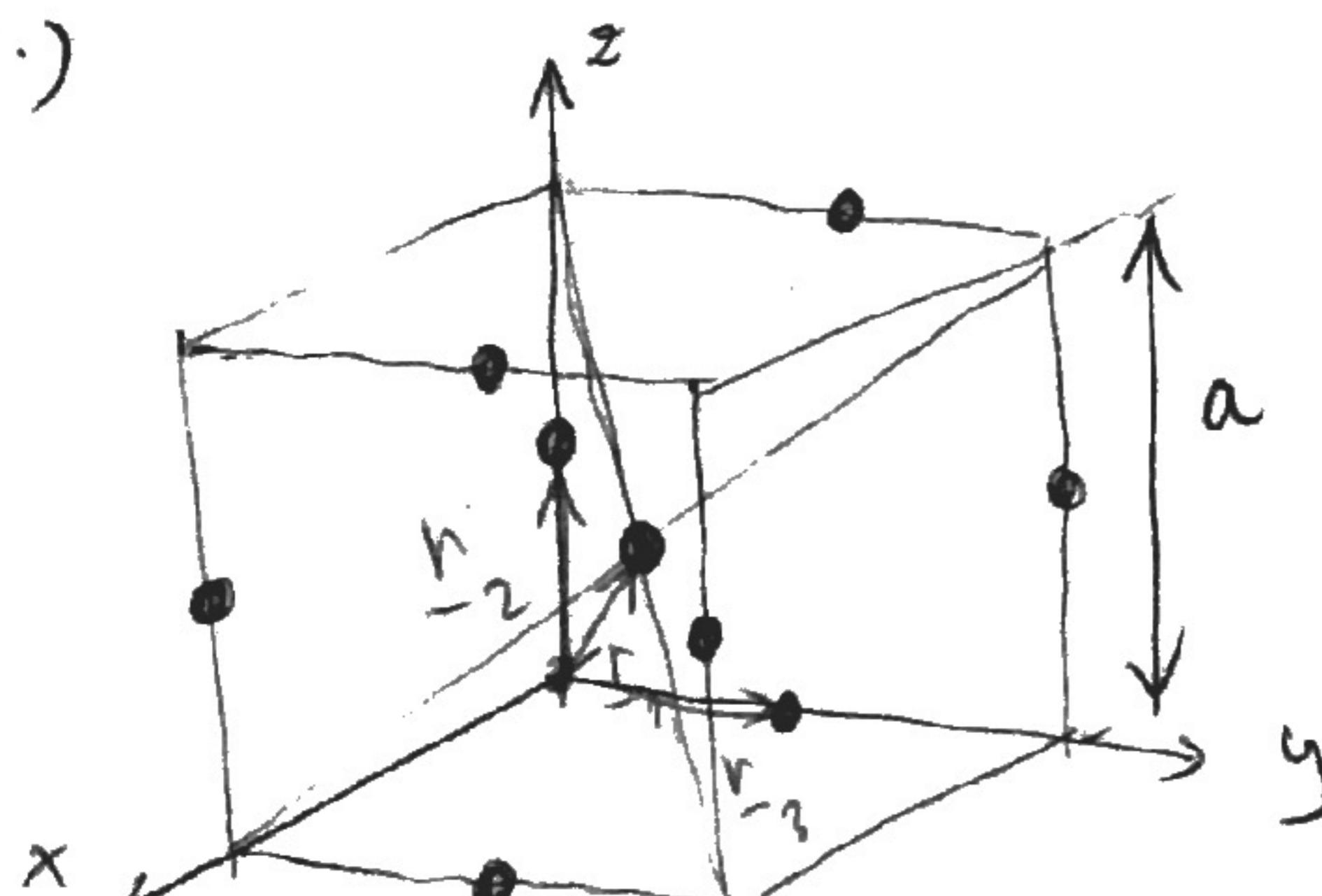
Többi három:

$$hkl = (2\bar{2}1) \rightarrow 1, 2, 1 \rightarrow 1, \frac{1}{2}, 1 \rightarrow \\ a.) \quad \rightarrow (2, 1, 2)$$

$$b.) \quad \infty, 1, -\frac{1}{2} \rightarrow (0, 1, \bar{2})$$

$$c.) \quad +\frac{1}{2}, \frac{1}{2}, -1 \rightarrow (2, 1, \bar{1})$$

2.)



A bázisban lévő atomok száma:

$$\frac{1}{4} \cdot 8 + 1 = 3$$

$$\text{Helyvekterek: } \underline{r}_1 = \left(\frac{a}{2}, \frac{a}{2}, \frac{a}{2}\right)$$

$$\underline{r}_2 = (0, 0, \frac{a}{2})$$

$$\underline{r}_3 = (0, \frac{a}{2}, 0)$$

10, ha jo
a bázis + részhár.

$$S(\underline{k}) = \sum_{\underline{r}} e^{i\underline{k} \cdot \underline{r}}, \text{ itt } \underline{k} = h\underline{b}_1 + k\underline{b}_2 + l\underline{b}_3, \|\underline{b}_i\| = \frac{2\pi}{a}$$

$$S(\underline{k}) = e^{i\pi(h+k+l)} + e^{i\pi l} + e^{i\pi \cdot k} \quad 14 \times 2 = 28 +$$

$$|S(\underline{k})|^2 = 9, \text{ ha } h, k, l \text{ mindenkor paros v. páratlan} \quad 5 \text{ az intenzitás} \\ + 2 \text{ ha null}$$

$$|S(\underline{k})|^2 = 1, \text{ ha egyet...} \quad + 5 \text{ a 2. rész}$$

22.

N	hkl	rel. Intensität
1	100	1/9
2	110	1/9
3	111	1
4	200	1
5	210	1/9
6	211	1/9

N	hkl	rel. Intensität
8	220	1
9	300, 221	1/9
10	301	1/9
11	311	1
12	222	1
13	320	1/9
14	321	1/9

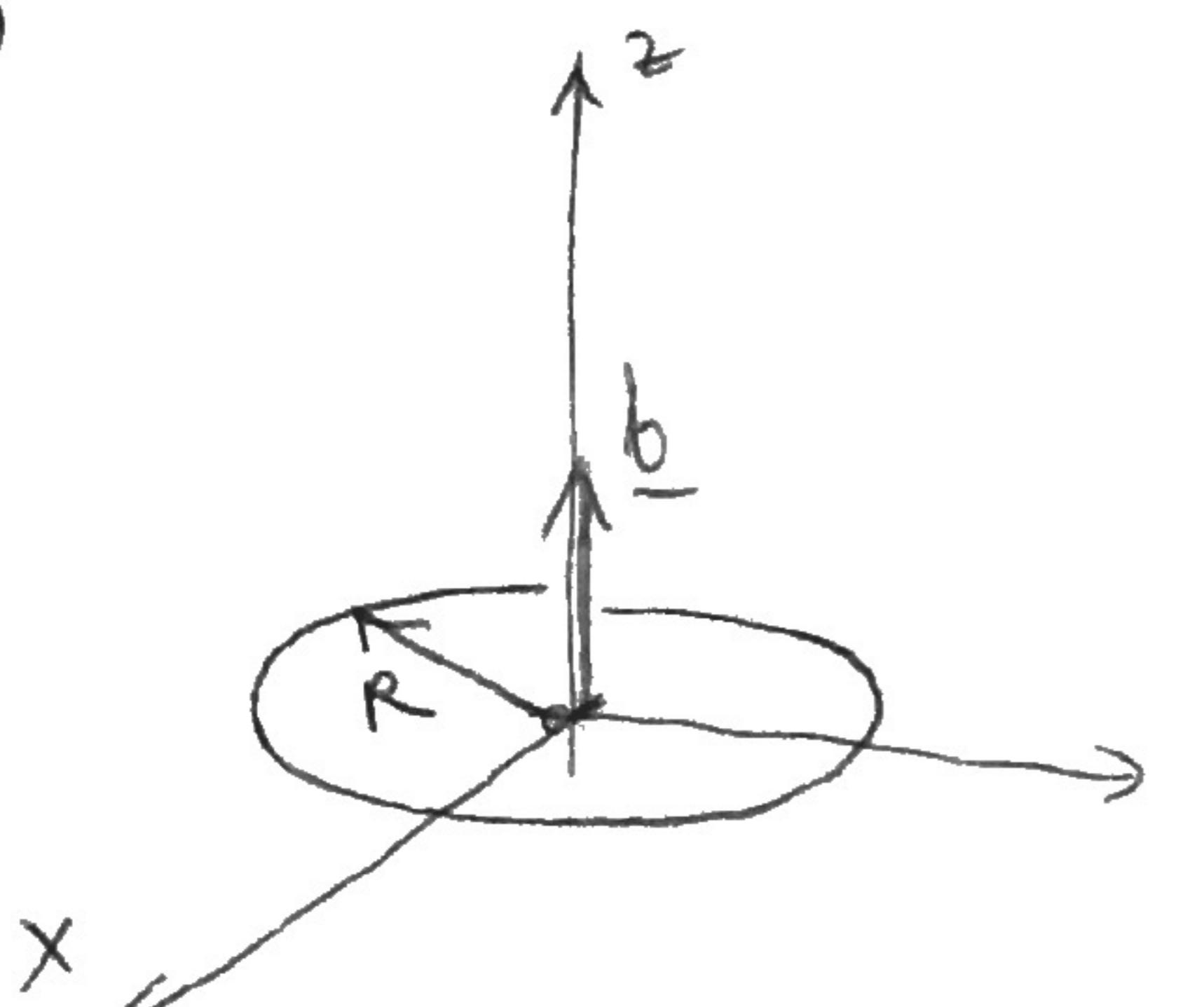
23.

$$2ds \sin\theta = \lambda, \quad d = \frac{a}{\sqrt{h^2+k^2+l^2}} = a$$

$$\left. \begin{array}{l} 2 \\ 2 \\ \end{array} \right\} 2a \sin\theta = \lambda$$

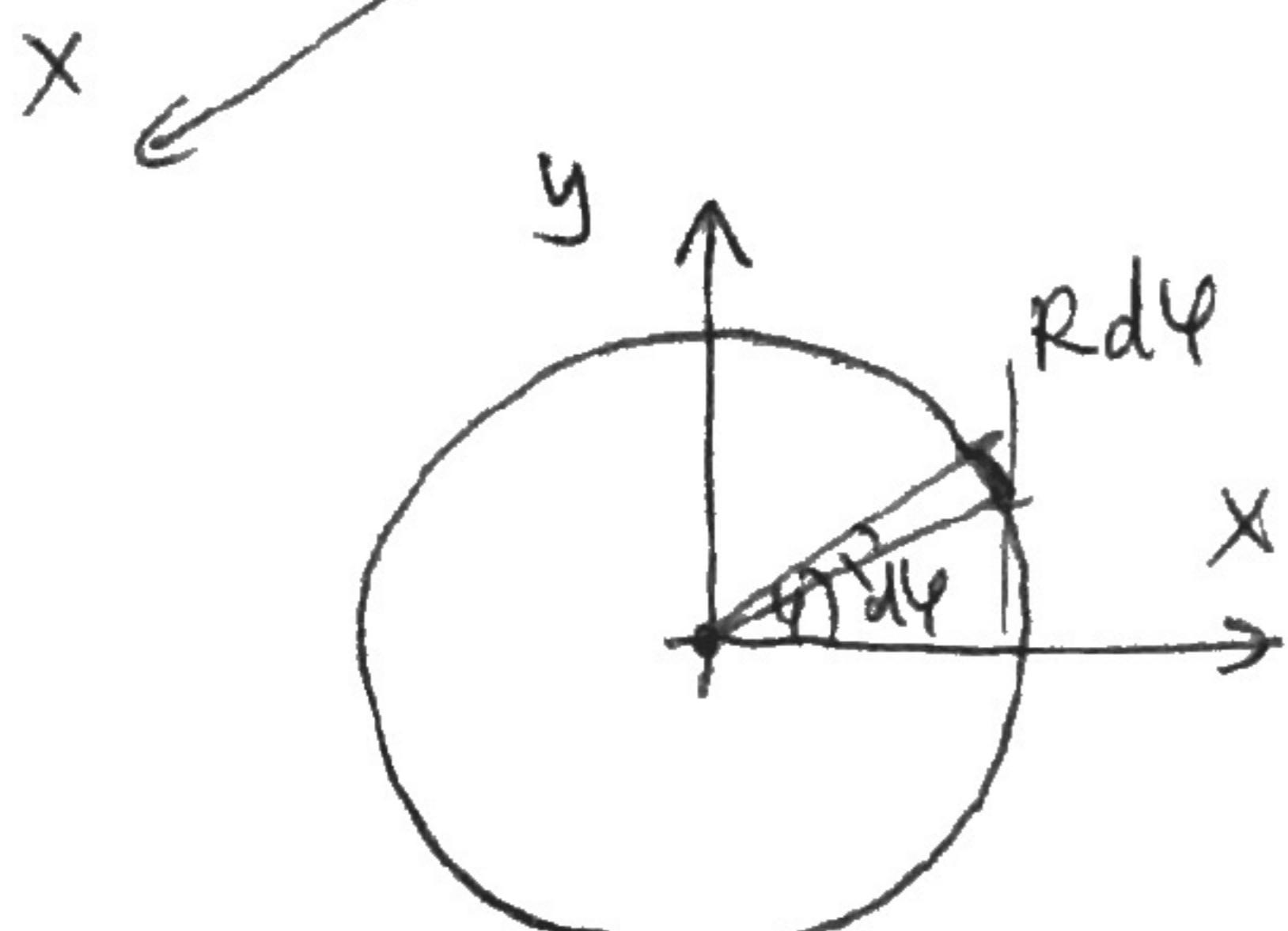
$$a = \frac{\lambda}{2 \sin\theta} = 1,997 \cdot 10^{-10} \text{ m}$$

3.)



$$\underline{b} = (0, 0, b)$$

$$\underline{\underline{b}} = \begin{pmatrix} 0 & 0 & \sigma_0 \\ 0 & 0 & 0 \\ \sigma_0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ b \end{pmatrix} = \begin{pmatrix} \sigma_0 b \\ 0 \\ 0 \end{pmatrix}$$

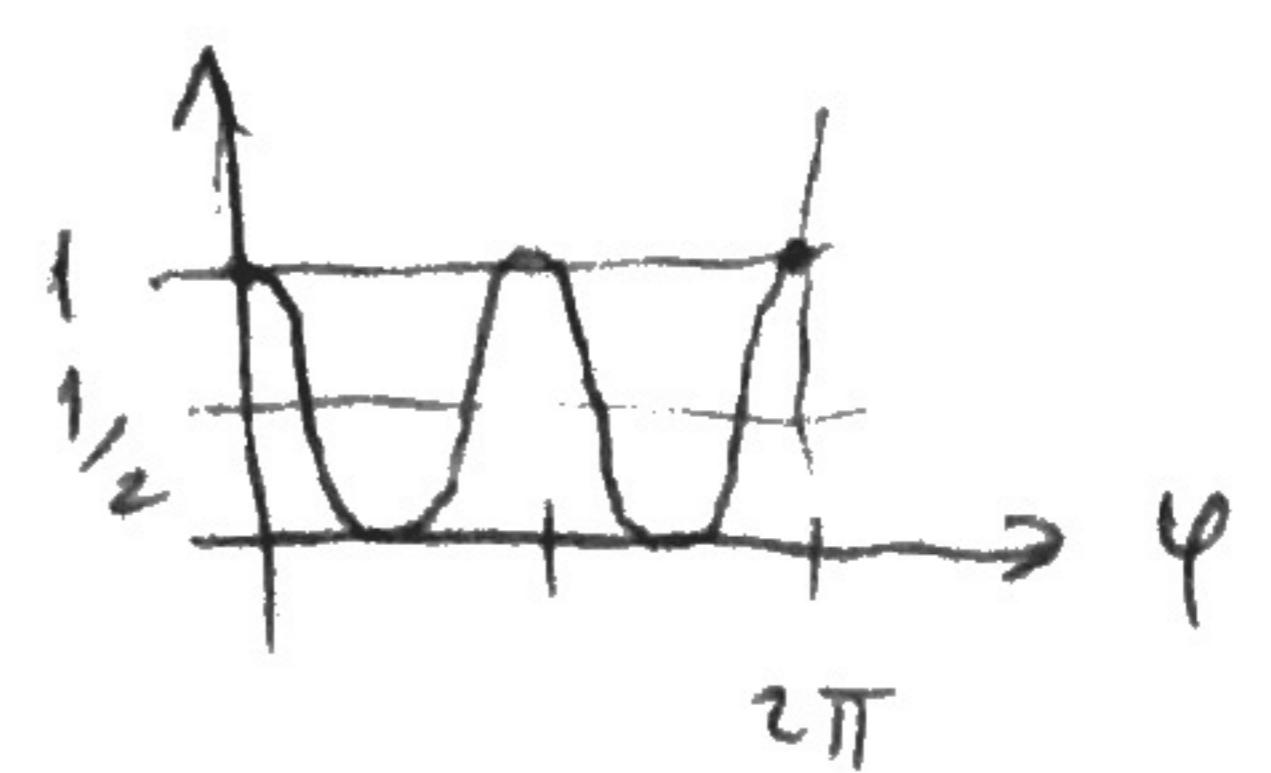


$$\underline{\Delta l} = \begin{pmatrix} -\sin\varphi \\ \cos\varphi \\ 0 \end{pmatrix} R d\varphi$$

$$\underline{\Delta F} = \underline{\Delta l} \times (\underline{\underline{b}}) = \begin{pmatrix} -\sin\varphi \\ \cos\varphi \\ 0 \end{pmatrix} \times \begin{pmatrix} \sigma_0 b \\ 0 \\ 0 \end{pmatrix} R d\varphi$$

$$\underline{dF} = \begin{pmatrix} 0 \\ 0 \\ -\sigma_0 b \cos\varphi \end{pmatrix} R d\varphi$$

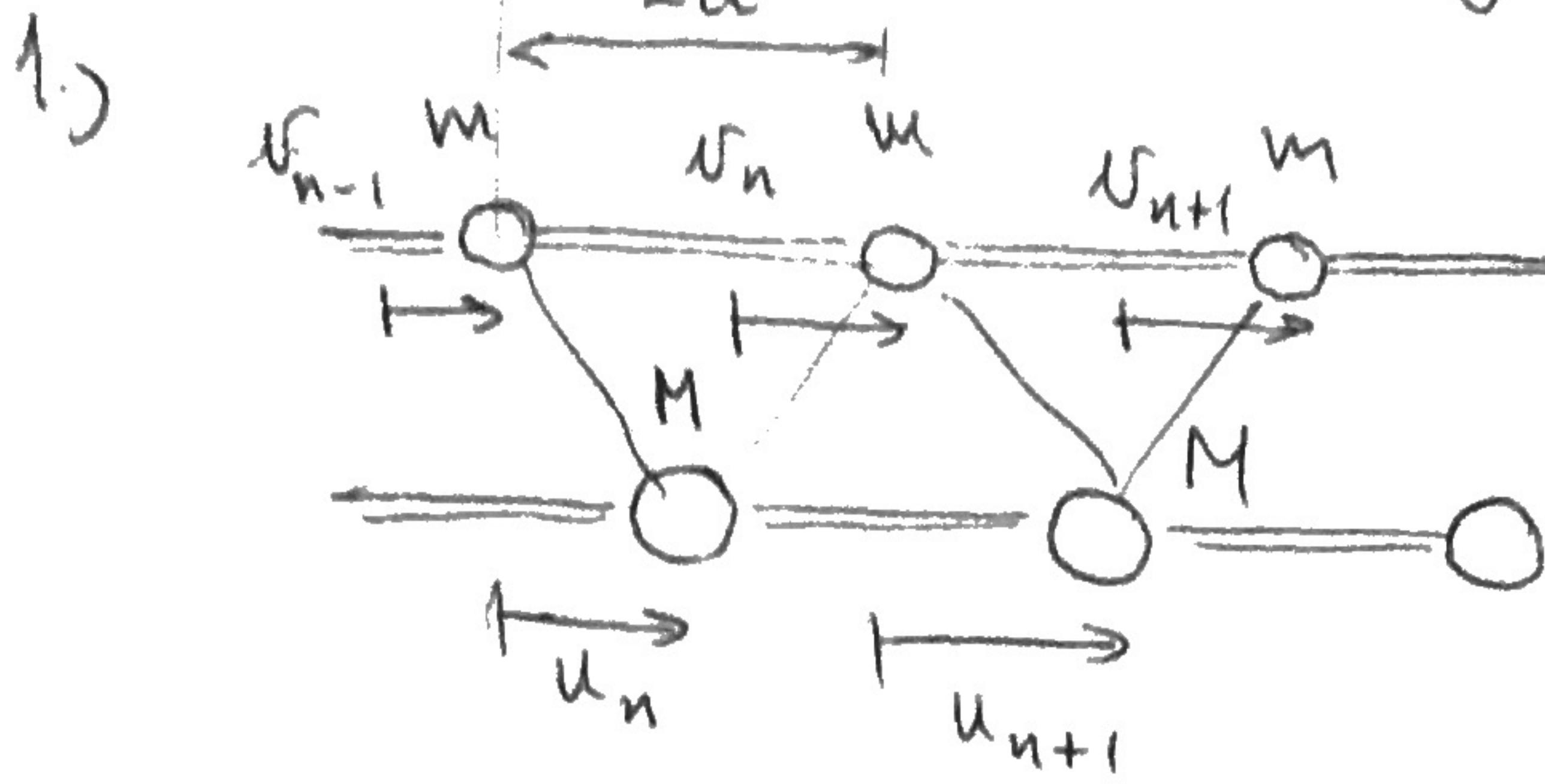
$$\underline{dJ} = \begin{pmatrix} \cos\varphi \\ \sin\varphi \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ -\sigma_0 b \cos\varphi \end{pmatrix} R^2 d\varphi$$



$$\underline{dJ} = \begin{pmatrix} -\sin\varphi \cos\varphi \\ \cos^2\varphi \\ 0 \end{pmatrix} R^2 \sigma_0 b d\varphi \rightarrow \underline{J} = R^2 \sigma_0 b \int_0^{2\pi} \begin{pmatrix} -\frac{1}{2} \sin 2\varphi \\ \cos^2\varphi \\ 0 \end{pmatrix} d\varphi \Rightarrow$$

$$|\underline{J}| = \underline{\underline{R}^2 \sigma_0 b}, \quad \text{, } \cancel{\text{ira y iralogn!}}$$

2. pótzár felügyeleti dolgozat



$$\Delta l = (v_n - u_n) \cdot \frac{1}{\sqrt{2}}$$

$$\cos^2 45^\circ = \frac{1}{2}$$

Mozgásvegyenletek:

$$\left\{ \begin{array}{l} M\ddot{v}_n = -D(v_n - u_n) \cdot \cos^2 45^\circ + D(u_{n+1} - v_n) \cdot \cos^2 45^\circ \\ M\ddot{u}_{n+1} = -D(u_{n+1} - v_n) \cos^2 45^\circ + D(v_{n+1} - u_{n+1}) \cos^2 45^\circ \end{array} \right.$$

$$\left. \begin{array}{l} v_n(t) = v(q) e^{iqn(2a)} e^{-i\omega t} \\ u_n(t) = u(q) e^{iqn(2a)} e^{-i\omega t} \end{array} \right\}$$

$$2M\ddot{v}_n = -D(2v_n - u_n - u_{n+1})$$

$$2M\ddot{u}_{n+1} = -D(2u_{n+1} - v_n - v_{n+1})$$

$$-2m\omega^2 v(q) = -D \cdot 2v(q) + D \cdot u(q) + Du(q)e^{iq \cdot 2a}$$

$$-2M\omega^2 u(q)e^{iq \cdot 2a} = -D \cdot 2u(q)e^{iq \cdot 2a} + Dv(q) + Dv(q)e^{iq \cdot 2a}$$

$$\begin{pmatrix} 2m\omega^2 - 2D & D(1 + e^{iq \cdot 2a}) \\ - & - \\ D(1 + e^{iq \cdot 2a}) & (2M\omega^2 - 2D)e^{iq \cdot 2a} \end{pmatrix} \begin{pmatrix} v(q) \\ u(q) \end{pmatrix} = \phi$$

$$(2m\omega^2 - 2D)(2M\omega^2 - 2D)e^{iq \cdot 2a} - D^2(1 + e^{iq \cdot 2a})^2 = \phi$$

~~$$4(m\omega^2 - D)(M\omega^2 - D) - D^2 \underbrace{(1 + e^{iq \cdot 2a})(1 + e^{-iq \cdot 2a})}_{= 2} = \phi$$~~

$$\begin{aligned} 2 + 2 \cos(2qa) &= 2(1 + \cos^2 qa - \sin^2 qa) = \\ &= 4 \cos^2 qa \end{aligned}$$

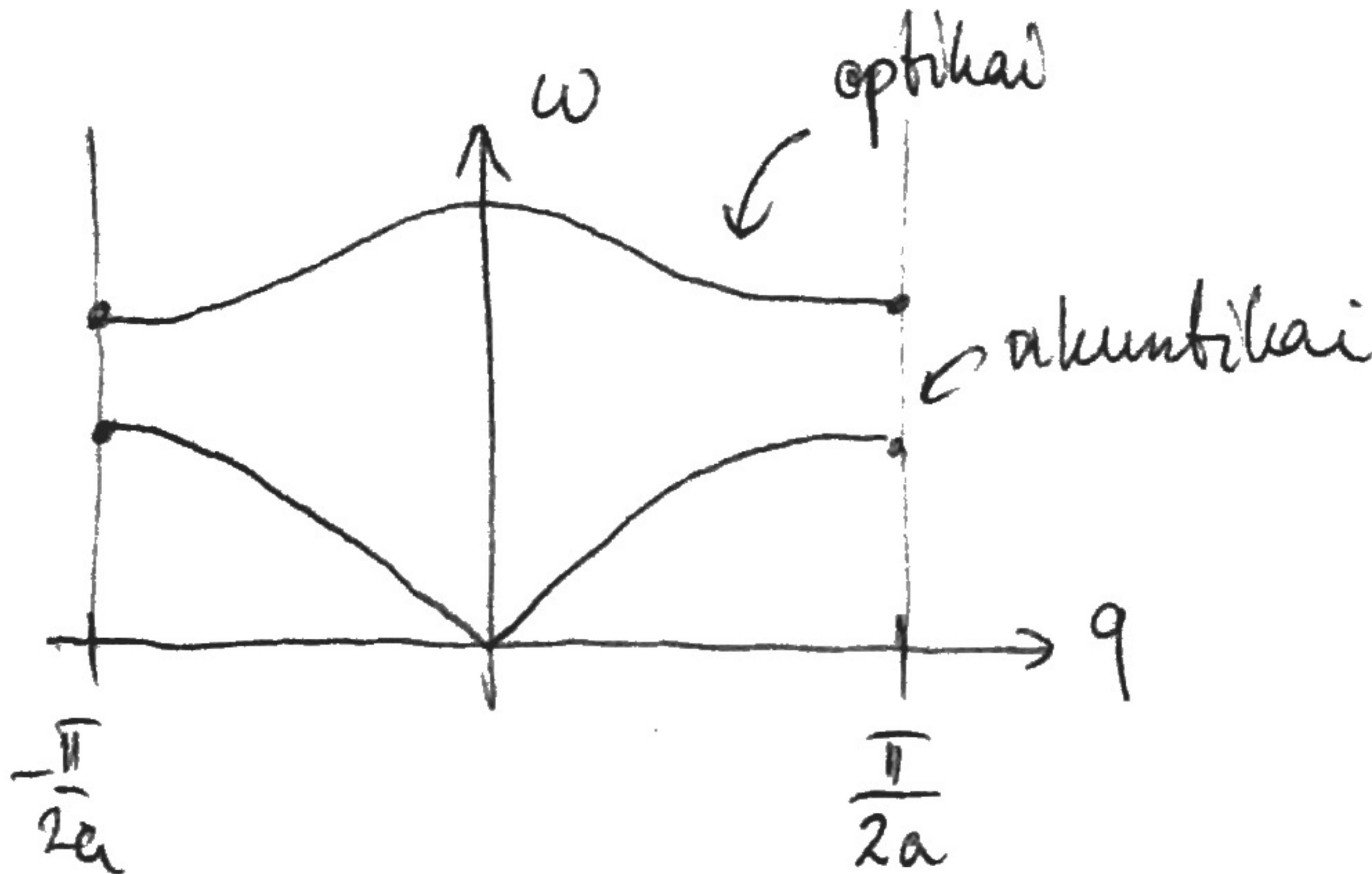
$$\underbrace{(m\omega^2 - D)(N\omega^2 - D)}_{(m\omega^2 - D)^2} - D^2 \cos^2 qa = \phi$$

$$mM\omega^4 - D(M+m)\omega^2 + D^2(1-\cos^2(qa)) = \phi$$

$\underbrace{\sin^2(qa)}$

$$\omega_{1,2}^2 = \frac{D(M+m) \pm \sqrt{D^2(M+m)^2 - 4mMD^2 \sin^2(qa)}}{2mM}$$

$$\omega_{1,2}^2 = \frac{1}{2} \left[D \left(\frac{1}{M} + \frac{1}{m} \right) \pm D \sqrt{\left(\frac{1}{M} + \frac{1}{m} \right)^2 - \frac{1}{Mm} \sin^2(qa)} \right]$$



2.) 3 akustikus 3 3D-s, 1 elemi celláként, pl. FCC vas.
Optikai

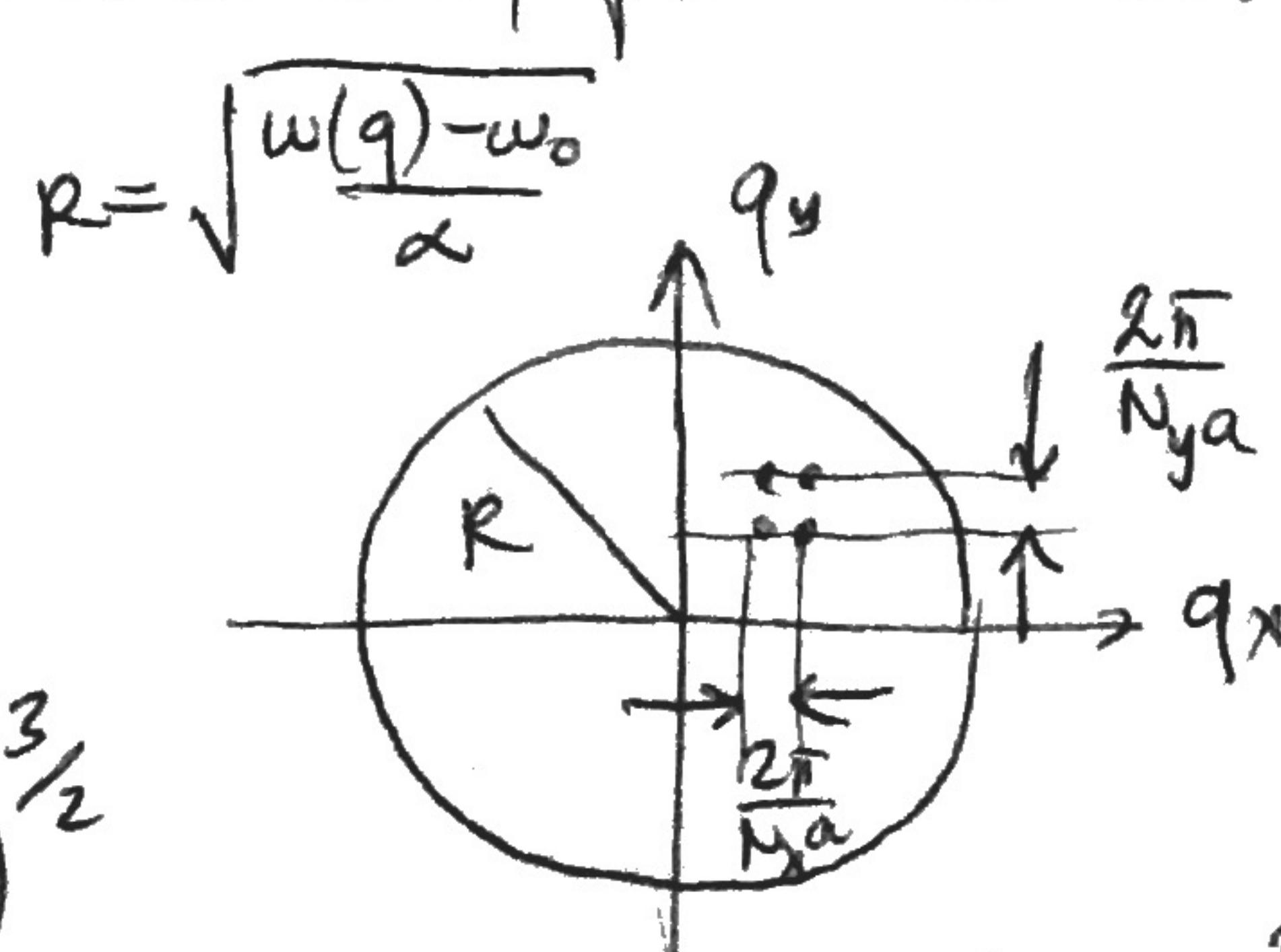
$$3.) \omega(q) = \omega_0 + \alpha q^2$$

$$\omega(q) - \omega_0 = \alpha(q_x^2 + q_y^2 + q_z^2)$$

$$\mathcal{N}(\omega) = \frac{1}{\frac{2\pi}{N_x a} \frac{2\pi}{N_y a} \frac{2\pi}{N_z a}} \cdot \frac{4\pi}{3} \cdot \left(\frac{\omega(q) - \omega_0}{\alpha} \right)^{3/2}$$

$$\mathcal{N}(\omega) = \frac{V}{6\pi^2} \cdot \left(\frac{\omega(q) - \omega_0}{\alpha} \right)^{3/2}$$

$$\frac{d\mathcal{N}}{d\omega} = \frac{V}{6\pi^2} \cdot \frac{3}{2} \cdot \left(\frac{\omega(q) - \omega_0}{\alpha} \right)^{1/2} = V \cdot g(\omega)$$



$$N_x N_y N_z a^3 = V$$

$$\Rightarrow g(\omega) = \frac{1}{4\pi^2} \cdot \sqrt{\frac{\omega(q) - \omega_0}{\alpha}} \cdot \frac{1}{\omega}$$

$$4.) V(x) = V_0 \sin^3\left(\frac{\pi}{d} \cdot x\right) \quad \text{periódus: } \frac{\pi}{d} \cdot a = 2\pi \\ a = 2d$$

$$V(x) = V_0 \cdot \left(e^{i \frac{\pi}{d} x} + e^{-i \frac{\pi}{d} x} \right)^3 \cdot \frac{1}{(2i)^3}$$

$$V(x) = V_0 \frac{i}{8} \cdot \left(e^{i \frac{\pi}{d} x} - e^{-i \frac{\pi}{d} x} \right)^3 = \frac{i V_0}{8} \left(e^{i \frac{\pi}{d} x} - e^{-i \frac{\pi}{d} x} \right) \left(e^{i \frac{\pi}{d} x} - e^{-i \frac{\pi}{d} x} \right) \left(e^{i \frac{\pi}{d} x} - e^{-i \frac{\pi}{d} x} \right)$$

$$V(x) = \frac{i V_0}{8} \left[\left(e^{i \frac{2\pi}{d} x} - 1 + e^{-i \frac{2\pi}{d} x} \right) \left(e^{i \frac{\pi}{d} x} - e^{-i \frac{\pi}{d} x} \right) \right]$$

$$V(x) = \frac{i V_0}{8} \left[e^{i \frac{3\pi}{d} x} - 3e^{i \frac{\pi}{d} x} + 3e^{-i \frac{\pi}{d} x} + e^{-i \frac{3\pi}{d} x} \right]$$

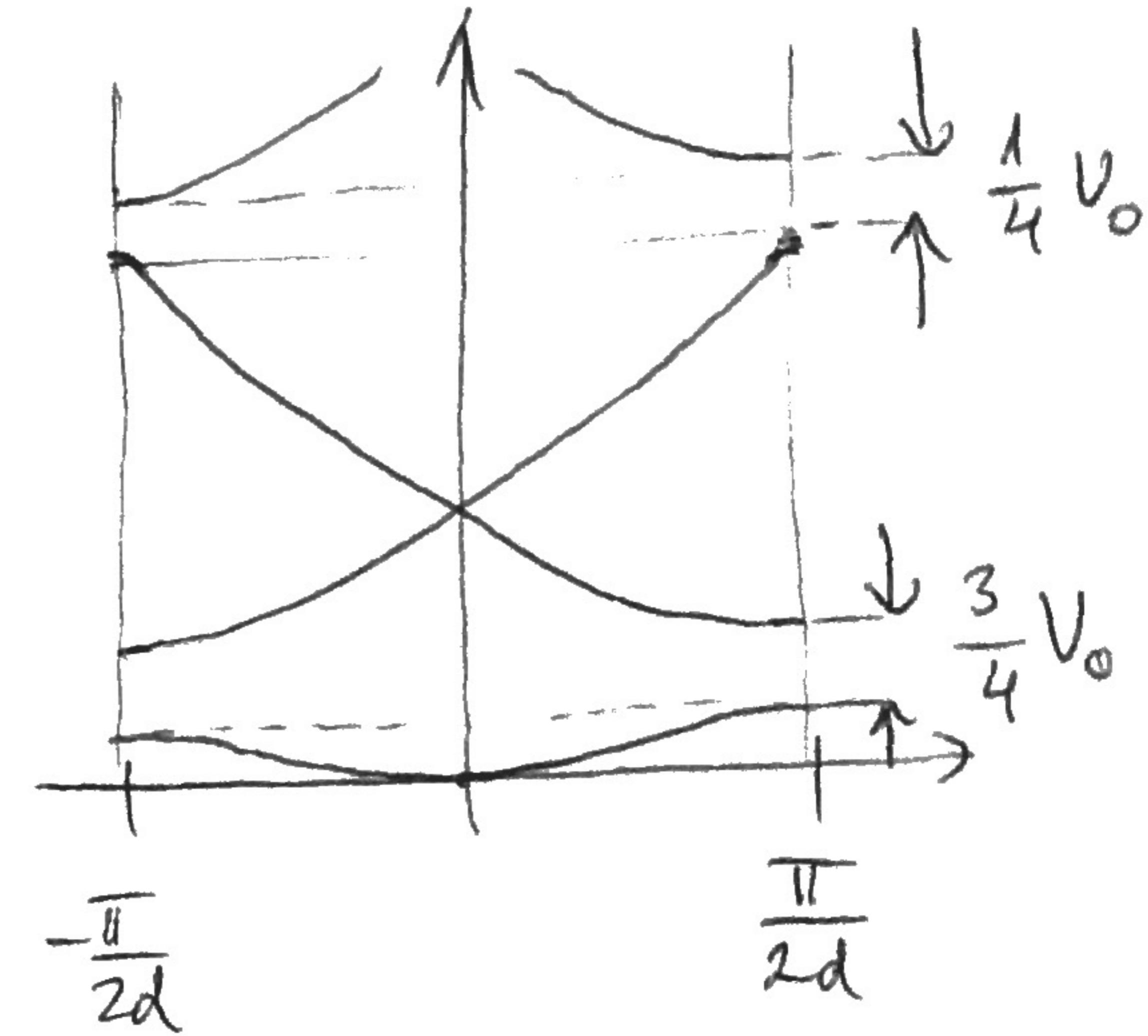
$$V(x) = \sum_G V(G) e^{i G x}, \quad G = n \cdot \frac{2\pi}{a} = n \cdot \frac{\pi}{d}$$

$$V\left(\frac{\pi}{d}\right) = -\frac{3i}{8} V_0 \quad \left. \begin{array}{l} \\ \end{array} \right\} \text{gap: } \frac{3}{4} V_0$$

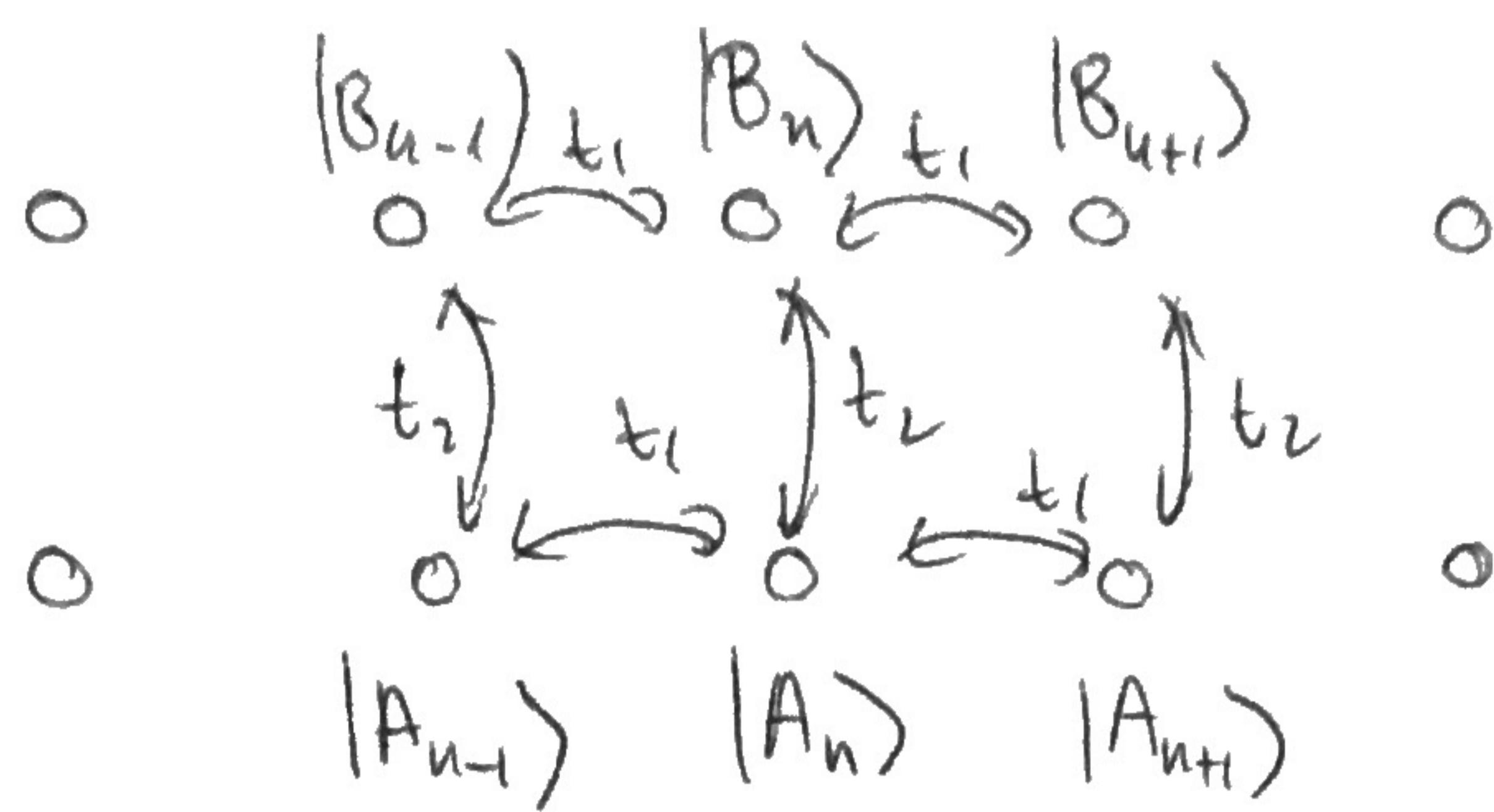
$$V\left(-\frac{\pi}{d}\right) = \frac{3i}{8} V_0$$

$$V\left(\frac{3\pi}{d}\right) = \frac{i}{8} V_0 \quad \left. \begin{array}{l} \\ \end{array} \right\} \text{gap: } \frac{1}{4} V_0$$

$$V\left(-\frac{5\pi}{d}\right) = -\frac{i}{8} V_0$$



5.)



$$\left(\begin{array}{c|cc|c} \varepsilon_A t_2 & & & \\ \hline t_1 & \varepsilon_B & 0 & t_1 \\ -\frac{t_1}{t_1} & 0 & \varepsilon_A & t_2 \\ \hline t_1 & t_2 & 0 & t_1 \\ \hline \varepsilon_A & & & \end{array} \right) \left(\begin{array}{c} A e^{ik(n-1)a} \\ B e^{ik(n-1)a} \\ A e^{ika} \\ B e^{ika} \\ A e^{ik(n+1)a} \\ B e^{ik(n+1)a} \end{array} \right) = E(k) \left(\begin{array}{c} . \\ A e^{ika} \\ B e^{ika} \end{array} \right)$$

$$A t_1 e^{-ika} + \varepsilon_0 A + B t_2 + t_1 A e^{ika} = E(k) A \quad (1)$$

$$B t_1 e^{-ika} + A t_2 + B \varepsilon_0 + B t_1 e^{ika} = E(k) B \quad (2)$$

Ergebnis:

$$\left(\begin{array}{cc} \varepsilon_0 - E(k) + 2t_1 \cos(ka) & t_2 \\ t_2 & \varepsilon_0 - E(k) + 2t_1 \cos(ka) \end{array} \right) \left(\begin{array}{c} A \\ B \end{array} \right) = \phi$$

$$[\varepsilon_0 - E(k) + 2t_1 \cos(ka)]^2 - t_2^2 = \phi$$

$$E(k) = \varepsilon_0 + 2t_1 \cos(ka) \pm t_2$$

