FROM HESSIAN MATRIX TO ION CHAINS

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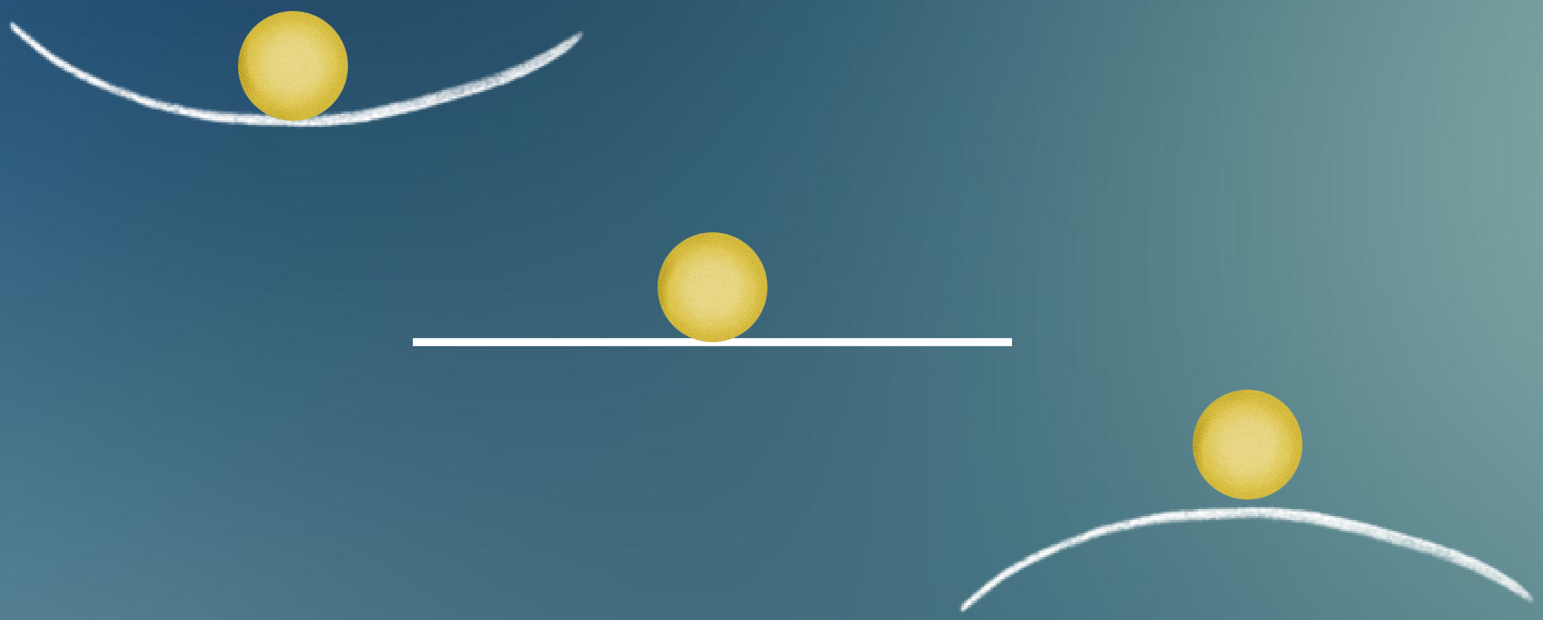
What is Hessian Matrix?

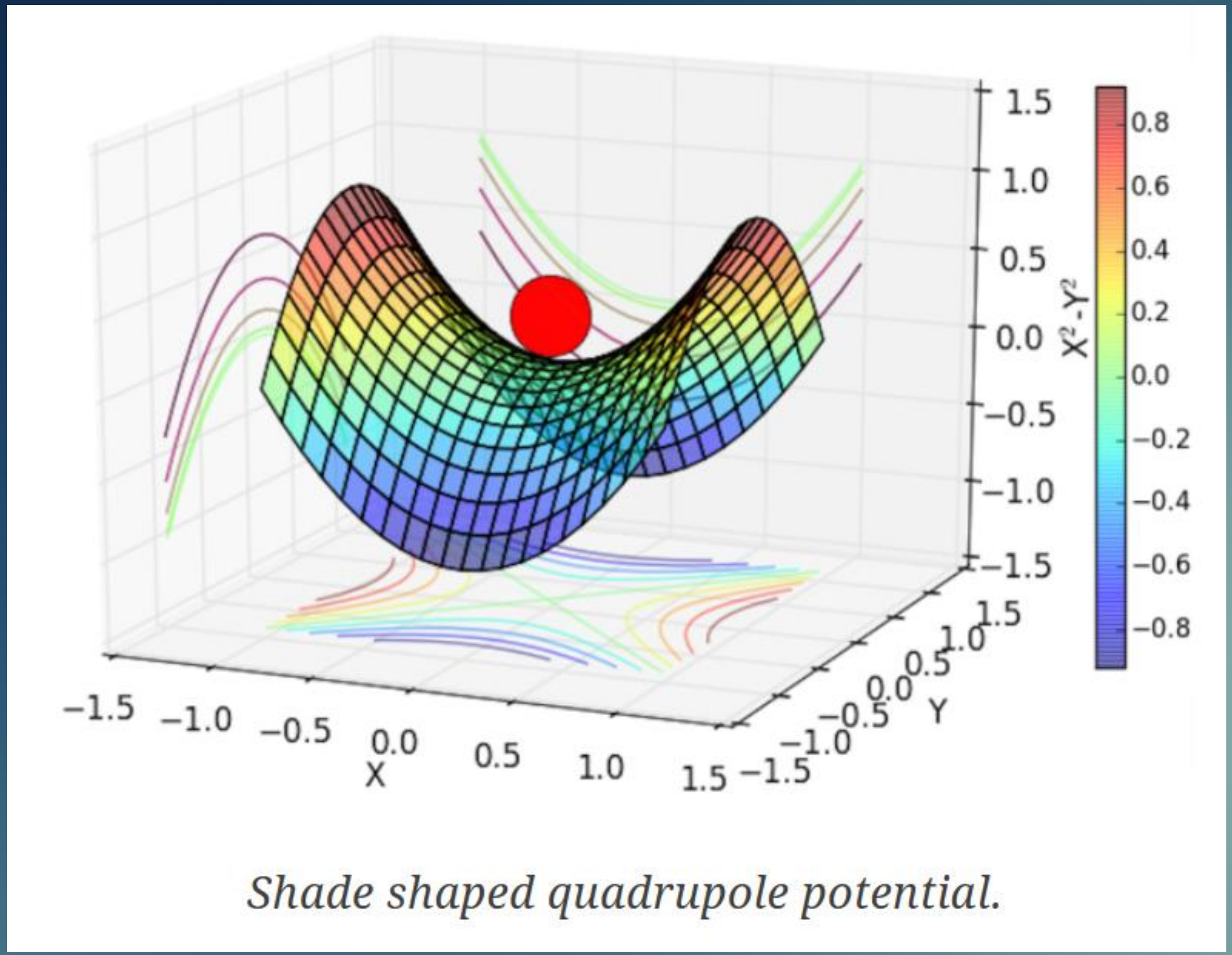
- second derivative of f (f'')
- index of stability
- prediction of motion



$$\mathbf{H}_f = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1\,\partial x_n} \\[2.2ex] \dfrac{\partial^2 f}{\partial x_2\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_2\,\partial x_n} \\[2.2ex] \vdots & \vdots & \ddots & \vdots \\[2.2ex] \dfrac{\partial^2 f}{\partial x_n\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

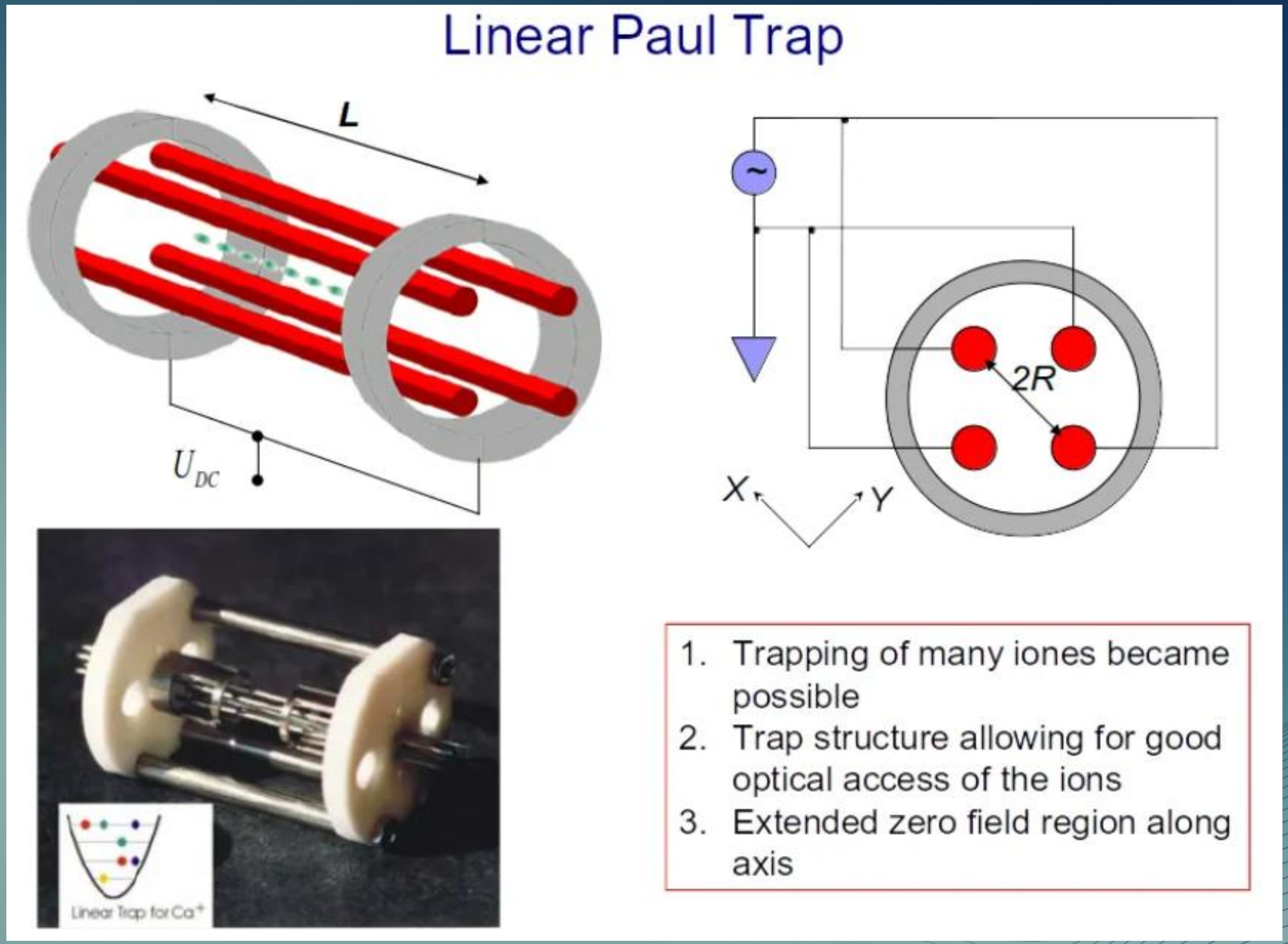
3 PARTICLES SYSTEM

Imagine few particle in a potential



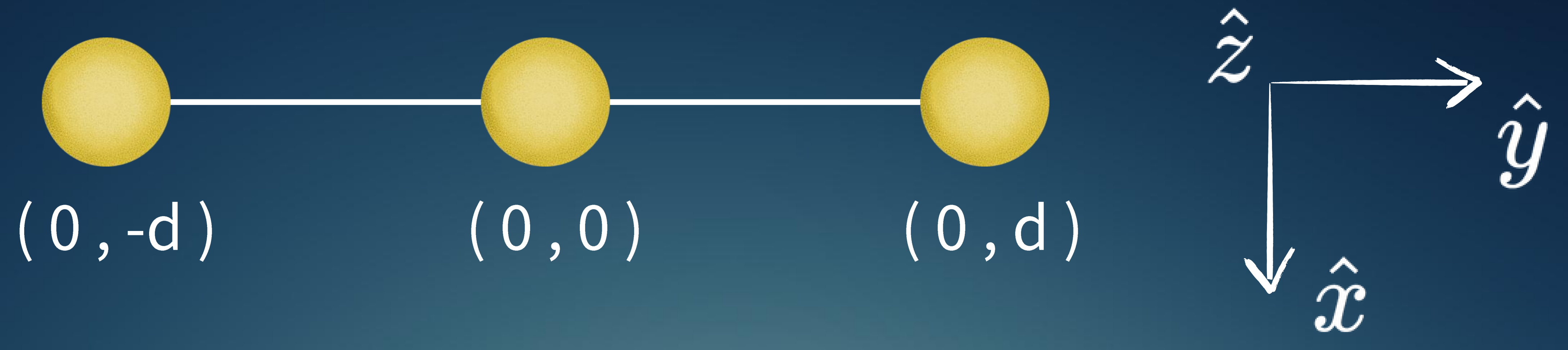
Shade shaped quadrupole potential.

POTENTIAL



PAUL TRAP

3 PARTICLES SYSTEM



potential : $V = \sum_{i=1}^{N} \frac{1}{2} m(\omega_x^2 x_i^2 + \omega_y^2 y_i^2) + \sum_{i>j}^{N} \frac{k_e Q^2}{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}}$

Fy = 0 for 1st and 3rd particle : $\frac{\partial V}{\partial y_1} = 0 = m\omega_y^2 d - \frac{k_e Q^2}{d^2} - \frac{k_e Q^2}{(2d)^2} => d = \sqrt[3]{\frac{5}{4} \frac{k_e Q^2}{m\omega_y^2}}$

constructure Hessian Matrix : $\hat{H} = \frac{\partial^2 V}{\partial x_i \partial x_j} = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}$

3 PARTICLES SYSTEM

$$H_{ii} = \frac{\partial^2 V}{\partial x_i^2}(x_i = 0) = m\omega_x^2 - \frac{k_e Q^2}{|y_i - y_j|^3} \quad H_{ij} = \frac{\partial^2 V}{\partial x_i \partial x_j}(x_i = x_j = 0) = \frac{k_e Q^2}{|y_i - y_j|^3}$$

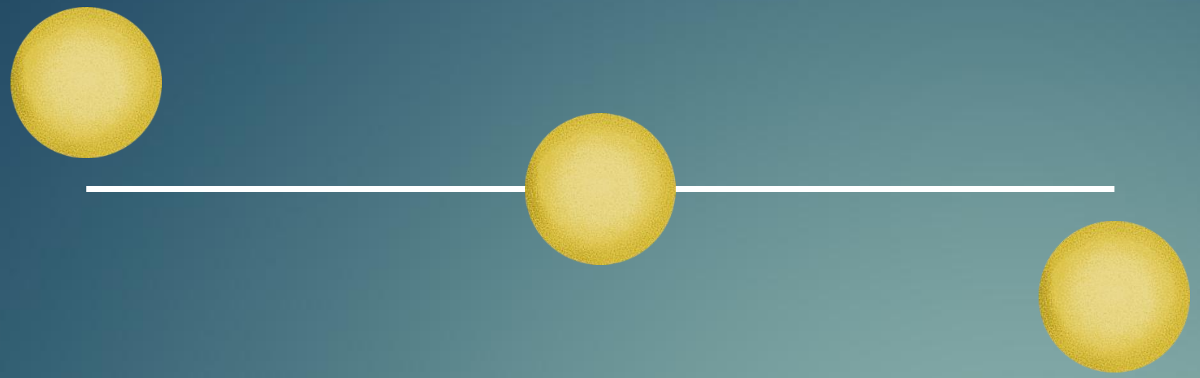
$$(\frac{k_e Q^2}{d^3} \equiv C) => \hat{H} = m\omega_x^2 I - C \begin{pmatrix} \frac{9}{8} & -1 & -\frac{1}{8} \\ -1 & 2 & -1 \\ -\frac{1}{8} & -1 & \frac{9}{8} \end{pmatrix}$$ (unstable when < 0)

$$\lambda = 1(V = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}) \qquad \lambda = \frac{5}{4}(V = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}) \qquad \lambda = 3(V = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix})$$

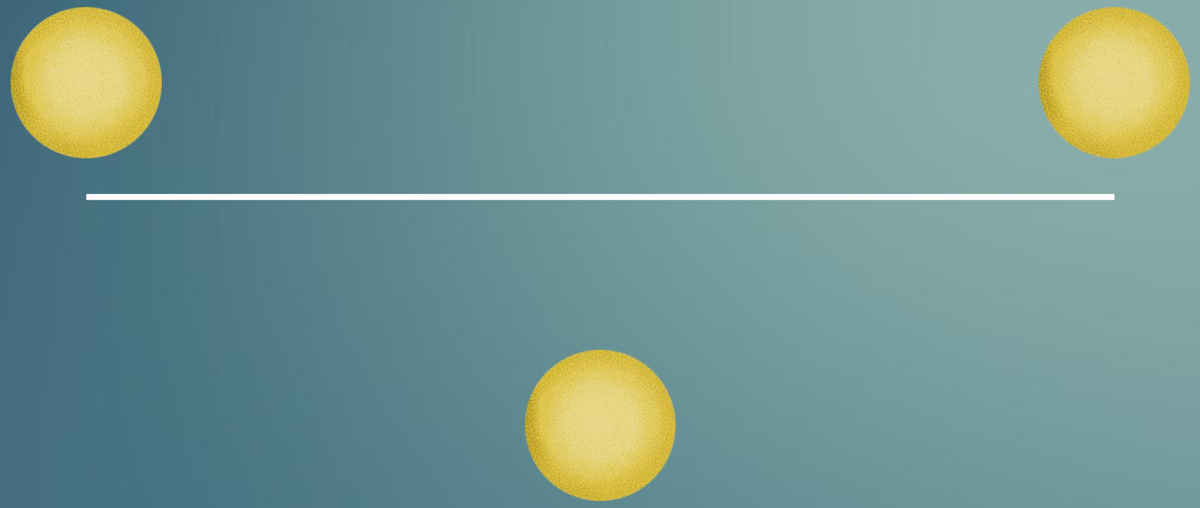
3 PARTICLES SYSTEM

$$\lambda = 0 (V = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix})$$

$$\lambda = \frac{5}{4} (V = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix})$$



$$\lambda = 3 (V = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix})$$

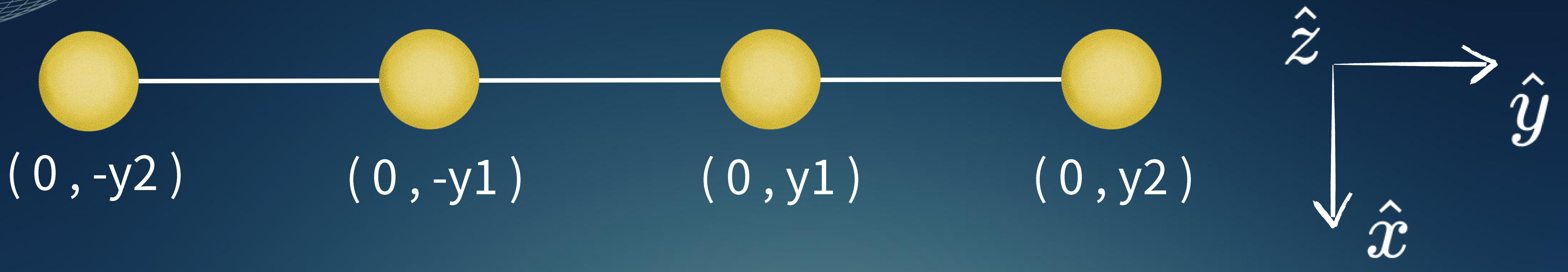


When potential is lower than internal energy, then structure from linear become zigzag.

$$m\omega_x^2 < 3\frac{k_e Q^2}{d^3}$$

$$d = \sqrt[3]{\frac{5}{4}\frac{k_e Q^2}{m\omega_y^2}}$$

4 PARTICLES SYSTEM



Similiar to 3 particle, so we do it again!

Fy = 0 for 3rd and 4th particle : $\frac{\partial V}{\partial y_3} = 0 = \frac{\partial V}{\partial y_4} => \frac{y_2}{y_1} = 1 + \sqrt{2}$

$$\left(\frac{k_e Q^2}{(2d)^3} \equiv C\right) => \hat{H} = m\omega_x^2 I - C \begin{pmatrix} 3.1 & -2.83 & -0.2 & -0.07 \\ -2.83 & 4.03 & -1 & -0.2 \\ -0.2 & -1 & -4.03 & -2.83 \\ -0.07 & -0.2 & -2.83 & 3.1 \end{pmatrix}$$

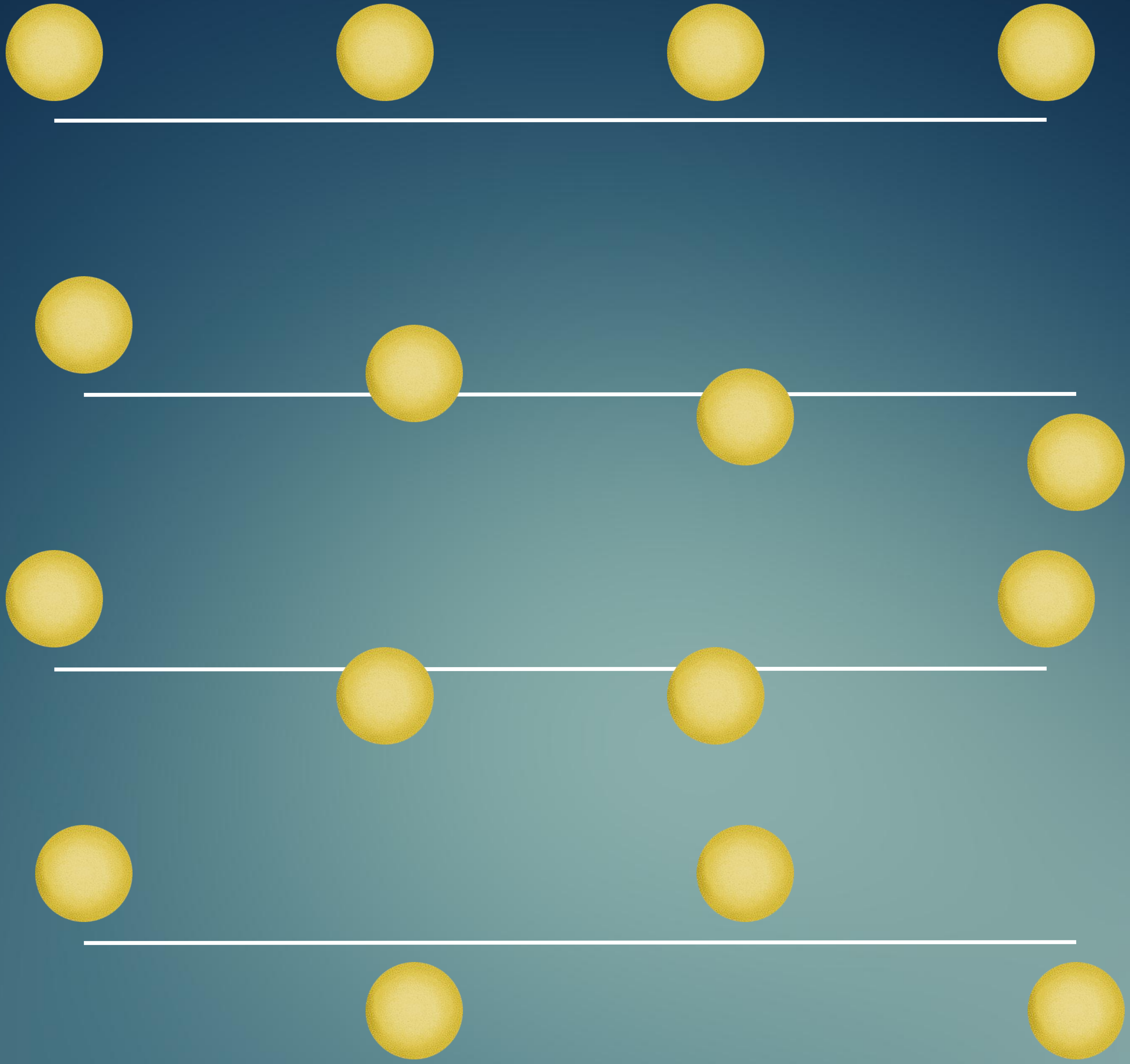
4 PARTICLES SYSTEM

$$\lambda = 0(V = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix})$$

$$\lambda = 1.21(V = \begin{pmatrix} 1 \\ 0.45 \\ -0.45 \\ -1 \end{pmatrix})$$

$$\lambda = 2.56(V = \begin{pmatrix} 1 \\ -0.5 \\ -0.5 \\ 1 \end{pmatrix})$$

$$\lambda = 4.41(V = \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix})$$

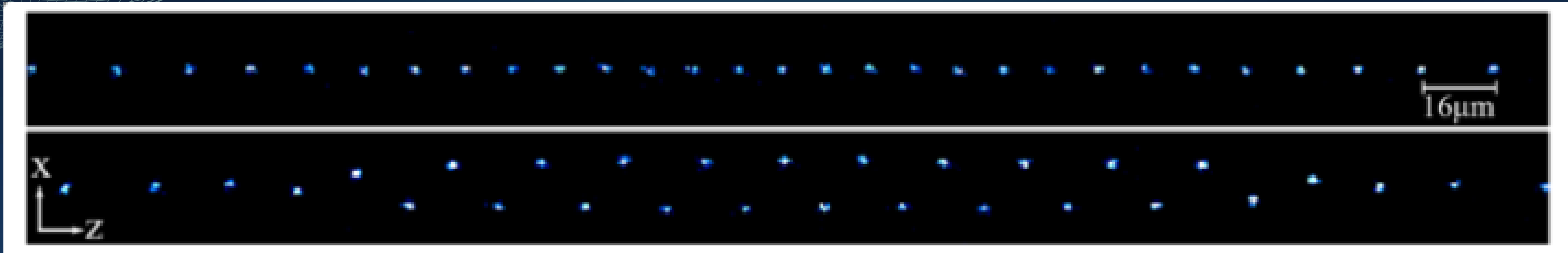


GENERALIZE

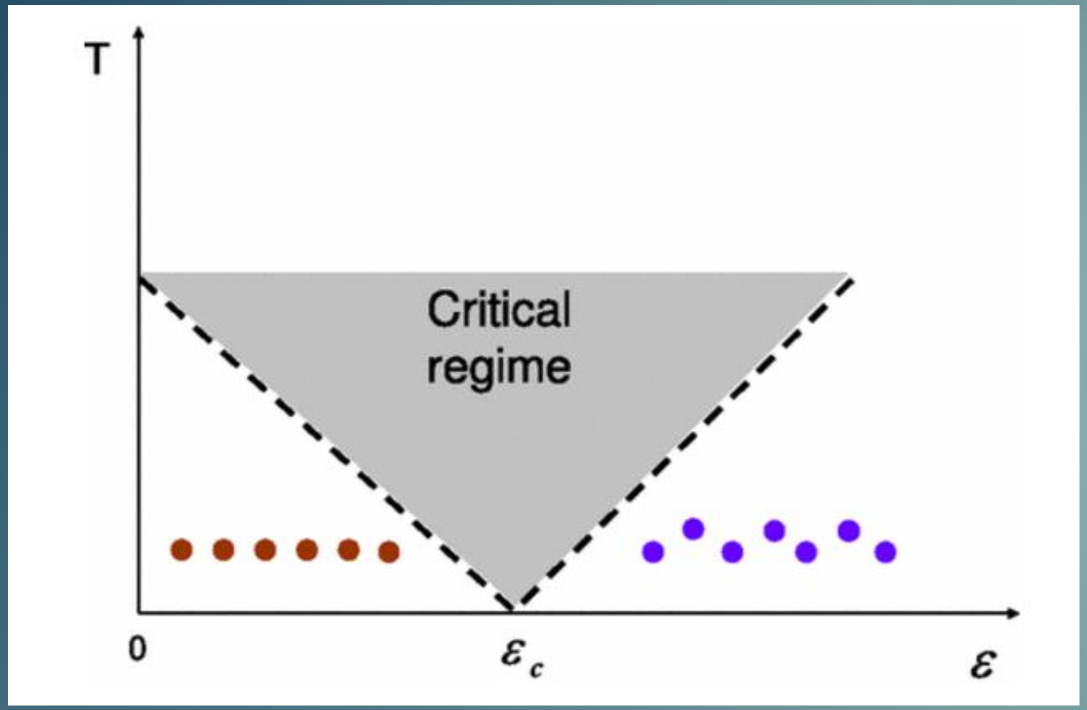
For more particles, the easiest structures are all "zigzag"!

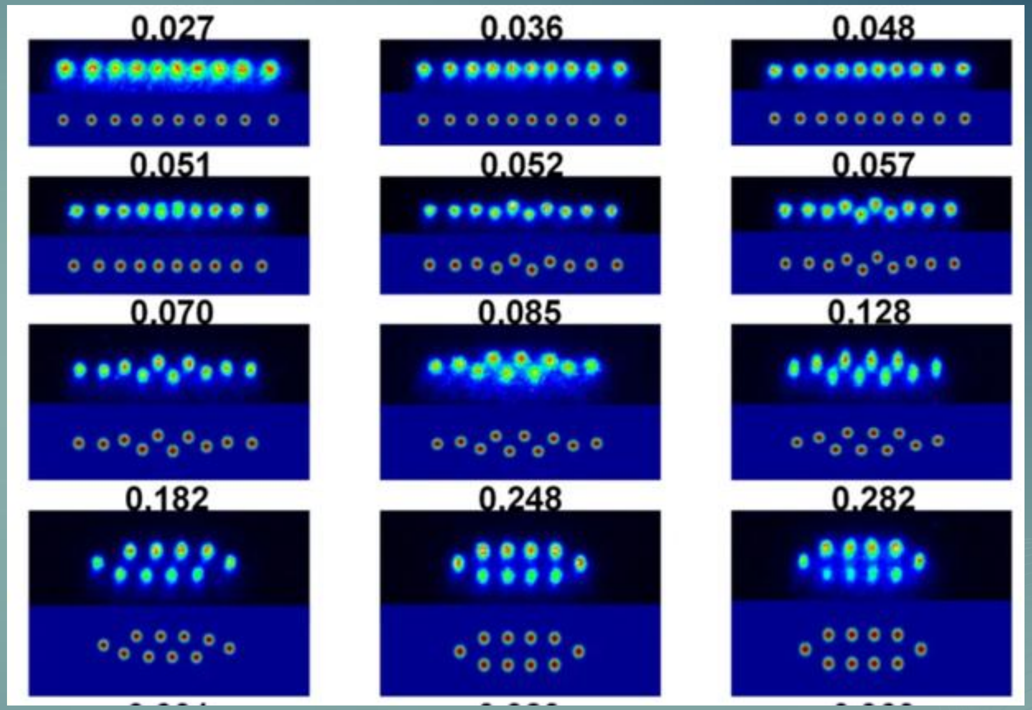
$$\lambda = 5.9, 7.4, 9.0, 10.6\ldots (V = \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} \ldots)$$

IN EXPERIMENTS



https://www.researchgate.net/figure/a-Experimental-pictures-of-the-linear-chain-top-and-of-the-zigzag-configuration_fig4_347535228





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THANK YOU