

PUNKTGRUPPEN UND KRISTALLE

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Slides: s.0hm.ch/ctBsD

2D Symmetrien

Algebraische Symmetrien

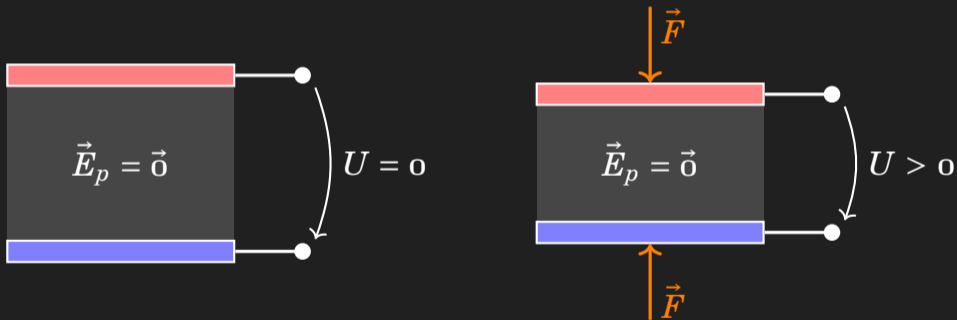
3D Symmetrien

Matrizen

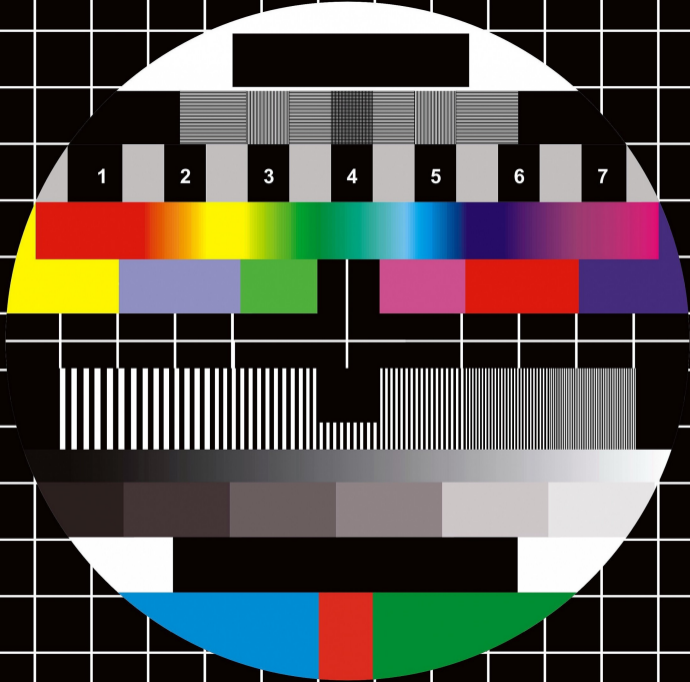
Kristalle

Anwendungen

- ▶ Was heisst *Symmetrie* in der Mathematik?
- ▶ Wie kann ein Kristall modelliert werden?
- ▶ Aus der Physik: Piezoelektrizität



2D Symmetrien



Algebraische Symmetrien

Produkt mit i

$$1 \cdot i = i$$

$$i \cdot i = -1$$

$$-1 \cdot i = -i$$

$$-i \cdot i = 1$$

Gruppe

$$G = \{1, i, -1, -i\}$$

$$= \{1, i, i^2, i^3\}$$

$$C_4 = \{1, r, r^2, r^3\}$$

Darstellung $\phi : C_4 \rightarrow G$

$$\phi(1) = 1 \quad \phi(r^2) = i^2$$

$$\phi(r) = i \quad \phi(r^3) = i^3$$

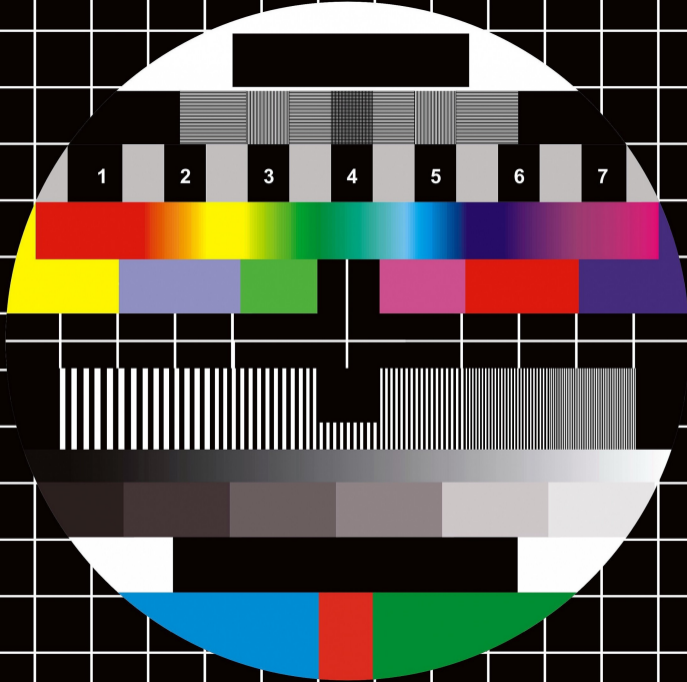
Homomorphismus

$$\begin{aligned} \phi(r \circ 1) &= \phi(r) \cdot \phi(1) \\ &= i \cdot 1 \end{aligned}$$

ϕ ist bijektiv $\implies C_4 \cong G$

$$\begin{aligned} \psi : C_4 &\rightarrow (\mathbb{Z}/4\mathbb{Z}, +) \\ \psi(1 \circ r^2) &= 0 + 2 \pmod{4} \end{aligned}$$

3D Symmetrien



Matrizen

Symmetriegruppe

$$G = \{1, r, \sigma, \dots\}$$

Matrixdarstellung

$$\begin{aligned}\Phi : G &\rightarrow O(3) \\ g &\mapsto \Phi_g\end{aligned}$$

Orthogonale Gruppe

$$O(n) = \{Q : QQ^t = Q^tQ = I\}$$

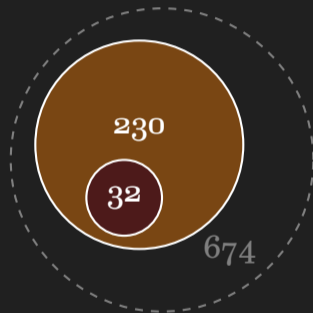
$$\Phi_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I$$

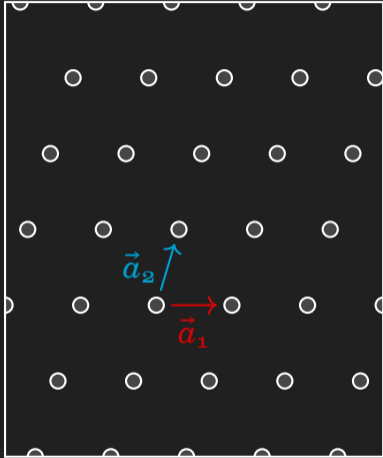
$$\Phi_\sigma = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\Phi_r = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Kristalle

Mögliche Kristallstrukturen





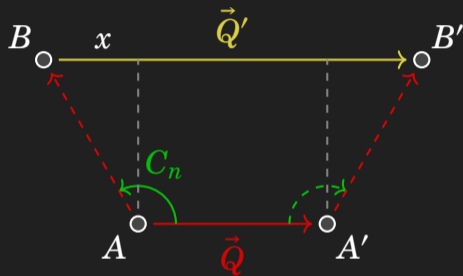
Kristallgitter: $n_i \in \mathbb{Z}$, $\vec{a}_i \in \mathbb{R}^3$

$$\vec{r} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

Invariant unter Translation

$$Q_i(\vec{r}) = \vec{r} + \vec{a}_i$$

Wie kombiniert sich Q_i mit der anderen Symmetrien?



Sei $q = |\vec{Q}|$, $\alpha = 2\pi/n$ und $n \in \mathbb{N}$

$$q' = nq = q + 2x$$

$$nq = q + 2q \sin(\alpha - \pi/2)$$

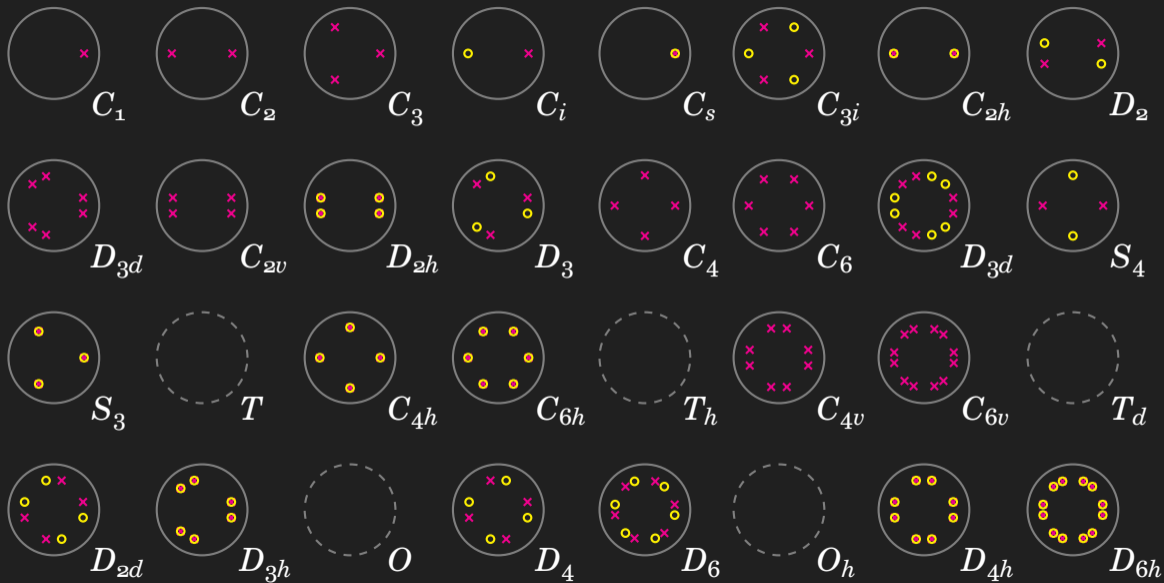
$$n = 1 - 2 \cos \alpha$$

Somit muss

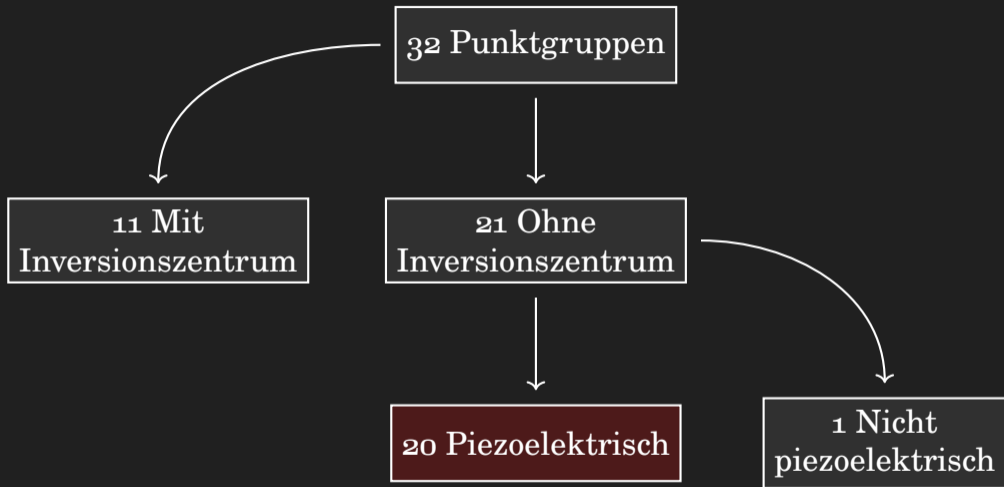
$$\alpha = \cos^{-1} \left(\frac{1-n}{2} \right)$$

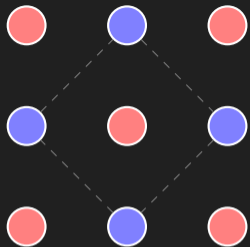
$$\alpha \in \{0^\circ, 60^\circ, 90^\circ, 120^\circ, 180^\circ\}$$

$$n \in \{1, 2, 3, 4, 6\}$$



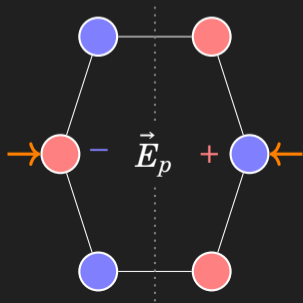
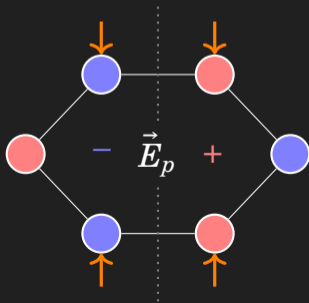
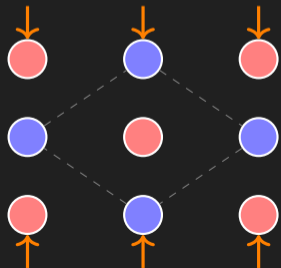
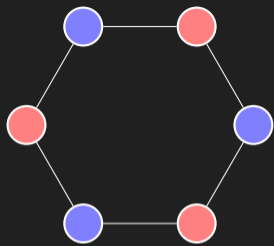
Anwendungen





Mit und Ohne Symmetriezentrum

Polarisation Feld \vec{E}_p



Licht in Kristallen

Symmetriegruppe und Darstellung

$$G = \{1, r, \sigma, \dots\}$$
$$\Phi : G \rightarrow O(n)$$

$$U_\lambda = \{v : \Phi v = \lambda v\}$$
$$= \text{null}(\Phi - \lambda I)$$

Helmholtz Wellengleichung

$$\nabla^2 \vec{E} = \varepsilon \mu \frac{\partial^2}{\partial t^2} \vec{E}$$

Ebene Welle

$$\vec{E} = \vec{E}_0 \exp \left[i \left(\vec{k} \cdot \vec{r} - \omega t \right) \right]$$

Anisotropisch Dielektrikum

$$(K\varepsilon) \vec{E} = \frac{k^2}{\mu \omega^2} \vec{E}$$

$$\vec{E} \in U_\lambda \implies (K\varepsilon) \vec{E} = \lambda \vec{E}$$