Punktgruppen und Kristalle

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10. Mai 2021

Slides: `s.0hm.ch/ctBsD`

2D Symmetrien

Algebraische Symmetrien

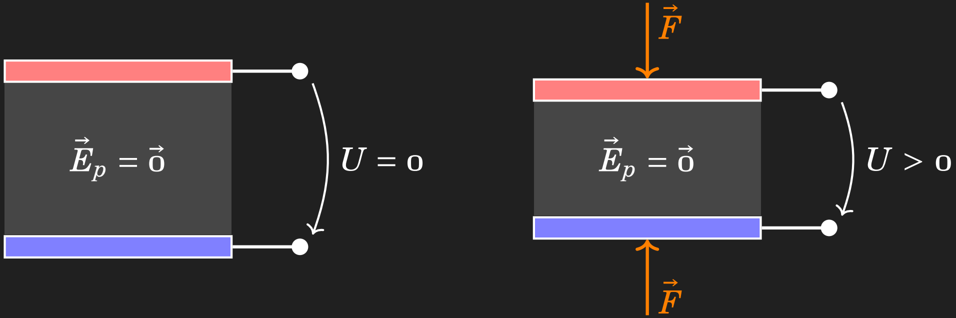
3D Symmetrien

Matrizen

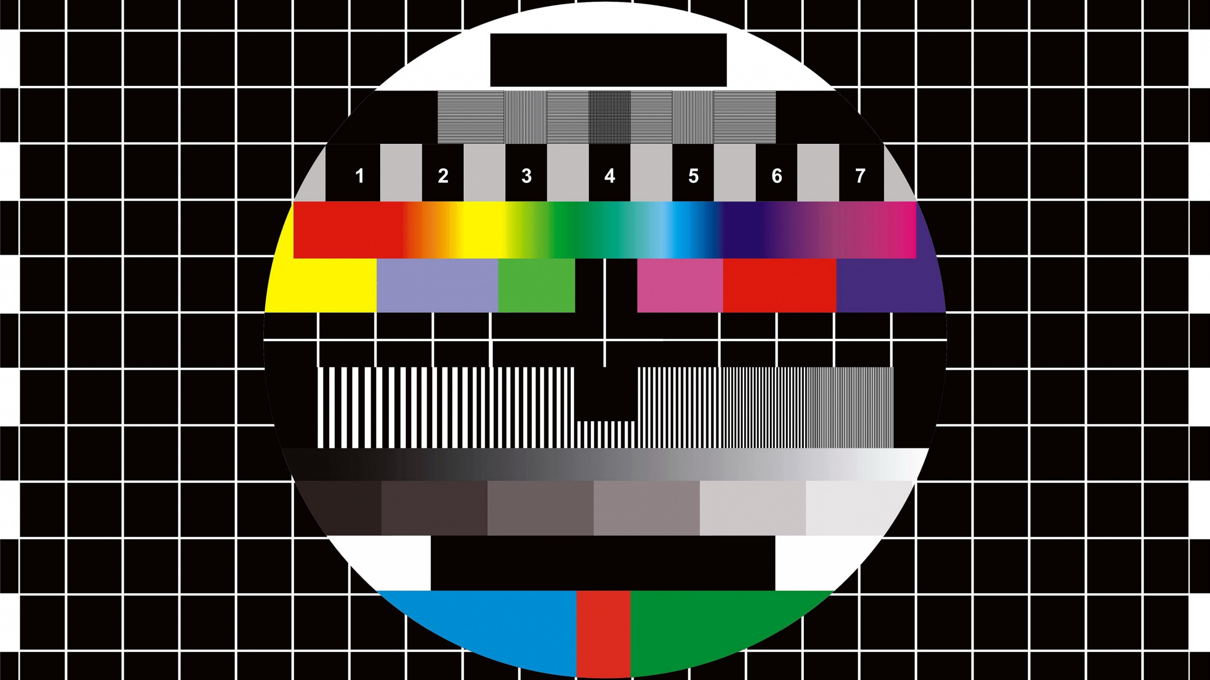
Kristalle

Anwendungen

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



2D Symmetrien


1
2
3
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Algebraische Symmetrien

Produkt mit i

$$
\begin{aligned}
1 \cdot i &= i \\
i \cdot i &= -1 \\
-1 \cdot i &= -i \\
-i \cdot i &= 1
\end{aligned}
$$

Gruppe

$$
\begin{aligned}
G &= \{1, i, -1, -i\} \\
&= \{1, i, i^2, i^3\} \\
C_4 &= \{\mathbb{1}, r, r^2, r^3\}
\end{aligned}
$$

Darstellung $\phi : C_4 \to G$

$$
\begin{aligned}
\phi(\mathbb{1}) &= 1 & \qquad \phi(r^2) &= i^2 \\
\phi(r) &= i & \qquad \phi(r^3) &= i^3
\end{aligned}
$$

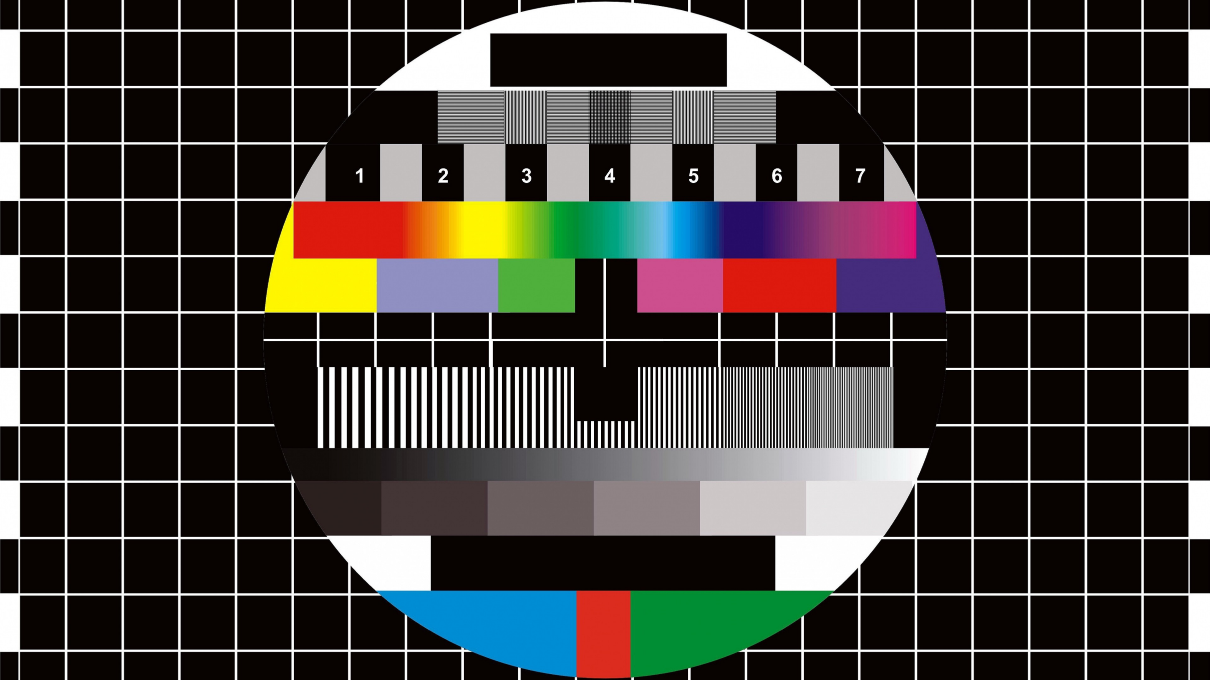
Homomorphismus

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

ϕ ist bijektiv $\implies C_4 \cong G$

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

3D Symmetrien


1
2
3
4
5
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Matrizen

Symmetriegruppe

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

Matrixdarstellung

$$\Phi : G \longrightarrow O(3)$$
$$g \mapsto \Phi_g$$

Orthogonale Gruppe

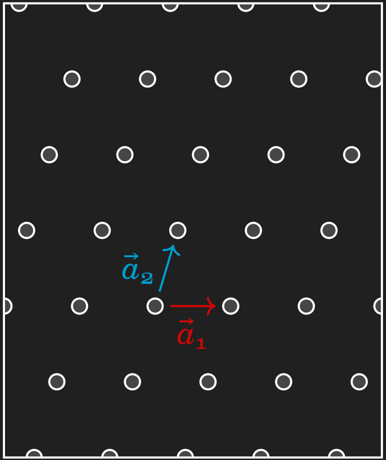
$$O(n) = \left\{Q : QQ^t = Q^t Q = I\right\}$$

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

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

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

Kristalle



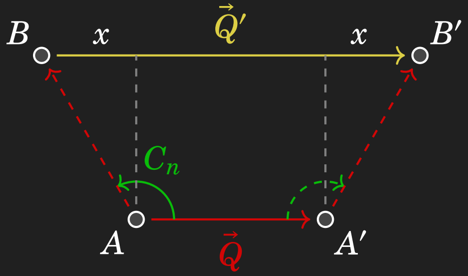
Kristallgitter: $n_i \in \mathbb{Z}, \quad \vec{a}_i \in \mathbb{R}^3$

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

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 $n \in \mathbb{N}$

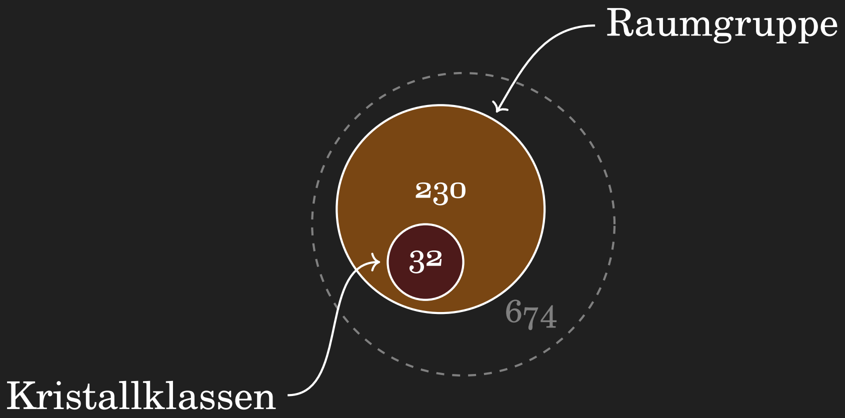
$$q' = nq = q + 2x$$
$$nq = q + 2q\sin(\alpha - \pi/2)$$
$$n = 1 - 2\cos\alpha$$

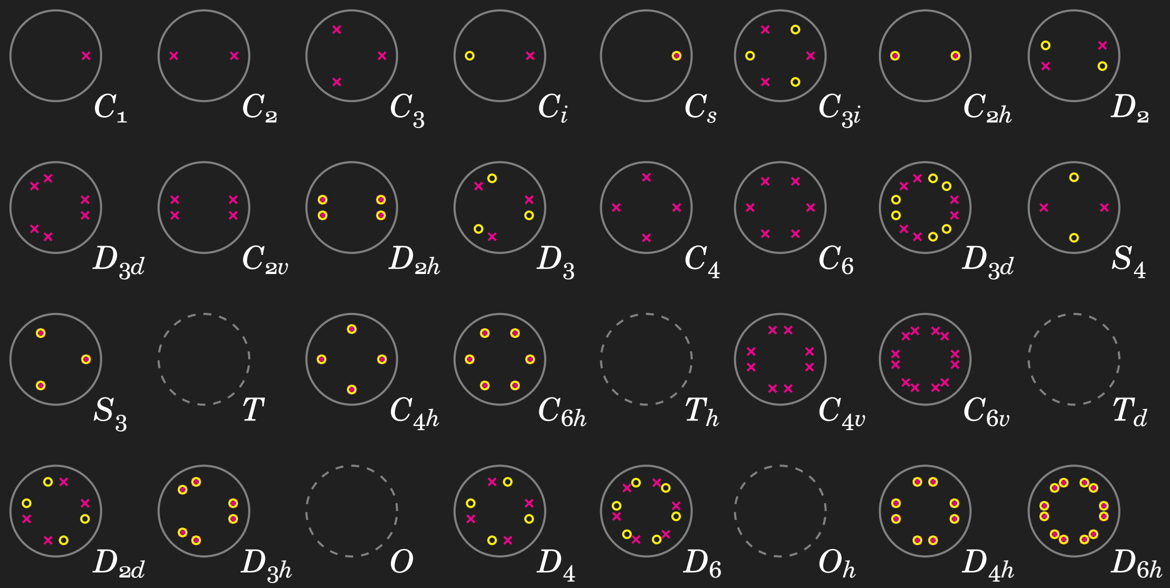
Somit muss

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

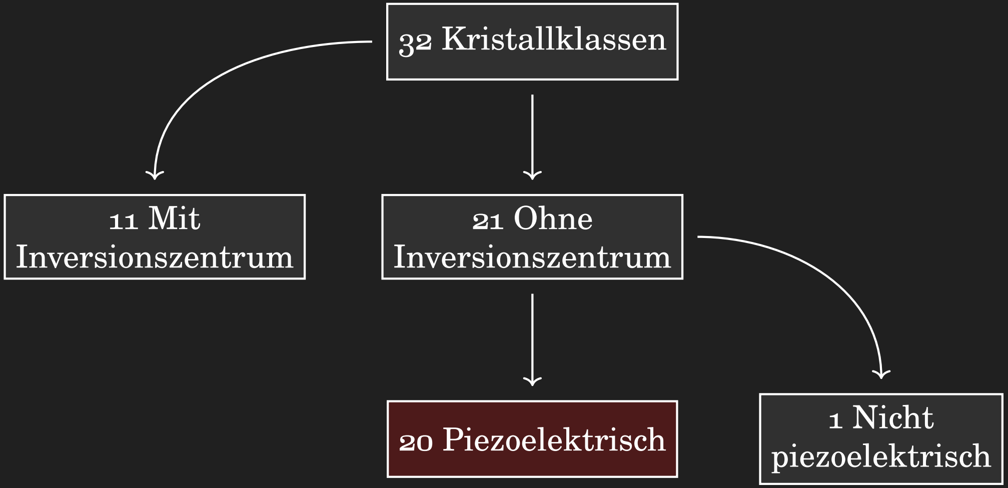
$$\alpha \in \{0, 60^\circ, 90^\circ, 120^\circ, 180^\circ\}$$
$$n \in \{1, 2, 3, 4, 6\}$$

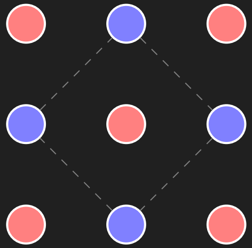
Mögliche Kristallstrukturen




C_1
C_2
C_3
C_i
C_s
C_{3i}
C_{2h}
D_2
D_{3d}
C_{2v}
D_{2h}
D_3
C_4
C_6
D_{3d}
S_4
S_3
T
C_{4h}
C_{6h}
T_h
C_{4v}
C_{6v}
T_d
D_{2d}
D_{3h}
O
D_4
D_6
O_h
D_{4h}
D_{6h}

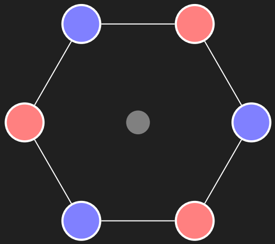
Anwendungen

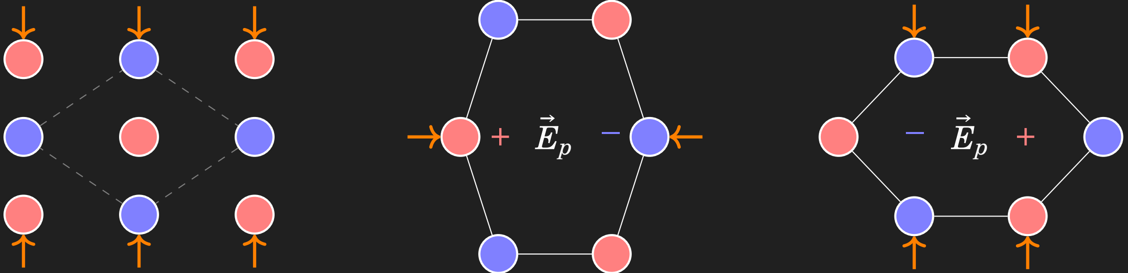

32 Kristallklassen
11 Mit Inversionszentrum
21 Ohne Inversionszentrum
20 Piezoelektrisch
1 Nicht piezoelektrisch



Mit und Ohne Symmetriezentrum

Polarisation Feld $\vec{E}_p$





Licht in Kristallen

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

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

Eingenraum

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

Symmetriegruppe und Darstellung

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

Kann man U_λ von G herauslesen?

$$U_\lambda \stackrel{?}{=} f\left(\bigoplus_{g \in G} \Phi_g \right)$$