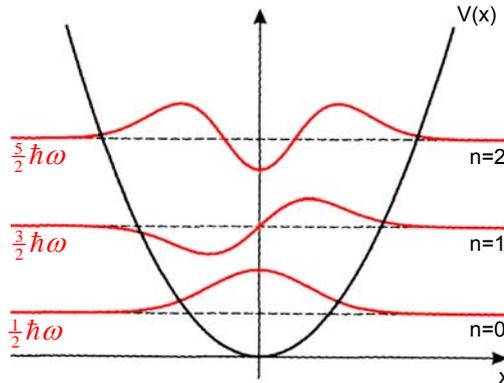


Energieeigenwerte

$$1\text{D: } E_n = (n + \frac{1}{2}) \cdot \hbar\omega; \quad n = 0, 1, 2, \dots$$

$$3\text{D: } E_n = (n_x + \frac{1}{2}) \cdot \hbar\omega_x + (n_y + \frac{1}{2}) \cdot \hbar\omega_y + (n_z + \frac{1}{2}) \cdot \hbar\omega_z$$

$$n_x, n_y, n_z = 0, 1, 2, \dots$$

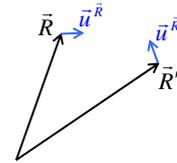
Kleine Fluktuationen der Atome um Gitterpositionen:

$$\vec{r}^{\vec{R}} = \vec{R} + \vec{u}^{\vec{R}}$$

3D Taylor-Entwicklung von (allg.) Potential um Gleichgewichtslage \vec{r}_0 :

$$f(\vec{r}_0 + \Delta\vec{r}) = f(\vec{r}_0) + \Delta\vec{r} \cdot \vec{\nabla} f(\vec{r}) \Big|_{\vec{r}=\vec{r}_0} + \frac{1}{2} [\Delta\vec{r} \cdot \vec{\nabla}]^2 f(\vec{r}) \Big|_{\vec{r}=\vec{r}_0} + \dots$$

$$= f(\vec{r}_0) + \frac{1}{2} \sum_{\alpha, \beta=x,y,z} \Delta r_\alpha \Delta r_\beta \cdot \frac{\partial^2 f(\vec{r})}{\partial r_\alpha \partial r_\beta} \Big|_{\vec{r}=\vec{r}_0}$$



Anwendung auf potentielle Energie des Kristalls:

$$U = \frac{1}{2} \sum_{\vec{R}, \vec{R}'} \phi(\vec{r}^{\vec{R}} - \vec{r}^{\vec{R}'}) = \underbrace{\frac{1}{2} \sum_{\vec{R}, \vec{R}'} \phi(\vec{R} - \vec{R}')}_{U_{Cl}} + \underbrace{\frac{1}{4} \sum_{\vec{R}, \vec{R}'} [(\vec{u}^{\vec{R}} - \vec{u}^{\vec{R}'} \cdot \vec{\nabla}]^2 \phi(\vec{R} - \vec{R}')}_{U_{harm}} + \dots$$

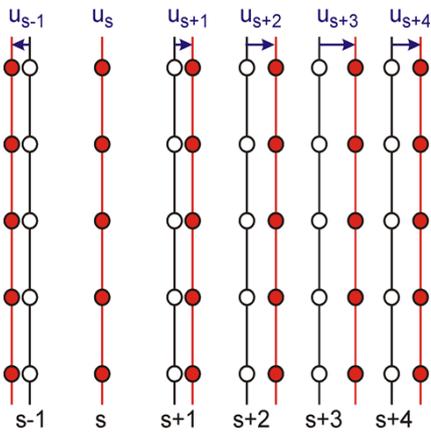
Harmonische Näherung: Abbruch nach Termen 2. Ordnung

$$U_{harm} = \frac{1}{4} \sum_{\substack{\vec{R}, \vec{R}' \\ \alpha, \beta=x,y,z}} (u_\alpha^{\vec{R}} - u_\alpha^{\vec{R}'}) \phi_{\alpha\beta}(\vec{R} - \vec{R}') (u_\beta^{\vec{R}} - u_\beta^{\vec{R}'}) \quad ; \quad \phi_{\alpha\beta}(\vec{r}) \equiv \frac{\partial^2 \phi(\vec{r})}{\partial r_\alpha \partial r_\beta}$$

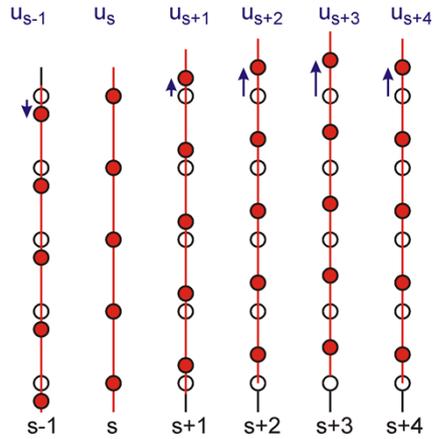
$$\text{Allgemeinere Form: } U_{harm} = \frac{1}{2} \sum_{\substack{\vec{R}, \vec{R}' \\ \alpha, \beta=x,y,z}} u_\alpha^{\vec{R}} D_{\alpha\beta}(\vec{R} - \vec{R}') u_\beta^{\vec{R}'} \quad ; \quad D_{\alpha\beta}(\vec{r}) \equiv \text{Kopplungskonstanten}$$

(nach Ashcroft/Mermin)

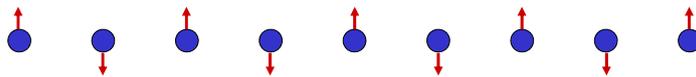
Longitudinale Wellen



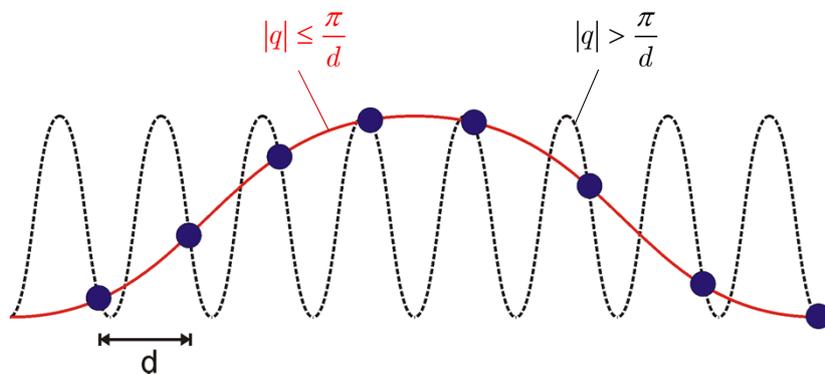
Transversale Wellen



Stehende Wellen, falls q auf Rand der 1. Brillouin Zone liegt („Bragg-Reflexion“):



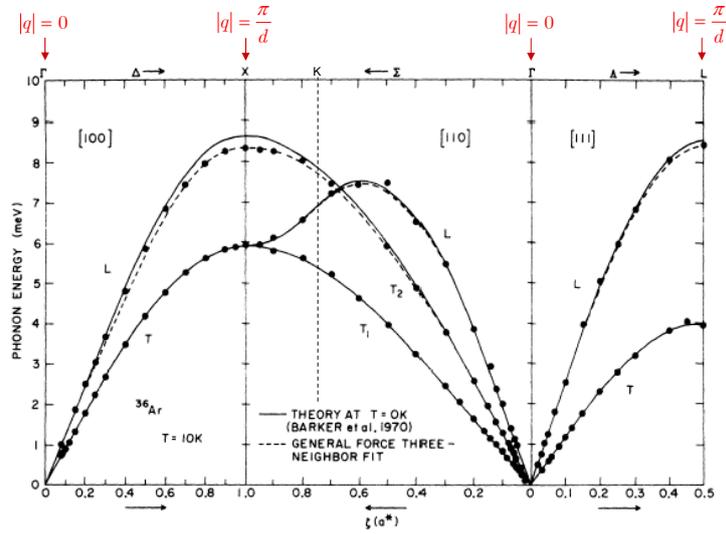
Alle möglichen Gitterschwingungen können durch Wellen mit q in der 1. Brillouin Zone beschrieben werden.



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Phononendispersionsrelation

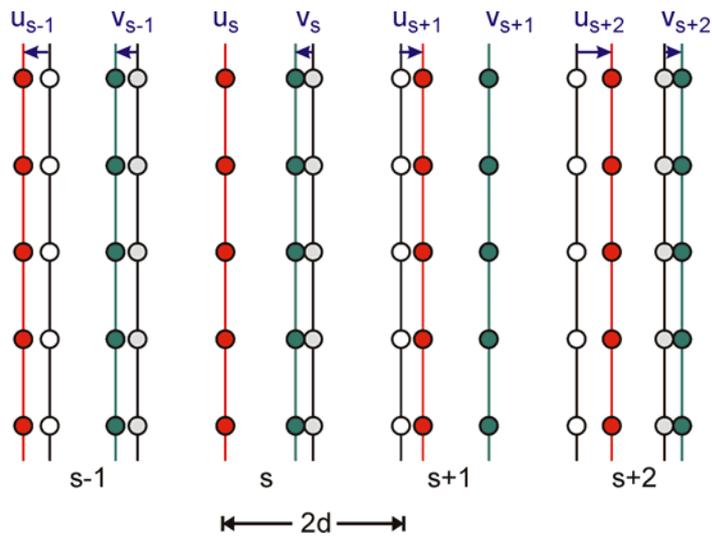
Beispiel: Dispersionsrelation für ^{36}Ar



Fujii, et al., PRB 10 (1974) 3647

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Gitterschwingungen mit 2 Atomen / EZ

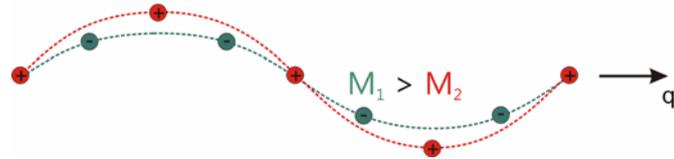


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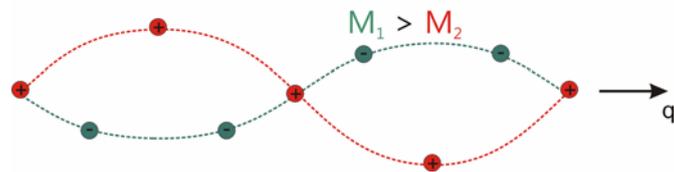
Akustische und optische Phononen

Mitte der Brillouinzone ($q = 0$)

Akustisches Phonon



Optisches Phonon

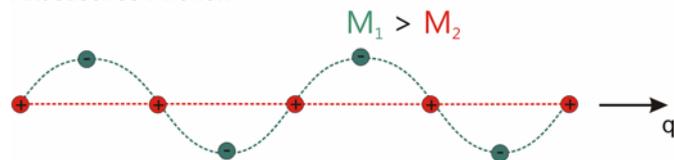


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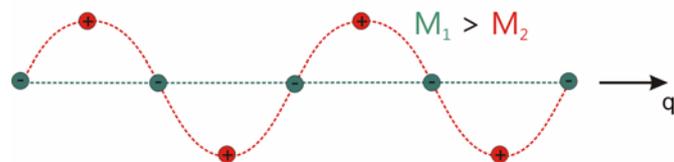
Akustische und optische Phononen

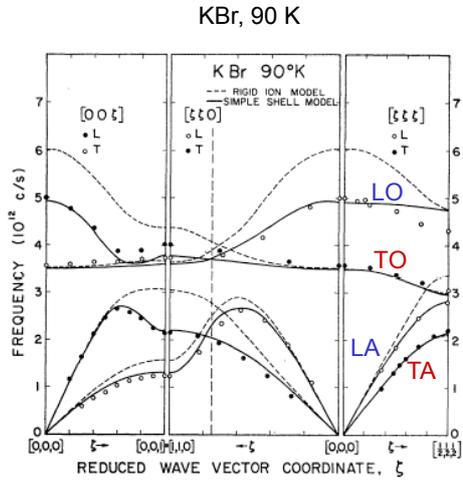
Rand der Brillouinzone ($q = 2\pi/d$)

Akustisches Phonon

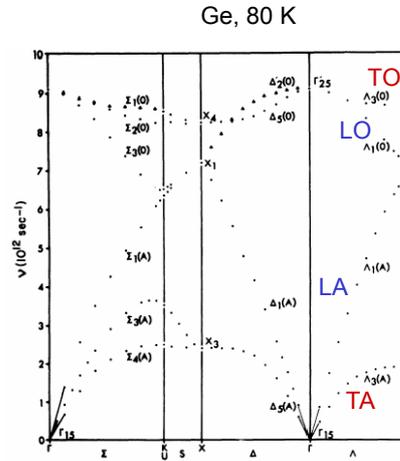


Optisches Phonon



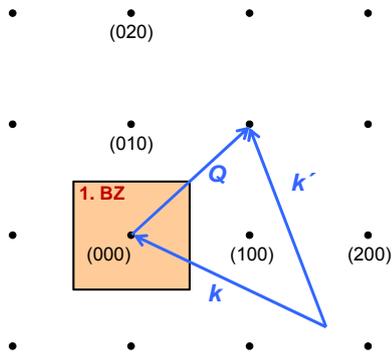


A.D.B. Wods, et al., Phys.Rev. 13 (1963) 1025



G. Nilson und G. Neling, PRB 3 (1971) 364

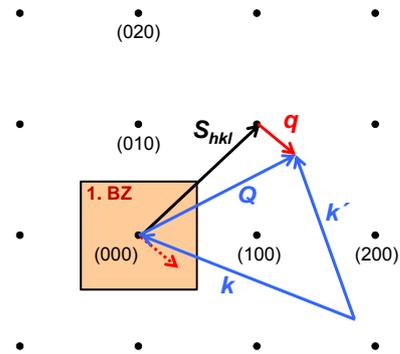
Elastische Streuung



$$E' = E$$

$$k' = k + G$$

Inelastische Streuung an Phonon mit Wellenvektor q und Frequenz $\omega(q)$

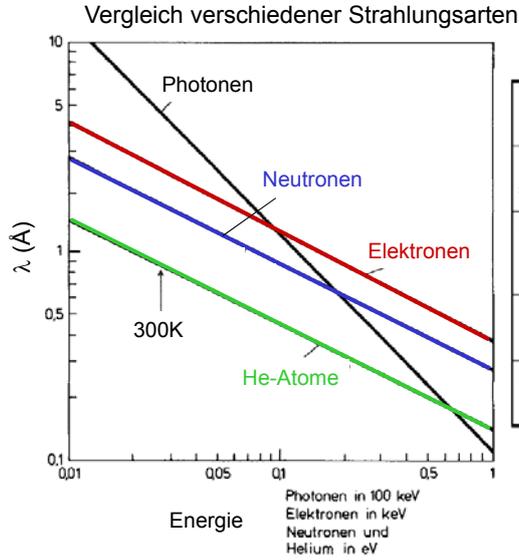


$$E' = E \pm \hbar \omega$$

$$k' = k + G \pm q$$

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Sonden für Streuexperimente

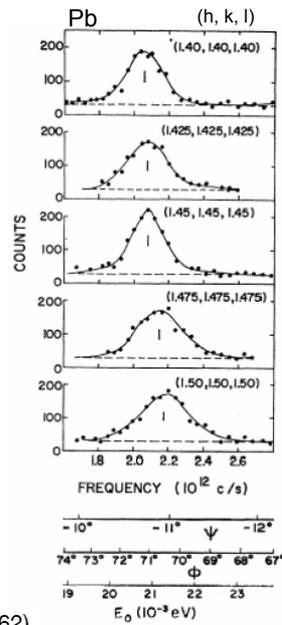
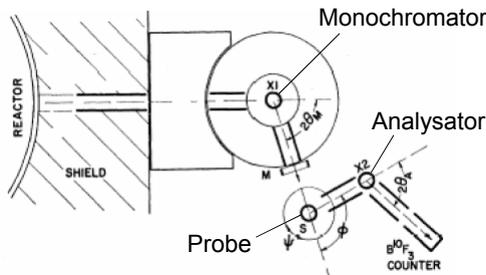


	$E (\lambda = 1 \text{ \AA})$	Wechselwirkung	Eindringtiefe
Röntgenstrahlung	12,4 keV	Elektronen	$\approx \mu\text{m}$ ($\approx 20 \text{ \AA}$)
Neutronen	80 meV	Kern magnet. Moment	$\approx \text{mm}$
Elektronen	144 eV	Elektronen	$\approx 10 \text{ \AA}$
He-Atome	20 meV	Elektronen	oberste Schicht

Nach Ibach/Lüth, 6. Aufl., S. 67

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Inelastische Neutronenstreuung

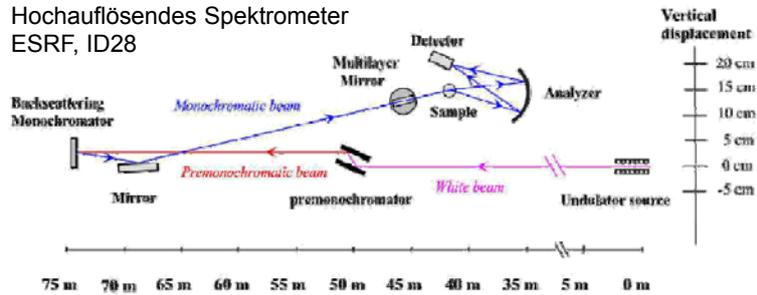


B. N. Brockhouse *et al.*, *Phys. Rev.* **128**, 1099 (1962)

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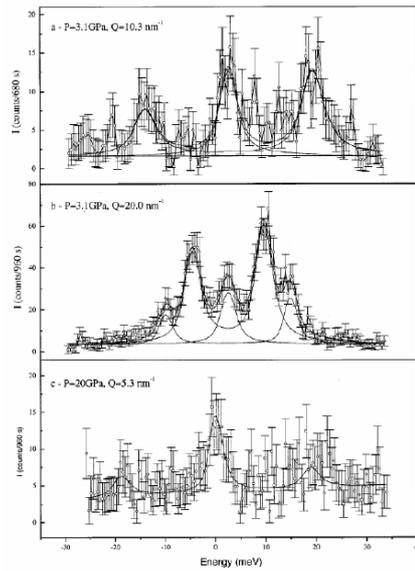
Inelastische Röntgenstreuung

Hochauflösendes Spektrometer
ESRF, ID28

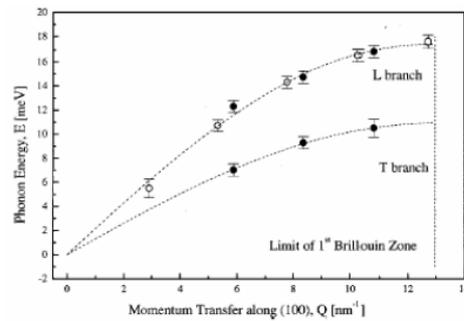


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Inelastische Röntgenstreuung



Messungen an Argon bei 20 GPa Druck
ESRF, ID 16



F. Occelli et al., *Phys. Rev. B* **63**, 224306 (2001)