Solid State Theory I+II **SS 2024**

Registration required: https://lv.physik.uni-kl.de/registration/
All material will be found online: https://www.physik.uni-kl.de/eggert/festkoerper/

Lectures: Mo. 11:45-13:45 in room 46-576 (starting 22.4.2024)
Thu. 10:00-11:30 in room 46-576
Sebastian Eggert, Office: 46-551, Tel.: 205-2375 e-mail: seggert

Excercises: Wed 13:45-15:15 in room 46-387 (starting 8.5.2024)
Larissa Schwarz, Office: 46-554, Tel.: 205-2299 e-mail: laschwar

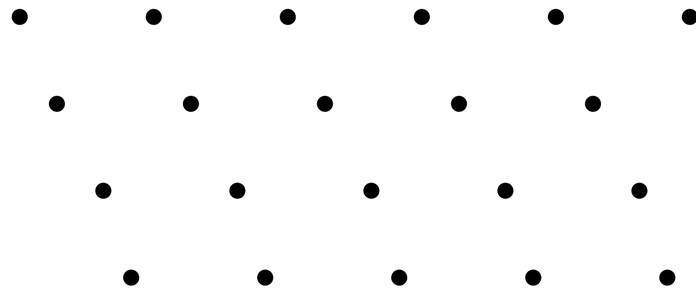
Suggested literature:
1. Ashcroft and Mermin: Solid State Physics, Saunders College, 1976.
2. Altland and Simon: Condensed Matter Field Theory (Cambridge)
3. Czycholl: Theoretische Festkörperphysik, Springer 2004
4. Kittel: Quantum Theory of Solids, Wiley, 1963. (Quantentheorie der Festkörper, Oldenburg)
5. Nolting: Grundkurs Theoretische Physik, Bd. 7: Vielteilchentheorie, Springer 2004.
6. Rössler: Solid State Theory, Springer 2004

Springer books are free of charge via the library.

Contents:

1. Lattices and Phonons: Fourier-Transformation, 2^{nd} Quantization, Phonon thermodynamics
2. Electrons: Calculating Band-Structure, Hubbard interaction
3. Superconductivity: Electron-Phonon-Interaction, BCS and Ginzburg-Landau Theory
4. Magnetism: Magnons, Phase Transitions, Quantum Hall Effect

<u>What is a solid?</u>



Def. 1.1 The Bravais lattice: Vectors of the form $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

$n_{1,} n_2, n_3$ are integers.

The **primitive vectors** $\vec{a}_1, \vec{a}_2, \vec{a}_3$ define the lattice.

The **unit cell** is the volume which is periodically repeated around each lattice point.

The **basis** is the content of the unit cell.

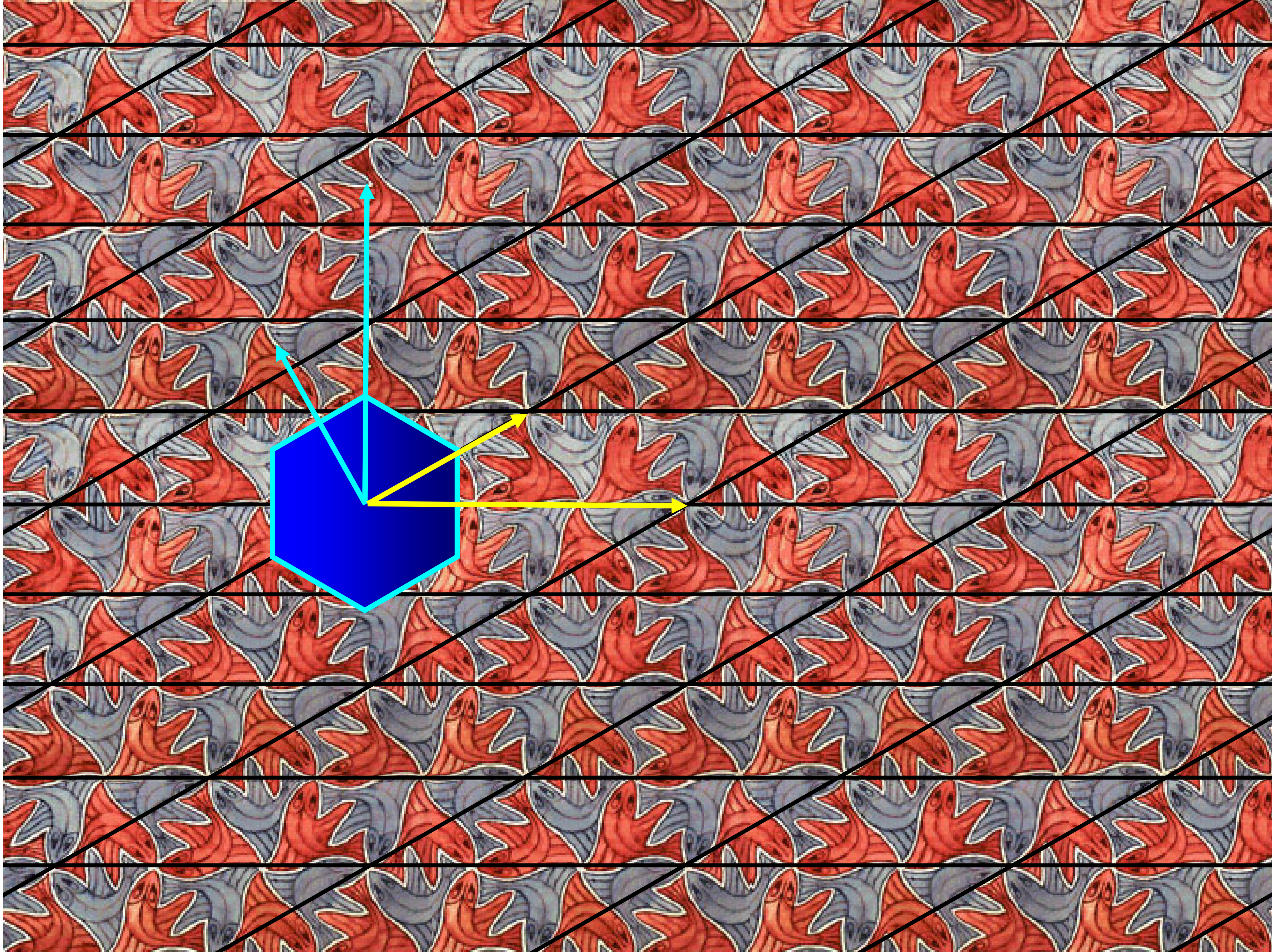
The **Wigner-Seitz unit cell** is the volume, which is closest to one lattice point.

Def. 1.2 The reciprocal lattice: Vectors $\vec{G}$ for which $\vec{R} \cdot \vec{G} = 2\pi m$ m is an integer

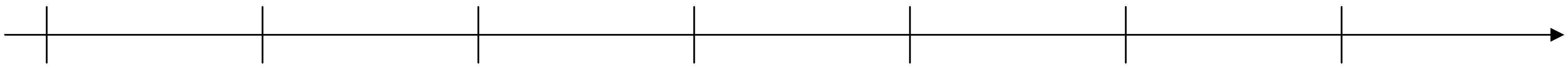
Claim: Vectors $\vec{G}$ is also a Bravais lattice.

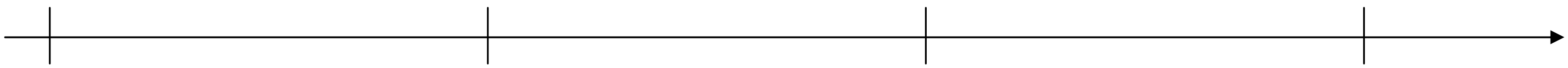
The **First Brillouin Zone (1BZ)** is the Wigner-Seitz unit cell in reciprocal space.

The **Bragg planes** are the half-planes between two reciprocal lattice points



One-dimensional example:





A discrete Fourier transformation is a linear map of a function on a Bravais lattice to the 1BZ

Def. 1.3 The 1D discrete Fourier transformation on a (finite) lattice

Given: A complex valued function $f(na)$ for discrete values, $n=1,2,...N$ integer

The Fourier transformation is $\tilde{f}_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikna} f(na)$ $\quad k = \frac{2\pi}{Na} m$ $\quad m = -N/2, \ldots, N/2-1$ integer

Claim: The inverse Fourier transformation is given by $f(na) = \frac{1}{\sqrt{N}} \sum_{k \in 1BZ} e^{-ikna} \tilde{f}_k$

Generalization to $N \to \infty$

$$\tilde{f}_k = \sqrt{\frac{a}{2\pi}} \sum_{n=-\infty}^{\infty} e^{ikna} f(na)$$

Inverse transformation:

$$f(na) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} e^{-ikna} \tilde{f}_k \, dk$$

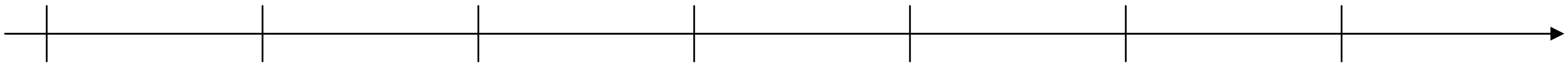
Generalization to $N \to \infty$ and $a \to 0$

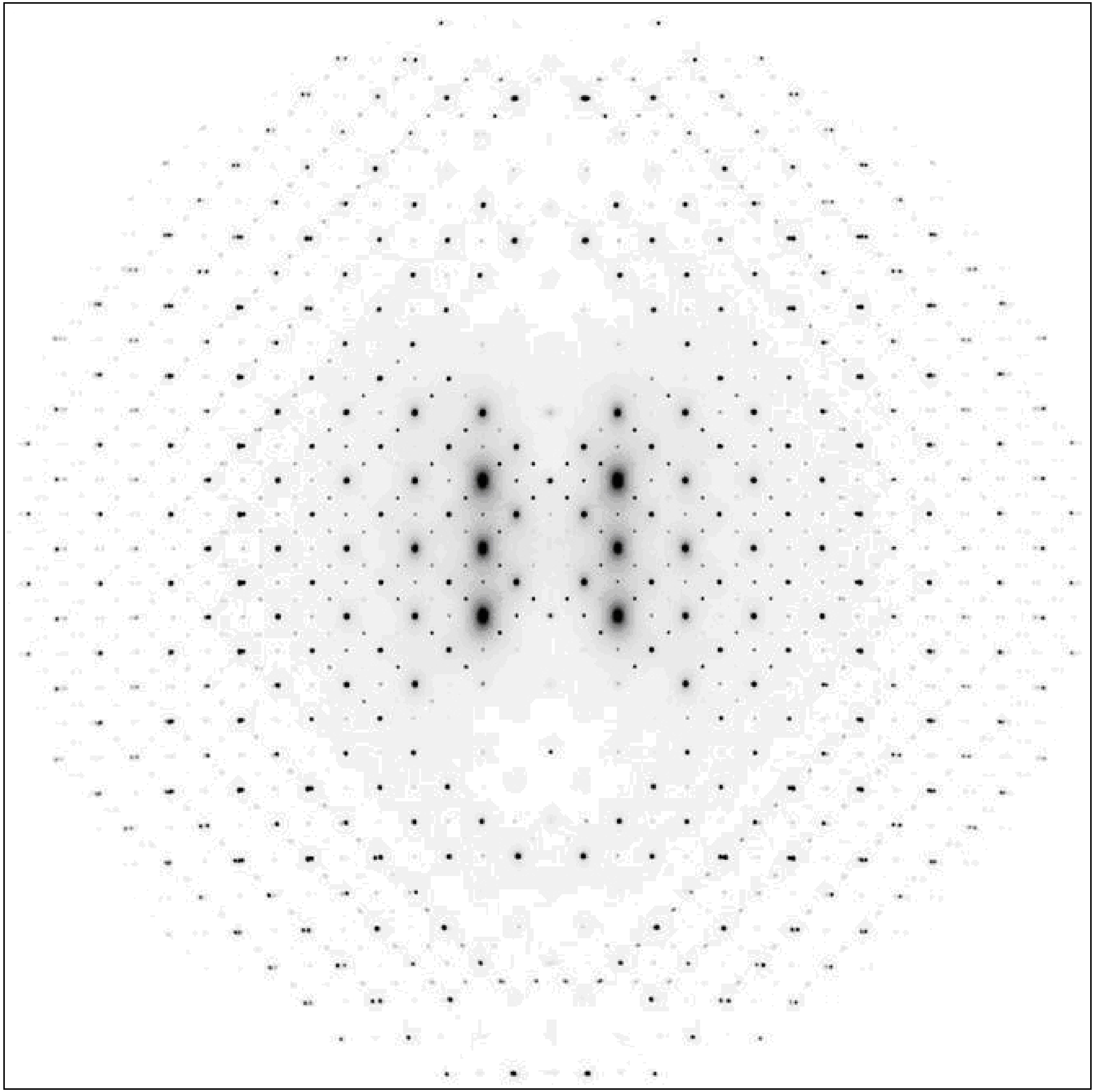
$$\tilde{f}_k = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} e^{ikx} f(x) dx$$

Inverse transformation:

$$f(x) = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \tilde{f}_k dk$$

Special case: $f(x) = f(x+a)$ is periodic on a lattice





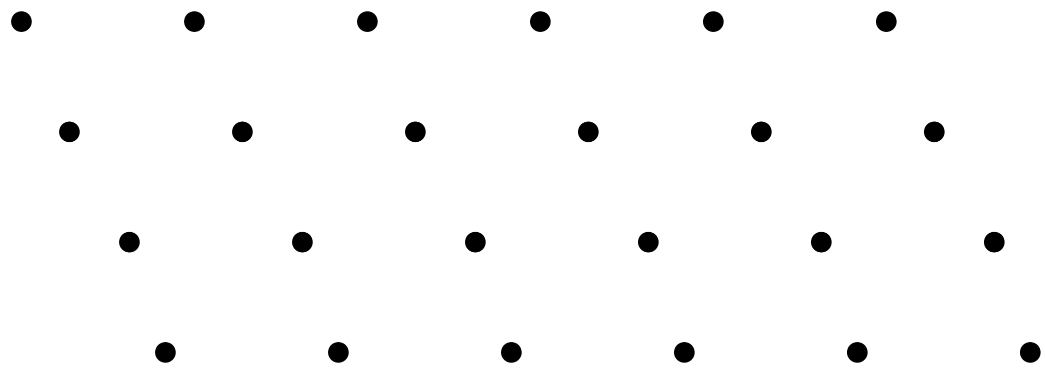
Fourier transformation on a **3D** Bravais lattice

$$\tilde{f}_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} f(\vec{R}) = \frac{1}{\sqrt{N}} \sum_{m_1=-\infty}^{\infty} e^{im_1\vec{k}\cdot\vec{a}_1} \sum_{m_2=-\infty}^{\infty} e^{im_2\vec{k}\cdot\vec{a}_2} \sum_{m_3=-\infty}^{\infty} e^{im_3\vec{k}\cdot\vec{a}_3} f(\vec{R})$$

Inverse transformation:

$$f(\vec{R}) = \frac{1}{\sqrt{N}} \sum_{\vec{k}\in V_{1BZ}} e^{-i\vec{k}\cdot\vec{R}} \tilde{f}_{\vec{k}}$$

Classical lattice vibrations



Each nuclear position $\vec{R}_j$

can be displaced by $\vec{u}_j(t)$

Born Oppenheimer approximation:

Electron configuration adjust much faster (instantaneously), so at any time the nuclear positions feel an effective electrostatic potential of their positions

$$V\left(\vec{R}_1 + \vec{u}_1(t), \vec{R}_2 + \vec{u}_2(t), \ldots, \vec{R}_N + \vec{u}_N(t)\right)$$

Harmonic approximation:

Taylor expansion to second order in displacements

$$V\left(\vec{R}_1+\vec{u}_1,\vec{R}_2+\vec{u}_2,\ldots,\vec{R}_N+\vec{u}_N\right)$$
$$\approx V\left(\vec{R}_1,\vec{R}_2,\ldots,\vec{R}_N\right)+\sum_j\sum_{\alpha=x,y,z}\frac{\partial V}{\partial R_j^\alpha}u_j^\alpha+\frac{1}{2}\sum_{j,l}\sum_{\alpha,\beta=x,y,z}\frac{\partial^2 V}{\partial R_j^\alpha\partial R_l^\beta}u_j^\alpha u_l^\beta$$

Def. 1.4 The dynamical Matrix $D_{j,l}^{\alpha\beta}=\frac{\partial^2 V}{\partial R_j^\alpha\partial R_l^\beta}$ couples the components of the displacements between sites j and l

Effective harmonic model:

$$H = \sum_j \frac{\vec{p}_j^{\,2}}{2m} + \frac{1}{2}\sum_{j,l}\sum_{\alpha\beta} D_{j,l}^{\alpha\beta} u_j^{\alpha} u_l^{\beta}$$

Quantum mechanical description: Momentum and displacement operators

$$u_j^\alpha \to \hat{X}_j^\alpha$$

$$p_j^\alpha \to \hat{P}_j^\alpha$$

$$[\hat{X}_j^\alpha, \hat{P}_l^\beta] = i\delta_{jl}\delta_{\alpha\beta}\hbar$$

Fourier transformation of operators on the lattice:

$$X_{\vec{k}}^\alpha = \frac{1}{\sqrt{N}} \sum_j e^{i\vec{k}\cdot\vec{R}_j} X_j^\alpha$$

inverse: $$X_j^\alpha = \frac{1}{\sqrt{N}} \sum_{\vec{k}\in V_{1BZ}} e^{-i\vec{k}\cdot\vec{R}_j} X_{\vec{k}}^\alpha$$

$$P_{\vec{k}}^\alpha = \frac{1}{\sqrt{N}} \sum_j e^{-i\vec{k}\cdot\vec{R}_j} P_j^\alpha$$

inverse: $$P_j^\alpha = \frac{1}{\sqrt{N}} \sum_{\vec{k}\in V_{1BZ}} e^{i\vec{k}\cdot\vec{R}_j} P_{\vec{k}}^\alpha$$

Commutators of Fourier transformed operators:

$$[\hat{X}^{\alpha}_{\vec{k}_1}, \hat{P}^{\beta}_{\vec{k}_2}] = \frac{1}{N}\sum_{j,l} e^{i\vec{k}_1\cdot\vec{R}_j} e^{-i\vec{k}_2\cdot\vec{R}_l} [\hat{X}^{\alpha}_{j}, \hat{P}^{\beta}_{l}]$$

Solution by Fourier transformation:

$$H = \sum_j \frac{\vec{P}_j^2}{2m} + \frac{1}{2}\sum_{j,l}\sum_{\alpha\beta} D_{j,l}^{\alpha\beta} X_j^{\alpha} X_l^{\beta}$$

Kinetic energy:

$$\sum_j \frac{\vec{P}_j^2}{2m} = \frac{1}{2m}\sum_j \sum_{\alpha=x,y,z} P_j^{\alpha} P_j^{\alpha} = \frac{1}{2mN}\sum_j \sum_{\alpha=x,y,z} \sum_{\vec{k}_1,\vec{k}_2\in V_{1BZ}} e^{i\vec{k}_1\cdot\vec{R}_j} P_{\vec{k}_1}^{\alpha} e^{i\vec{k}\cdot_2\vec{R}_j} P_{\vec{k}_2}^{\alpha} =$$

Coupling of dynamical matrix:

$$\frac{1}{2}\sum_{j,l}\sum_{\alpha\beta} D_{j,l}^{\alpha\beta} X_j^{\alpha} X_l^{\beta} = \frac{1}{2N}\sum_{j,l}\sum_{\alpha\beta} D_{j,l}^{\alpha\beta} \sum_{\vec{k}_1,\vec{k}_2\in V_{1BZ}} e^{-i\vec{k}_1\cdot\vec{R}_j} X_{\vec{k}_1}^{\alpha} e^{-i\vec{k}\cdot_2\vec{R}_l} X_{\vec{k}_2}^{\beta}$$

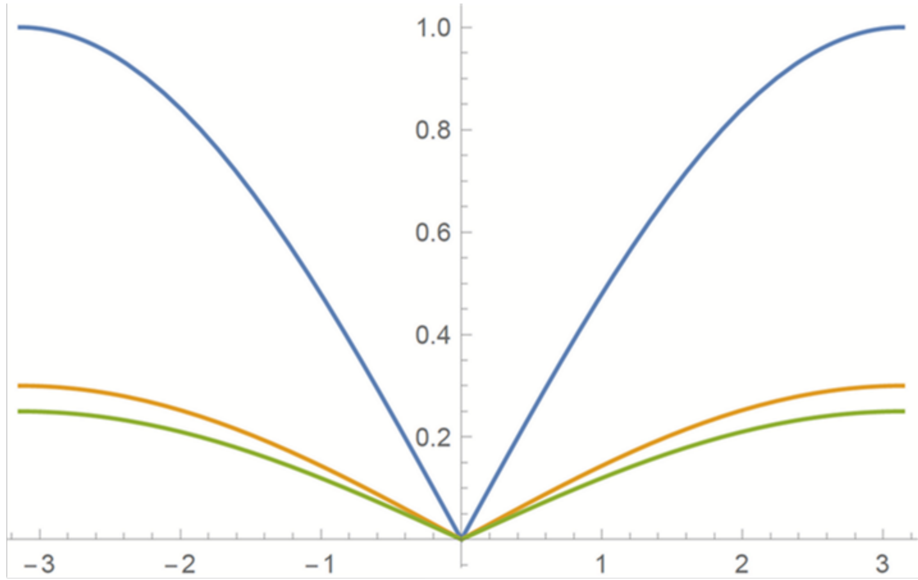
Define Fourier transformation of $D_{i,l}^{\alpha\beta} = D^{\alpha\beta}(\vec{R}_j - \vec{R}_l) = D^{\alpha\beta}(\Delta\vec{R}_{jl})$

$$\sum_{j,l} e^{-i\vec{k}_1\cdot\vec{R}_j} e^{-i\vec{k}\cdot_2\vec{R}_l} D_{j,l}^{\alpha\beta} = \sum_{\vec{R}_j,\Delta\vec{R}_{jl}} e^{-i\vec{k}_1\cdot\vec{R}_j} e^{-i\vec{k}\cdot_2(\vec{R}_j-\Delta\vec{R}_{jl})} D^{\alpha\beta}(\Delta\vec{R}_{jl}) =$$

Decoupled model in Fourier space:

$$H = \sum_{\vec{k}\in V_{1BZ}} \left(\sum_{\alpha} \frac{P^{\alpha}_{\vec{k}} P^{\alpha}_{-\vec{k}}}{2m} + \frac{1}{2} \sum_{\alpha\beta} D^{\alpha\beta}(\vec{k}) X^{\alpha}_{\vec{k}} X^{\beta}_{-\vec{k}} \right)$$

Properties of the dynamical matrix: Transverse and longitudinal modes



Define creation and annihilation operators for independent oscillators

$$H=\sum_{\vec{k}\in V_{1BZ}}\sum_{\alpha}\left(\frac{P_{\vec{k}}^{\alpha}P_{-\vec{k}}^{\alpha}}{2m}+\frac{1}{2}\widetilde{D}^{\alpha}(\vec{k})X_{\vec{k}}^{\alpha}X_{-\vec{k}}^{\alpha}\right)=\sum_{\vec{k}\in V_{1BZ}}\sum_{\alpha}\left(\frac{P_{\vec{k}}^{\alpha}P_{-\vec{k}}^{\alpha}}{2m}+\frac{1}{2}m(\omega_{\vec{k}}^{\alpha})^{2}X_{\vec{k}}^{\alpha}X_{-\vec{k}}^{\alpha}\right)$$

$$\hat{a}_{\vec{k}}^{\alpha}=\sqrt{\frac{m\omega_{\vec{k}}^{\alpha}}{2\hbar}}X_{\vec{k}}^{\alpha}+i\sqrt{\frac{1}{2m\omega_{\vec{k}}^{\alpha}\hbar}}P_{-\vec{k}}^{\alpha} \qquad (\hat{a}_{\vec{k}}^{\alpha})^{\dagger}=\sqrt{\frac{m\omega_{\vec{k}}^{\alpha}}{2\hbar}}X_{-\vec{k}}^{\alpha}-i\sqrt{\frac{1}{2m\omega_{\vec{k}}^{\alpha}\hbar}}P_{\vec{k}}^{\alpha}$$

Commutation relations:

$$[\hat{a}_{\vec{k}_1}^{\alpha},(\hat{a}_{\vec{k}}^{\beta})^{\dagger}]=$$

Inverse:

$$P_{\vec{k}}^{\alpha} = i\sqrt{\frac{m\hbar\omega_{\vec{k}}^{\alpha}}{2}}\left((\hat{a}_{\vec{k}}^{\alpha})^{\dagger} - \hat{a}_{-\vec{k}}^{\alpha}\right) \qquad X_{\vec{k}}^{\alpha} = i\sqrt{\frac{\hbar}{2m\omega_{\vec{k}}^{\alpha}}}\left((\hat{a}_{-\vec{k}}^{\alpha})^{\dagger} + \hat{a}_{\vec{k}}^{\alpha}\right)$$

$$H = \sum_{\vec{k}\in V_{1BZ}}\sum_{\alpha}\left(\frac{P_{\vec{k}}^{\alpha}P_{-\vec{k}}^{\alpha}}{2m} + \frac{1}{2}m(\omega_{\vec{k}}^{\alpha})^{2}X_{\vec{k}}^{\alpha}X_{-\vec{k}}^{\alpha}\right) =$$

Dynamics of a phonon mode:

$$H = \sum_{\vec{k}\in V_{1BZ}} \sum_{\alpha} H_{\vec{k}}^{\alpha} \qquad H_{\vec{k}}^{\alpha} = \hbar\omega_{\vec{k}}^{\alpha}\left((\hat{a}_{\vec{k}}^{\alpha})^{\dagger}\hat{a}_{\vec{k}}^{\alpha} + \tfrac{1}{2}\right)$$

$$i\hbar\partial_t \hat{a}_{\vec{k}}^{\alpha} = [\hat{a}_{\vec{k}}^{\alpha}, H_{\vec{k}}^{\alpha}] = \hbar\omega_{\vec{k}}^{\alpha}\hat{a}_{\vec{k}}^{\alpha}$$

$$\hat{a}_{\vec{k}}^{\alpha}(t) = e^{-i\omega_{\vec{k}}^{\alpha}t}\left(\sqrt{\frac{m\omega_{\vec{k}}^{\alpha}}{2\hbar}}X_{\vec{k}}^{\alpha} + i\sqrt{\frac{1}{2m\omega_{\vec{k}}^{\alpha}\hbar}}P_{-\vec{k}}^{\alpha}\right)$$