Visualisation of Concepts in Condensed Matter Physics

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Outline

- Introduction
- Background
- Lattices and crystal structure
- The reciprocal lattice and scattering
- Band structure

Introduction

Background

Bloch's theorem

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r}) = \sum_{\mathbf{G}} u_{\mathbf{G},\mathbf{k}} e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}}$$

Lattices and crystal structure

$$\mathbf{R} = \sum_{i=1}^{d} n_i \mathbf{a}_i$$

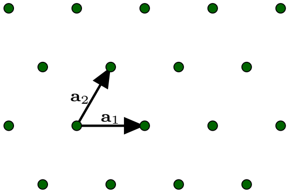

Figure: A triangular lattice. $\mathbf{a}_1 = a \cdot (1, 0)$, $\mathbf{a}_2 = a \cdot (1/2, \sqrt{3}/2)$

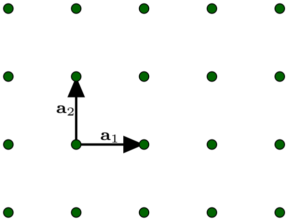

Figure: A square lattice. $\mathbf{a}_1 = a \cdot (1, 0), \mathbf{a}_2 = a \cdot (0, 1)$

Lattices and crystal structure

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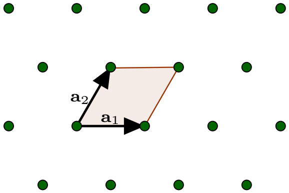

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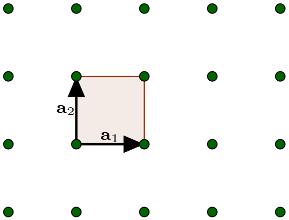

Figure: A square lattice. $\mathbf{a}_1 = a \cdot (1,0), \mathbf{a}_2 = a \cdot (0,1)$

Lattices and crystal structure

$$\mathbf{r}_{atom,i} = \mathbf{R} + \mathbf{r}_{basis,i}$$

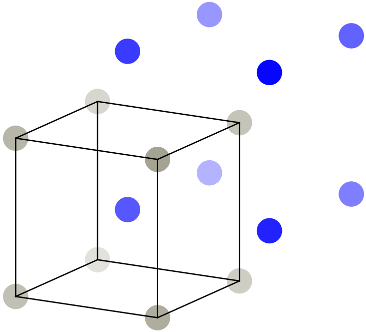

Figure: Conventional unit cell of a bcc lattice. Two atoms, one (grey) at $a \cdot (0, 0, 0)$ and one (blue) at $a \cdot (1/2, 1/2, 1/2)$

Lattices and crystal structure

Reciprocal lattice and scattering

$$e^{i\mathbf{G}\cdot\mathbf{R}} = 1,$$

$$\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3, \quad \mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$

$$\mathbf{b}_1 = \frac{2\pi\, \mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \quad \mathbf{b}_2 = \frac{2\pi\, \mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)},$$

$$\mathbf{b}_3 = \frac{2\pi\, \mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)},$$

Fermi's Golden Rule

$$\Gamma(\mathbf{k}', \mathbf{k}) = \frac{2\pi}{\hbar} | \langle \mathbf{k}' | V | \mathbf{k} \rangle |^2 \delta(E_{\mathbf{k}'} - E_{\mathbf{k}}), \tag{1}$$