Visualisation of Concepts in Condensed Matter Physics

Nikolai Plambech Nielsen
Niels Bohr Institute

Supervised by Mark Spencer Rudner

Outline

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

Introduction / Background

Periodic medium. Discrete translational symmetry

$$[\hat{T}_{\mathbf{R}}, \hat{H}] = 0, \quad V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r}),$$

Introduction / Background

Periodic medium. Discrete translational symmetry

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Bloch's theorem:

$$\begin{aligned}\psi(\mathbf{r}) &= e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r}), \quad u(\mathbf{r} + \mathbf{R}) = u(\mathbf{r}), \\ &= \sum_{\mathbf{G}} u_{\mathbf{G},\mathbf{k}} e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}}.\end{aligned}$$

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Crystal momentum. One dimension, spacing of a:

$$k \to k + \frac{2\pi}{a}, \quad -\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$$

Lattices and crystal structure

The lattice [1]

$$\mathbf{R} = \sum_{i=1}^{d} n_i \mathbf{a}_i, \quad n_i \in \mathbb{Z}$$

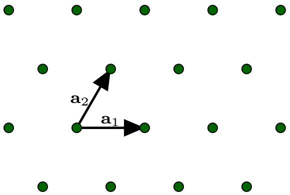


Figure: A triangular lattice. $\mathbf{a}_1 = a \cdot (1,0)$, $\mathbf{a}_2 = a \cdot (1/2, \sqrt{3}/2)$.

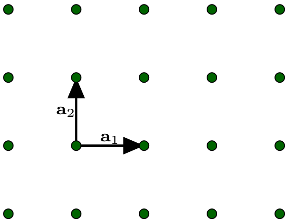
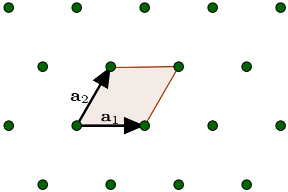


Figure: A square lattice. $\mathbf{a}_1 = a \cdot (1,0), \mathbf{a}_2 = a \cdot (0,1)$.

Lattices and crystal structure

The unit cell

$$\mathbf{R} = \sum_{i=1}^{d} n_i \mathbf{a}_i, \quad n_i \in \mathbb{Z}$$



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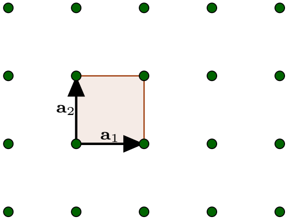

Figure: A square lattice. $\mathbf{a}_1 = a \cdot (1, 0), \mathbf{a}_2 = a \cdot (0, 1)$.

Lattices and crystal structure

The basis

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

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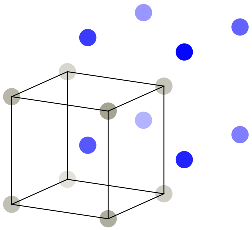

Figure: Simple cubic lattice with a two atom basis. One (grey) at $a \cdot (0,0,0)$ and one (blue) at $a \cdot (1/2, 1/2, 1/2)$.

Lattices and crystal structure

Demonstration

Reciprocal lattice and scattering

The reciprocal lattice

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

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3, \quad h, k, l \in \mathbb{Z}$$

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij},\ [2]$$

Reciprocal lattice and scattering

Scattering

Free particles:

$$E_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}, \quad E_{\mathbf{k}'} = \frac{\hbar^2 \mathbf{k}'^2}{2m}$$

Fermi's Golden Rule: [1]

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

Reciprocal lattice and scattering

Scattering

$$
\begin{aligned}
\langle \mathbf{k}' | V | \mathbf{k} \rangle &= \int_{-\infty}^{+\infty} \frac{e^{-i\mathbf{k}'\cdot\mathbf{r}}}{\sqrt{L^3}} V(\mathbf{r}) \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{L^3}} \, \mathrm{d}\mathbf{r}, \\
&= \frac{1}{L^3} \int_{-\infty}^{+\infty} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} \, V(\mathbf{r}) \, \mathrm{d}\mathbf{r}.
\end{aligned}
$$

Reciprocal lattice and scattering

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&= \frac{1}{L^3}\int_{-\infty}^{+\infty} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}\, V(\mathbf{r})\,\mathrm{d}\mathbf{r}. \\
V(\mathbf{r}+\mathbf{R}) &= V(\mathbf{r}), \quad \mathbf{r} = \mathbf{R}+\mathbf{x}, \\
\langle \mathbf{k}'|V|\mathbf{k}\rangle &= \frac{1}{L^3}\sum_{\mathbf{R}} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}} S(\mathbf{k}'-\mathbf{k}), \\
S(\mathbf{k}'-\mathbf{k}) &= \int_{\substack{\text{unit-}\\\text{cell}}} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}} V(\mathbf{x})\,\mathrm{d}\mathbf{x},
\end{aligned}
$$

Reciprocal lattice and scattering

Scattering

$$\langle \mathbf{k}' | V | \mathbf{k} \rangle = \int_{-\infty}^{+\infty} \frac{e^{-i\mathbf{k}'\cdot\mathbf{r}}}{\sqrt{L^3}} V(\mathbf{r}) \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{L^3}} \, \mathrm{d}\mathbf{r},$$

$$= \frac{1}{L^3} \int_{-\infty}^{+\infty} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} V(\mathbf{r}) \, \mathrm{d}\mathbf{r}.$$

$$V(\mathbf{r}+\mathbf{R}) = V(\mathbf{r}), \quad \mathbf{r} = \mathbf{R} + \mathbf{x},$$

$$\langle \mathbf{k}' | V | \mathbf{k} \rangle = \frac{1}{L^3} \sum_{\mathbf{R}} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}} S(\mathbf{k}'-\mathbf{k}),$$

$$S(\mathbf{k}'-\mathbf{k}) = \int_{\substack{\text{unit-}\\\text{cell}}} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}} V(\mathbf{x}) \, \mathrm{d}\mathbf{x},$$

$$\sum_{\mathbf{R}} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}} = \begin{cases} N, & \mathbf{k}'-\mathbf{k} = \mathbf{G}, \\ 0, & \mathbf{k}'-\mathbf{k} \neq \mathbf{G}. \end{cases}$$

Reciprocal lattice and scattering

Scattering conditions

$$|\mathbf{k}| = |\mathbf{k}'|, \quad \mathbf{k}' - \mathbf{k} = \mathbf{G}.$$

Reciprocal lattice and scattering

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$$I \propto |S(\mathbf{G})|^2. \text{ [1]}$$

Reciprocal lattice and scattering

Neutron scattering on a cubic lattice with a basis

$$V(\mathbf{x}) = \sum_{\text{atoms } j} f_j \, \delta(\mathbf{x} - \mathbf{x}_j),$$

$$S(\mathbf{G}) = \sum_{\text{atoms } j} f_j e^{i\mathbf{G}\cdot\mathbf{x}_j}.$$

Reciprocal lattice and scattering

Systemic absences

$$S(\mathbf{G}) = S_{hkl} = \sum_{\text{atoms } j} f_j e^{2\pi i(hx_j + ky_j + lz_j)}$$

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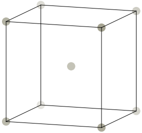
bcc ($h + k + l$ even)

$$S_{hkl} = f(1 + (-1)^{h+k+l})$$



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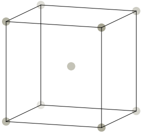
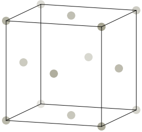


fcc (h, k, l all even or odd)

$$S_{hkl} = f(1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)})$$



Reciprocal lattice and scattering

Demonstration

Band structure

Introduction

2 dimensional square lattice.

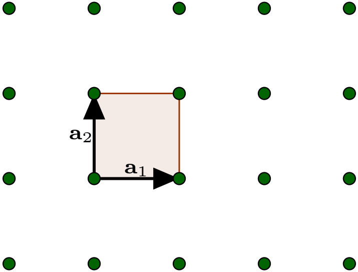


Figure: A square lattice. $\mathbf{a}_1 = a \cdot (1,0), \mathbf{a}_2 = a \cdot (0,1)$.

Band structure

Introduction

2 dimensional square lattice.

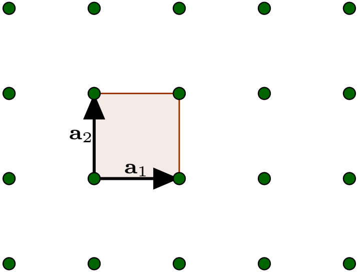


Figure: A square lattice. $\mathbf{a}_1 = a \cdot (1, 0), \mathbf{a}_2 = a \cdot (0, 1)$.

First Brillouin zone: $-\pi/a \leq k_i \leq \pi/a$

Band structure

Fourier transform the Schrödinger equation

$$V(\mathbf{r}+\mathbf{R}) = V(\mathbf{r}) \quad \Leftrightarrow \quad V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}},$$

$$V_{\mathbf{G}} = \frac{1}{a^2} \int_{\substack{\text{unit-}\\ \text{cell}}} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}} V(\mathbf{x})\ \mathrm{d}\mathbf{x},$$

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$$\sum_{\mathbf{G}} \left[\frac{\hbar^2 \mathbf{k}^2}{2m} \delta_{\mathbf{G},0} + V_{\mathbf{G}} \right] \tilde{\psi}(\mathbf{k}-\mathbf{G}) = E\tilde{\psi}(\mathbf{k}).$$

Band structure

Matrix equation and notation

$$V_{\mathbf{G}} = V_{[m_1,m_2]}, \quad \mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2,$$

$$|\psi\rangle = \begin{pmatrix} \vdots \\ \tilde{\psi}(\mathbf{k}-\mathbf{G}_1) \\ \tilde{\psi}(\mathbf{k}) \\ \tilde{\psi}(\mathbf{k}+\mathbf{G}_1) \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \psi_{[0,-1]} \\ \psi_{[0,0]} \\ \psi_{[0,1]} \\ \vdots \end{pmatrix},$$

Band structure

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$$T = \frac{\hbar^2}{2m} \begin{pmatrix} \ddots & & & & \\ & (\mathbf{k}-\mathbf{G}_1)^2 & & & \\ & & \mathbf{k}^2 & & \\ & & & (\mathbf{k}+\mathbf{G}_1)^2 & \\ & & & & \ddots \end{pmatrix}.$$

Band structure

The potential matrix

$$
\begin{aligned}
[m_1, m_2] \in \{&[-1,-1],[-1,0],[-1,1],\\
&[0,-1],[0,0],[0,1],\\
&[1,-1],[1,0],[1,1]\}.
\end{aligned}
$$

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\end{aligned}
$$

$$
\begin{aligned}
E\psi_{[-1,0]} &= \sum_{m_1'=-\infty}^{\infty}\sum_{m_2'=-\infty}^{\infty} V_{[m_1',m_2']}\ \psi_{[-1-m_1',-m_2']},\\
&= \dots + V_{[-2,-1]}\psi_{[1,1]} + V_{[-2,0]}\psi_{[1,0]} + V_{[-2,1]}\psi_{[1,-1]} + \dots\\
&\quad + V_{[-1,-1]}\psi_{[-2,1]} + V_{[-1,0]}\psi_{[-2,0]} + V_{[-1,1]}\psi_{[-2,-1]} + \dots\\
&\quad + V_{[0,-1]}\psi_{[-1,1]} + V_{[0,0]}\psi_{[-1,0]} + V_{[0,1]}\psi_{[-1,-1]} + \dots\\
&\quad + V_{[1,-1]}\psi_{[0,1]} + V_{[1,0]}\psi_{[0,0]} + V_{[1,1]}\psi_{[0,-1]} + \dots .
\end{aligned}
$$

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\end{aligned}
$$

Row $[m_1, m_2]$, column $[m_1', m_2']$: $V_{[m_1-m_1', m_2-m_2']}$.

Band structure

Specific potentials

$$V_{\text{dirac}}(\mathbf{r}) = V_0 a^2 \sum_{\mathbf{R}} \delta(\mathbf{r} - \mathbf{R}), \quad V_{\text{dirac},\mathbf{G}} = V_0,$$

Band structure

Specific potentials

$$V_{\text{dirac}}(\mathbf{r}) = V_0 a^2 \sum_{\mathbf{R}} \delta(\mathbf{r} - \mathbf{R}), \quad V_{\text{dirac},\mathbf{G}} = V_0,$$

$$V_{\text{harmonic}}(\mathbf{r}) = V_0 \left[\cos\left(\frac{2\pi}{a}x\right) + \cos\left(\frac{2\pi}{a}y\right)\right],$$

$$V_{\text{harmonic},\mathbf{G}} = \begin{cases} \frac{V_0}{2} & \text{if } [m_1, m_2] \in \{[0,1],[0,-1],[1,0],[-1,0]\}, \\ 0 & \text{else.} \end{cases}$$

Band structure

Specific potentials

$$m_1, m_2 \in \{-1, 0, 1\}$$

$$V_{\text{harmonic}} = \frac{V_0}{2} \begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}.$$

Band structure

Dimensionless quantities

Define $k_0 \equiv 2\pi/a, E_0 \equiv \hbar^2 k_0^2/m$:

$$\sum_{\tilde{\mathbf{G}}} \left[\frac{\tilde{\mathbf{k}}^2}{2} \delta_{\tilde{\mathbf{G}},0} + \tilde{V}_{\tilde{\mathbf{G}}} \right] \tilde{\psi}(\tilde{\mathbf{k}} - \tilde{\mathbf{G}}) = \tilde{E} \tilde{\psi}(\tilde{\mathbf{k}}),$$

Band structure

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$$\sum_{\tilde{\mathbf{G}}} \left[\frac{\tilde{\mathbf{k}}^2}{2} \delta_{\tilde{\mathbf{G}},0} + \tilde{V}_{\tilde{\mathbf{G}}} \right] \tilde{\psi}(\tilde{\mathbf{k}} - \tilde{\mathbf{G}}) = \tilde{E} \tilde{\psi}(\tilde{\mathbf{k}}),$$

$$\tilde{\mathbf{G}} \equiv \mathbf{G}/k_0 = m_1 \hat{\mathbf{x}} + m_2 \hat{\mathbf{y}},$$
$$\tilde{\mathbf{k}} \equiv \mathbf{k}/k_0, \quad -\frac{1}{2} \leq \tilde{\mathbf{k}}_i \leq \frac{1}{2}$$
$$\tilde{V}_{\tilde{\mathbf{G}}} \equiv V_{\mathbf{G}}/E_0, \quad \tilde{E} \equiv E/E_0$$

Band structure

Demonstration

Discussion

- 3 (4) programs
  - Lattice plotting
  - (Plotting of Lattice planes)
  - Scattering simulation
  - Band structure of 2D materials
- command line interface - convert to graphical user interface
- Problems with Matplotlib

References

[1] S. H. Simon, *The Oxford Solid State Basics*. Oxford University Press, 2013.

[2] C. Kittel, *Introduction to Solid State Physics*. John Wiley and Sons, 2005.