Section 8
Brillouin Zone and Reciprocal Lattice

8.2 2D Problems

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Section 8
Brillouin Zone and Reciprocal Lattice

One Video Segment

- 8.1 1D Problems
  - » Brillouin Zone
  - » Solution strategy
  - » Reciprocal Lattice

One Video Segment

- 8.2 2D Problems
  - » Reciprocal Lattice Recipe
  - » Examples - Square and Hexagonal

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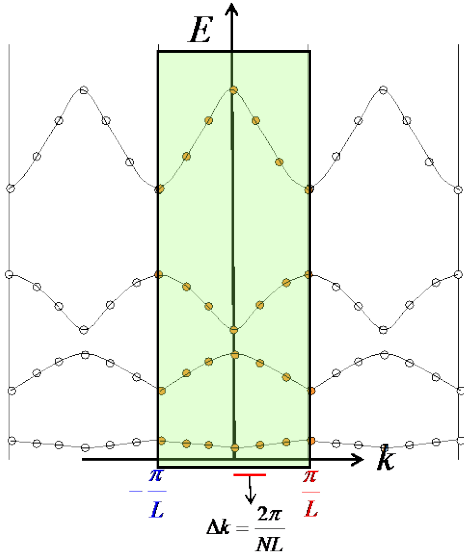
- 8.3 3D Problems



$$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$$

$$\sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = f(\mathbf{r})$$

Prasad Sarangapani, Arun Goud Akkala, Sebastian Steiger, Hong-Hyun Park, Yosef Borga, Tillmann Christoph Kubis, Michael Povolotskyi, Gerhard Klimeck (2014), "Brillouin Zone Viewer," https://nanohub.org/resources/brillouin. (DOI: 10.4231/D3DB7VQ35).

Reciprocal Space in 1D

A 1D **periodic** function: $f(x) = f(x + nL)$

can be expanded in a Fourier series:

$$f(x) = \sum_n A_n \, e^{i2\pi nx/L} = \sum_k A_k \, e^{ikx} \quad k = \frac{2\pi n}{L}$$

The Fourier components are defined on a discrete set of periodically arranged points (analogy: frequencies) in a reciprocal space to physical coordinate space.

There are multiple notations in the literature:

$$f(x) = \sum_g A_g \, e^{ikx} \quad g = \frac{2\pi n}{L}$$

$$f(r) = \sum_g A_g \, e^{ikr} \quad g = \frac{2\pi n}{L}$$

Fourier Expansion of any Periodic Function in 2D

$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$ $\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$

$\boldsymbol{a}_1, \boldsymbol{a}_2$ Primitive Bravais Lattice Vectors

n_1, n_2 Any integer $n_1, n_2 \in \mathbb{Z}$

$$\sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = f(\mathbf{r})$$

Fourier expansion

f_m Fourier coefficients

$\boldsymbol{G}_m = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2$ => Reciprocal Space Basis

What is the Reciprocal Space Basis – Given a Bravais Lattice?

$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$ with $\sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = f(\mathbf{r})$

Results in: $\sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = \sum_m f_m e^{i\mathbf{G}_m \cdot (\mathbf{r} + \mathbf{R}_n)} = e^{i\mathbf{G}_m \cdot \mathbf{R}_n} \sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}}$

This requires that: $e^{i\mathbf{G}_m \cdot \mathbf{R}_n} = 1$ => $\mathbf{G}_m \cdot \mathbf{R}_n = 2\pi N \quad N \in \mathbb{Z}$

https://en.wikipedia.org/wiki/Reciprocal_lattice

Reciprocal Space of a 2D Bravis Lattice

$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$ $\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$ $\boldsymbol{a}_1, \boldsymbol{a}_2$ Primitive Bravais Lattice Vectors

n_1, n_2 Any integer $n_1, n_2 \in \mathbb{Z}$

$\sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = f(\mathbf{r})$ Fourier expansion

f_m Fourier coefficients

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What is the Reciprocal Space Basis – Given a Bravais Lattice?

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=> Reciprocal Space Basis $\boldsymbol{G}_m = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2$

Is the Fourier Transform of Bravais Lattice $\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$

$$\boldsymbol{b}_1 = 2\pi \frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2}{\boldsymbol{a}_1 \cdot \bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2} \qquad \boldsymbol{b}_2 = 2\pi \frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1}{\boldsymbol{a}_2 \cdot \bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1} \qquad \bar{\bar{\boldsymbol{R}}} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \qquad \cos\theta = \boldsymbol{a}_1 \cdot \boldsymbol{a}_2$$

https://en.wikipedia.org/wiki/Reciprocal_lattice

Reciprocal Space of a 2D Square Lattice

$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$ $\quad$ $\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$ $\quad$ $\boldsymbol{a}_1, \boldsymbol{a}_2$ Primitive Bravais Lattice Vectors

n_1, n_2 Any integer $\quad n_1, n_2 \in \mathbb{Z}$

$$\sum_m f_m e^{i\mathbf{G}_m \cdot \mathbf{r}} = f(\mathbf{r})$$

f_m Fourier coefficients

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This is the full 2D Recipe!

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This is the full 2D Recipe!

Example of a square lattice: $\boldsymbol{a}_1 = a\begin{pmatrix}1\\0\end{pmatrix}$ $\boldsymbol{a}_2 = a\begin{pmatrix}0\\1\end{pmatrix}$

=> $\cos\theta = \boldsymbol{a}_1 \cdot \boldsymbol{a}_2 = 0$ => $\theta = 90$ => $\bar{\bar{\boldsymbol{R}}} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

$$\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1 = a\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = a\begin{pmatrix}0\\1\end{pmatrix} = \boldsymbol{a}_2$$

$$\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2 = a\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = a\begin{pmatrix}-1\\0\end{pmatrix} = -\boldsymbol{a}_1$$

https://en.wikipedia.org/wiki/Reciprocal_lattice

Reciprocal Space of a 2D Square Lattice

$$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n)$$

$$\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$$

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$$\boldsymbol{b}_1 = 2\pi\frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2}{\boldsymbol{a}_1\cdot\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2} \quad \boldsymbol{b}_2 = 2\pi\frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1}{\boldsymbol{a}_2\cdot\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1} \quad \bar{\bar{\boldsymbol{R}}} = \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix} \quad \cos\theta = \boldsymbol{a}_1\cdot\boldsymbol{a}_2$$

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$$\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1 = a\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \mathrm{a}\begin{pmatrix}0\\1\end{pmatrix} = \boldsymbol{a}_2$$

$$\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2 = a\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \mathrm{a}\begin{pmatrix}-1\\0\end{pmatrix} = -\boldsymbol{a}_1$$

$$\boldsymbol{b}_1 = 2\pi\frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2}{\boldsymbol{a}_1\cdot\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_2} = 2\pi\frac{\mathrm{a}\begin{pmatrix}-1\\0\end{pmatrix}}{a\begin{pmatrix}1\\0\end{pmatrix}\cdot\mathrm{a}\begin{pmatrix}-1\\0\end{pmatrix}} = \frac{2\pi}{a}\begin{pmatrix}1\\0\end{pmatrix} \qquad \boldsymbol{b}_2 = 2\pi\frac{\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1}{\boldsymbol{a}_2\cdot\bar{\bar{\boldsymbol{R}}}\boldsymbol{a}_1} = 2\pi\frac{\mathrm{a}\begin{pmatrix}0\\1\end{pmatrix}}{a\begin{pmatrix}0\\1\end{pmatrix}\cdot\mathrm{a}\begin{pmatrix}0\\1\end{pmatrix}} = \frac{2\pi}{a}\begin{pmatrix}0\\1\end{pmatrix}$$

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\begin{pmatrix}1\\0\end{pmatrix} \qquad \boldsymbol{b}_2 = \frac{2\pi}{a}\begin{pmatrix}0\\1\end{pmatrix}$$

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Reciprocal Space of a 2D Square Lattice

$$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n) \qquad \boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$$

$\boldsymbol{a}_1, \boldsymbol{a}_2$ Primitive Bravais Lattice Vectors

n_1, n_2 Any integer $\quad n_1, n_2 \in \mathbb{Z}$

$$\boldsymbol{G}_m = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2$$

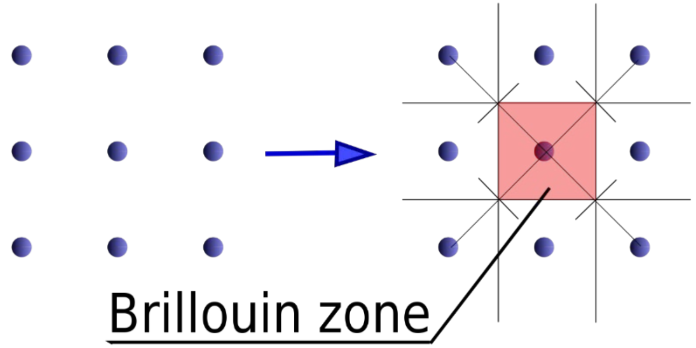
=> Reciprocal Space Basis

$$\boldsymbol{b}_1 = 2\pi \frac{\overline{\overline{\boldsymbol{R}}}\boldsymbol{a}_2}{\boldsymbol{a}_1 \cdot \overline{\overline{\boldsymbol{R}}}\boldsymbol{a}_2} \qquad \boldsymbol{b}_2 = 2\pi \frac{\overline{\overline{\boldsymbol{R}}}\boldsymbol{a}_1}{\boldsymbol{a}_2 \cdot \overline{\overline{\boldsymbol{R}}}\boldsymbol{a}_1} \qquad \overline{\overline{\boldsymbol{R}}} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \qquad \cos\theta = \boldsymbol{a}_1 \cdot \boldsymbol{a}_2$$

Example of a square lattice: $\boldsymbol{a}_1 = a\begin{pmatrix}1\\0\end{pmatrix} \quad \boldsymbol{a}_2 = a\begin{pmatrix}0\\1\end{pmatrix}$

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\begin{pmatrix}1\\0\end{pmatrix} \qquad \boldsymbol{b}_2 = \frac{2\pi}{a}\begin{pmatrix}0\\1\end{pmatrix}$$

Square ⇔ Square



Wigner Seitz algorithm
=> unit cell in reciprocal space.

https://en.wikipedia.org/wiki/Reciprocal_lattice
https://upload.wikimedia.org/wikipedia/commons/thumb/2/22/Brillouin_zone.svg/

Reciprocal Space of a 2D Hexagonal Lattice

$$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}_n) \qquad \boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$$

$\boldsymbol{a}_1, \boldsymbol{a}_2$ Primitive Bravais Lattice Vectors

n_1, n_2 Any integer $n_1, n_2 \in \mathbb{Z}$

$$\boldsymbol{G}_m = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2$$ => Reciprocal Space Basis

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Example of a square lattice: $\boldsymbol{a}_1 = a\begin{pmatrix}1\\0\end{pmatrix}$ $\boldsymbol{a}_2 = a\begin{pmatrix}0\\1\end{pmatrix}$

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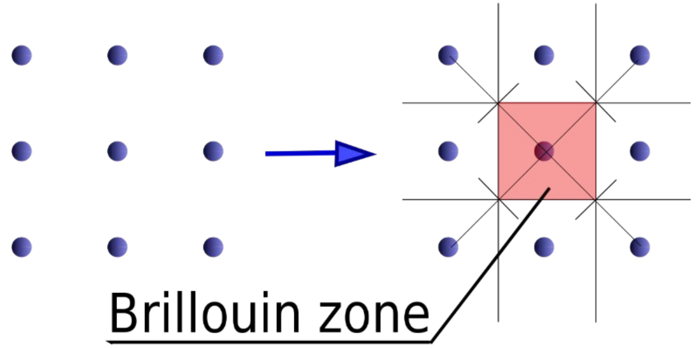
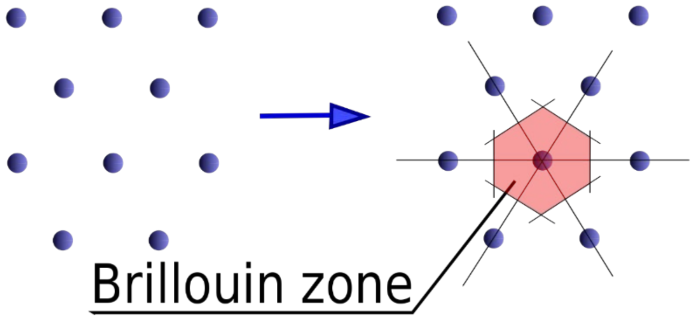


Example of a hexagonal lattice:

Wigner Seitz algorithm

=> unit cell in reciprocal space.



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Reciprocal Spaces of 2D Bravais Lattices

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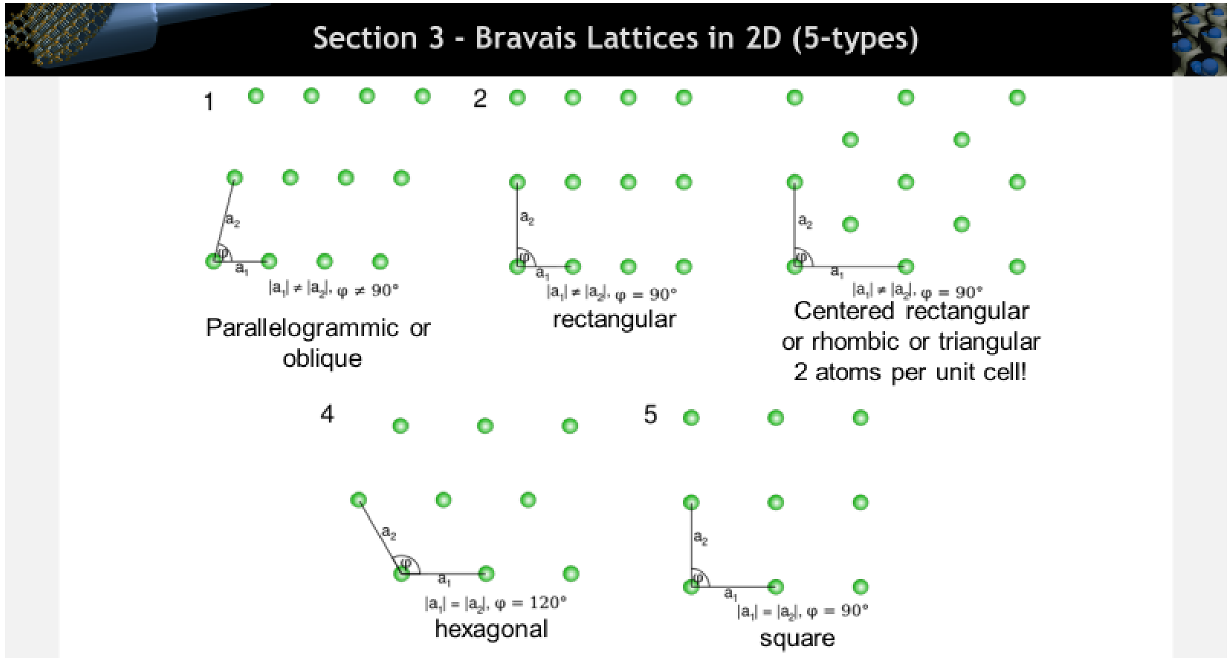
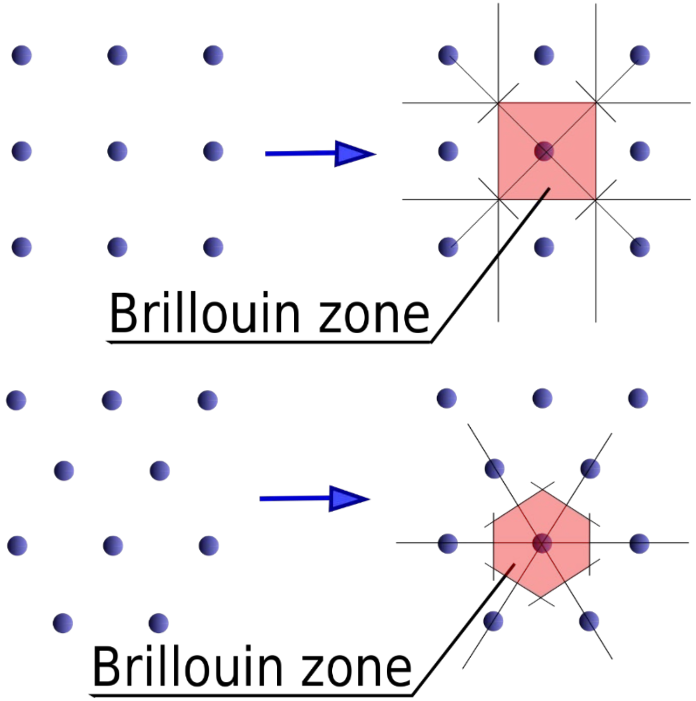
The number of lattices to “test students” on is limited!





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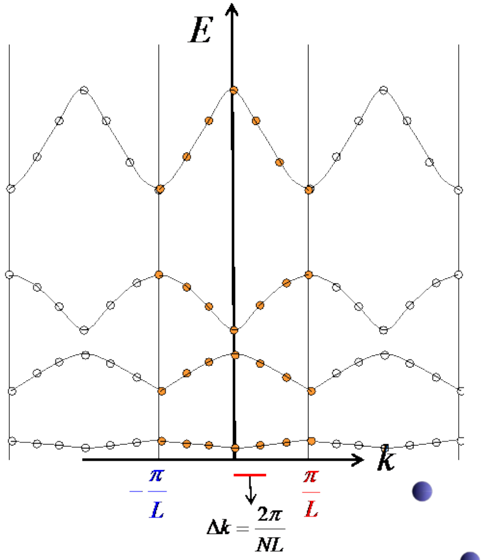
- 8.3 3D Problems



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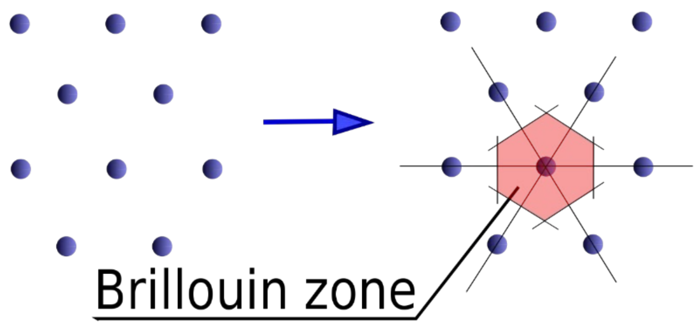

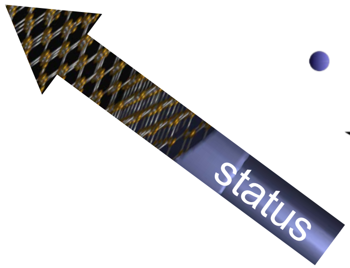

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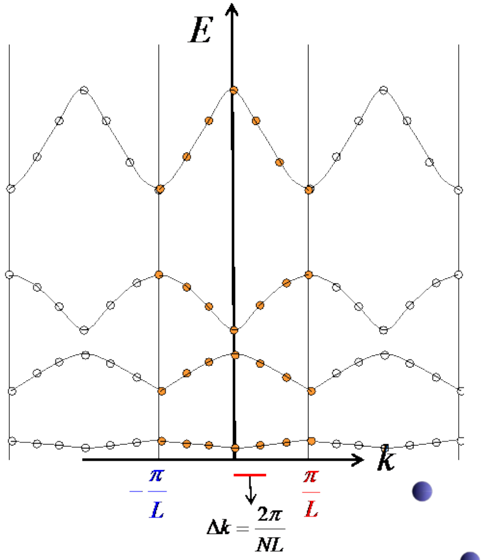

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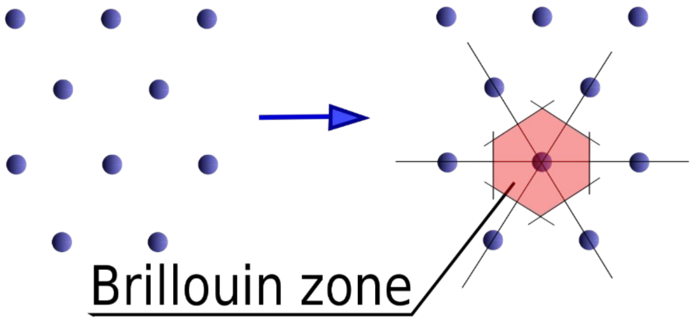

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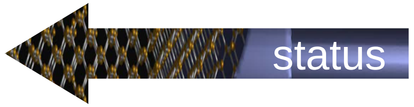

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