Symmetry properties

$$\mathcal{H} = \frac{\hat{\vec{p}}^2}{2m} + V(\hat{\vec{r}})$$

periodic potential $V(\vec{r} + \vec{a}) = V(\vec{r})$

crystal symmetry:

$$\begin{aligned} \vec{r}\,' &= \{g|\vec{a}\}\vec{r} \\ &= g\vec{r} + \vec{a} \end{aligned}$$

$\{g|\vec{a}\} \in \mathcal{R}$ space group

$g \in \mathcal{P}$ point group

related symmetry operator $\hat{S}_{\{g|\vec{a}\}}$ with $[\hat{S}_{\{g|\vec{a}\}}, \mathcal{H}] = 0$

Bloch theorem

$$\hat{S}_{\{E|\vec{a}\}}\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}(\vec{r} - \vec{a}) = e^{-i\vec{k}\cdot\vec{a}}\psi_{\vec{k}}(\vec{r})$$

translation

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u_{\vec{k}}(\vec{r})$$

with $u_{\vec{k}}(\vec{r} + \vec{a}) = u_{\vec{k}}(\vec{r})$

Bloch function

$$\mathcal{H}\psi_{\vec{k}}(\vec{r}) = \epsilon_{\vec{k}}\psi_{\vec{k}}(\vec{r})$$

$\vec{k}$ pseudo-momentum (quantum number)

Symmetry properties

Bloch states: $|\vec{k}\rangle$ with $\psi_{\vec{k}}(\vec{r}) = \langle \vec{r}|\vec{k}\rangle$

$$\hat{S}_{\{g|\vec{a}\}}|\vec{k}\rangle = \lambda_{\{g|\vec{a}\}}(\vec{k})|g\vec{k}\rangle$$

$$\mathcal{H}|\vec{k}\rangle = \epsilon_{\vec{k}}|\vec{k}\rangle$$

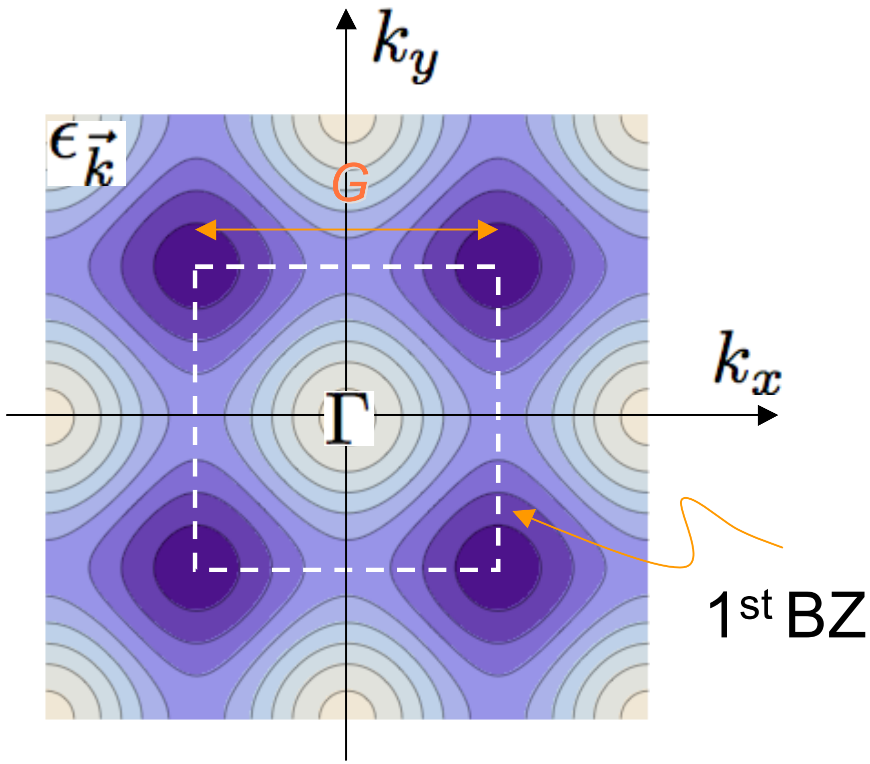
$$\begin{cases} |\lambda_{\{g|\vec{a}\}}(\vec{k})| = 1 \\ \lambda_{\{E|\vec{a}\}}(\vec{k}) = e^{-i\vec{k}\cdot\vec{a}} \end{cases}$$

$$\mathcal{H}|\vec{k}\rangle = \mathcal{H}\hat{S}^{-1}\hat{S}|\vec{k}\rangle = \lambda\hat{S}^{-1}\mathcal{H}|g\vec{k}\rangle$$

$$= \epsilon_{g\vec{k}}\lambda\hat{S}^{-1}|g\vec{k}\rangle = \epsilon_{g\vec{k}}|\vec{k}\rangle$$

$\epsilon_{g\vec{k}} = \epsilon_{\vec{k}}$ point group

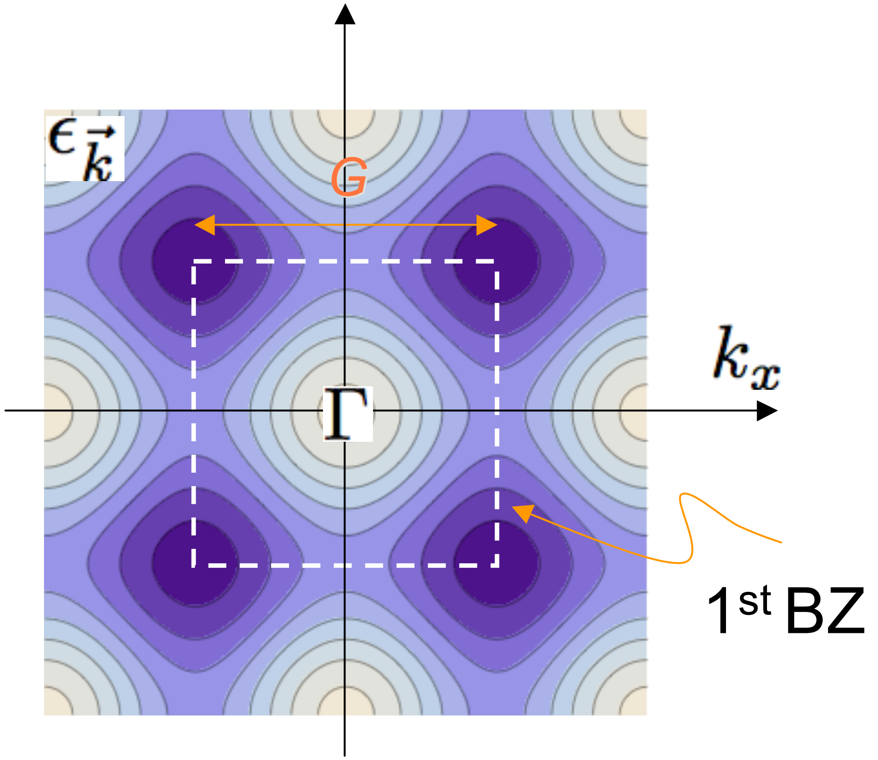
$\epsilon_{\vec{k}+\vec{G}} = \epsilon_{\vec{k}}$ translation



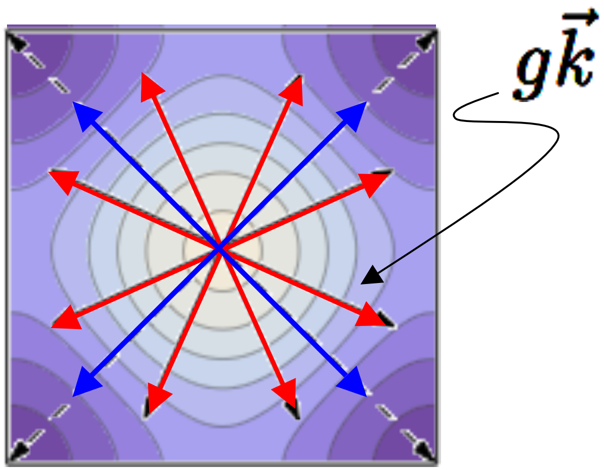
Symmetry properties

$$\epsilon_{g\vec{k}} = \epsilon_{\vec{k}}$$ point group

$$\epsilon_{\vec{k}+\vec{G}} = \epsilon_{\vec{k}}$$ translation



star of $\vec{k}$



little group of $\vec{k}$

$$g'\vec{k} = \vec{k} \qquad g' \in \mathcal{P}' \subset \mathcal{P}$$

subgroup leaving $\vec{k}$ invariant

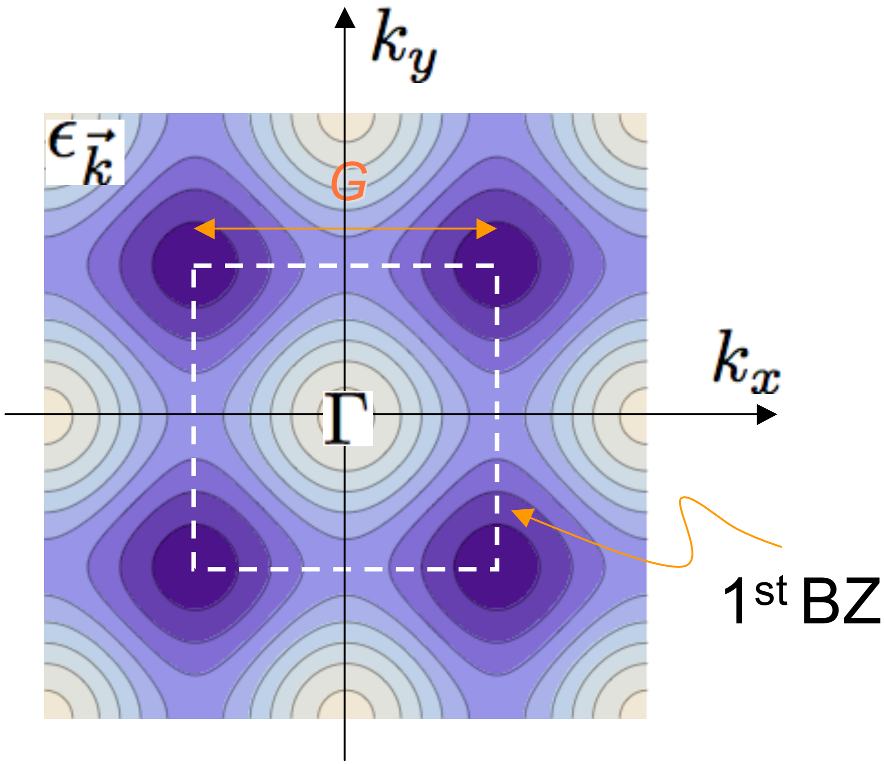
Symmetry properties

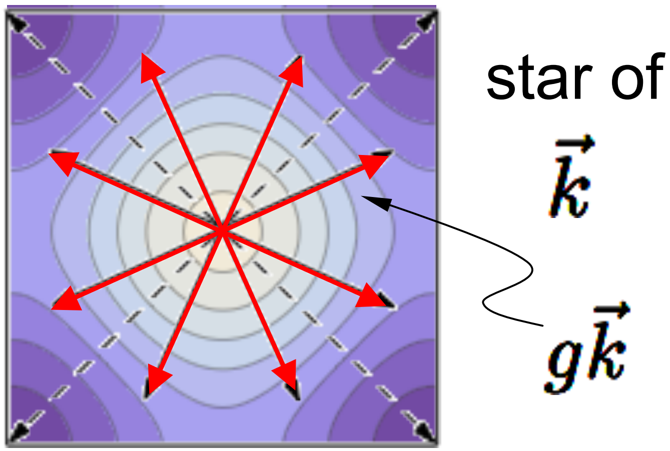
$$\hat{S}_{\{g|\vec{a}\}}|\vec{k}\rangle = \lambda_{\{g|\vec{a}\}}(\vec{k})|g\vec{k}\rangle$$

$$|\lambda_{\{g|\vec{a}\}}(\vec{k})| = 1$$

$$\epsilon_{\vec{k}+\vec{G}} = \epsilon_{\vec{k}}$$

$$\epsilon_{g\vec{k}} = \epsilon_{\vec{k}}$$





little group of $\vec{k}$

$$g'\vec{k} = \vec{k} \qquad g' \in \mathcal{P}' \subset \mathcal{P}$$