General Problem:

Study (linear) wave equation, e.g Maxwell equations, Elasticity equations, (Schrödinger equation) in a region of space filled by regular tiling (discrete translational symmetry), see Image

Two possible approaches:

- Top-down (Band theory): Derive general properties of solutions based on symmetries.
  (Powerfull in combination with finite elements solver)

- Bottom-up (Tight-binding): Start from solutions of building **block** (ex. single WGMR) to find solutions for the full system
  (Possible if the full system is made of weakly interacting subsystems)

Top-down approach (band theory)

I have to solve (generalized) eigenvalue problem

$$\Theta(r)\,\vec{\Psi} = \lambda(\omega)\,B(r)\,\vec{\Psi} \qquad (i)$$

$\lambda(\omega)$: frequency

! $\vec{\Psi}$ can be vector

e.g. for Maxwell equation $\mathrm{Re}\,\Psi$ = Magnetic field

$$\Theta(r)\vec{\Psi} = \nabla \times \left(\frac{1}{\varepsilon(r)} \nabla \times \vec{\Psi} \right) \qquad \lambda(\omega) = \frac{\omega^2}{c^2}$$

$B(r) = 1$

For Elasticity equation $\mathrm{Re}\,\Psi$ = displacement ...

$B(r)$ = density, $\lambda(\omega) = \omega^2$, $\Theta(r)$ = bulky :)

Translational invariance $\Rightarrow$

- Equivalent points (e.g. centers of hexagons) form Bravais lattice spanned by two primitive lattice vectors

$$\vec{a}_\mu = n_1 \vec{a}_1 + n_2 \vec{a}_2$$

- Unit cell: smallest region that allows to tile the whole space (not uniquely defined)
- Wigner-Seitz cell: unit-cell with the same point symmetries of the lattice

$$\Rightarrow \Theta(\vec{r} + \vec{a}_\mu) = \Theta(r) \text{ and } B(\vec{r} + \vec{a}_\mu) = B(r)$$

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Bloch Theorem: I can find a set of solutions of (i) that are also eigenstates of translations by a lattice vector

$$T_{\vec a}\vec\Psi_{n,\vec K}(\vec r) = \Psi_{\underbrace{n}_{\text{band index}},\underbrace{\vec K}_{\text{quasimomentum}}}(\vec r - \vec a) = \lambda_{\vec a}(K)\Psi_{n,\vec K} = e^{i\vec K\cdot\vec a}\vec\Psi_{n,\vec K}$$

$\forall$ lattice vector $\vec a$

I can write the eigenvalues $\lambda_{\vec a}(K)$ in the form $e^{i\vec K\cdot\vec a}$ because $|\lambda_{\vec a}(K)| \overset{!}{=} 1$ otherwise wavefunction would explode and because

$$T_{\vec a_1} T_{\vec a_2} = T_{\vec a_1+\vec a_2} \Rightarrow \lambda_{\vec a_1}(K)\lambda_{\vec a_2}(K) \overset{!}{=} \lambda_{\vec a_1+\vec a_2}(K)$$

$\Rightarrow$ linear dependence on $\vec a$ in the exponent

Note that

$$e^{i\vec K\cdot\vec a} = e^{i(\vec K+\vec b)\cdot\vec a} \quad \text{if } \vec b\cdot\vec a = 2\pi\times\text{Integer}$$

$\Rightarrow$ Quasimomentum $\vec K$ defined modulus a vector $\vec b$, all possible $\vec b$ form reciprocal lattice

$$\vec b = n_1\vec b_1 + n_2\vec b_2 \quad \text{where } \vec b_i\cdot\vec a_j = 2\pi\delta_{ij}$$

see slides for geometrical interpretation

$\Rightarrow$ All inequivalent quasimomenta can be chosen within Wigner-Seitz cell of reciprocal lattice, i.e. the Brillouin zone, see slides.