Beyond LCAO-MO

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Plane Waves

- useful for periodic materials
- but first a bit on Fourier transform

Bloch's theorem

potential experienced is periodic

$$V(r) = V(r+R)$$

we can then expand our basis with a periodic function

$$\psi(r) = e^{ikr} f(r)$$

$$f(r) = \sum_G c_i e^{iGr}$$

$$c_i = (\frac{\hbar^2}{2m}) |k+G|^2$$

We can include infinite waves within the cell, but the ones with less kinetic energy are more important, so a cut-off energy is set, G_{max}. **check the gif in this directory for a visuzlization of a fourier transform**

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Other basis sets

Here are a list of other basis sets used that I don't know enough about to explain

- wavelets
- real-space

Codes

- Pisces: grid-based
- Crystal, VASP: Gaussian basis function DFT
- Quantum Espresso: plane waves