Interactions: additional energy if two quantum numbers are occupied

$$\hat{H}_{\text{int}} = \sum_{\alpha\beta} H_{\alpha\beta} \hat{n}_\alpha \hat{n}_\beta$$

General two-body operators:

Product of single particle operators:

Continuous quantum numbers $\left|\varphi\right\rangle = \int d^3\vec{r}\,\left|\vec{r}\right\rangle\left\langle\vec{r}\middle|\varphi\right\rangle = \int d^3\vec{r}\;\varphi(\vec{r})\left|\vec{r}\right\rangle$

Define fermionic field operators $\hat{\Psi}^\dagger(\vec{r})$ to create particle at position $\vec{r}$

$$\left|\vec{r}\right\rangle = \hat{\Psi}^\dagger(\vec{r})\left|0\right\rangle$$

Anti-commutation relations: $\left\{\hat{\Psi}(\vec{r}_1), \hat{\Psi}^\dagger(\vec{r}_2)\right\} = \delta(\vec{r}_1 - \vec{r}_2)$

Operators in continuous real space

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})$$

Expressed in terms of field operators:

$$\hat{H} = \int d^3\vec{r}\, \hat{\Psi}^\dagger(\vec{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\hat{\Psi}(\vec{r})$$

Momentum space

Momentum states are plane waves: $$|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3\vec{r}\ e^{i\vec{p}\cdot\vec{r}/\hbar} |\vec{r}\rangle$$

Define momentum creation operators:

$$\hat{c}^\dagger(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int d^3\vec{r}\ e^{i\vec{k}\cdot\vec{r}} \hat{\Psi}^\dagger(\vec{r})$$

Kinetic energy becomes “diagonal”

$$\hat{H}_{kin} = -\frac{\hbar^2}{2m} \int d^3\vec{r}\ \hat{\Psi}^\dagger(\vec{r}) \nabla^2 \hat{\Psi}(\vec{r})$$

Potential $U(\vec{r})$: scattering in k-space

$$\hat{H}_{pot} = \int d^3\vec{r}\ U(\vec{r})\hat{\Psi}^\dagger(\vec{r})\hat{\Psi}(\vec{r})$$

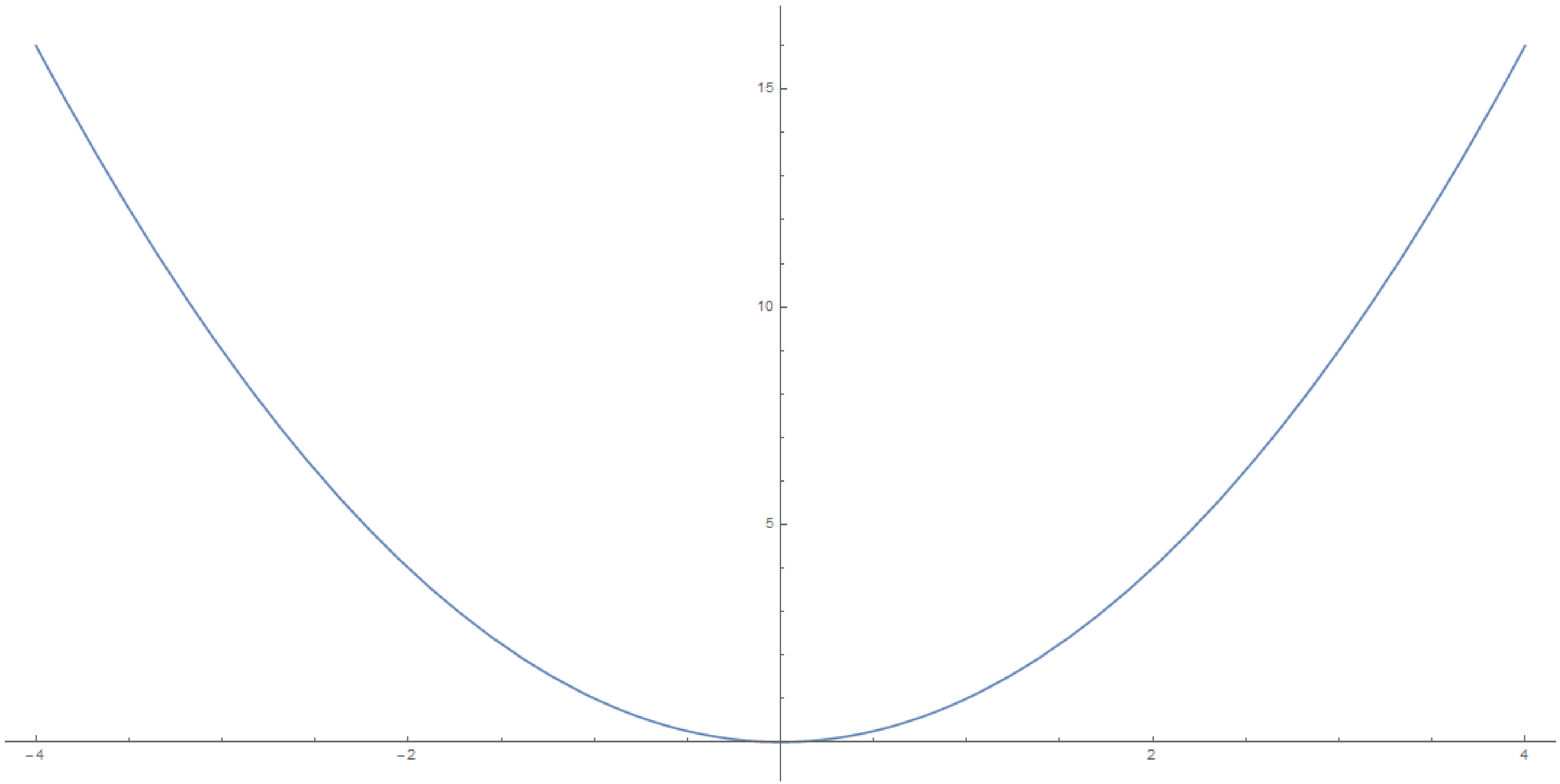
Periodic Potential $U(\vec{r}) = U(\vec{r} + \vec{R})$

$$\tilde{U}(\Delta\vec{k}) = \frac{1}{(2\pi)^3} \int d^3\vec{r}\ e^{-i\Delta\vec{k}\cdot\vec{r}} U(\vec{r})$$

Scattering in reciprocal space: Extended Zone Scheme

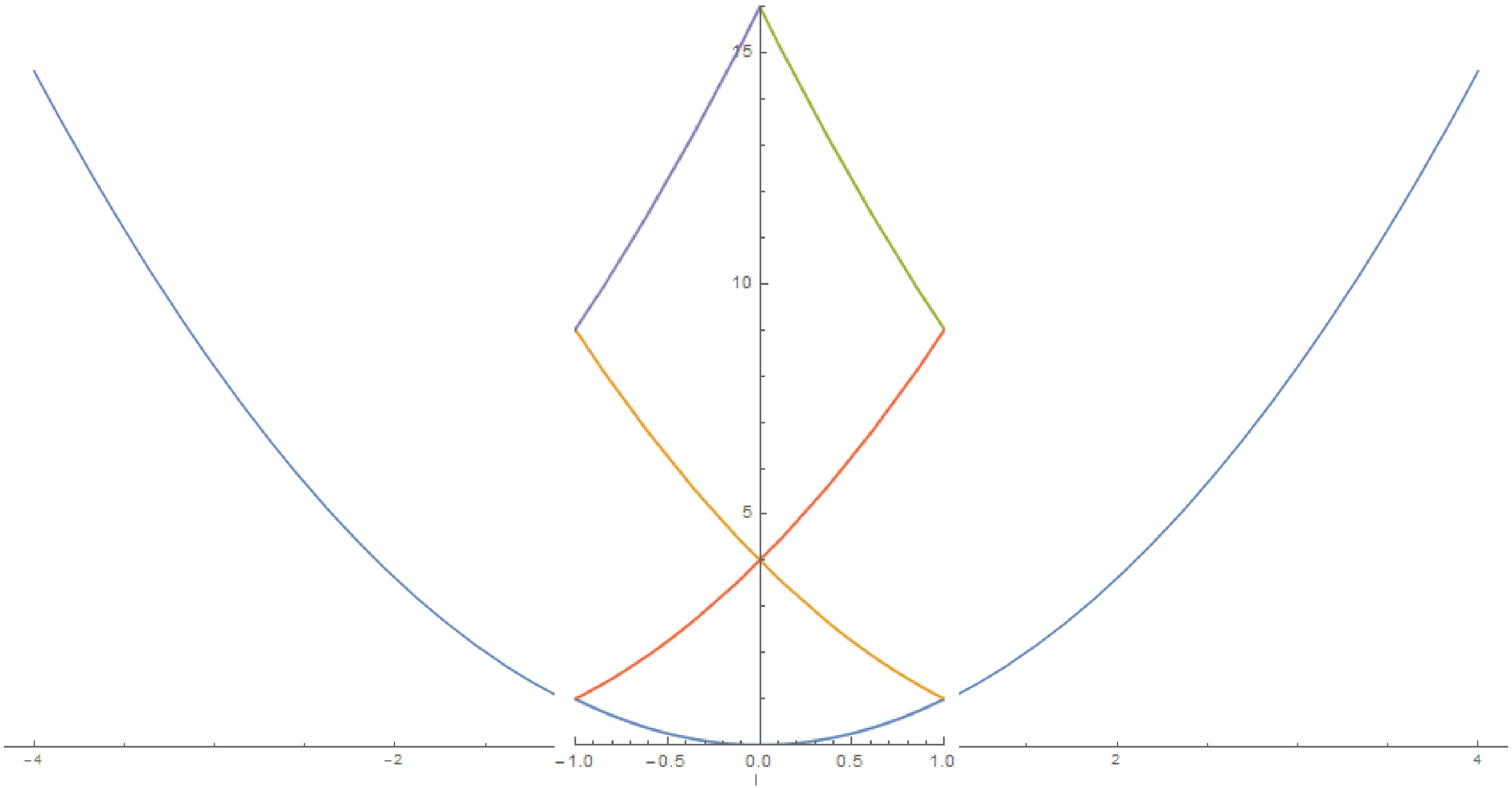
$$\hat{H} = \hat{H}_{kin} + \hat{H}_{pot} = \frac{\hbar^2}{2m}\int d^3\vec{k}\ \left|\vec{k}\right|^2 \hat{c}^\dagger(\vec{k})\hat{c}(\vec{k}) + \int d^3\vec{k}\ \sum_{\vec{G}} \hat{c}^\dagger(\vec{k}+\vec{G})U(\vec{G})\hat{c}(\vec{k})$$

$$U(\vec{G}) = \frac{1}{V_U}\int_{V_U} d^3\vec{r}\ e^{-i\vec{G}\cdot\vec{r}}U(\vec{r})$$



Reduced Zone Scheme

$$\hat{H} = \sum_{\vec{G}} \int_{1BZ} d^3\vec{k} \left(\frac{\hbar^2}{2m} \left| \vec{k} - \vec{G} \right|^2 \hat{c}^\dagger(\vec{k} - \vec{G}) \hat{c}(\vec{k} - \vec{G}) + \sum_{\vec{G}'} \hat{c}^\dagger(\vec{k} - \vec{G} + \vec{G}') U(\vec{G}') \hat{c}(\vec{k} - \vec{G}) \right)$$



Bloch solution for each $\vec{k}$ in 1BZ: Bands

$$\hat{H}_{\vec{k}} = \sum_{\vec{G}} \left(\frac{\hbar^2}{2m} \left| \vec{k} - \vec{G} \right|^2 \hat{c}^\dagger(\vec{k} - \vec{G}) \hat{c}(\vec{k} - \vec{G}) + \sum_{\vec{G}'} \hat{c}^\dagger(\vec{k} - \vec{G} + \vec{G}') U(\vec{G}') \hat{c}(\vec{k} - \vec{G}) \right)$$

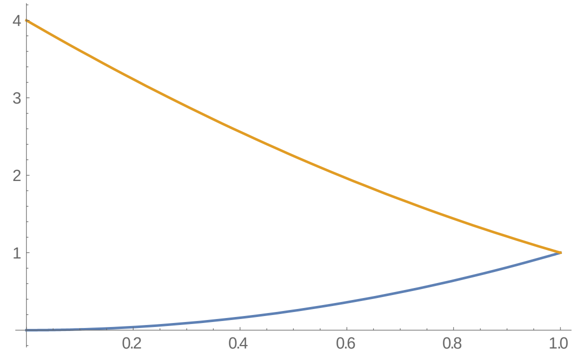
For solution:

$$\hat{H}_{\vec{k}} \left| \psi_{\vec{k},\alpha} \right\rangle = \varepsilon_\alpha(\vec{k}) \left| \psi_{\vec{k},\alpha} \right\rangle$$

Find superposition of plane waves:

$$\left| \psi_{\vec{k},\alpha} \right\rangle = \sum_{\vec{G}} \lambda_{\vec{k},\alpha}(\vec{G}) \hat{c}^\dagger(\vec{k} - \vec{G}) \left| 0 \right\rangle = \sum_{\vec{G}} \lambda_{\vec{k},\alpha}(\vec{G}) \left| \vec{k} - \vec{G} \right\rangle$$

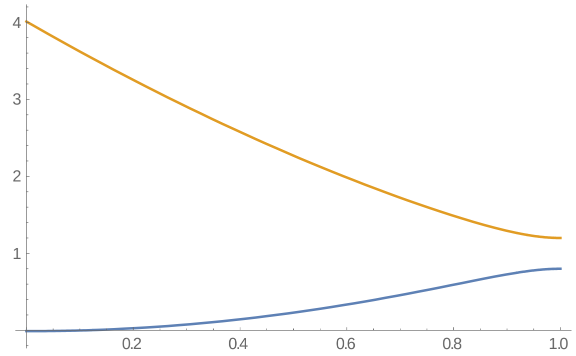
Solution are plane waves as $U \to 0$
Start with only reduced basis of superposition of few plane waves:



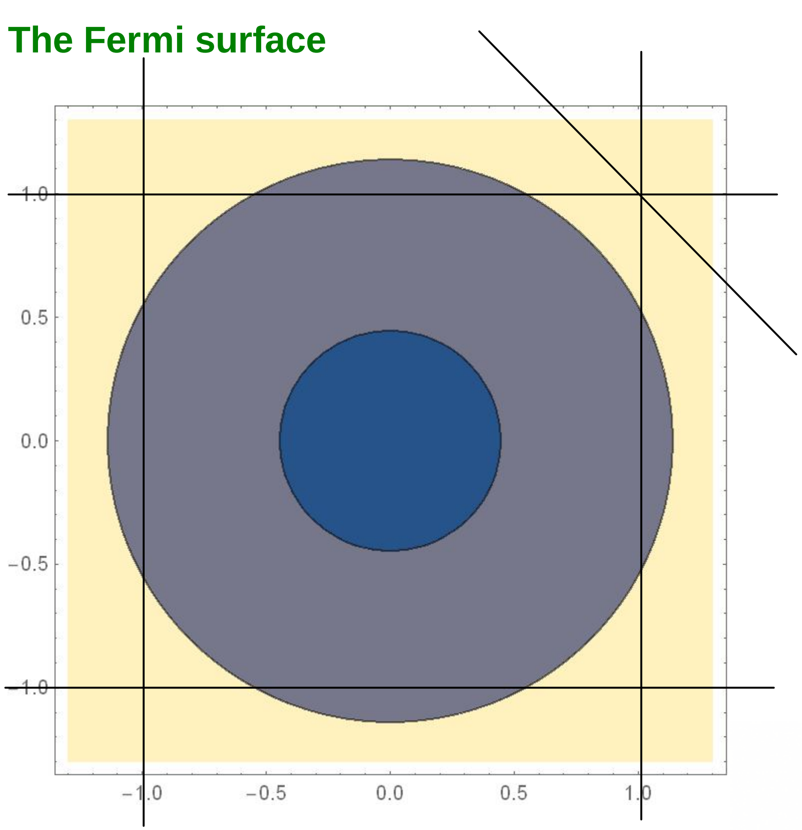
$$\hat{H}_{\vec{k}} \to \begin{pmatrix} \frac{\hbar^2}{2m}|\vec{k}|^2 & U(\vec{G}) \\ U(-\vec{G}) & \frac{\hbar^2}{2m}|\vec{k}-\vec{G}|^2 \end{pmatrix}$$

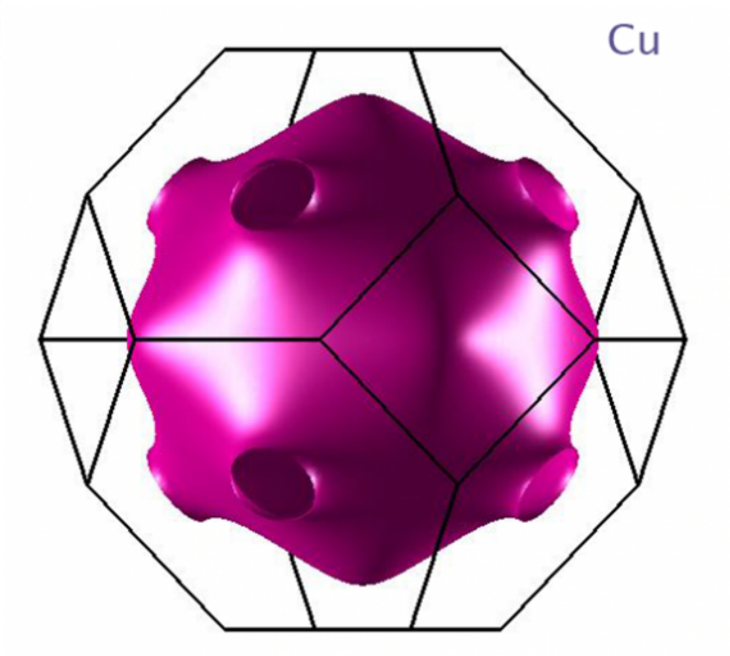
In units of $\frac{\hbar^2}{2m}=1$: Two bands

$$\varepsilon_{\pm}(\vec{k}) \approx \frac{1}{2}\left(|\vec{k}|^2 + |\vec{k}-\vec{G}|^2 \pm \sqrt{\left(|\vec{k}|^2 - |\vec{k}-\vec{G}|^2\right)^2 + |U|^2}\right)$$



The Fermi surface





Wavefunction of the solution: Bloch theorem

$$\psi_{\vec{k},\alpha}(\vec{r}) = \left\langle \vec{r} \middle| \psi_{\vec{k},\alpha} \right\rangle = \frac{1}{(2\pi)^{3/2}} \sum_{\vec{G}} \lambda_{\vec{k},\alpha}(\vec{G}) \exp(\vec{k} - \vec{G}) \cdot \vec{r}$$

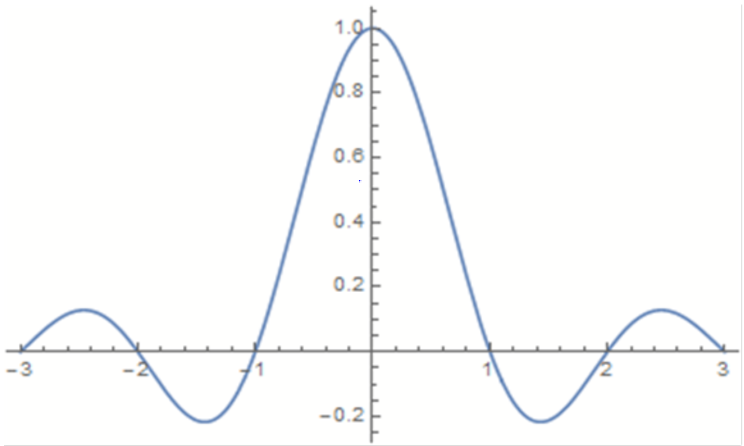
$$\psi_{\vec{k},\alpha}(\vec{r} + \vec{R}) =$$

Define Wannier functions

$$\tilde{\psi}_{\vec{R},\alpha}(\vec{r}) = \frac{1}{\sqrt{V_{1BZ}}} \int_{V_{1BZ}} d^3\vec{k}\, e^{-i\vec{k}\cdot\vec{R}} \psi_{\vec{k},\alpha}(\vec{r}) = \frac{1}{(2\pi)^{3/2}\sqrt{V_{1BZ}}} \sum_{\vec{G}} \int_{V_{1BZ}} d^3\vec{k}\, e^{i(\vec{k}-\vec{G})\cdot(\vec{r}-\vec{R})} \lambda_{\vec{k},\alpha}(\vec{G})$$

Example: "Free" 1D Fermions U=0

$$\left|\psi_{k,\alpha}\right\rangle = \left|k - \alpha \frac{2\pi}{a}\right\rangle$$



Hamiltonian in terms of Wannier orbitals: Hopping

$$\hat{H}_{\vec{k}} = \sum_{\alpha} \varepsilon_{\alpha}(\vec{k}) \hat{\Psi}^{\dagger}_{\vec{k},\alpha} \hat{\Psi}_{\vec{k},\alpha}$$

$$\hat{\Psi}^{\dagger}_{\vec{k},\alpha} = \frac{1}{\sqrt{V_{1BZ}}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \hat{\Psi}^{\dagger}_{\vec{R},\alpha}$$