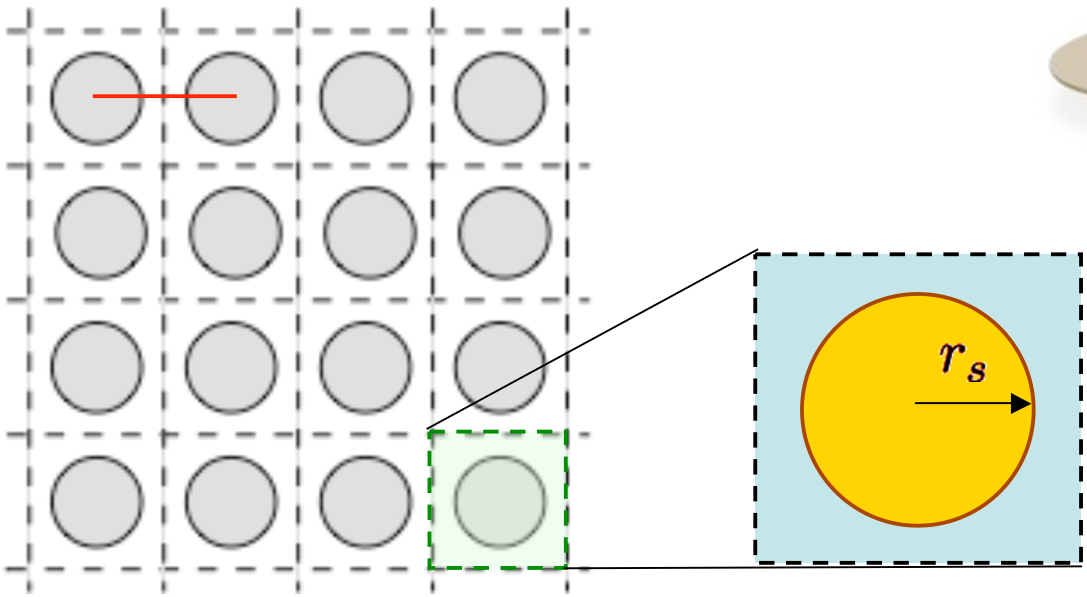
Augmented plane wave — muffin tin potential

strategy

- split real space lattice up in Wigner-Seitz cells (analog Brillouin zones)
- insert circle around each atom contained completely within each WS cell
- solve spherically symmetric problem in sphere
- match with plane wave solution outside of sphere

muffin tin

muffin tin potential



Wigner Seitz cell

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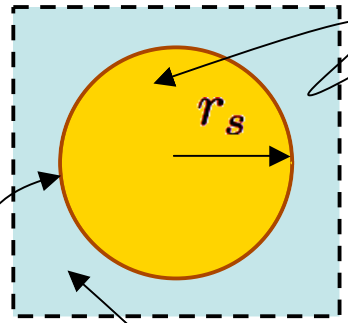
Wigner Seitz cell



$|\vec{r}| < r_s$

spherical wave function

$$\varphi(\vec{r}) = \frac{u_l(r)}{r} Y_{lm}(\theta, \phi)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) - E\right] u_l(r, E) = 0$$

$|\vec{r}| > r_s$

plane wave

$$e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(kr) Y^*_{lm}(\hat{k}) Y_{lm}(\hat{r})$$

j_l: spherical Bessel function

$|\vec{r}| = r_s$

wave function matching

$$A(\vec{k}, \vec{r}, E) = \begin{cases} \dfrac{4\pi}{\sqrt{\Omega_{UC}}} \sum_{l,m} i^l j_l(kr_s) \dfrac{r_s u_l(r, E)}{r u_l(r_s, E)} Y^*_{lm}(\hat{k}) Y_{lm}(\hat{r}), & r < r_s, \\ \dfrac{4\pi}{\sqrt{\Omega_{UC}}} \sum_{l,m} i^l j_l(kr) Y^*_{lm}(\hat{k}) Y_{lm}(\hat{r}), & r > r_s, \end{cases}$$

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superposition as for "*nearly free electron approximation*"

$$\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} c_{\vec{G}}(\vec{k}) A(\vec{k}+\vec{G},\vec{r},E)$$

$$\Rightarrow \quad \sum_{\vec{G}} \langle A_{\vec{k}}(E)|\mathcal{H}-E|A_{\vec{k}+\vec{G}}(E)\rangle c_{\vec{G}}(\vec{k}) = 0$$

challenge: calculation of matrix elements

$$\langle A_{\vec{k}}(E)|\mathcal{H}-E|A_{\vec{k}'}(E)\rangle = \left(\frac{\hbar^2 \vec{k}\cdot\vec{k}'}{2m} - E\right)\Omega_{UC}\delta_{\vec{k},\vec{k}'} + V_{\vec{k},\vec{k}'}$$

$$V_{\vec{k},\vec{k}'} = 4\pi r_s^2 \Bigg[-\left(\frac{\hbar^2 \vec{k}\cdot\vec{k}'}{2m} - E\right)\frac{j_1(|\vec{k}-\vec{k}'|r_s)}{|\vec{k}-\vec{k}'|} + \sum_{l=0}^{\infty}\frac{\hbar^2}{2m}(2l+1)P_l(\hat{k}\cdot\hat{k}')j_l(kr_s)j_l(k'r_s)\frac{u_l'(r_s,E)}{u_l(r_s,E)} \Bigg]$$

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superposition as for "*nearly free electron approximation*"

$$\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} c_{\vec{G}}(\vec{k}) A(\vec{k}+\vec{G}, \vec{r}, E)$$

$$\Rightarrow \quad \sum_{\vec{G}} \langle A_{\vec{k}}(E) | \mathcal{H} - E | A_{\vec{k}+\vec{G}}(E) \rangle c_{\vec{G}}(\vec{k}) = 0$$

advantage: • rapid convergence

- need only a few tens of $\vec{G}$-vectors
- need angular momentum only up to $l = 5$

• interpolation between weakly bound states and tight-binding limit