Summary of electron in a periodic potential: different basis systems

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

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

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

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

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

$$\Psi^\dagger_{\vec{k},\alpha} = \sum_{\vec{G}}\lambda_{\vec{k},\alpha}(\vec{G})\hat{c}^\dagger(\vec{k}-\vec{G})$$

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

$$\tilde{\Psi}_{\vec{R},\alpha}(\vec{r}) = \frac{1}{\sqrt{V_{1BZ}}}\int_{V_{1BZ}} d^3\vec{k}e^{-i\vec{k}\cdot\vec{R}}\Psi^\dagger_{\vec{k},\alpha}$$

$$t_\alpha(\Delta\vec{R}) = \frac{1}{V_{1BZ}}\int_{V_{1BZ}} d^3\vec{k}\;\varepsilon_\alpha(\vec{k})^{i\vec{k}\cdot\Delta\vec{R}}$$

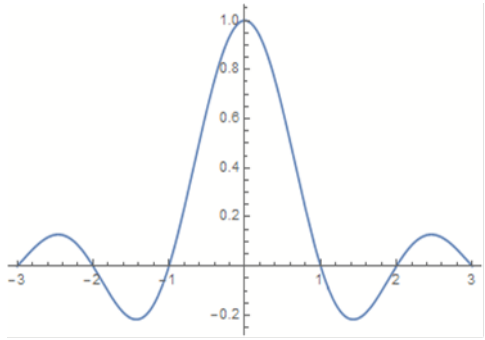
$$\hat{H} = \int_{1BZ} d^3\vec{k}\,\hat{H}_{\vec{k}} = \sum_\alpha\sum_{\vec{R},\Delta\vec{R}} t_\alpha(\Delta\vec{R})\tilde{\Psi}^\dagger_{\vec{R}+\Delta\vec{R},\alpha}\tilde{\Psi}_{\vec{R},\alpha}$$

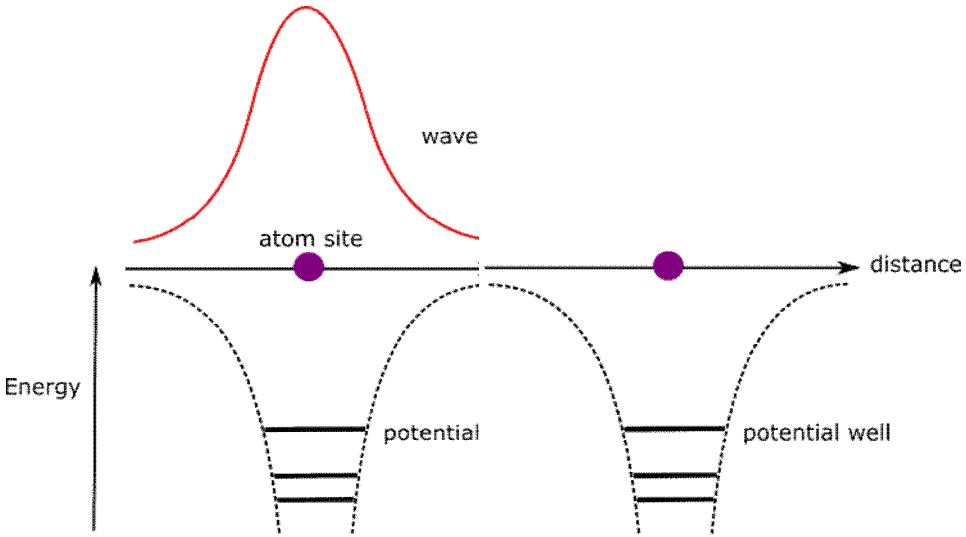
Tight binding approximation

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

Hopping integrals $t_\alpha(\Delta\vec{R})$ are Fourier transformation of dispersion but also matrix elements:

$$t_\alpha(\Delta\vec{R}) = \left\langle \tilde{\psi}_{\vec{R}+\Delta\vec{R},\alpha} \middle| \hat{H} \middle| \tilde{\psi}_{\vec{R},\alpha} \right\rangle$$



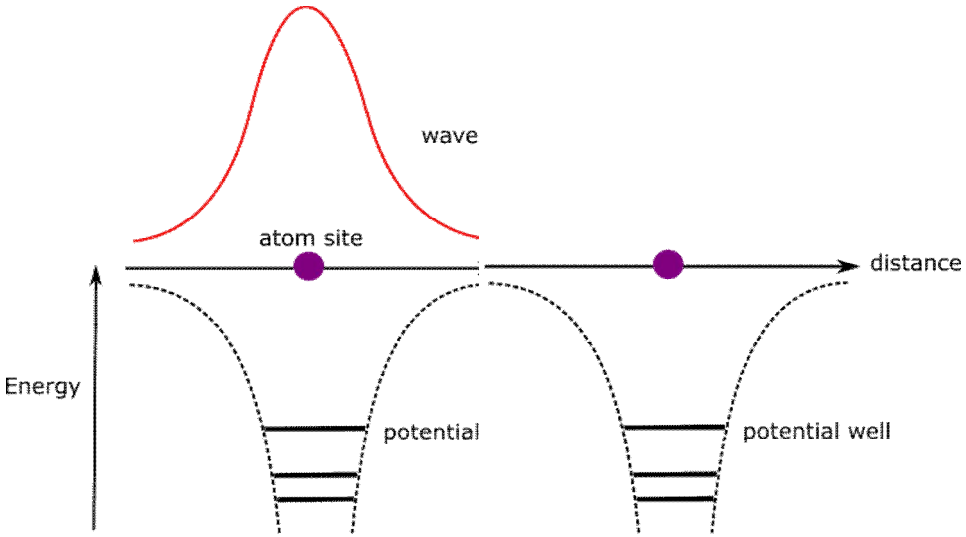


In the limit of very strong potential, Wannier functions are similar to atomic orbitals $\left|\tilde{\psi}_{\vec{R},\alpha}\right\rangle \approx \left|\psi^{atom}_{\vec{R},\alpha}\right\rangle$

Ansatz: Linear combination of atomic orbitals (LCOA)

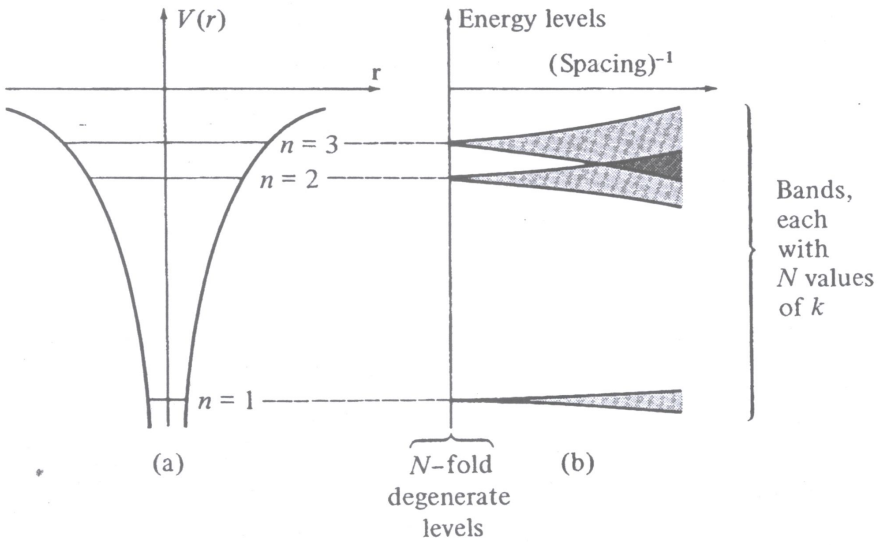
Simplest case: Hopping of one single orbital

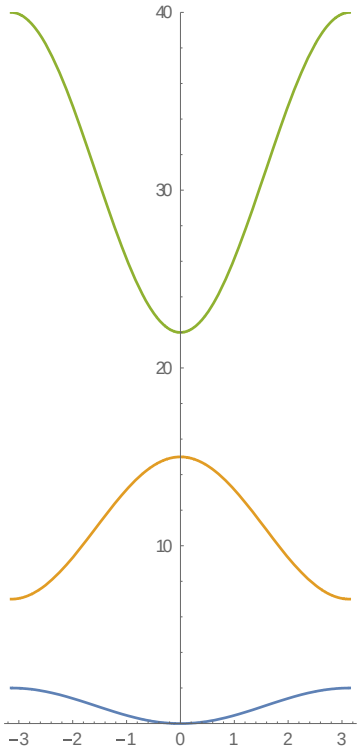
$$t_\alpha(\Delta\vec{R}) \approx \left\langle \psi^{atom}_{\vec{R}+\Delta\vec{R},\alpha} \middle| \hat{H} \middle| \psi^{atom}_{\vec{R},\alpha} \right\rangle = \left\langle \psi^{atom}_{\vec{R}+\Delta\vec{R},\alpha} \middle| \left(\hat{H}^{atom} + \hat{H}^{rest}\right) \middle| \psi^{atom}_{\vec{R},\alpha} \right\rangle$$

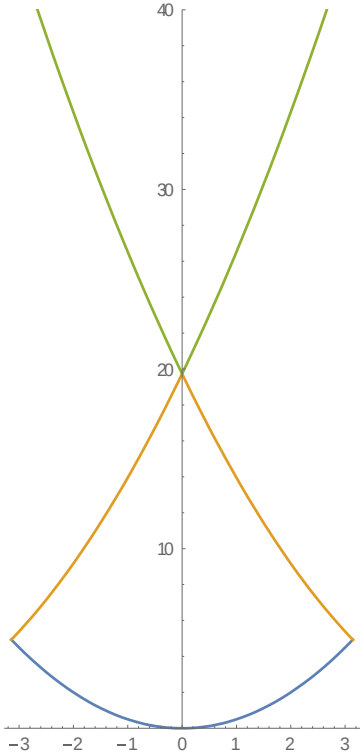


Tight binding approximation

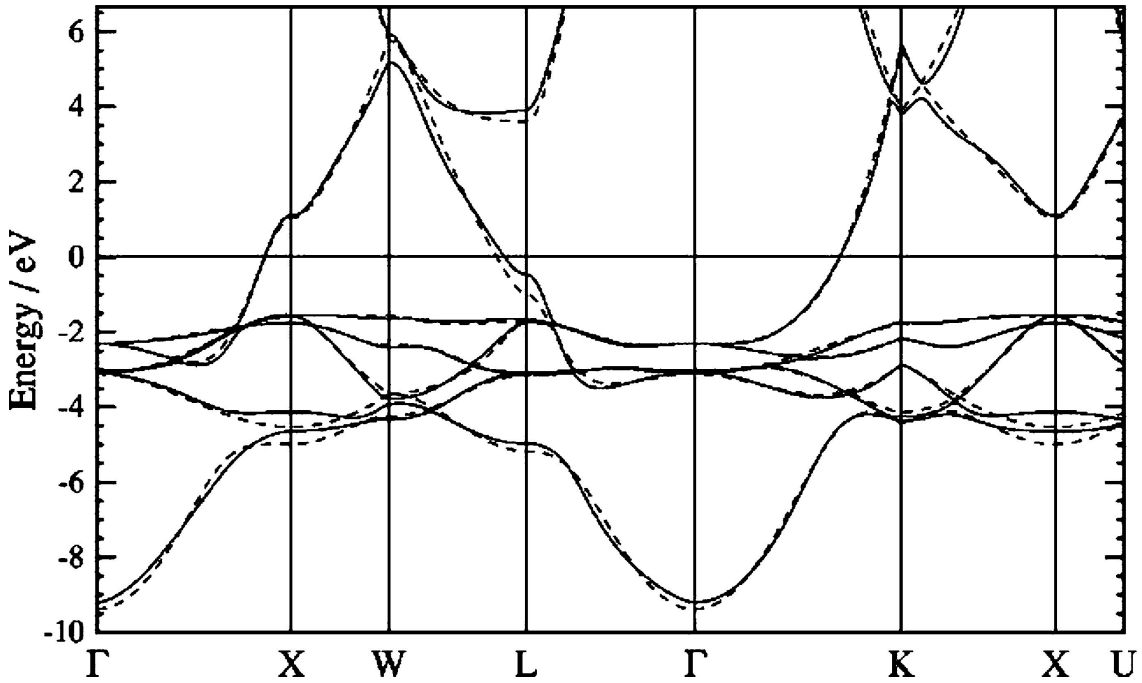
$$\hat{H} = \sum_{\alpha} \sum_{\vec{R},\Delta\vec{R}} t_{\alpha}(\Delta\vec{R}) \left| \psi^{atom}_{\vec{R}+\Delta\vec{R},\alpha} \right\rangle \left\langle \psi^{atom}_{\vec{R},\alpha} \right|$$

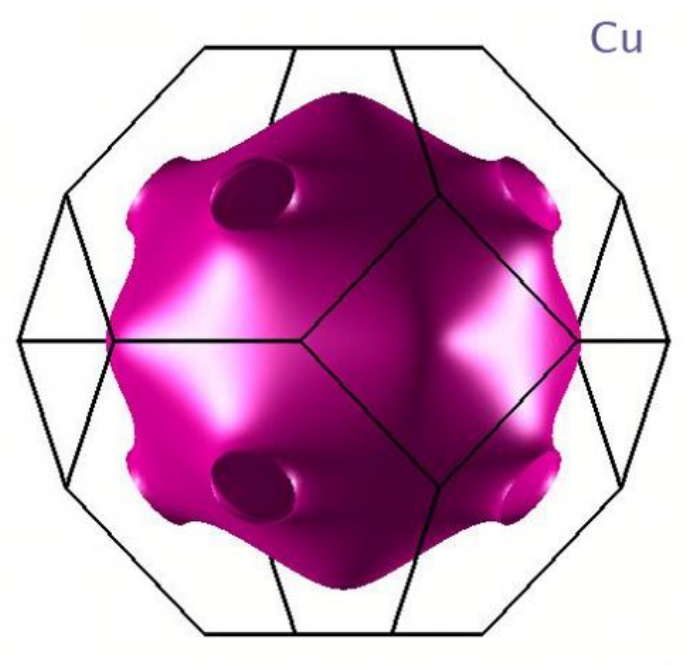






Real band structure: Estimates

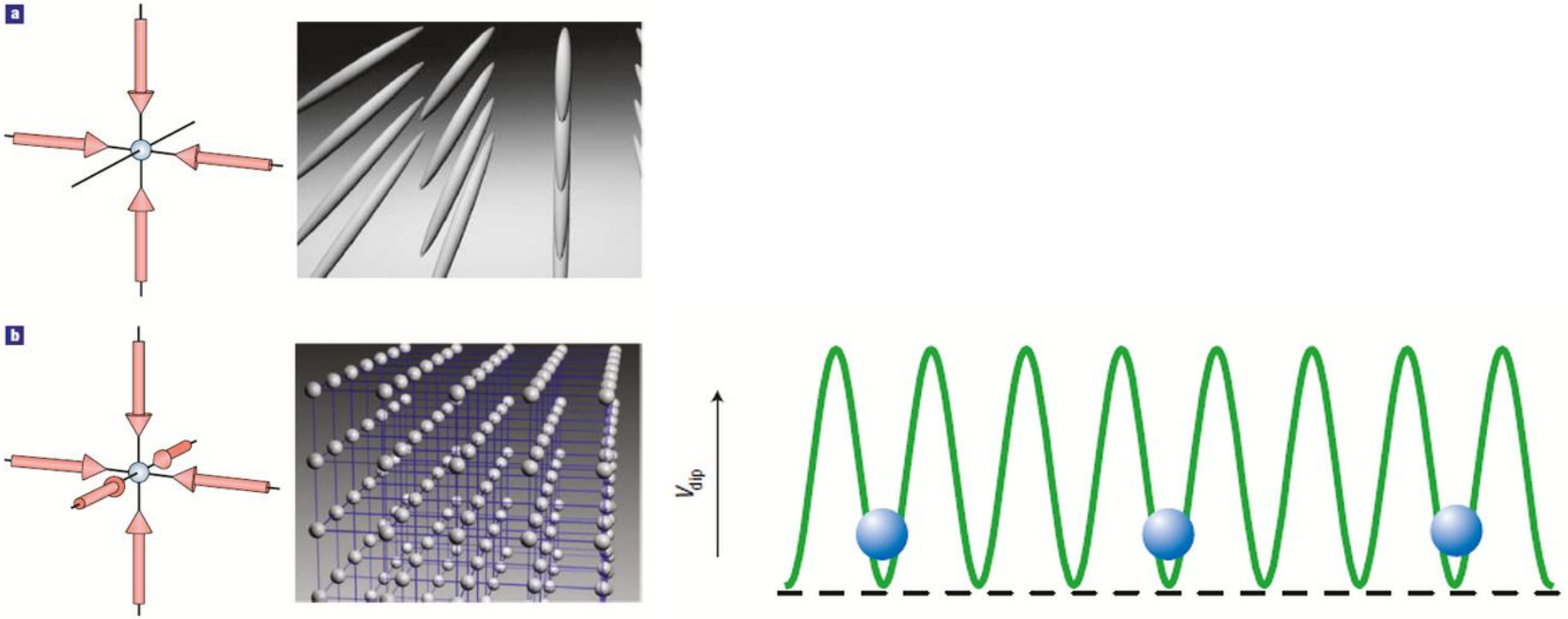




Real band structure in ultracold gases

Immanuel Bloch, Nature Phys. V1, p 23 (2005)

Wilhelm Zwerger, J. Opt B: Quantum Semiclass. Opt. 5, S9 (2003).



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

$$= \hat{H}_x + \hat{H}_y + \hat{H}_z$$

$$\hat{H}_x = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U\sin^2\frac{\pi x}{a}$$

Müller-Kirsten: *Introduction to Quantum Mechanics*, World Scientific
Martin Holthaus, J. Phys. B: At. Mol. Opt. Phys. **49**, 013001 (2006)

The Mathieu equation

$$\hat{H}_{1D} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + U \sin^2 k_a r$$

Define $\tau = k_a r$

$$\left(\frac{\partial^2}{\partial \tau^2} + a - 2p\cos\tau \right) \varphi_{1D}(\tau) = 0$$