From Bloch to Maximally Localized Wannier Functions

- Bloch functions depend on crystal momentum and describe particle which is spread out over the whole lattice → an alternative basis is provided by maximally localized Wannier functions

$$w_n(x - x_i) = \sqrt{\frac{a}{2\pi}} \int_{\mathrm{BZ}} dk e^{-ikx} \phi_k^{(n)}(x)$$

$$\phi_k^{(n)}(x) \mapsto e^{i\theta(q,n)} \phi_k^{(n)}(x)$$ not uniquely defined

$$|w_n(x)| \sim e^{-h_n x}$$ for each band there exists only one real maximally localized Wannier function which is either symmetric or antisymmetric about x=0 or x=a/2

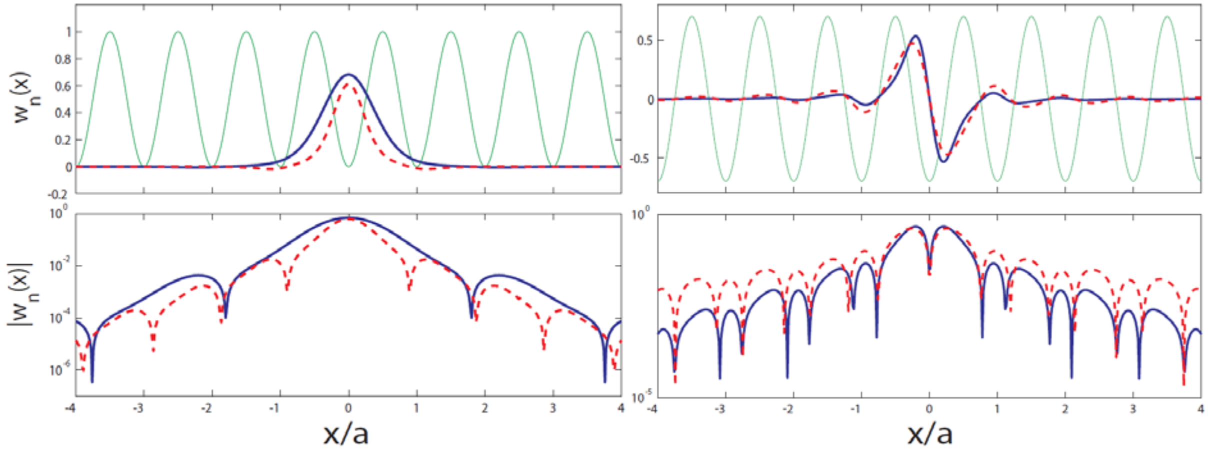

Figure 2.3. *Wannier Functions $w_n(x)$ in units $\sqrt{2\pi/a}$ for $n = 0$ (left) and $n = 1$ (right), plotted for $V_0 = 10E_R$ (solid line) and $V_0 = 5E_R$ (dashed line). The lower plots show the absolute version of the Wannier functions on a logarithmic scale. The position of the periodic potential is indicated on the upper plots.*