

DERIVATION OF EFFECTIVE MASS APPROXIMATION

Bloch functions:

$$H|\psi_{n\mathbf{k}}\rangle = \epsilon_{n\mathbf{k}}|\psi_{n\mathbf{k}}\rangle \quad [1]$$

Forward and reverse Wannier transform pair:

$$|\psi_{n\mathbf{k}}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{r}} |w_{n\mathbf{R}}\rangle \quad [2a]$$

$$|w_{n\mathbf{R}}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} |\psi_{n\mathbf{k}}\rangle \quad [2b]$$

Wannier matrix elements:

$$\langle w_{n\mathbf{R}} | w_{n'\mathbf{R}'} \rangle = \delta_{\mathbf{R},\mathbf{R}'} \delta_{nn'} \quad [3]$$

$$\langle w_{n\mathbf{R}} | H_0 | w_{n'\mathbf{R}'} \rangle = E_n(\mathbf{R}' - \mathbf{R}) \delta_{nn'} \quad [4]$$

where $\epsilon_{n\mathbf{k}}$ and $E_n(\mathbf{R})$ are related by

$$E_n(\mathbf{R}) = \frac{1}{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} \epsilon_{n\mathbf{k}} \quad [5a]$$

$$\epsilon_{n\mathbf{k}} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} E_n(\mathbf{R}) \quad [5b]$$

Consider wavepacket:

$$|\psi(t)\rangle = \sum_{n'\mathbf{R}'} f_{n'}(\mathbf{R}', t) |w_{n'\mathbf{R}'}\rangle \quad [6]$$

Time-dependent Schroedinger equation for wavepacket:

$$(H_0 + U) |\psi(t)\rangle = i\hbar \frac{d}{dt} |\psi(t)\rangle \quad [7]$$

Goal: Find equation of motion for envelope function $f_n(\mathbf{R}, t)$.

Substitute [6] into [7] and multiply on the left by $\langle w_{n\mathbf{R}} | :$

$$\begin{aligned} \sum_{n'\mathbf{R}'} \langle w_{n\mathbf{R}} | H_0 + U | w_{n'\mathbf{R}'} \rangle f_{n'}(\mathbf{R}', t) \\ = i\hbar \sum_{n'\mathbf{R}'} \langle w_{n\mathbf{R}} | w_{n'\mathbf{R}'} \rangle \frac{d}{dt} f_{n'}(\mathbf{R}', t) \end{aligned} \quad [8]$$

Using [3] and [4] we get

$$\sum_{n'\mathbf{R}'} \left[E_n(\mathbf{R}' - \mathbf{R}) \delta_{nn'} + U_{nn'}(\mathbf{R}, \mathbf{R}') \right] f_{n'}(\mathbf{R}', t) = i\hbar \frac{d}{dt} f_n(\mathbf{R}, t) \quad [10]$$

where

$$U_{nn'}(\mathbf{R}, \mathbf{R}') = \langle w_{n\mathbf{R}} | U(\mathbf{r}) | w_{n'\mathbf{R}'} \rangle \quad [11]$$

Up to here, everything is exact. Now introduce **approximation**:

$$\begin{aligned} U_{nn'}(\mathbf{R}, \mathbf{R}') &\simeq U(\mathbf{R}) \langle w_{n\mathbf{R}} | w_{n'\mathbf{R}'} \rangle \\ &= U(\mathbf{R}) \delta_{nn'} \delta_{\mathbf{R}, \mathbf{R}'} \end{aligned} \quad [12]$$

Then (with $\mathbf{R}'' = \mathbf{R}' - \mathbf{R}$)

$$\sum_{\mathbf{R}''} E_n(\mathbf{R}'') f_n(\mathbf{R} + \mathbf{R}'', t) + U(\mathbf{R}) f_n(\mathbf{R}, t) = i\hbar \frac{d}{dt} f_n(\mathbf{R}, t) \quad [13]$$

Regarding $E_n(\mathbf{R})$ as being defined by [5a], the Wannier functions have disappeared! Letting $\mathbf{R} \rightarrow \mathbf{r}$ (continuum limit), $\mathbf{R}'' \rightarrow \mathbf{R}$, and restoring t -dependence to U , the final result is usually written as

$$\sum_{\mathbf{R}} E_n(\mathbf{R}) f_n(\mathbf{r} + \mathbf{R}, t) + U(\mathbf{r}, t) f_n(\mathbf{r}, t) = i\hbar \frac{d}{dt} f_n(\mathbf{r}, t) \quad [14]$$