Bloch to Wannier

$$\boxed{\begin{aligned} H\psi_{nk} &= E_{nk}\psi_{nk} \\ \psi_{nk} &= \frac{1}{\sqrt{N_k}} e^{ikx} u_{nk} \end{aligned}} \quad (1)$$

(1) $\Rightarrow$ $\psi_{nk}(x) = \psi_{nk}(x+N_k a)$; $\psi_{nk}(x) = \psi_{nk+G}(x)$; $E_{nk} = E_{nk+G}$

$N_k a \to$ BvK Cell, $\quad u_{nk}(x) = u_{nk}(x+a)$; $a \to$ Cell.

$N_k \to$ # of allowed k in 1BZ

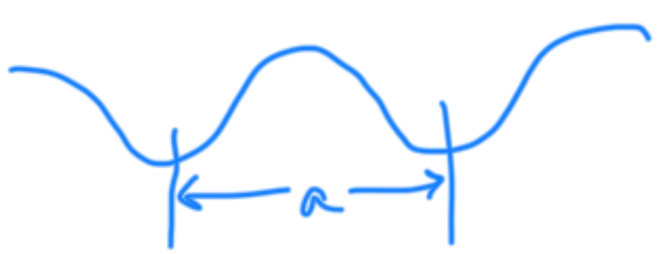
(1) $\Rightarrow$ $$\boxed{\begin{aligned} &\int_{\text{BvK cell}} \psi^*_{nk}\psi_{n'k'}\, dx = \delta_{nn'}\delta_{kk'} \\ &\int_{\text{cell}} u^*_{nk} u_{n'k}\, dx = \delta_{nn'} \end{aligned}}$$

(1) $\Rightarrow$ $\int_{\text{cell}} u^*_{nk} u_{n'k}\, dx = \delta_{nn'}$; $\int_{\text{Cell}} u^*_{nk} u_{nk'}\, dx \neq 0$

Recall Fourier expansion of periodic fn:

If $f(x+ma) = f(x)$, $m \in \mathbb{Z}$, then $f(x) = \sum_{n=-\infty}^{+\infty} c_n e^{i n \frac{2\pi}{a} x}$ (not normalized)

$$c_n = \frac{1}{a}\int_{-a/2}^{a/2} f(x)\, e^{-i n \frac{2\pi}{a} x}\, dx$$



Recall the identity $\Psi_{k+mG_0} = \Psi_k$ $\rightarrow$ periodic in $\vec{k}$ space, $m \in \mathbb{Z}$

$\therefore$ for all x : $\Psi_k(x) = \sum_{n=-\infty}^{+\infty} W_n(x)\, e^{in\left(\frac{2\pi}{G_0}\right)k}$ $\longrightarrow$ Fourier expansion in k space.

$$= \sum_{n=-\infty}^{+\infty} W_n(x)\, e^{in\frac{2\pi}{\frac{2\pi}{a}}k} = \sum_{n=-\infty}^{+\infty} W_n(x)\, e^{inak}$$

Inverse:

Wannier fn : $W_n(x) = \frac{1}{G_0}\int_{BZ} e^{-inak}\, \Psi_{\vec{k}}(x)\, dk$ (not normalized)

writing $n \to R_n = na$

$$\Rightarrow W_{m,R_n}(x) = A \int_{BZ} e^{-iR_nk}\, \Psi_{m\vec{k}}(x)\, dk \rightarrow \text{Wannier fn}$$

m $\uparrow$ band index

$A \rightarrow$ normalization constant

$$\int_{BvK} W^*_{jR_l} W_{mR_n}\, dx = A^2 \int_{BZ} dk \int_{BZ} dk'\, e^{+i(R_nk - R_lk')} \int_{BvK} \Psi^*_{jk}\Psi_{mk'}\, dx$$

$$= A^2 \int_k\int_{k'} e^{i(\quad)}\, \delta_{jm}\delta_{kk'}\, dk\, dk'$$

$$= A^2 \left(\frac{2\pi}{Na}\right)^2 \sum\sum e^{i(R_nk - R_lk')}\, \delta_{jm}\delta_{kk'}$$

$$= A^2\left(\frac{2\pi}{Na}\right)^2 \sum_k e^{ik(R_n - R_l)} \delta_{jm}$$

$$= A^2\left(\frac{2\pi}{Na}\right)^2 N \quad \delta_{jm} \text{ for } R_l = R_n$$

Implying normalized $W_{mR_n}(x)$ as:

$$\boxed{\begin{aligned} W_{mR_n}(x) &= \frac{a}{2\pi}\sqrt{N}\int_{1BZ} e^{-iR_n k}\psi_{mk}(x)\, dk \quad \text{—— 1D} \\ \Big[\text{In 3D: } W_{mR_n}(\vec{r}) &= \frac{\Omega^3}{8\pi^3}\sqrt{N}\int_{1BZ} e^{-i\vec{R}_n\vec{k}}\psi_{m\vec{k}}(\vec{r})\, d^3k\Big] \quad \text{—— 3D}\end{aligned}}$$

$$= \frac{a}{2\pi}\sqrt{N}\sum_k e^{-iR_n k}\psi_{mk}(x)\left(\frac{2\pi}{Na}\right) \quad (\text{in 1D})$$

$$\boxed{\begin{aligned} &= \frac{1}{\sqrt{N}}\sum_k e^{-iR_n k}\psi_{mk}(x) \quad \text{—— 1D} \\ \Big[\text{In 3D: } W_{mR_n}(\vec{r}) &= \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{-i\vec{R}_n\cdot\vec{k}}\psi_{m\vec{k}}(\vec{r})\Big] \quad \text{—— 3D}\end{aligned}}$$

$$\Rightarrow \boxed{\int_{BvK} W^*_{mR_p}(\vec{r})\, W_{nR_q}(\vec{r})\, d^3r = \delta_{R_pR_q}\delta_{mn}}$$

Inverse

let $\psi_{mk}(x) = B \sum_{n=-\infty}^{+\infty} W_{m R_n}(x)\, e^{i R_n k}$

Orthonormalization of ψ:

$$\int_{BZ k} \psi^*_{mk}(x)\, \psi_{lk'}(x)\, dx = B^2 \sum_{R_p} \sum_{R_q} e^{-i(R_p k - R_q k')} \int_{BZk} W^*_{mR_p}(x)\, W_{lR_q}(x)\, dx$$

$$= B^2 \sum_{R_p R_q} e^{-i(R_p k - R_q k')}\, \delta_{R_p R_q}\, \delta_{ml}$$

$$= B^2 \sum_{R_p} e^{-i R_p (k-k')}\, \delta_{ml}$$

$$= B^2 N\, \delta_{ml} \quad \text{if } k = k'$$

$$\Rightarrow \psi_{mk}(x) = \frac{1}{\sqrt{N}} \sum_{R_n} W_{mR_n}(x)\, e^{i R_n k}$$

$$\boxed{\Rightarrow \int_{BZk} \psi^*_{mk}(\vec{r})\, \psi_{nk'}(\vec{r})\, d^3r = \delta_{mn}\, \delta_{kk'}}$$

How does $W_{mR_n}(x)$ look like?

... the cell periodic

Let us consider nearly free electron where ... (1 in case of free electrons)
part u_k of the Bloch function are rather flat.

$$W_{mR_n}(x) = \frac{a}{2\pi}\sqrt{N}\int_{BZ} e^{ik(x-R_n)} u_{m\vec{k}}(x)\, dk$$

$$\approx \frac{a\sqrt{N}}{2\pi}\int_{BZ} e^{ik(x-R_n)}\, dk$$

as we approach free electron limit

$U_{m\vec{k}}(x) \to 1$ for all x.

$$= a\sqrt{N}\,\delta(x-R_n)$$

However if an arbitrarily chosen phase $e^{i\theta_{mk}}$ accompanies $u_{mk}(x)$ then the outcome of the integration will not be δ fn in real sp.

Thus WF localization will vary with different choices of gauge $\{e^{i\theta_{nk}}\}$ for $\{u_{nk}\}$.

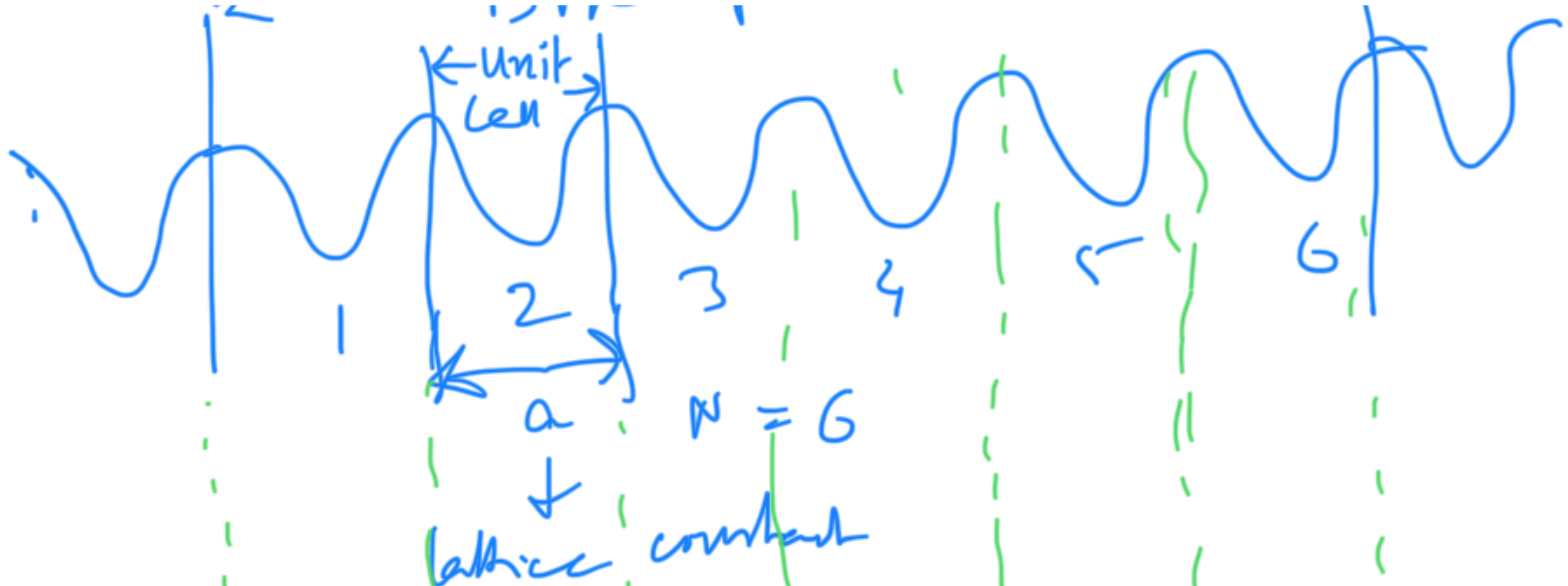
$$\Rightarrow W_{nR}(x) = \frac{a}{2\pi}\sqrt{N}\int_{1BZ} e^{i\theta_{nk}} e^{-i\vec{k}\cdot\vec{R}} \psi_{n\vec{k}}(x)\, dk$$

A central issue is to find the choice of gauge $e^{i\theta_{nk}}$ which leads to the maximum localization of the WFs.

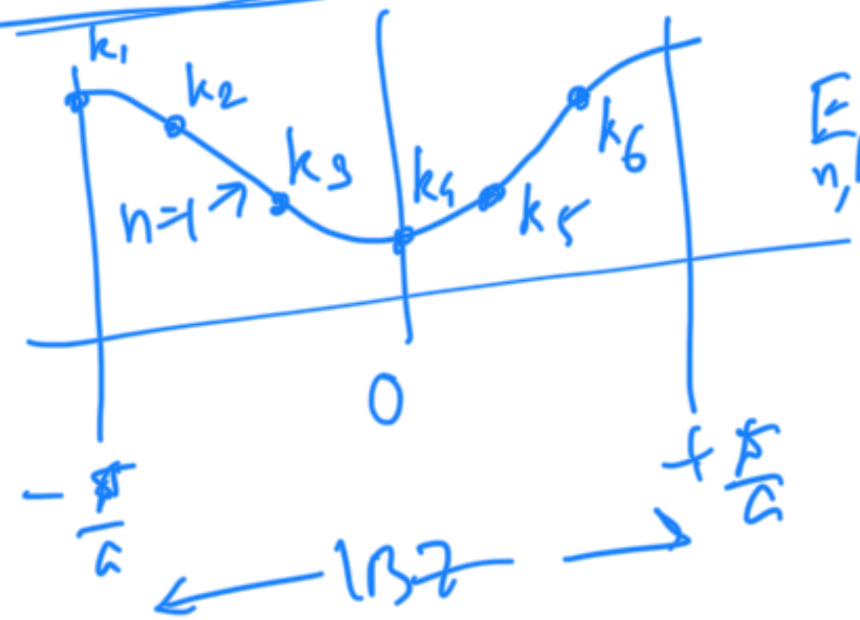
← BvK supercell →

Schematically:

for $V(x) = V(x+a)$:

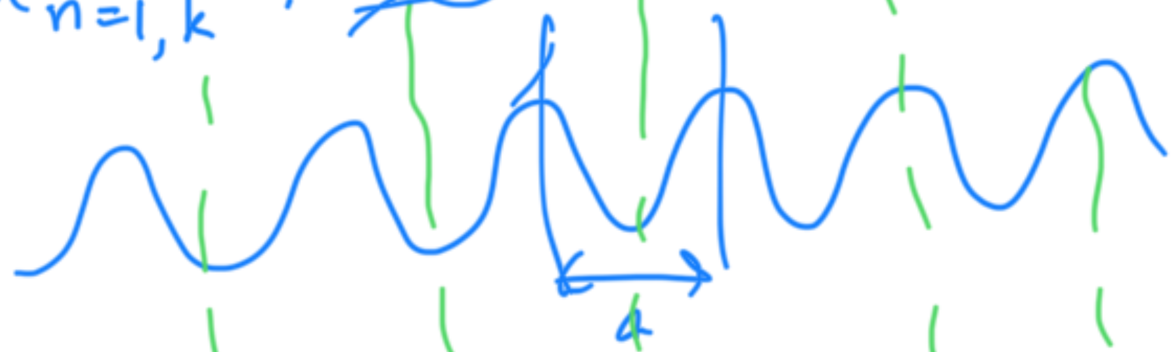


$\Rightarrow$ Band str:

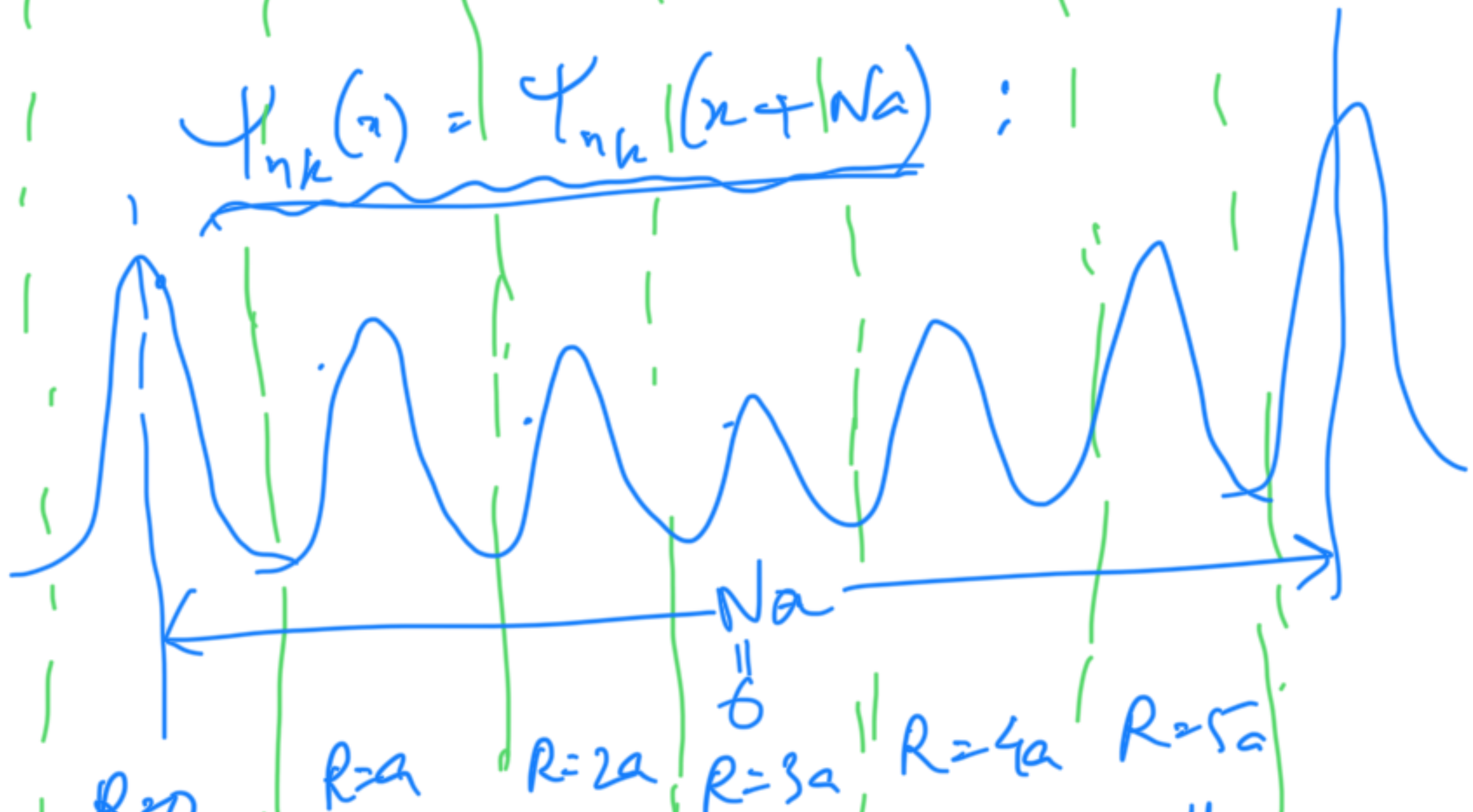


$E_{n,k} = E_{n,-k}$

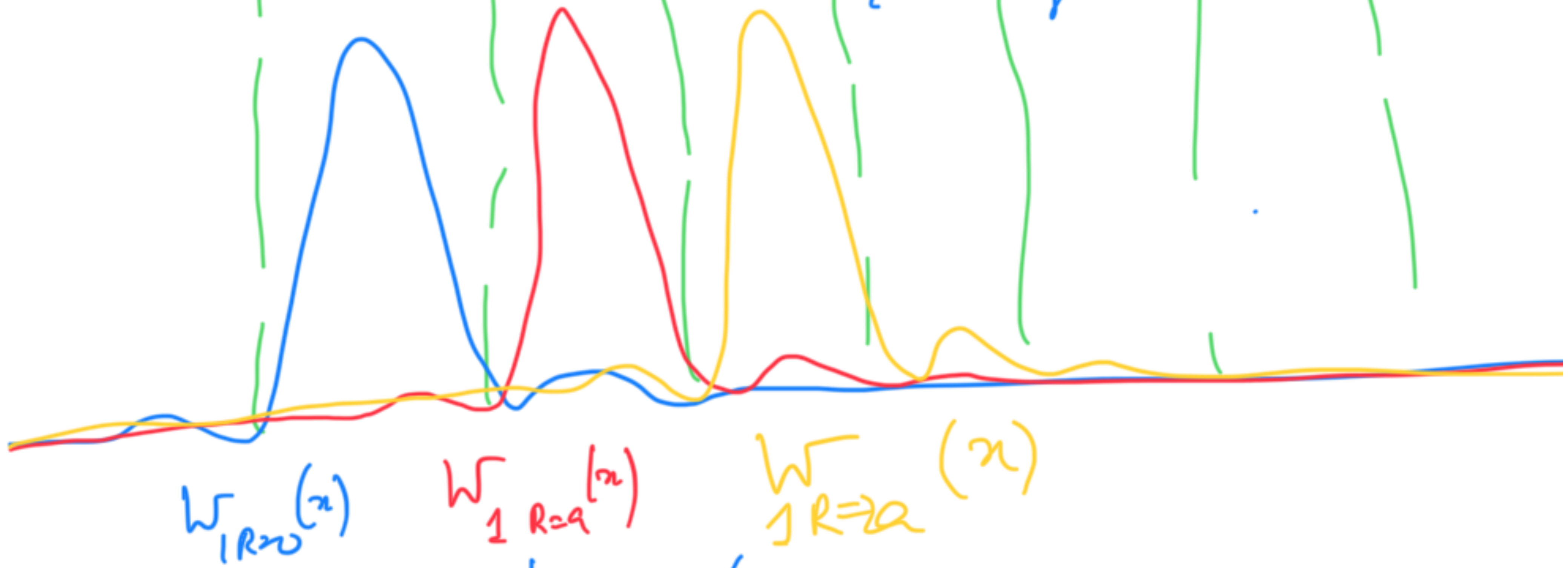
$u_{n=1,k}$: $u_{nk}(x) = u_{nk}(x+a)$:



$\psi_{nk}(x) = \psi_{nk}(x+Na)$:



$W_{n,R}(x)$ (assuming we know the choice of gauge with maximally localize the WS



Identical shape but shifted by lattice constant "a".