Differential equation eigenvalue problem.

I. Look up the math text : the operator and BC

$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+V(\vec{r})\right)u_{n,\vec{k}}(\vec{r})=E_n(\vec{k})u_{n,\vec{k}}(\vec{r})$$

$$u_{n,\vec{k}}(\vec{r}+\vec{R})=u_{n,\vec{k}}(\vec{r})$$

II. Fourier expansion

$$u_{n,\vec{k}}(\vec{r})=\sum_{\lambda=1}^{\infty}C(\vec{G}_\lambda)e^{i\vec{G}_\lambda\cdot\vec{r}}=\sum_{\lambda=1}^{\infty}C_\lambda e^{i\vec{G}_\lambda\cdot\vec{r}}=\sum_{\vec{G}}^{\infty}C(\vec{G})e^{i\vec{G}\cdot\vec{r}}$$

Matrix eigenvalue problem.

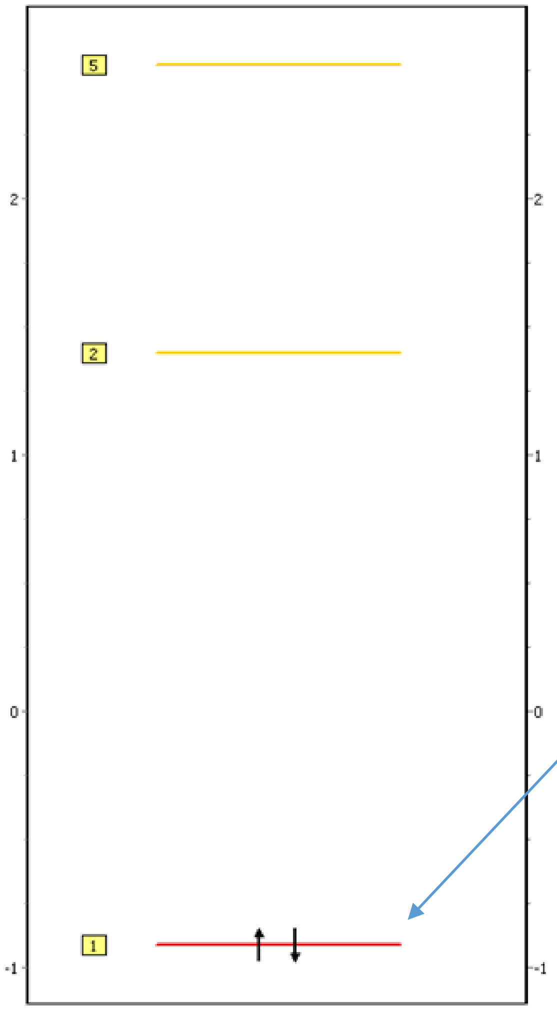
III. Now we have matrix eigenvalue problem

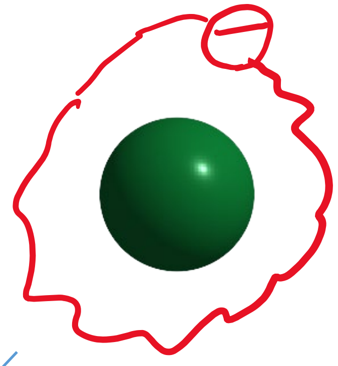
$$\sum_{\lambda}\left(\frac{1}{2}(-i\vec{G}_{\mu}+\vec{k})^{2}\delta_{\mu\lambda}+V(\vec{G}_{\mu}-\vec{G}_{\lambda})\right)C_{\lambda}=E_{n}(\vec{k})C_{\mu}$$

IV. Prove that the energy eigenvalues are periodic function in the reciprocal space.

$$E_{n}(\vec{k})=E_{n}(\vec{k}+\vec{G})$$

The electron in the atom, isolated system



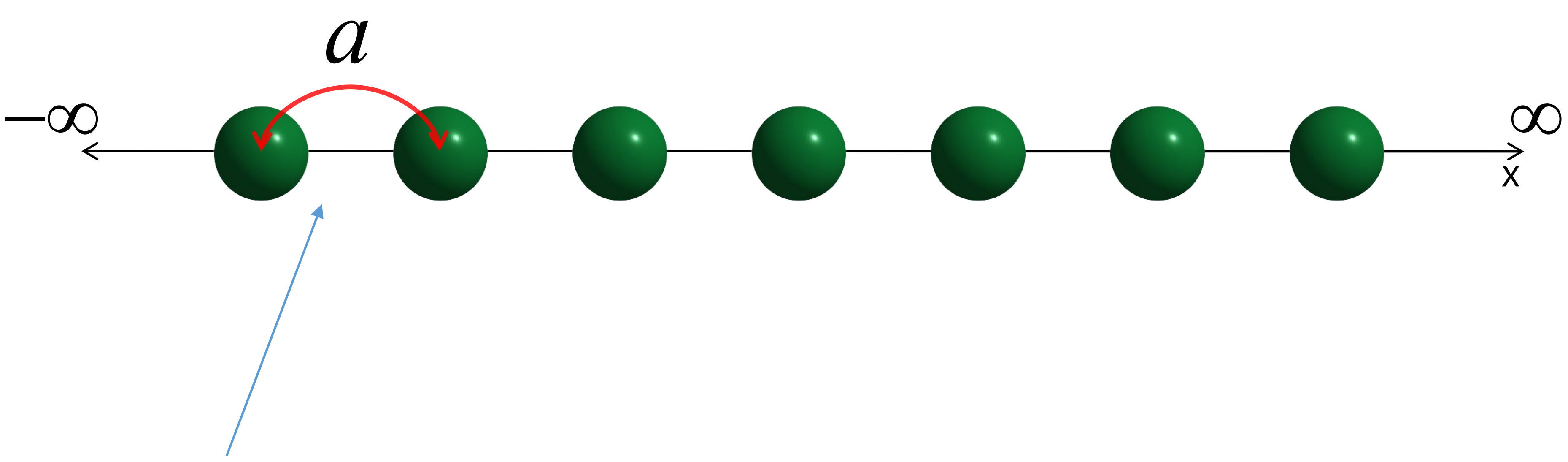


$$\varphi_n(\vec{r})$$

$$\text{Momentum} = \langle \varphi_n | \hat{\mathbf{p}} | \varphi_n \rangle = ???$$

$$\text{Angular momentum} = \langle \varphi_n | \hat{\mathbf{L}} | \varphi_n \rangle = ???$$

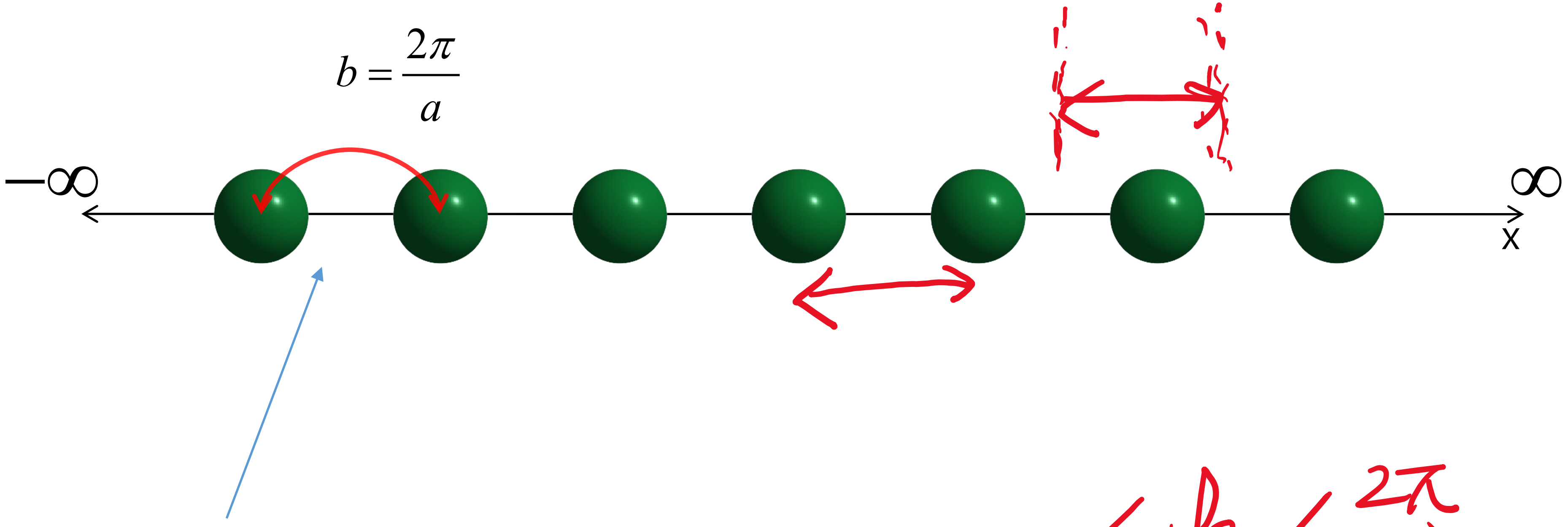
[Example] A one-dimensional lattice



Unit cell ?
Lattice constant

Remember !!! The reciprocal lattice

$$b = \frac{2\pi}{a}$$



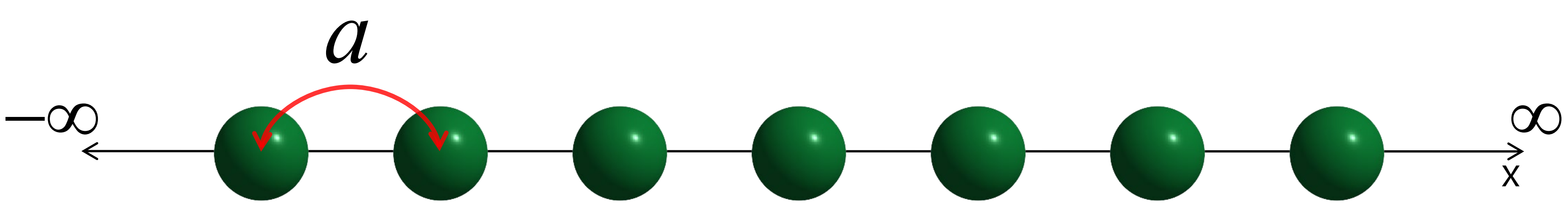
Unit cell of the reciprocal
Lattice constant

$$0 \le k < \frac{2\pi}{a}$$

or $-\frac{\pi}{a} \le k < \frac{\pi}{a}$

or ......

[Example] tight-binding limit



$$\psi_{n,k}(x)=\sum_{R} e^{ikR}\varphi_n\left(x-R\right)$$

$$\psi_{n,k}(x)=\sum_{l=-\infty}^{\infty} e^{ikla}\varphi_n\left(x-la\right)$$

Show that it is the Bloch translation eigenstate

$$\psi_{n,k}(x+R)=e^{ikR}\psi_{n,k}(x)$$

The energy band structure

band width

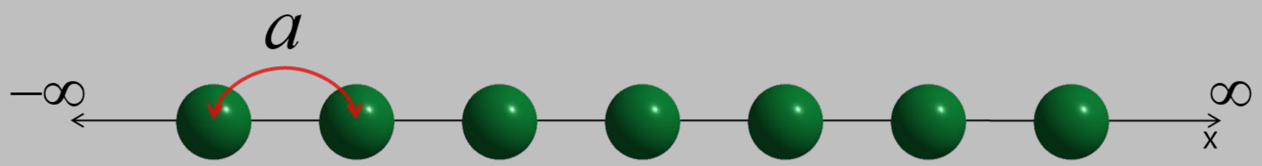
The energy band structure

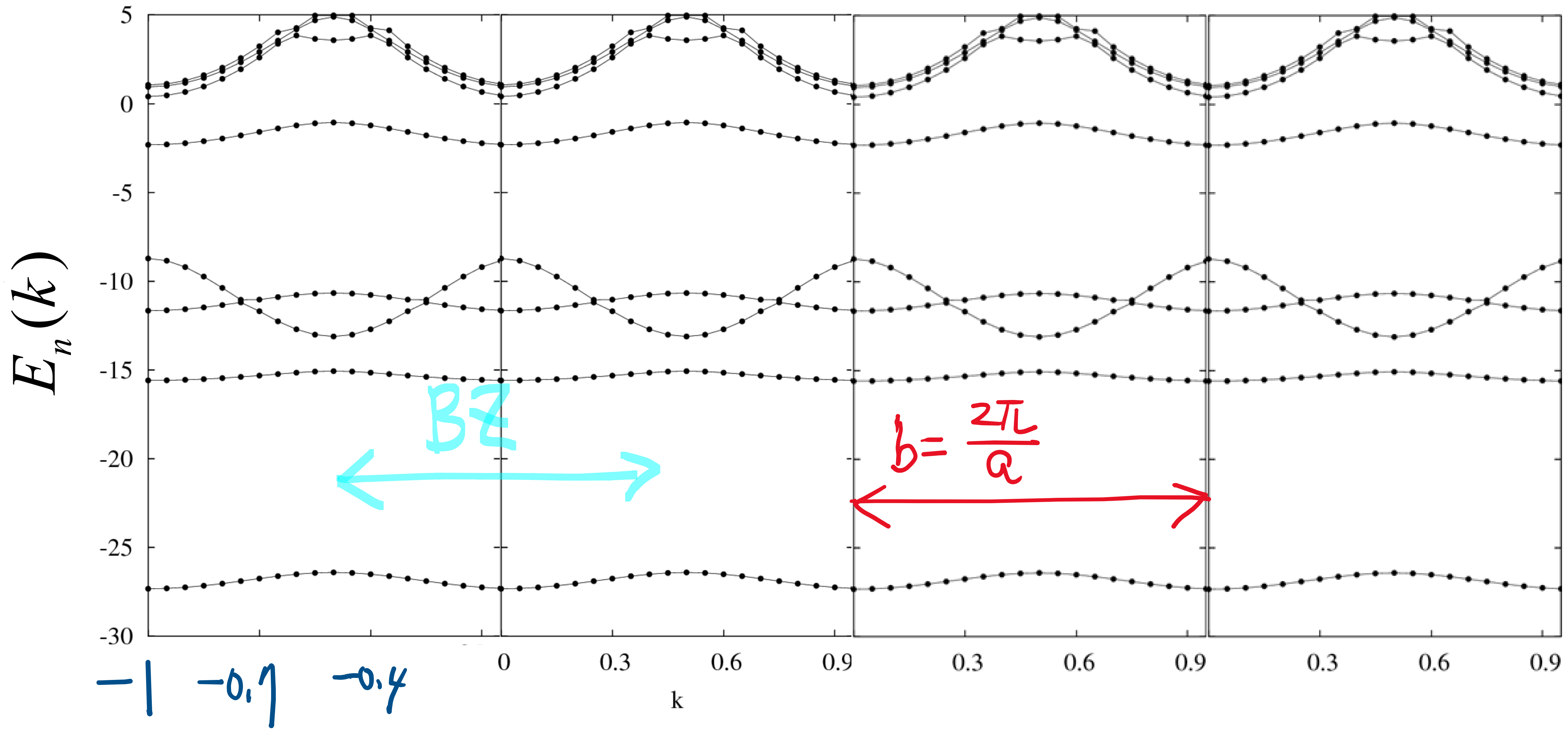
I. The eigenvalue

$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+V(\vec{r})\right)u_{n,\vec{k}}(\vec{r})=E_n(\vec{k})u_{n,\vec{k}}(\vec{r})$$

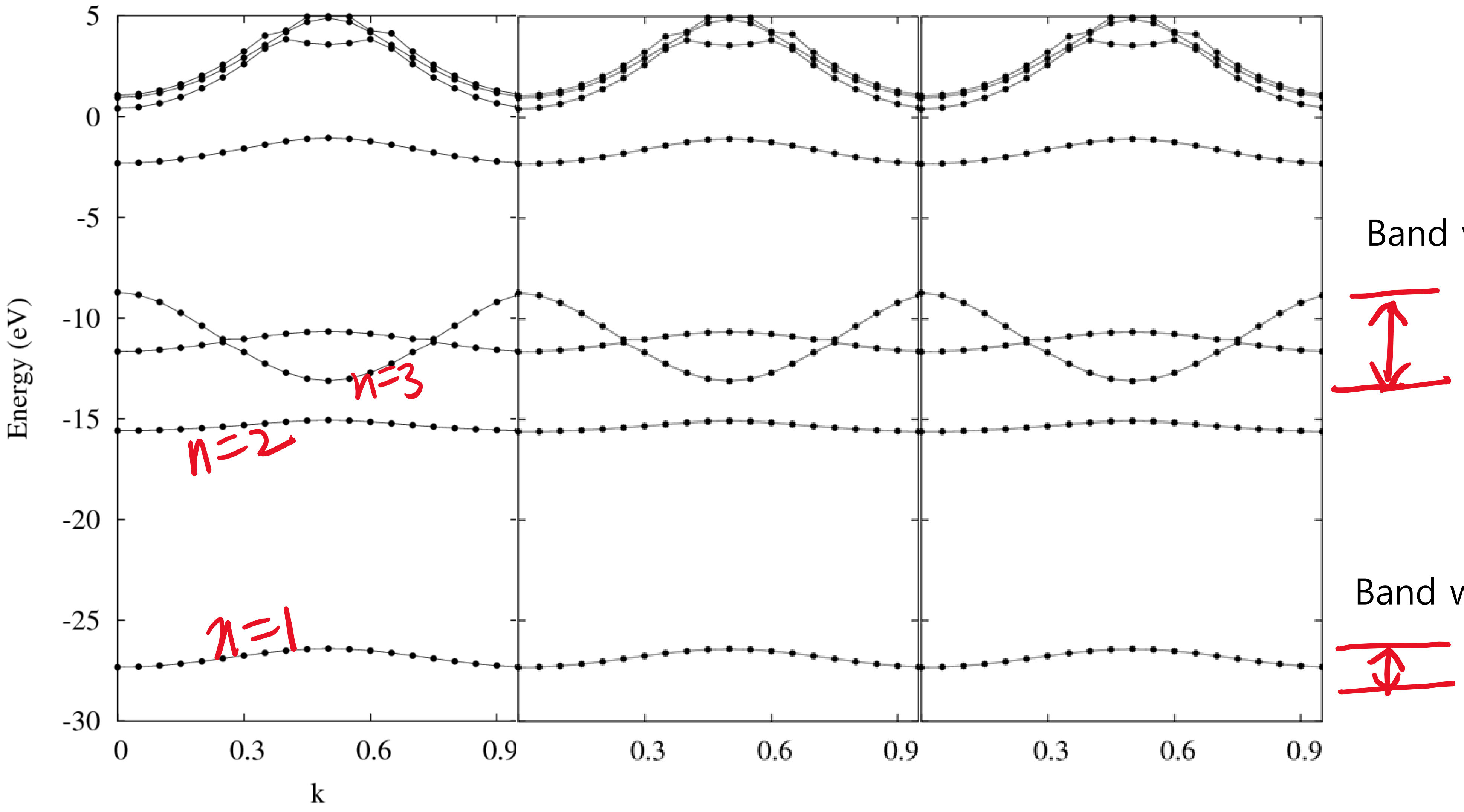
$$E_n(\vec{k})=E_n(\vec{k}+\vec{G})$$

The eigenvalue constitutes the band structure


a
−∞
∞
x


$E_n(k)$
5
0
-5
-10
-15
-20
-25
-30
0
0.3
0.6
0.9
0.3
0.6
0.9
0.3
0.6
0.9
k
BZ
$b = \frac{2\pi}{a}$
−1
−0,7
−0,4

The energy band structure



Band width of the 3rd band

Band width of the 1st band