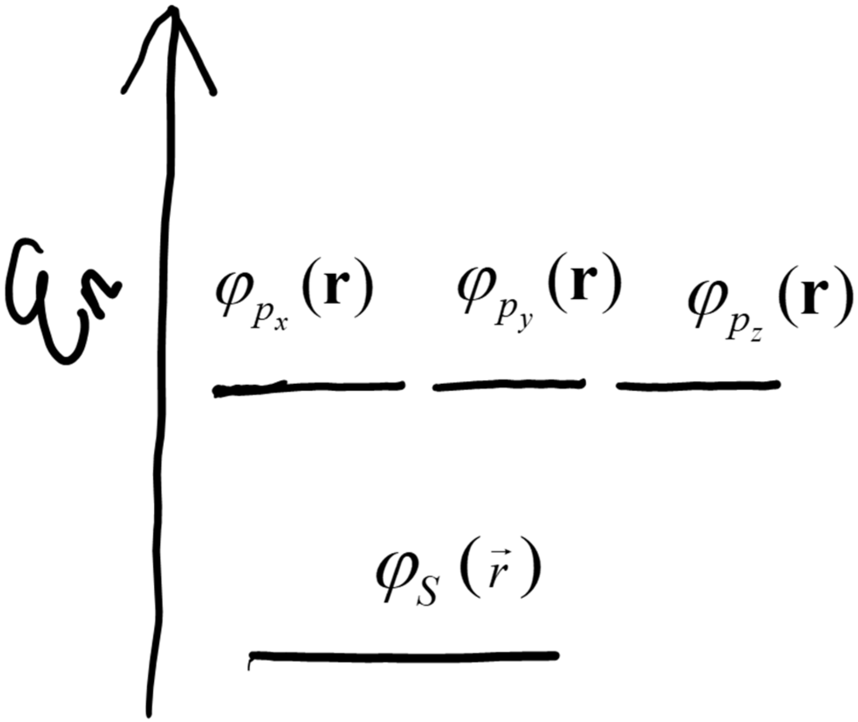
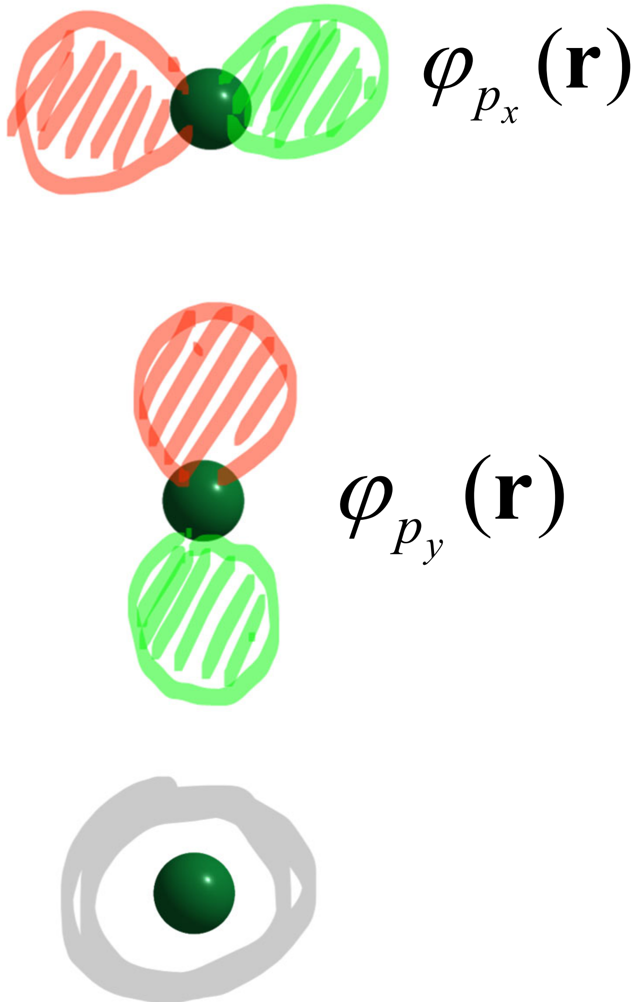
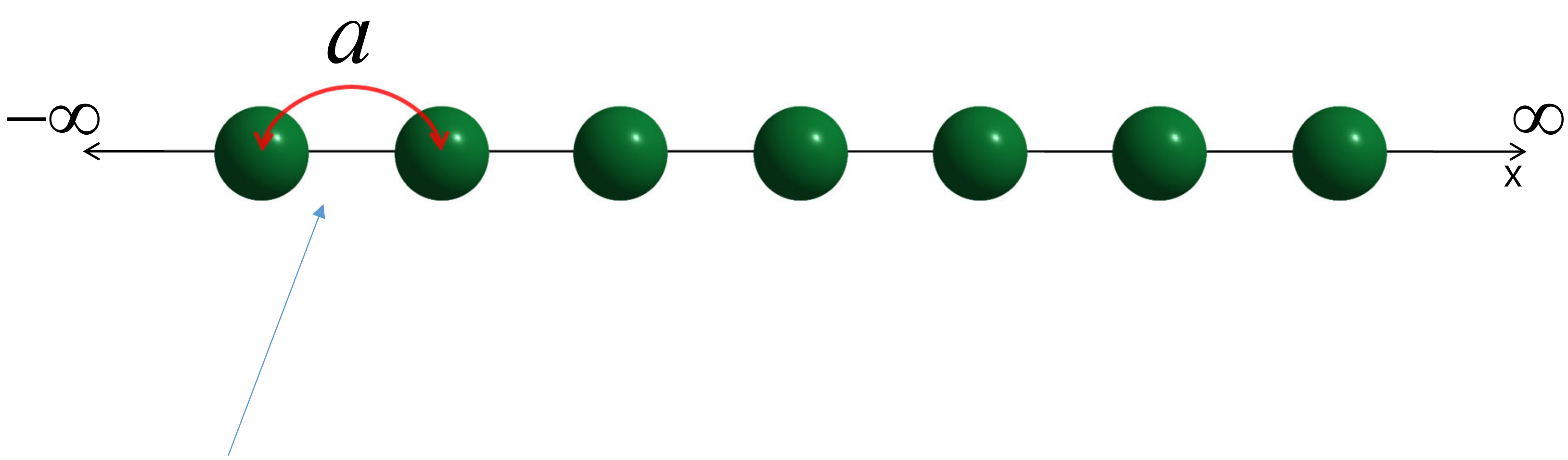
Suppose we have an atom





The lattice consisting of this atom



Unit cell ?
Lattice constant

The Bloch state

I. The simultaneous eigenstate of $\widehat{H}$ and $\hat{T}[\vec{R}]$

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

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

II. Tight-binding limit, it is well described by the linear sum

$$\psi_{n,\vec{k}}(\vec{r}) = \sum_{\vec{R}} A_n e^{i\mathbf{k}\cdot\mathbf{R}}\varphi_n(\vec{r} - \vec{R})$$

The Bloch state

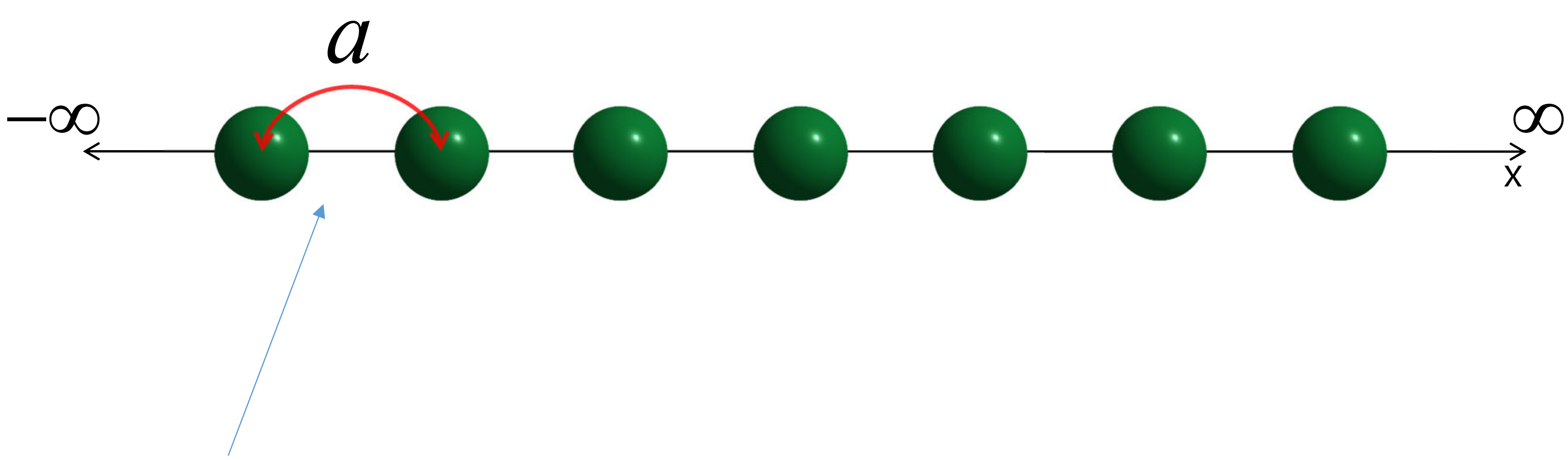
III. Show that it is indeed the translation eigenstate

$$\psi_{n,\vec{k}}(\vec{r}) = \sum_{\vec{R}} A_n e^{i\mathbf{k}\cdot\mathbf{R}} \varphi_n(\vec{r} - \vec{R})$$

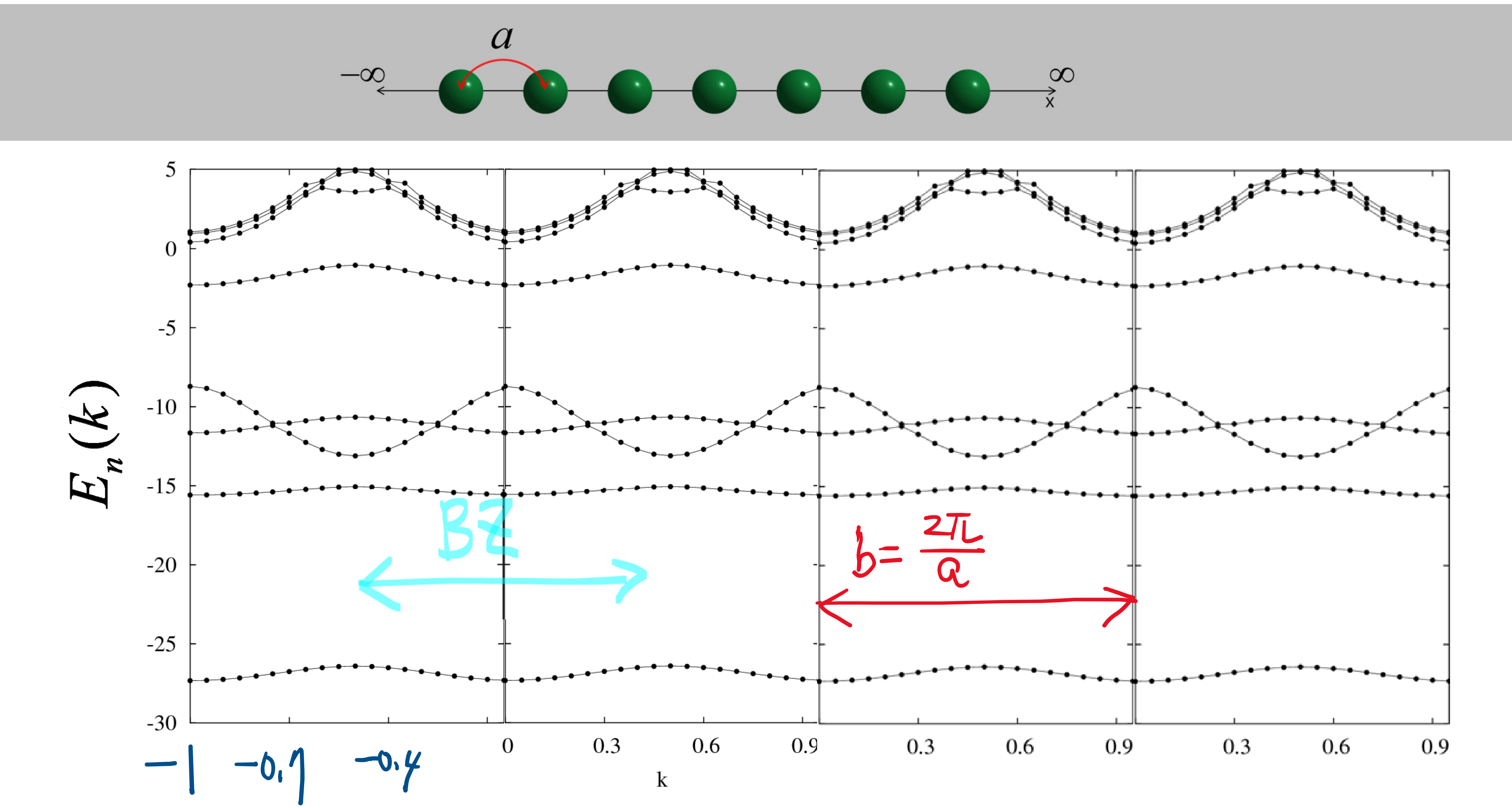
$$\hat{T}(\vec{R})\psi_{n,\vec{k}}(\vec{r}) = \psi_{n,\vec{k}}(\vec{r} + \vec{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n,\vec{k}}(\vec{r})$$

IV. Tight-binding limit, it is well described by the linear sum

Think of one-dimensional energy band structure

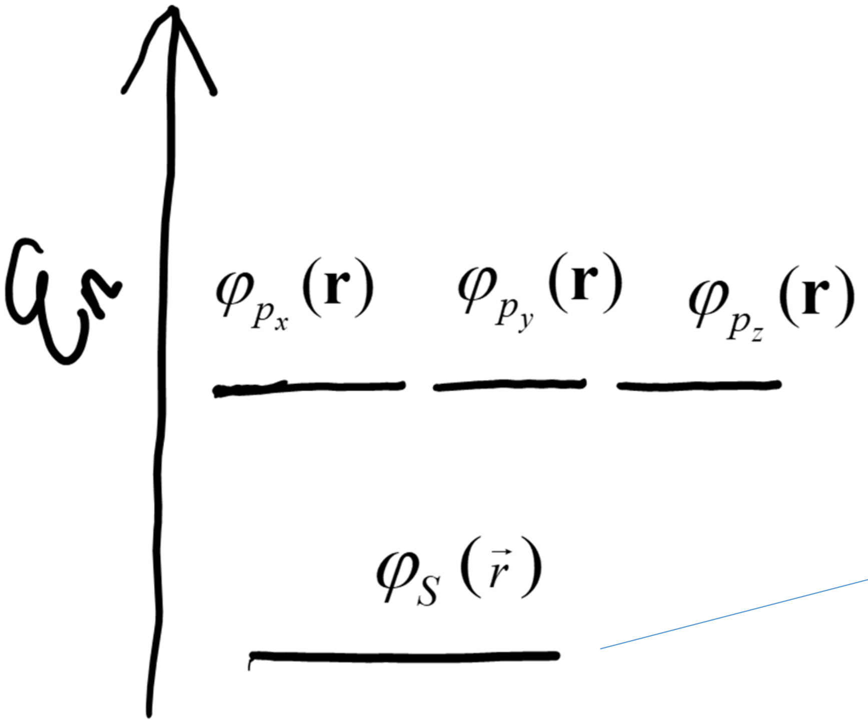


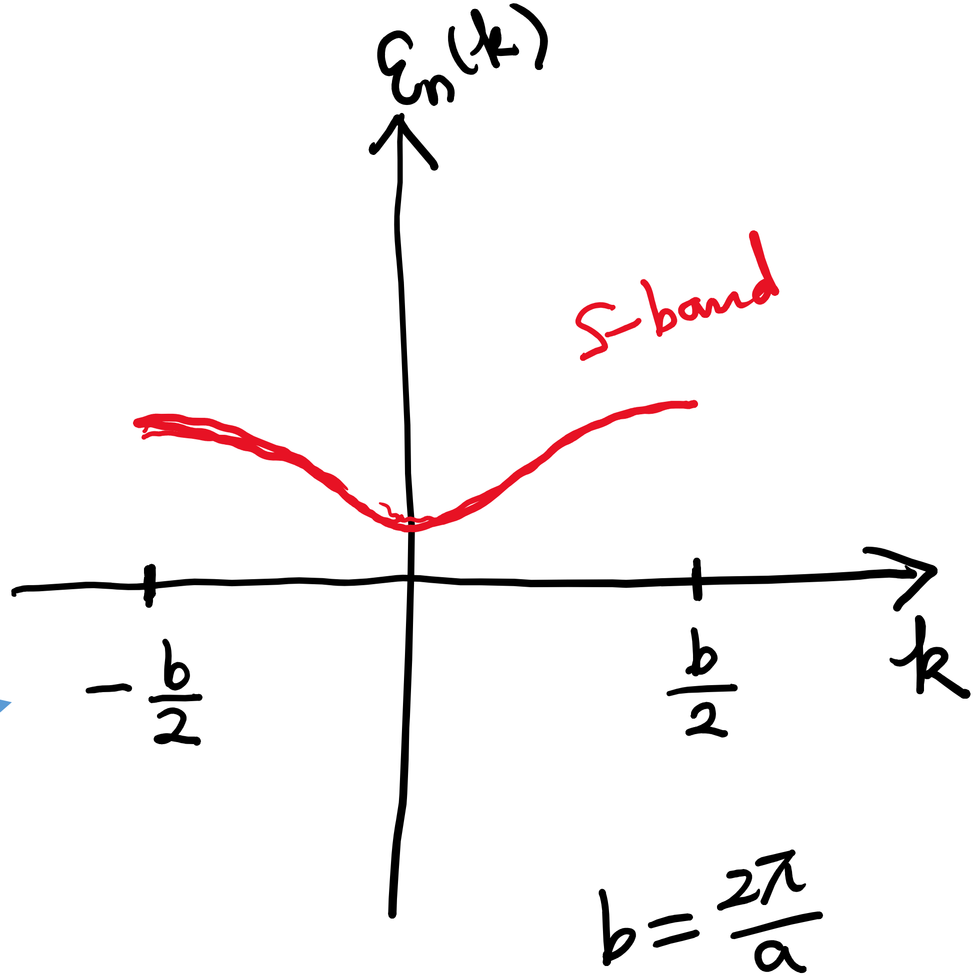
Unit cell ?
Lattice constant



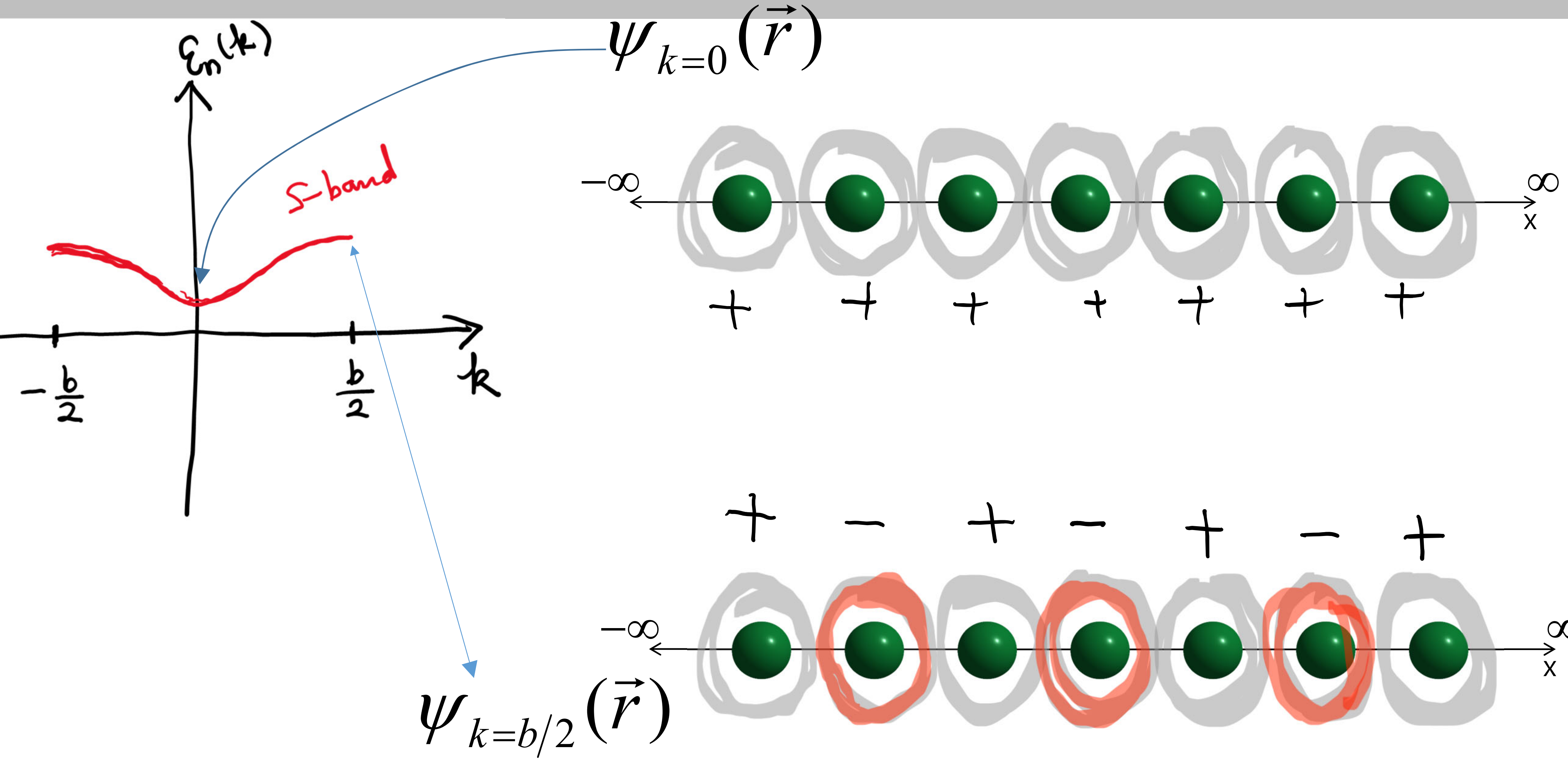
a
−∞
∞
x
$E_n(k)$
5
0
-5
-10
-15
-20
-25
-30
0
0.3
0.6
0.9
k
BZ
$b = \frac{2\pi}{a}$
-1
-0.7
-0.4

Suppose we have an atom





The shape of s-band wavefunction at each k



Suppose we have an atom