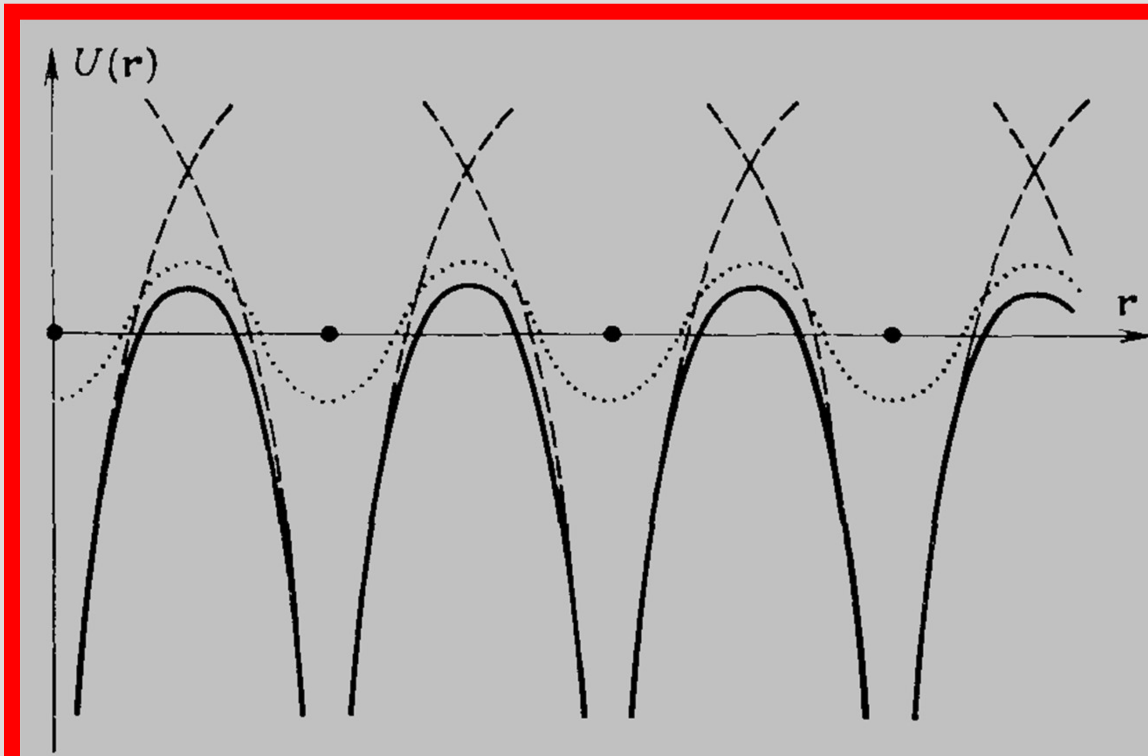
# فصل 7

## ترازهای الکترونی در یک پتانسیل تناوبی

- قضیه بلوخ
- ساختار نواری
- مدل کرونینگ پنی

# THE PERIODIC POTENTIAL




$$H\psi = \left( -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right) \psi = \mathcal{E} \psi$$

# BLOCH'S THEOREM

*Theorem.*[1] The eigenstates $\psi$ of the one-electron Hamiltonian $H = -\hbar^2\nabla^2/2m + U(\mathbf{r})$, where $U(\mathbf{r} + \mathbf{R}) = U(\mathbf{r})$ for all $\mathbf{R}$ in a Bravais lattice, can be chosen to have the form of a plane wave times a function with the periodicity of the Bravais lattice:

$$\boxed{\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})}$$

$$\boxed{u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})}$$

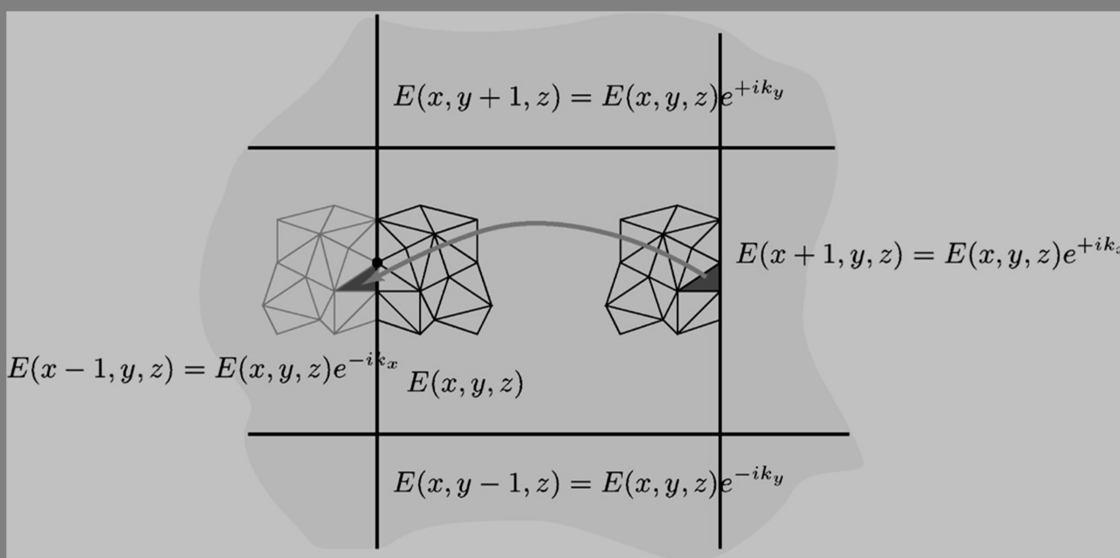
$$\Rightarrow \boxed{\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r})}$$

Bloch's theorem is sometimes stated in this alternative form:[3] the eigenstates of $H$ can be chosen so that associated with each $\psi$ is a wave vector $\mathbf{k}$ such that

$$\boxed{\psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r})}$$

*'When I started to think about it, I felt that the main problem was to explain how the electrons could sneak by all the ions in a metal....
By straight Fourier analysis I found to my delight that the wave differed from the plane wave of free electrons only by a periodic modulation'*

*F. BLOCH*



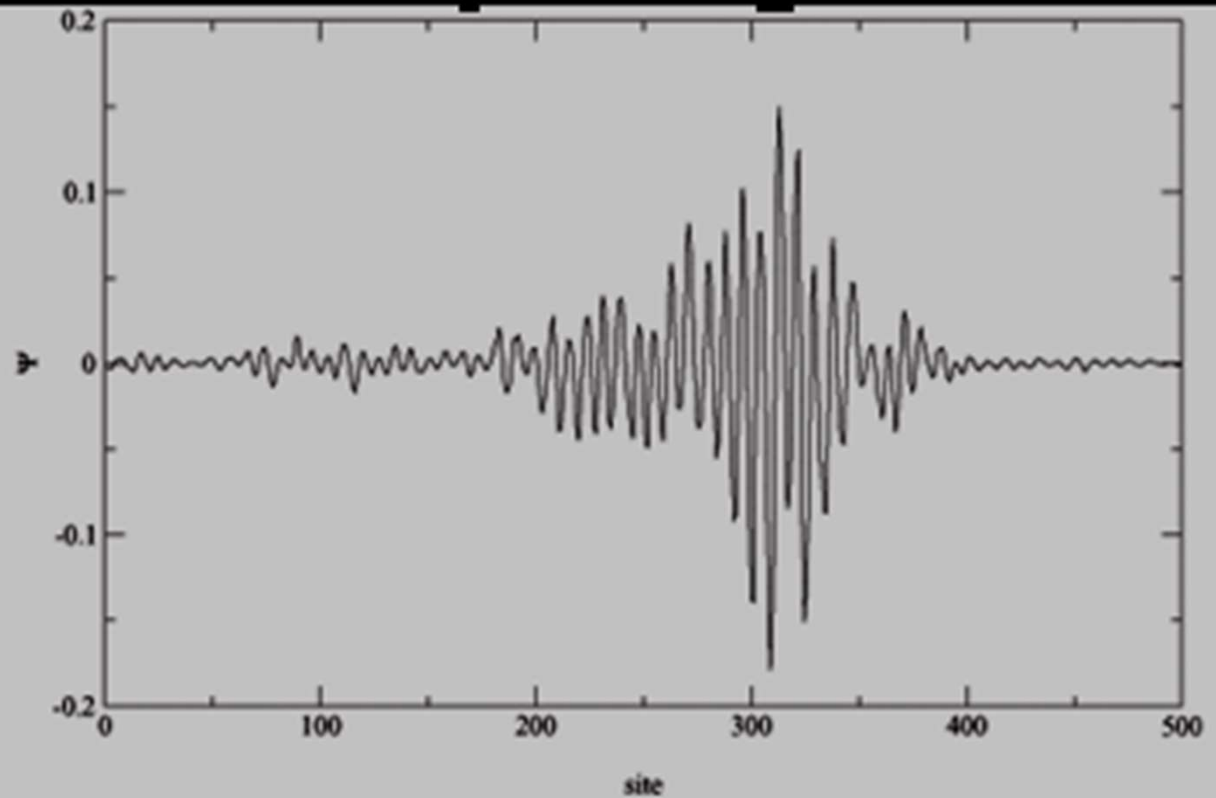




FIG. 4. Wave function of a delocalized state with energy close to 10.5 eV.

# Proof of Bloch's Theorem

$$T_{\mathbf{R}}\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{R})$$

$$T_{\mathbf{R}}H(\mathbf{r})\psi(\mathbf{r}) = \mathbf{H}(\mathbf{r}+\mathbf{R})\psi(\mathbf{r}+\mathbf{R}) = \mathbf{H}(\mathbf{r})\psi(\mathbf{r}+\mathbf{R}) = \mathbf{H}(\mathbf{r})\mathbf{T}_{\mathbf{R}}\psi(\mathbf{r})$$

Translation operator commutes with Hamiltonain.

$$\boxed{[\mathbf{H}, \mathbf{T}_{\mathbf{R}}] = 0}$$

so they share the same eigenstates

$$H\psi(\mathbf{r}) = \mathbf{E}\psi(\mathbf{r}) \qquad T_{\mathbf{R}}\psi(\mathbf{r}) = \mathbf{c}(\mathbf{R})\psi(\mathbf{r})$$

$$T_{\mathbf{R}}T_{\mathbf{R}'}\psi(\mathbf{r}) = \mathbf{c}(\mathbf{R})\mathbf{T}_{\mathbf{R}'}\psi(\mathbf{r}) = \mathbf{c}(\mathbf{R})\mathbf{c}(\mathbf{R}')\psi(\mathbf{r})$$

$$T_{\mathbf{R}}T_{\mathbf{R}'}\psi(\mathbf{r}) = \mathbf{T}_{\mathbf{R}+\mathbf{R}'}\psi(\mathbf{r}) = \mathbf{c}(\mathbf{R}+\mathbf{R}')\psi(\mathbf{r})$$

$$\boxed{c(\mathbf{R}+\mathbf{R}') = \mathbf{c}(\mathbf{R})\mathbf{c}(\mathbf{R}')}$$

**We can always write:** $c(\mathbf{a}_i) = e^{2\pi i x_i}$

Now let $\mathbf{a}_i$ be three primitive vectors for the Bravais lattice.

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

**We had proved that:** $\boxed{c(\mathbf{R}+\mathbf{R}') = c(\mathbf{R})c(\mathbf{R}')}$

**Thus:** $C(\mathbf{R}) = C(n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3) = C(n_1\mathbf{a}_1)C(n_2\mathbf{a}_2)C(n_3\mathbf{a}_3)$

$$C(n_i a_i) = C(a_i)^{n_i}$$

**Why ?**

$$C(n_i\mathbf{a}_i) = C(\underbrace{\mathbf{a}_i + \mathbf{a}_i + \ldots + \mathbf{a}_i}_{n_i}) = \underbrace{C(\mathbf{a}_i)C(\mathbf{a}_i)\ldots C(\mathbf{a}_i)}_{n_i} = C(a_i)^{n_i}$$

$$\Rightarrow \quad c(\mathbf{R}) = c(\mathbf{a}_1)^{n_1} c(\mathbf{a}_2)^{n_2} c(\mathbf{a}_3)^{n_3}$$

$$C(\mathbf{R}) = \exp\{2\pi i x_1\}^{n_1} \exp\{2\pi i x_2\}^{n_2} \exp\{2\pi i x_3\}^{n_3}$$

$$C(\mathbf{R}) = \exp\{2\pi i x_1\}^{n_1} \exp\{2\pi i x_2\}^{n_2} \exp\{2\pi i x_3\}^{n_3}$$

$$C(\mathbf{R}) = \exp\{2\pi i n_1 x_1\} \ \exp\{2\pi i n_2 x_2\} \ \exp\{2\pi i n_3 x_3\}$$

$$C(\mathbf{R}) = \exp\{2\pi i (n_1 x_1 + n_2 x_2 + n_3 x_3)\}$$

$$\boxed{c(\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}}$$

$$\mathbf{K.R} = 2\pi i (n_1 x_1 + n_2 x_2 + n_3 x_3)\}$$

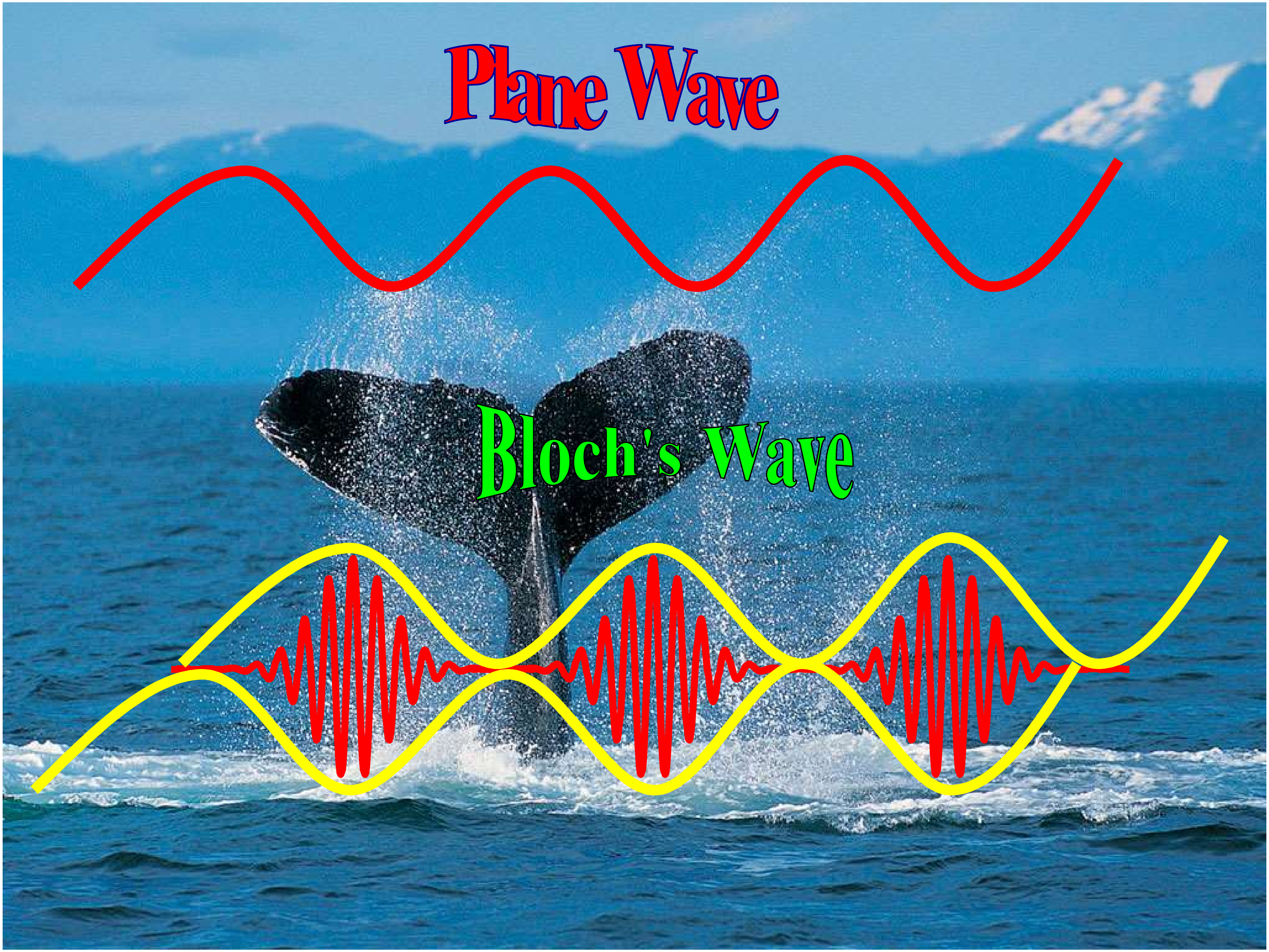
Why ?

$$\mathbf{k} = x_1\mathbf{b}_1 + x_2\mathbf{b}_2 + x_3\mathbf{b}_3 \qquad \mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

$$\boxed{T_{\mathbf{R}}\psi = \psi(\mathbf{r}+\mathbf{R}) = c(\mathbf{R})\,\psi = e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r})}$$

☺


Plane Wave
Bloch's Wave