فصل 7
ترازهای الکترونی در یک پتانسیل تناوبی
قضیه بلور
ساختار نواری
مدل کروینگ پنی
THE PERIODIC POTENTIAL

\[ H \psi = \left( -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right) \psi = \xi \psi \]
**Theorem.** The eigenstates $\psi$ of the one-electron Hamiltonian $H = -\hbar^2 \nabla^2 / 2m + U(r)$, where $U(r + R) = U(r)$ for all $R$ 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:

\[
\psi_{nk}(r) = e^{i \mathbf{k} \cdot \mathbf{r}} u_{nk}(r)
\]

\[
\psi_{nk}(r + R) = e^{i \mathbf{k} \cdot \mathbf{R}} \psi_{nk}(r)
\]

\[
u_{nk}(r + R) = u_{nk}(r)
\]

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

\[
\psi(r + R) = e^{i \mathbf{k} \cdot \mathbf{R}} \psi(r)
\]
‘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

\[ T_R \psi(r) = \psi(r + R) \]

\[ T_R H(r) \psi(r) = H(r + R) \psi(r + R) = H(r) \psi(r + R) = H(r) T_R \psi(r) \]

Translation operator commutes with Hamiltonain.

\[ [H, T_R] = 0 \]

so they share the same eigenstates

\[ H \psi(r) = E \psi(r) \]
\[ T_R \psi(r) = c(R) \psi(r) \]

\[ T_R T_{R'} \psi(r) = c(R) T_{R'} \psi(r) = c(R) c(R') \psi(r) \]

\[ T_R T_{R'} \psi(r) = T_{R + R'} \psi(r) = c(R + R') \psi(r) \]

\[ c(R + R') = c(R) c(R') \]
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.

Thus:

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

We had proved that:

\[ c(\mathbf{R} + \mathbf{R}') = c(\mathbf{R})c(\mathbf{R}') \]

Thus:

\[ C(\mathbf{R}) = C(n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3) = C(n_1 \mathbf{a}_1)C(n_2 \mathbf{a}_2)C(n_3 \mathbf{a}_3) \]

\[ C(n_i \mathbf{a}_i) = C(\mathbf{a}_i)^{n_i} \]

Why?

\[ C(n_i \mathbf{a}_i) = C(\mathbf{a}_i + \mathbf{a}_i + \ldots + \mathbf{a}_i) = C(\mathbf{a}_i)^{n_i} \]

\[ C(\mathbf{R}) = c(\mathbf{R}) \]

\[ = c(\mathbf{a}_1)^{n_1}c(\mathbf{a}_2)^{n_2}c(\mathbf{a}_3)^{n_3} \]

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

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

\[ c(R) = e^{ik \cdot R} \]

\[ K \cdot R = 2\pi i(n_1 x_1 + n_2 x_2 + n_3 x_3) \]

\[ k = x_1 b_1 + x_2 b_2 + x_3 b_3 \hspace{1cm} R = n_1 a_1 + n_2 a_2 + n_3 a_3 \]

\[ b_i \cdot a_j = 2\pi \delta_{ij} \]

\[ T_R \psi = \psi (r + R) = c(R) \psi = e^{ik \cdot R} \psi (r) \]
Plane Wave

Bloch's Wave