

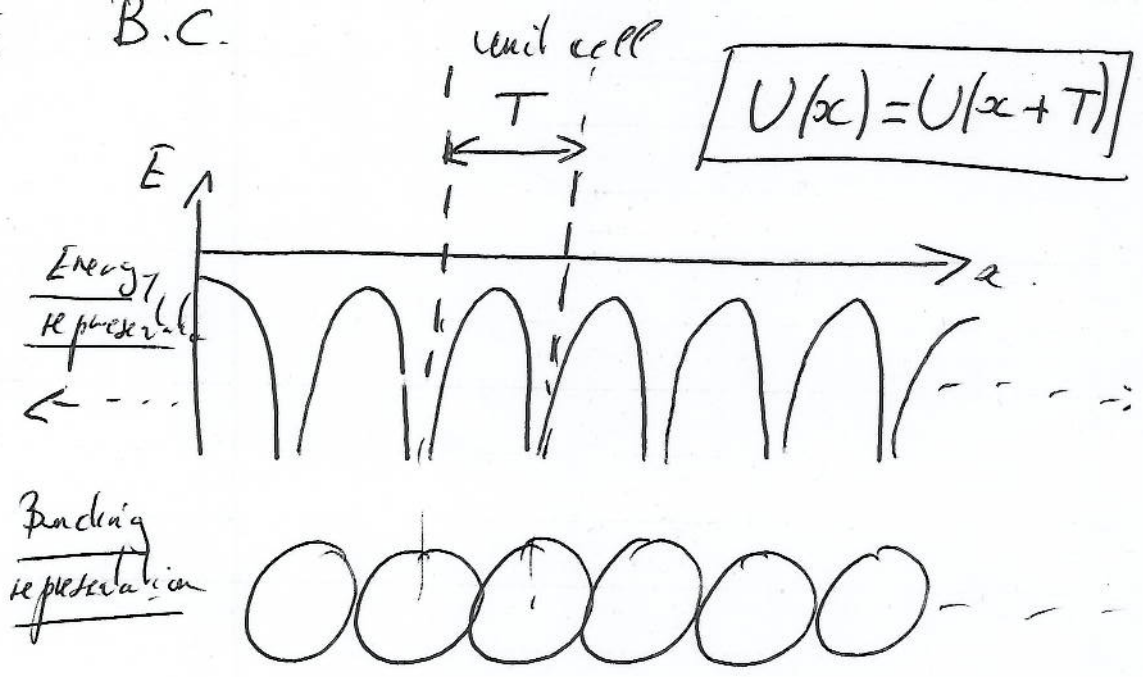
⑥ Infinite systems

we are considering a crystal system

(crystalline structure where atoms are placed in high ordered structure).

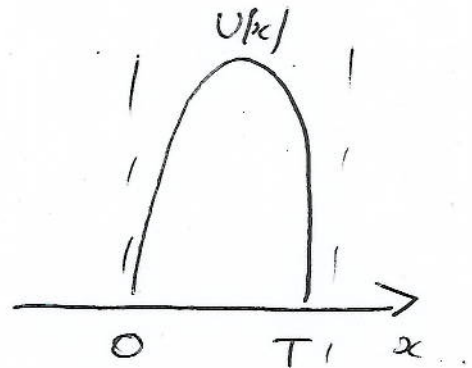
The potential is then periodic and we can obtain all the properties of the crystal while solving the Schrödinger equation only in one unit cell with appropriate B.C.

Example 1D



so let us consider only $U(x)$.

where $x \in [0, T]$



What are the B.C for $\psi(x)$ at $x=0, x=T$?

(i) First form of the Bloch theorem.

$$\text{if } U(x) = U(x+t) \Rightarrow \psi_R(x+t) = \psi_R(x) e^{ikT}$$

in our case we need to solve for a given $k \in \left[\frac{-\pi}{T}, \frac{\pi}{T} \right]$.

$$\left\{ \begin{array}{l} -\frac{\hbar^2}{2m} \frac{d^2 \psi_R(x)}{dx^2} + U(x) \psi_R(x) = E_k \psi_R(x), \quad x \in [0, T] \\ \text{and } \psi_R(T) = \psi_R(0) e^{ikT}. \end{array} \right.$$

(ii) Second form of the Bloch theorem.

$\psi(x)$ can be factored into a Bloch function $u_k(x)$

and a plane wave e^{ikx} .

$$\left\{ \begin{array}{l} \psi_R(x) = u_k(x) e^{ikx} \\ u_k(x+T) = u_k(x). \end{array} \right.$$

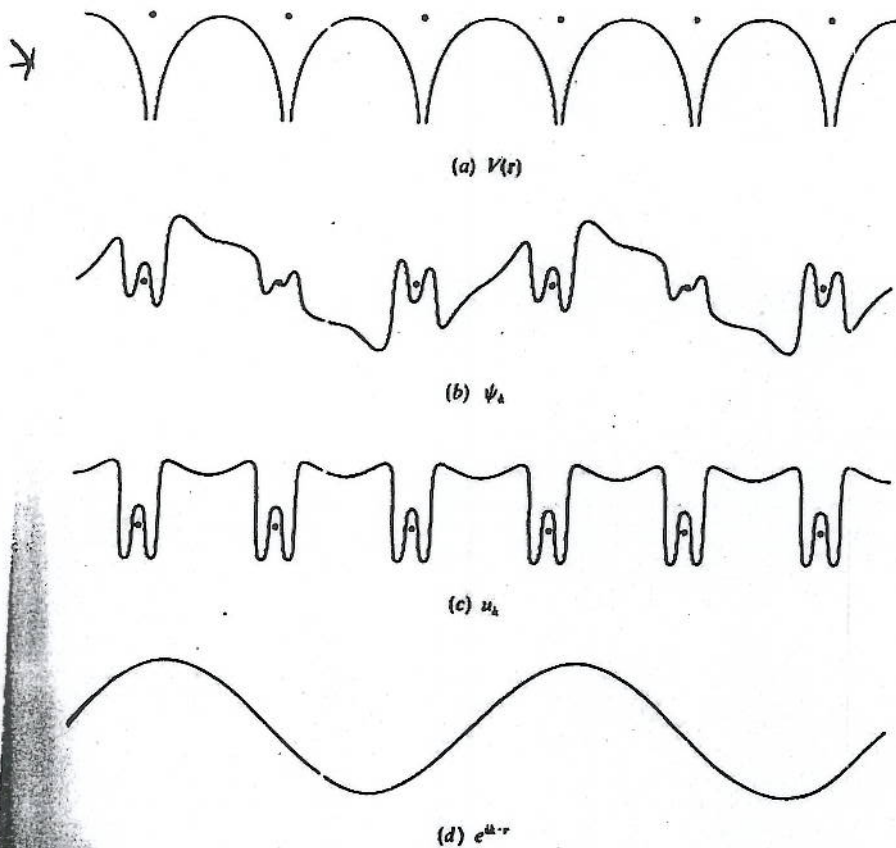


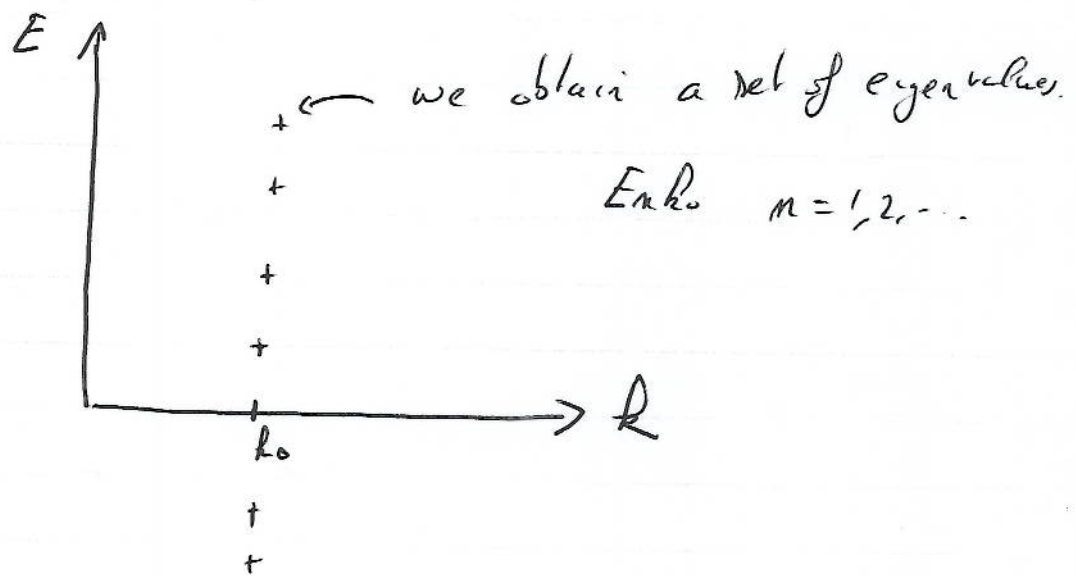
Fig. 2.1 A schematic representation of electronic eigenstates in a crystal. (a) The potential plotted along a row of atoms. (b) A sample eigenstate; the state itself is complex but only the real part is shown. This state can be inserted into Bloch function (c), which has the periodicity of the lattice, and (d) a plane wave, the real part of which is shown.

So we need to solve for a given $k \in [-\frac{\pi}{T}; \frac{\pi}{T}]$

$$\begin{cases} -\frac{\hbar^2}{2m} (\Delta + 2i\vec{k} \cdot \vec{\nabla} - k^2) \psi_k + U \psi_k = E_k \psi_k & x \in [0, T] \\ \text{and } \psi_k(T) = \psi_k(0) \Rightarrow \text{periodic B.C.} \end{cases}$$

iii) Numerical procedure (Bandstructure calculations).

For a given k , we get to solve an eigenvalue problem to obtain a set of eigenvalues $\{E_k^m\}$ and eigenvectors $\{\psi_k^m\}$ $m=1, 2, 3, \dots$



Then we repeat for all $k(s)$ and obtain the

dispersion relation, $-\frac{\pi}{T} < k < \frac{\pi}{T} \Rightarrow$ because of periodicity, First Brillouin zone

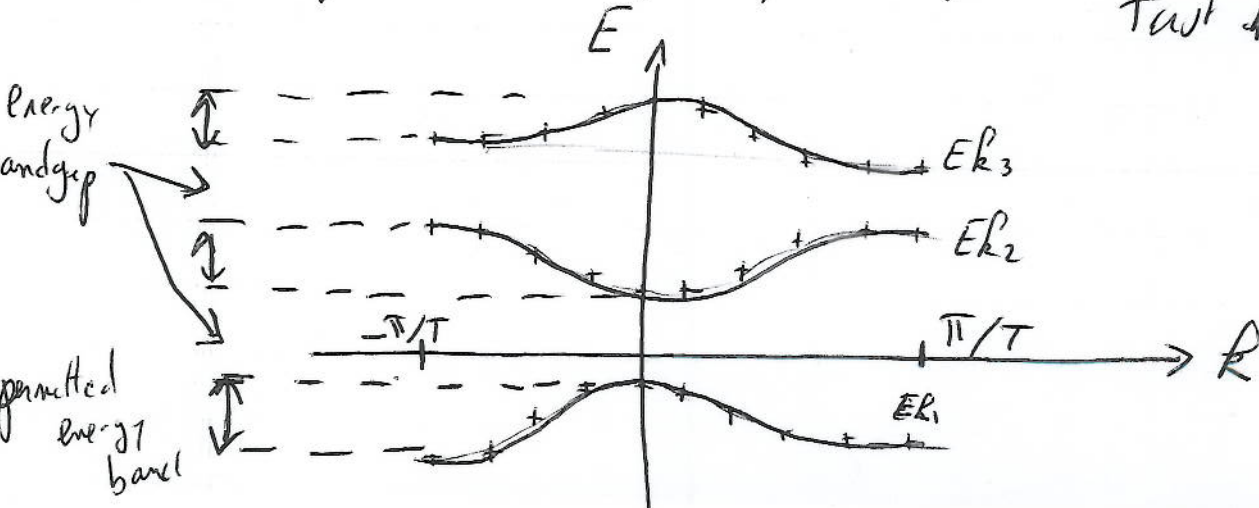
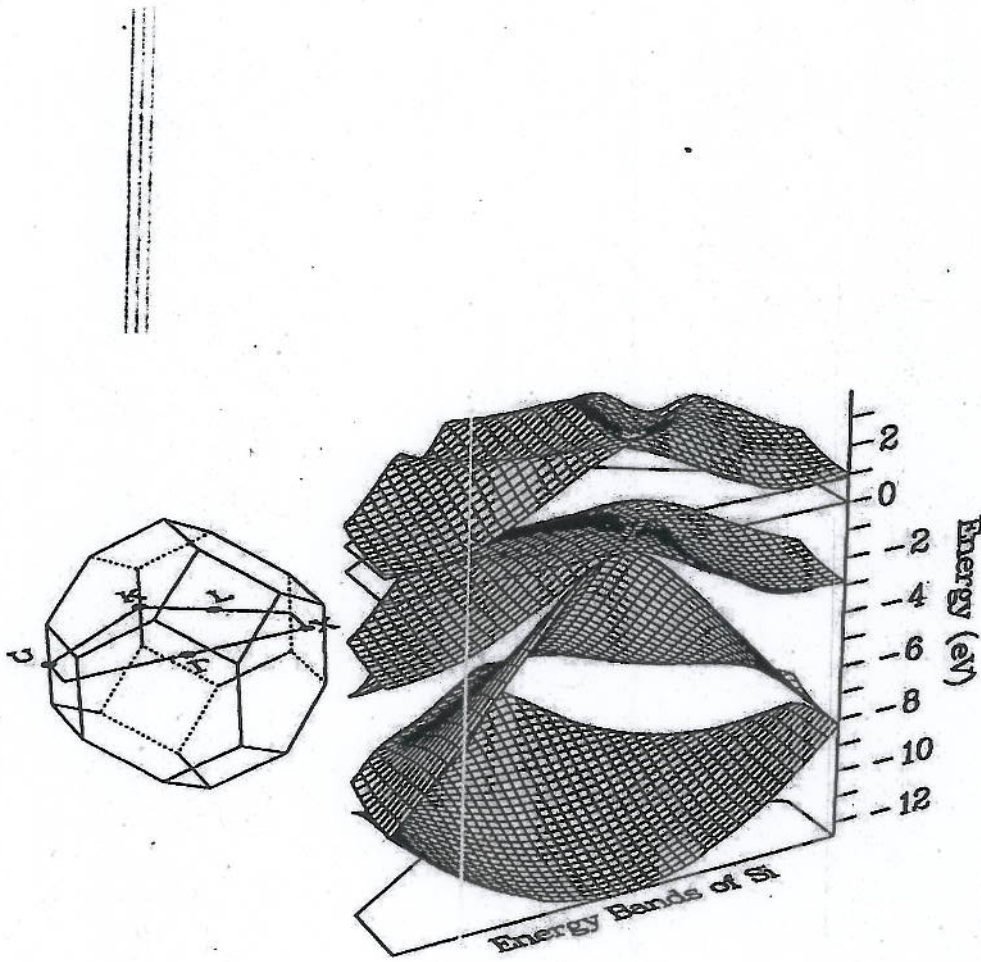


Figure 1: Perspective plot of the energy band structure of silicon. The figure to the left shows the Brillouin zone, and the two-dimensional section over which the energy bands are displayed. The energy bands are plotted to the right. The four surfaces lying below 0 eV are the valence bands, and the upper surface is the lowest conduction band. The maximum valence band energy occurs at $k = 0$, which on this figure is the center of the front boundary of the Brillouin-zone section. The minimum conduction-band energy occurs along the front boundary of the section, near the left and right ends. Thus, Si has an indirect-gap band structure.



$$E_g = 1.12 \text{ eV}$$

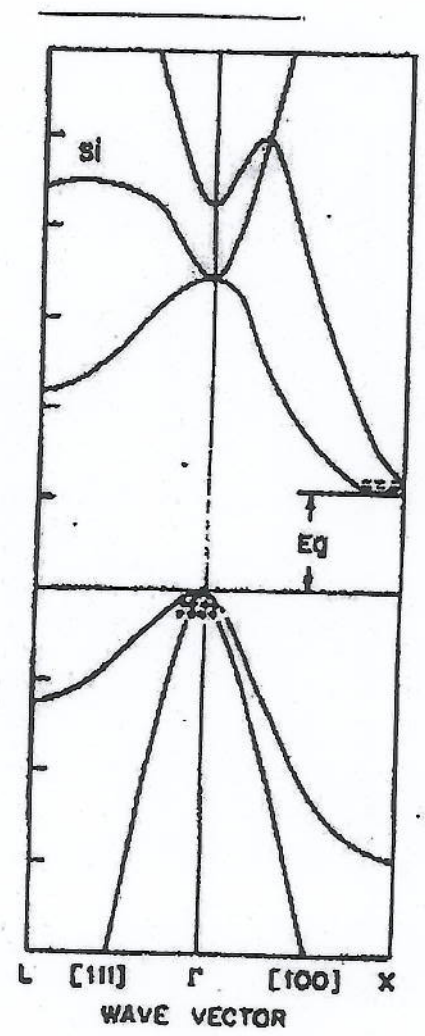
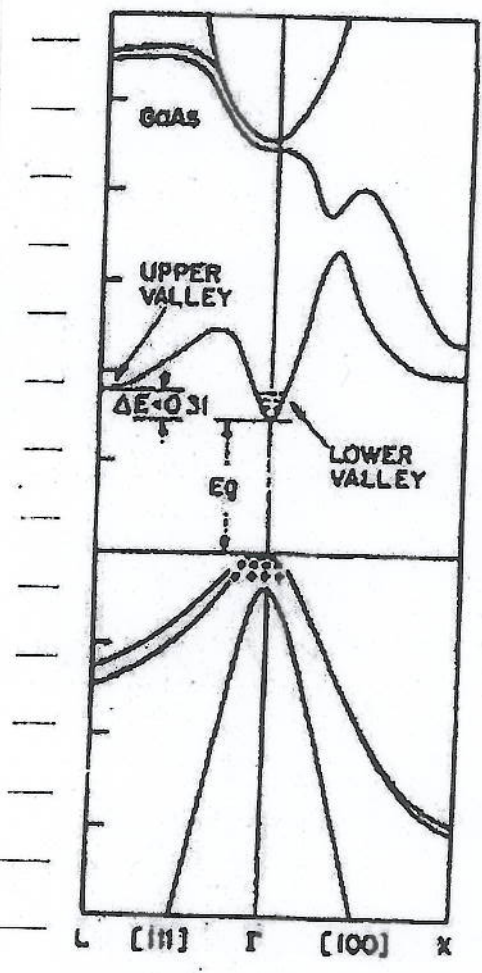
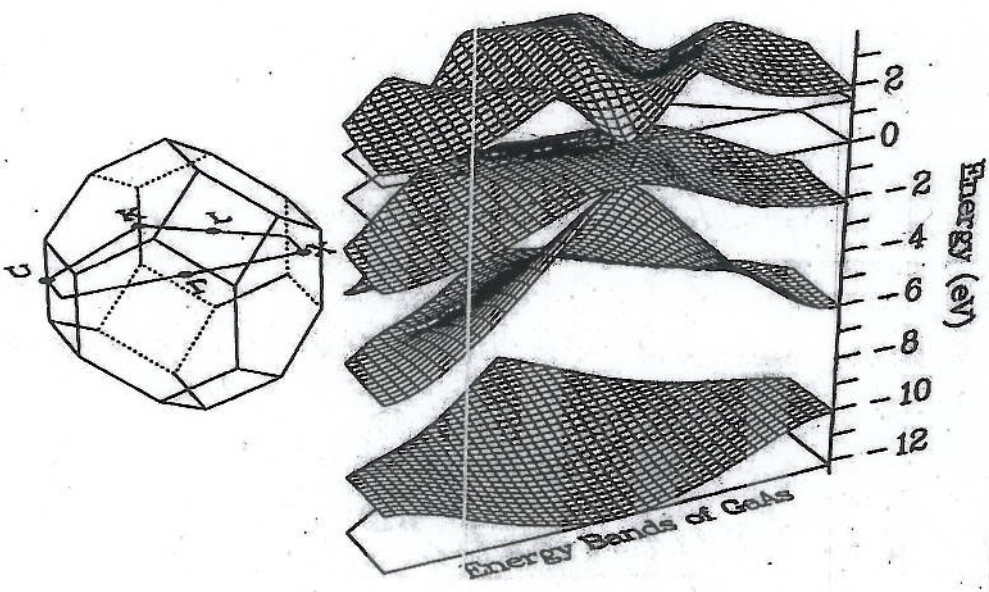


Figure 2: Perspective plot of the energy band structure of gallium arsenide. The conventions of the figure are the same as those of Fig. 1. The conduction-band minimum of GaAs occurs at $k = 0$, and thus GaAs has a direct-gap band structure.



$E_g = 1.42 \text{ eV}$