The electronic states in this system are most simply described by the Effective Mass Approximation (EMA). As long as one considers states of same symmetry across the heterojunction (see Fig 2.1), e.g., Γ valley electrons in both GaA and AlₓGa₁₋ₓAs, the motion of particles relative to the band edge is determined by the envelope function equation:

\[
\begin{bmatrix}
-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m^*_\perp(z)} \frac{\partial}{\partial z} - \frac{\hbar^2}{2m^*_\parallel} \nabla^2 + V_{\text{eff}}(z)
\end{bmatrix} \psi(\vec{r}, z) = \varepsilon \psi(\vec{r}, z).
\]  

(1)

Here \( m^*_\perp(z) \) = effective mass perpendicular to the heterojunction interface

\( m^*_\parallel \) = effective mass parallel to the interface

\( \vec{r} \) = position vector parallel to the interface

\( z \) = position perpendicular to the interface

The EMA is valid only if \( \psi(\vec{r}, z) \) vary slowly over the dimensions comparable to the unit cell of the crystal.

The kinetic energy operator for motion perpendicular to the interface has been chosen to make the Hamiltonian Hermitian so that the eigen values are real.

The effective potential is assumed to vary only in the direction perpendicular to the interface, and it comprises of several terms:

\[ V_{\text{eff}}(E) = E_c + V_D(z) + V_{ee}(z) \]

where \( E_c(z) \) = heterojunction conduction band discontinuity

\( V_D(z) \) = electrostatic potential due to ionized donors and acceptors

\( V_{ee}(z) \) = self consistent Hartree and exchange potentials due to free electrons

Since the potential is only \( z \) dependent, the solution of eqn. (1) is separable i.e.

\[ \psi(\vec{r}, z) = \frac{1}{\sqrt{A}} e^{i\vec{k} \cdot \vec{r}} \phi(z). \]

(2)

Here, \( A = \) area parallel to the interface and \( \vec{k} \) = wave vector parallel to the interface and the function \( \phi(z) \) must satisfy the equation

\[
\begin{bmatrix}
-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m^*_\perp(z)} \frac{\partial}{\partial z} + V_{\text{eff}}(z)
\end{bmatrix} \phi_n(z) = \varepsilon_n \phi_n(z)
\]

(3)

and the total energy relative to the band minima (or maxima) is (assuming parabolic bands)

\[
\varepsilon_{n, \vec{k}} = \frac{\hbar^2 k^2}{2m^*_\parallel} + \varepsilon_n
\]

(4)

Continuity of wave function requires \( \phi_n(z) \) to be continuous, and conservation of probability current.
requires \( \frac{1}{m^*_l(z)} \partial \phi_n \) to be continuous across interfaces. Note that solution of (3) allows both bound as well as propagating states.

**Quantum Well**

![Schematic Quantum well structure for heterojunction](image)

In the simplest energy band picture for a quantum well made of AlGaAs-GaAs-Al-Ga-As structures, the band gap difference is distributed between the valence and conduction band in such a way that both electrons and holes are confined to the smaller band gap GaAs layer. Such a heterojunction is called Type I system. At 300 K, the band gap of Al\(_x\)Ga\(_{1-x}\)As is found empirically as (at \( \Gamma \) point in k-space)

\[
E_g^\Gamma(x) = 1.424 + 1.245x \ eV, \quad \text{for } x < 0.35
\]

where \( x \) is the Al mole-fraction.

The actual fraction of the band gap difference \( \Delta E_c \) is not known accurately, and one usually finds

\[
\Delta E_c \approx 0.65 \times \left[ E_{AlGaAs} - E_{GaAs} \right].
\]

If one assumes a low carrier density \( < 10^{14} \text{ m}^{-2} \) and low doping, then the terms \( V_D(z) \) and \( V_{es}(z) \) in \( V_{eff}(z) \) may be neglected and \( m^*_l(z) \) treated as a constant = \( m^*_l \), so that the problem of Eqn.(3) is reduced to that of a simple finite square well of width \( L \) (say). If now one assumes the potential barrier \( \Delta E_c \) large compared with the bound states (i.e., states deep inside the well) \( \in \), then regarding the barrier as infinite, one gets

\[
\phi_n(z) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi z}{L} \right), \quad n = 1, 2, 3, \ldots
\]

\[
\in = \frac{\hbar^2 \pi^2}{2m^*_l L^2}.
\]

Typically, \( \in \) varies from several hundred meV for \( L < 50 \text{ nm} \) to several meV for \( L \sim 100 \text{ nm} \) for low values of \( n \).

Since the motion in the plane parallel to the interface is free, whereas that in the direction perpendicular to the interface is confined (i.e., bound in the well), such a system is referred to as a quasi-two dimensional electron gas (to be denoted as 2 DEG). For each solution 'n', there exists a continuum of two dimensional states called "sub-bands" (sometimes referred to as modes, in analogy with standing waves in em wave guides).