CHAPTER 1

BASIC PROPERTIES OF TWO-DIMENSIONAL ELECTRON GAS
1.1 INTRODUCTION

Advances in miniaturization technology made it possible to fabricate artificial semiconductor heterostructures whose chemical composition and shapes are controlled with nanostructure accuracy. Properties of these structures are based on quantum effects, the very nature of matter and energy itself. These quantum semiconductor structures provide us with new ways to investigate condensed matter physics under the conditions of reduced dimensionality (two, one and zero). Because of the possibility of tailoring the properties of these systems for specific purposes, the quantum structures have potential or revolutionary applications in the electronic and optoelectronic devices.

After the pioneering work by Esaki and Tsu [1.1] for the transport properties and Dingle [1.2] for optical properties, the field of two-dimensional quantum well heterostructures got sudden impulse and break through in the fundamental physics and applications at the end of 1970's with the discovery of quantum Hall effect in Si/SiO$_2$ inversion layers [1.3]. There are several reviews on the electronic properties of semiconductor heterostructures starting with the celebrated Ando, Fowler and
Stern [1.4] continuing with conference proceedings, book chapters and books. Few of them are mentioned in references[1.5-1.11].

Si-MOSFET (metal-oxide semiconductor field effect transistor) is the device in which a two-dimensional electron gas (2DEG) was first realized. During 1970's it was the prominent test structure for examining a 2DEG. In this structure 2DEG is formed at the Si/SiO₂ interface, due to the creation of an inversion layer by application of a sufficiently strong positive bias to the gate electrode. Electrons in this well are free to move only in the plane parallel to the interface. Electronic properties of the 2DEG in Si-MOSFETs have been reviewed by Ando, Fowler and Stern [1.4].

Subsequently, higher quality 2D systems such as GaAs/GaAlAs heterojunctions (HJs), quantum wells (QWs) and multiple quantum wells (MQWs) were fabricated using molecular beam epitaxy and metal organic chemical vapour deposition techniques.

A heterojunction structure is formed when lattice matched two different semi-infinite semiconductors are joined. Doping one or both constituents a space charge region is established that leads to band bending at the interface forming a nearly
triangular potential well in the smaller band gap material. Carriers in this well form a 2DEG. The spatial extent of 2DEG is typically 30-100 Å and surface carrier density is of the order of $10^{12}$ cm$^{-2}$. In HJ carrier concentration is controlled by doping unlike in case of MOSFET. Usually, spacer layer (undoped larger band gap layer of few nm thickness) is used between impurities and the interface to reduce scattering due to impurities to achieve very high mobilities. Most of the HJ devices are fabricated from III-V compounds. GaAs/Ga$_{1-x}$Al$_x$As is one of the prominent heterostructures with the Al mole fraction $x = 0.3$.

A quantum well (QW) is formed when a smaller band gap semiconductor layer ($\approx 10$ nm) sandwiched between two thick layers of larger band gap semiconductors. Carriers remain in smaller band gap semiconductor. It is similar to 'particle in a box' problem in quantum mechanics. We describe QW in detail in section 1.2 as it is the system of primary interest in our study.

Multiple quantum well (MQW) is essentially made of many single quantum wells grown one over the other with the barrier region so thick that there is no interaction between the neighbouring wells. Properties of each QW are going to be
MQWs form a superlattice (SL), with new periodicity along the growth axis, when barriers are so thin that there is finite interaction between the neighbour wells [1.1]. The quantized energy levels in QWs now get broadened resulting into formation of minibands separated by miniband gaps. Electron gas in SL form a quasi-3DEG system.

Quantum systems such as quantum well wires (QWW), quantum point contacts (narrow constrictions), quantum boxes and quantum dots which are of still lower dimensionality are achieved in 2DEG by additional lateral confinements (see for example references [1.9 - 1.11]) with split gate techniques and nanoscale lithographic techniques. Due to the huge success of physics and devices of 2DEG systems it was natural to continue to diminish systems' dimensionality which have given new exciting results.

In this thesis we present some of the important optical and transport properties of 2DEG in QW. To study any physical property of a QW it is essential to know its electronic structure. In section 1.2 we describe a quantum well along with the shape of its potential well. In section 1.3 we give eigen functions and energy eigenvalues of a 2DEG in QW.
Electronic properties of a QW are strongly modified when a magnetic field is applied perpendicular to the interface. Electron gas becomes zero-dimensional. All physical properties show oscillatory behaviour as a function of magnetic field. In section 1.4 we discuss eigen functions and eigenvalues of 2DEG in a quantizing magnetic field. The density of states (DOS), an important property governing almost all optical and transport properties, is discussed in section 1.5. The properties that we are going to study will involve electron-phonon interactions. These are discussed in section 1.6.

1.2 QUANTUM WELL

Quantum well is considered to be the simplest quantum situation in which two-dimensional electron gas is realized. It consists of a single layer of material A embedded between two thick layers of materials B where B has a band gap larger than A. Both materials are lattice matched and band gap discontinuities are such that both types of carriers are confined in material A. The thickness of the layers of the material B is much greater than the penetration length of the confined wavefunction. This situation is exemplified by the
pairs of the materials GaAs/GaAlAs, GaInAsP/InP, GaInAs/AlInAs, GaSb/AlSb etc. They are also called type - 1 quantum wells as the minimum of conduction band lies above the maximum of the valence band of the sandwiched layer material. A range of materials now grown in ultrathin layers is too wide to be listed.

At the junctions of these systems the electron structure can be modelled as a steplike change (discontinuity) in the conduction and valence band edges. The height of the discontinuities, which are also called conduction band and valence band offsets, depend upon the bulk band structures of the constituent materials and on their relative positions. A QW can be thought as made up of two single heterojunctions. In fact each heterojunction has triangular potential well and when quantum well is formed the bottom is curved upwards. This gradually becomes almost a rectangular potential well with flat bottom as the width of the sandwiched layer becomes smaller and also curvature is smaller for lightly doped materials. A QW may be considered rectangular [1.5,1.8] for all practical purposes.

By far the most frequently used materials are GaAs and Ga\(_{1-x}\)Al\(_x\)As with \(x = 0.3\) to ensure that potential barrier in
the conduction band is large and the alloy is still a direct-gap material. Abrupt nature of interface is well satisfied in GaAs/AlAs structures. A sample consisting of a thin layer of GaAs of width $L$ sandwiched between thick layer of $\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}$ is shown in figure 1.1(a). A buffer layer of undoped GaAs (about 1 $\mu$m thickness) is first grown on semi insulating GaAs substrate. Layers of GaAlAs and GaAs of different thickness are grown alternately. At the interface conduction and valence band offsets are of the order of $\Delta E_c \approx 300$ meV and $\Delta E_v \approx 200$ meV, respectively, for Al mole fraction $x = 0.3$. The schematic band diagram of this structure is shown in figure 1.1(b).

Modulation doping is made possible in this structure. The dopants are placed in larger band gap GaAlAs layer keeping the smaller band gap layer close to the intrinsic region. On thermal or optical excitation the carriers are collected in the GaAs layer as it is region of least energy. Hence material layer with smaller energy gap is called active layer. The separation of the carriers in the well from the donors in the barriers by few nanometers reduces the scattering of carriers by impurities. Enhanced mobility as large as $\approx 10^6 \text{ cm}^2\text{V}^{-1}\text{S}^{-1}$ is achieved which is mainly lattice limited. The electron
Fig. 1.1 (a) A GaAs/Ga$_{1-x}$Al$_x$As quantum well with width $L$. (b) The electronic structure of GaAs/Ga$_{1-x}$Al$_x$As quantum well. The horizontal lines show the confined levels in the well. $E_g$ is the energy gap of respective material. $\Delta E_C$ and $\Delta E_V$ are the conduction band and valence band offsets, respectively.
densities are of the order of $10^{12}$ cm$^{-2}$.

In the above examples the difference in the lattice constants of the two constituents materials is of the order of fraction of a percent or less. However, it is possible to grow high quality layers of materials when lattice mismatch is as large as several percent. The most notable example of practical importance is Si$_{1-x}$Ge$_x$/Si strained quantum well with $x = 0.5$. These quantum wells allow photodetectors in the 1.77 μm range. Si$_{0.5}$Ge$_{0.5}$ is an alloy with 50% of Si and 50% of Ge. Band diagram of this structure is shown in figure 1.2. The advantage of silicon based structures is that it is compatible with other silicon based devices. Moreover, silicon and germanium are technologically well understood.

We focus our study on GaAs/GaAlAs and SiGe/Si quantum wells.

1.3 EIGEN FUNCTIONS AND ENERGY EIGENVALUES

Electronic states and band structure calculations are required to interpret the experimental findings. On the contrary, experimental techniques such as transport and optics have brought and keep bringing a wealth of information on the electronic states of heterostructures. There are different
Fig. 1.2 The band diagram for a $\text{Si}_{0.5}\text{Ge}_{0.5}/\text{Si}$ quantum well structure. The horizontal lines show the positions of confined levels in the wells.
methods such as envelope function approximation, empirical tight binding and pseudopotential formalisms to calculate the electronic states in quantum well. It is assumed that Bloch nature of the states is still preserved. Envelope function description of electron states [1.12] taking crystal potential into account by means of effective mass approximation is a versatile method that has proved to be accurate.

In a quantum well the potential energy in the growth direction is function of z only. The electron wavefunction \( \Psi_{pk}(r,z) \) can be written as the product of the Bloch function \( u_k(r,z) \), a plane wavefunction \( \exp(ik \cdot r) \) in the x-y plane and a z-dependent factor \( \xi_p(z) \).

\[
\Psi_{pk}(r,z) = u_k(r,z) A^{-1/2} \exp(ik \cdot r) \xi_p(z), \tag{1.3.1}
\]

where \( r = (x,y) \) and \( k = (k_x, k_y) \) are the two-dimensional position vector and the wave vector, respectively, of the electron in the plane of the layer. \( \xi_p(z) \) is determined to a first approximation by the Schrödinger like equation

\[
\left( -\frac{\hbar^2}{2m_z} \frac{d^2}{dz^2} + V(z) \right) \xi_p(z) = E \xi_p(z), \tag{1.3.2}
\]

where \( m_z \) is the electron effective mass in the z-direction,
$V(z)$ is the potential in the z-direction and $E_p$ is the so-called confinement energy of the carriers. Therefore the early description of energy level scheme by simple confinement in quantum well due to energy band discontinuities in Dingle's work can be well justified.

In the infinitely deep well approximation, the solution of equation (1.3.2) demands that the wavefunction must vanish in confining barrier and hence at the interface because of the continuity equation. Taking the origin of the abscissa at the interface, the solution of equation (1.3.2) can evidently be

$$
\xi_p(z) = \left( \frac{2}{L} \right)^{1/2} \sin \left( \frac{p\pi z}{L} \right) \tag{1.3.3}
$$

with $p = 1, 2, 3, \ldots$.

The confining energy, from equation (1.3.2) $E_p$ is then given by

$$
E_p = p^2 E_o, \tag{1.3.4}
$$

where

$$
E_o = \frac{\hbar^2}{2m^*L^2}. \tag{1.3.4a}
$$

Usually $m_z$ is taken to be equal to $m^*$, the effective mass of
the electron energy levels and wavefunctions of an infinitely deep QWs are shown in figure 1.1(b).

Since motion parallel to the interface is free, the energy eigenvalues associated with the wavefunction (1.3.1) are given by

$$E_{p\kappa} = E_p + E_k$$  \hspace{1cm} (1.3.5)

with

$$E_k = \frac{\hbar^2 k^2}{2m^*}.$$  \hspace{1cm} (1.3.6)

Thus the 3D continuum breaks up into series of subbands each associated with 2D continuum. $E_0$ acts as bottom of 2D subband. The relation (1.3.5) is true in the parabolic approximation. The dispersion relation for this quasi two-dimensional (Q2D) electron gas is shown in figure 1.3. The real band structure over the entire Brillouin zone is a complex one [1.13]. However, only the carriers at the band extrema are involved in transport and optical processes and thus the relation (1.3.5) is still valid. It is evident from equation (1.3.5) that the band structure near the extrema is highly anisotropic unlike the case of bulk semiconductors. In figures 1.4(a) and 1.4(b) we have shown the band structure of bulk GaAs and SiGe,
Fig. 1.3 The energy of the 2D subbands, as a function of the wave vector. For each parabola, \( E_p \) (\( p = 1, 2, 3, \ldots \)) are the lowest points.
Fig. 1.4a Dispersion curves limiting the conduction band and valence band in GaAs. $E_g$ - Energy gap, $E_g^* = 1.43 \text{ eV}$, $0.35 \text{ eV}$, $0.5 \text{ eV}$. $\Gamma$ - Conduction band, VB - Valence band.
Fig. 1.4b  Electronic band structure for Si$_{0.5}$Ge$_{0.5}$ alloy grown in the strained-layer mode on a Si(001) substrate.
respectively.

In most of the III-V compound semiconductors the conduction band minimum is at the zone centre (Γ-point) and they have the spherical constant energy surfaces [1.13]. The transport theory of these materials is simpler on account of this.

For a finite well case the Schrödinger like equation (1.3.2) can be solved exactly [1.9], to yield wavefunctions and energies, with continuity conditions that at the interface the $\chi_p (z)$ and $(1/m^*)(\partial \chi_p (z) / \partial z)$ should be continuous. The effective potential in the growth direction as seen by the electron can be written as

$$ V(z) = \begin{cases} V_0', & \text{if} \ z < L/2 \\ 0, & - L/2 < z < L/2 \\ V_0, & \text{if} \ z > L/2 \end{cases} \quad (1.3.7) $$

where $V_0$ is height of the potential barrier. With origin of the coordinate system chosen at the center of the well, the QW has an inversion symmetry of the well and hence the solutions for wavefunctions can only be even or odd. Therefore they can be written as
\( \xi_p(z) = \begin{cases} 
A \cos(kz) & \text{for } |z| < L/2 \\
B \exp[-k(z - L/2)] & \text{for } z > L/2 \\
B \exp[k(z + L/2)] & \text{for } z < -L/2 
\end{cases} \) 

(1.3.8)

or

\( \xi_p(z) = \begin{cases} 
A \sin(kz) & \text{for } |z| < L/2 \\
B \exp[-k(z - L/2)] & \text{for } z > L/2 \\
B \exp[k(z + L/2)] & \text{for } z < -L/2 
\end{cases} \) 

(1.3.9)

where

\[
E_p = \left\{ \begin{array}{ll}
\frac{\hbar^2 k^2}{2m_A^*} - V_0, \\
-(\frac{\hbar^2 k^2}{2m_B^*}),
\end{array} \right.
\] 

(1.3.10)

\( m_A^* \) and \( m_B^* \) are electron effective masses of layer A and B, respectively. For the solution of equation (1.3.8) continuity conditions at \( z = \pm L/2 \) yield

\( A \cos(kzL/2) = B \) 

(1.3.11)

\( \left( \frac{k}{m_A^*} \right) \sin(kzL/2) = \frac{kB}{m_B^*} \). 

(1.3.12)
Therefore

\[(k_z / m^*_A) \tan(k_z L/2) = k/m^*_B \]  

(1.3.13)

Similarly, equation (1.3.9) gives

\[(k_z / m^*_A) \cot(k_z L/2) = -k/m^*_B \]  

(1.3.14)

Simple graphical solutions of equations (1.3.13) and (1.3.14) can be developed if \(m^*_A = m^*_B\). Using equation (1.3.10), equations (1.3.13) and (1.3.14) can be transformed to

\[
\cos(k_z L/2) = k_z/k_0 \quad \text{for } \tan k_z L/2 > 0 \quad (1.3.15) \\
\sin(k_z L/2) = k_z/k_0 \quad \text{for } \tan k_z L/2 < 0 \quad (1.3.16) 
\]

where \(k_0^2 = 2m^*_V / \hbar^2\). By plotting \(\cos(k_z L/2)\) and \(\sin(k_z L/2)\) as a function of \(k_z\), solutions are located at the intersections of the straight line with slope \(k_0^{-1}\) with these curves. The limiting case of infinitely high barriers can be found again by putting \(k_0 = \infty\).

In order to calculate hole levels in quantum wells a successive perturbation approach is used. It is shown that
valence band degeneracy of the bulk GaAs is lifted due to confinement potential and separate heavy and light hole bands are formed. In each of these bands the energy spectrum of holes is given by equations of the types (1.3.5) with \( m^* \) replaced by \( m_{hh} \) and \( m_{lh} \), the heavy and light holes masses, respectively. They are given by

\[
\begin{align*}
  m_{hh} &= \frac{m_0}{\gamma_1 - 2\gamma_2}, \\
  m_{lh} &= \frac{m_0}{\gamma_1 + 2\gamma_2},
\end{align*}
\]

(1.3.17)

where \( m_0 \) is free electron mass, \( \gamma_1 \) and \( \gamma_2 \) are the Kohn - Luttinger parameters.

1.4 QUASI-TWO-DIMENSIONAL ELECTRON GAS IN A QUANTIZING MAGNETIC FIELD

As in 3D electrons, the transport measurements under quantizing magnetic fields (i.e., \( \omega_c \tau \gg 1 \), where \( \omega_c \) is cyclotron frequency and \( \tau \) is collision time) provide a large amount of information regarding Q2D electron gas [1.4, 1.5]. These studies have opened a new era of quantum Hall effects, a major area in solid state physics.

If a strong magnetic field \( B \) is applied perpendicular to the plane of Q2D electron gas, free translational motion of
the electrons in the plane gets quantized into series of Landau levels due to Lorentz force. The effect is more dramatic, as the z-motion of the carriers is also frozen by the confining potential leading to completely confined quantum regions of the system. Such systems provide an ideal tool for the study of quantum transport phenomena. Almost all physical properties show oscillatory behaviour as a function of magnetic field. In real systems the Landau levels are broadened due to scattering by phonons, impurities, surface roughness and other scattering mechanisms. In the simplest approximation the broadening of the levels is described by level width $\Gamma$. In very large magnetic fields $\hbar \omega_c \gg \Gamma$.

The Schrödinger equation of an unbounded Q2D electron gas in a magnetic field, in the effective mass approximation, is written as

$$\left[ \frac{1}{2 m^*} \left( p + \frac{eA}{c} \right)^2 + V(z) \right] \Psi = E \Psi, \quad (1.4.1)$$

where $p = -i\hbar \nabla$ is the momentum operator, $V(z)$ is the confining potential in the z-direction, $A$ is the vector potential due to magnetic field. Using the gauge for the vector potential
For the magnetic field along the z-direction, the wavefunctions are given by \[1.4\]

$$
\Psi_{npk_y} = L_y^{-1/2} \hat{\Phi}_n(x - x_o) \exp(ik_y y) \xi_p(z), \quad (1.4.2)
$$

where \(n\) is the Landau quantum number, \(L_y\) and \(k_y\) are, respectively, sample dimension and electron wavevector in the y-direction, \(\hat{\Phi}_n\) is the normalized simple harmonic oscillator wavefunction:

$$
\hat{\Phi}_n(x) = \left[ 2^n n! \pi^{1/2} \right]^{-1/2} \exp(-x^2/2l^2) H_n(x/l) \quad (1.4.3)
$$

\(H_n\) is the Hermite polynomial, \(l = (\hbar/eB)^{1/2}\) is the classical cyclotron radius of the lowest oscillator \((n = 0)\) and \(\xi_p(z)\) is the normalized wavefunction due to the confining potential \(V(z)\). In equation (1.4.2) \(\hat{\Phi}_n\) is centered at \(x_o(k_y) = l^2 k_y\). In the gauge chosen electron states in the y-direction are plane waves and are localized in the x-direction.

Energy eigenvalues corresponding to states (1.4.2) are

$$
E_{np} = (n + \frac{1}{2}) \hbar \omega_c + E_p, \quad (1.4.4)
$$
where \( n = 0, 1, 2, \ldots \), \( \omega_c = \frac{eB}{m^*} \) is the cyclotron frequency and \( E_p \) is the energy of the \( p \)th subband. Thus the energy level structure of the Q2D electron gas is made up of the ladder of cyclotron levels for each of the confined state. This is shown in figure 1.5.

The number of states on each circle i.e., degeneracy of each Landau level can be found from number of cyclotron orbits in the crystal. This is found by ascertaining the condition that

\[
0 < x_o(k_y) < L_x \quad \text{i.e.,} \quad 0 < k_y < \left( \frac{m^* \omega_c L_x}{\hbar} \right) \quad (1.4.5)
\]

and that the density of the states in the \( k_y \) - direction is \( \frac{L_y}{2\pi} \). It means that the number of possible states in the range \( 0 \) and \( \left( \frac{m^* \omega_c L_x}{\hbar} \right) \) is \( \frac{L_y \omega_c}{2\pi \hbar} \). Hence number of states per unit area is \( \left( \frac{m^* \omega_c}{2\pi \hbar} \right) = \frac{eB}{\hbar} \). Each Landau level contains \( N_L = \frac{eB}{\hbar} \) states per unit area per spin. If the spin splitting is not resolved \( N_L = 2\left( \frac{eB}{\hbar} \right) \) has to be taken. Similar to the case of 3D, this degeneracy is equal to the number of 2D states contained in the energy spacing between consecutive Landau levels. Using the above results for the degeneracy, if
Fig.1.5 Energy levels of 2D electron gas in a quantum well in a magnetic field. $n$ - Landau quantum number.
electron areal density is $n_s$, the number of filled Landau levels is given by Landau level filling factor

$$\gamma = \frac{n_s}{(eB/h)/2} \begin{cases} 2nl^2n_s & \text{for spin resolved case.} \\ \pi l^2n_s & \text{for spin unresolved case.} \end{cases}$$

This dimensionless number $\gamma$ indicates how many of the successive Landau levels are filled. If the carrier density does not change with the magnetic field then the Fermi level $E_F$ will lie, at $T = 0$, in the $n$th Landau level (for the spin unresolved) which is given by

$$n = \text{Int} \left[ \frac{n_s}{2N_L} \right].$$

$E_F$ will exhibit sawtooth oscillations making a discontinuous jumps each time an integer number of Landau levels are filled. Equations (1.4.6) and (1.4.7) imply that for even integral values of $\gamma$, $E_F$ lies in the orbital gap between the Landau levels whereas for odd $\gamma$, $E_F$ coincides with a given Landau level.
1.5 DENSITY OF STATES

Density of states (DOS) of two-dimensional electron gas is an interesting property on which most of the transport and optical properties depend. In a quantum well besides the quantization of energy along z-axis the density of states is bidimensional. From the usual calculations the density of states of a Q2D electron gas per unit area, for dispersion relation (1.3.5), is given by

\[ \rho_{\text{Q2D}} = \sum_{p,k} \delta(E - E_{p,k}) \]

\[ = \frac{m^*}{\pi \hbar^2} \sum_p \theta(E - E_p). \quad (1.5.1) \]

In this equation the summation is over all bound states and \( \theta(x) \) is the unit step function

\[ \theta(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0. \end{cases} \quad (1.5.2) \]

Thus we see that the DOS of a Q2D electron gas of a given quantum state \( E_p \) is independent of \( E \) and thickness of the well.
The DOS is evidently step like, the jumps occurring at energies corresponding to subband energies which is characteristic of Q2D electron gas. At zero temperature all states are filled up to Fermi energy level $E_F$ which remains still as a good approximation at finite temperature if thermal energy $k_B T \ll E_F$. Since DOS in a subband is constant the electron areal density $n_s$ is linearly related to $E_F$ by $n_s = \left( \frac{E_F}{m^*/(nk^2)} \right)$ and Fermi wavevector $k_F$ is related to $n_s$ by $k_F = \left( \frac{2\pi n_s}{\hbar} \right)^{1/2}$. It is interesting to compare Q2D DOS with 3D case. In 3D case $\rho(E) \propto E^{1/2}$ and it can be shown that, for infinitely deep well approximation, $\rho_{3D} \propto \rho_{2D}$. The DOS for Q2D and 3D cases are shown in figure 1.6. As the number of occupied subbands increases the DOS approaches the $E^{1/2}$ dependence. However, it may be noted that usually lowest subband is occupied.

We find that DOS of Q2D electron gas is finite even at the bottom of the Q2D level whereas it tends to zero in the bulk case. This has fundamental consequences on the properties of a Q2D system. All the dynamical phenomena such as scattering rates etc, remain finite at low kinetic energy. A Q2D system is truly two-dimensional when one deals with only one electric subband. As more number of subbands come into play the system loses gradually its two-dimensionality.
Fig. 1.6 Density of States: 2D electron gas in a quantum well (solid curve) and bulk (dashed curve).
DOS of a Q2D electron gas in a magnetic field is much more dramatic. Neglecting the broadening of the Landau levels by disorders the DOS can be approximated by

\[
\rho(E) = \sum_{k_y,p,n} \delta(E - E_{np})
\]

\[
= \frac{1}{n l^2} \sum_{p,n} \delta(E - E_{np}). \tag{1.5.3}
\]

In this equation spin degeneracy is taken into account. This will be resolved in strong magnetic fields as a result of Zeeman splitting of the Landau levels.

It is clear from above equation that, in a magnetic field, the DOS is effectively 0D form. Due to complete quantization of \( E_{np} \) DOS shows a series of equidistant \( \delta \)-function peaks at \( E = E_{np} \) as shown in figure 1.7. However, due to scattering by disorders the Landau levels are broadened leading to non zero DOS between the peaks. Broadening of Landau levels is described by either Lorentzian or Gaussian function with width of the level \( \Gamma \). Broadened DOS is shown in figure 1.7. In weak magnetic fields large number of Landau levels are
Fig. 1.7 Density of States of a 2D electron gas in a magnetic field with Broadened Landau levels. $E_F$ is Fermi level.
going to be occupied and one recovers the result of Q2D of zero field. In the case of strong magnetic fields, where \( \Gamma/(h\omega_c) \ll 1 \) (quantum limit), the Landau levels remain separated. The simple estimate of the \( \Gamma \) is given by [1.4]

\[
\Gamma = \frac{h}{\tau},
\]

(1.5.4)

where \( \tau \) is the scattering time determined from the zero mobility \( \mu = e\tau/m \). However, self consistent calculations of \( \Gamma \) give [1.4]

\[
\Gamma = \sqrt{\frac{\hbar}{m} \frac{e}{2\pi c}} \sqrt{\frac{B}{\mu}}
\]

(1.5.5)

for the case of short range scatters. Thus, measurements of width of line will help to determine scattering rate and life of electrons.

1.6 ELECTRON - PHONON INTERACTIONS

Electron - phonon interactions are important in determining the transport properties and some of the optical properties [1.13]. In bulk III-V semiconductors it is well established that electrons interact with acoustic phonons, polar optical phonons and non-polar optical phonons [1.13]. Interaction with acoustic phonons is via acoustic deformation
potential and piezoelectric potential. Interaction with polar optical modes is through the Fröhlich interaction and with non-polar optical phonons it is through the optical deformation potential. In non-polar semiconductors such as Si, Ge etc electrons interact with acoustic phonons via deformation potential and with non-polar optical phonons through the optical deformation potential. This is true in case of QWs formed from the respective semiconductor materials. However, the electron-phonon matrix elements are modified in QWs [1.14, 1.15].

1.6.1 Q2D Electron - Bulk Phonon Interactions

In layered structures such as GaAs/AlAs QWs not only electronic structure but also lattice mode structure is changed. More often this complicated structure of lattice modes is ignored assuming that phonons are not influenced by the layered structures. As a result of this assumption the Q2D electron in the well interact with the phonons of 3D nature with the coupling strengths characteristic of the bulk material used for the layer forming the well region [1.14, 1.15].

The Hamiltonian for the electron-phonon interaction is given by [1.13]
\[ H_{\text{el-ph}} = \sum_Q C_Q \left( a_Q \exp(iQ \cdot R) - a_Q^\dagger \exp(-iQ \cdot R) \right), \]

\[ = \mathcal{V}_s \]  

(1.6.1)

where \( C_Q \) is the strength of the electron-phonon interaction, \( Q = (q, q_z) \) and \( R = (r, z) \) are, respectively the 3D phonon wavevector and position vectors. \( a_Q \) and \( a_Q^\dagger \) are the phonon annihilation and creation operators, respectively. \( C_Q \) has different forms for different types of electron-phonon couplings.

For electron interaction with acoustic phonons via acoustic deformation potential coupling, \( C_Q \), is given by

\[ |C_Q|^2 = \left( \frac{\hbar}{2\rho \omega_Q V} \right) Q^2 E_1^2, \]  

(1.6.2)

where \( \omega_Q \) is the frequency of the acoustic phonon, \( E_1 \) the acoustic deformation potential constant of the material, \( \rho \) the mass density and \( V \) the volume of the semiconductor. It is only the longitudinal acoustic phonon in the long wave length region which get coupled to electrons through this interaction.
mechanism. Hence the dispersion $\omega_Q = v_s Q$, where $v_s$ is the velocity of longitudinal acoustic modes, is taken.

For electron - acoustic phonon interaction via piezoelectric coupling, $C_Q$, is given by \[1.14\]

For longitudinal modes and

\[ |C_{Ql}|^2 = \frac{(\epsilon h_{14})^2 \hbar \omega_Q}{2 \rho \nu \nu_l^2 Q^2} A_l \]  \hspace{1cm} (1.6.3)

for longitudinal modes and

\[ |C_{Qt}|^2 = \frac{(\epsilon h_{14})^2 \hbar \omega_Q}{2 \rho \nu \nu_t^2 Q^2} A_t \]  \hspace{1cm} (1.6.4)

for transverse modes, where

\[ A_l = \frac{9q^2 q_z^2}{2Q^6} \]  \hspace{1cm} (1.6.5)

and

\[ A_t = \frac{(8q^2 q_z^4 + q^6)}{4Q^6} \]  \hspace{1cm} (1.6.6)

In equation (1.6.3) and (1.6.4) the subscripts $l$ and $t$ to the respective quantities indicate longitudinal and transverse
modes. Generally at very low temperatures electron scattering is governed by acoustic phonons.

In case of electron interaction with non-polar optical phonons, optical phonons are assumed to be dispersionless i.e., \( \omega_Q = \omega_o \), and \( C_Q \) is given by

\[
|C_Q|^2 = \frac{\hbar^2 D^2_o}{2 \rho \sqrt{h \omega_o}},
\]

where \( D_o \) is the non-polar optical deformation potential constant. Usually this interaction is weaker in polar semiconductors. In non-polar semiconductors it is a dominant electron scattering mechanism at higher temperatures.

In polar semiconductors electron interaction with longitudinal polar optical phonons is through the Fröhlich Hamiltonian and \( C_Q \) in this case is given by

\[
|C_Q|^2 = \frac{2\pi e^2 h \omega_{LO}}{V\epsilon'} \frac{1}{q^2 + q_z^2},
\]

where \( \omega_{LO} \) is the polar optical phonon frequency of the well material and \( \epsilon' = \left( \varepsilon_{\infty}^{-1} - \varepsilon_{s}^{-1} \right)^{-1} \) with \( \varepsilon_{\infty} \) and \( \varepsilon_{s} \) being the high
frequency and static dielectric constants, respectively, of the well material. $\omega_{LO}$ is assumed to be dispersionless. This is the dominant scattering mechanism at temperatures greater than 50 K.

In our studies we use Hamiltonian given by equation (1.6.1), with appropriate $C_Q$ for different types of electron-phonon coupling, wherever we consider interaction of Q2D electron gas with 3D phonons.

1.6.2 Q2D Electron-Confined LO Phonon Interaction

In the QW structure fabricated from the polar (weakly ionic) semiconductors (for eg. GaAs/AlAs QW) electron interaction with polar optical phonons is important. It has been clearly established that in such structure changes of longitudinal optical (LO) phonon states take place similar to electron and hole states (see for eg. a review by Ridley ref. [1.16]). In these QWs LO phonon branches of the two materials, unlike the acoustic branches, and TO branches, do not overlap and hence LO phonons of a given layer are heavily damped in the other layer. Hence LO phonons can be considered to be confined to the respective material layers. In GaAs/AlAs or GaAs/GaAlAs QWs GaAs is the active layer which acts as a `quantum well for
LO phonons' resulting in the quantization of z-component of phonon wavevector in the direction of confinement. Besides, there exists other phonon states called 'interface optical phonons' which have no electronic counterparts. These are localized in the vicinity of interfaces. Their frequency lie in the forbidden gap between LO and TO bulk phonon frequencies.

Modified LO phonon structures and existence of interface phonons have been evidenced by means of Raman scattering measurements [1.16-1.19] and by high resolution energy loss spectroscopy [1.20] in GaAs/AlAs and GaAs/GaAlAs SLs. Recently Zhu et al [1.21] have observed substantial enhancement in electron mobility in GaAs/AlAs MQW structures in which optical phonon modes are confined. Experimental [1.22,1.23] and theoretical [1.24] investigations of I-V characteristics of phonon assisted tunneling in GaAs/GaAlAs double barrier tunneling structures in the presence of quantizing magnetic field have indicated electron relaxation through emission of confined and interface phonons.

Electron scattering rates due to confined and interface phonons are calculated in GaAs/AlAs QWs [1.25-1.28] and SLs [1.29] in the presence of applied electric field and in presence of quantizing magnetic field [1.30]. Free carrier
absorption [1.31] and phonon assisted cyclotron resonance are also studied [1.32] with confined LO phonon structure and interface phonons.

From the foregoing discussions it is obvious that electron optical phonon interaction must be treated properly in QWs in describing any of the physical properties.

Several theories (see for eg. [1.16]) have been proposed for interaction of the electron confined LO phonon in QW structures depending upon the way the vibrational modes are treated. Widely employed models in literature are dielectric continuum models or microscopic lattice dynamical models. Of the two different macroscopic continuum models, one corresponds to the 'slab modes' of a free ionic slab [1.33,1.34] and the other to the 'guided modes' of a model layered structure [1.35]. Different boundary conditions imposed on the electrostatic potential or vibrational amplitude of the phonons at the interfaces make the two models differ. The problem of physically correct boundary conditions can not be solved within the macroscopic models, but must be approached within microscopic lattice dynamic models. A microscopic lattice dynamical model for describing phonon modes in SL has been proposed by Huang and Zhu (HZ) [1.36]. They have given
analytic approximations based on their numerical solutions. The HZ model has received a wide acceptance and best describes the electron-phonon interaction in Q2D systems \[1.37\]. Electron intra- and inter subband scattering rates due to confined LO phonons are calculated in GaAs QWs, in zero magnetic field \[1.25,1.38\], using above three models. Estimates based on HZ model are found to be in good agreement with experimental results \[1.39,1.40\]. However, clear acceptance of any of these modes is not yet established and none of the above three models are to be excluded in the electronic properties of QWs.

Fröhlich interaction Hamiltonian describing the electron confined LO phonon interaction is given by \[1.33,1.34\]

\[
H_{el-ph} = \left( \frac{4\pi e^2 \hbar \omega_{LO}}{V_e} \right)^{1/2} \sum_{q, m \alpha = \pm} \exp(iq \cdot r) \ t_{m\alpha}(q) \ u_{m\alpha}(z)
\]

\[
\times \left[ a_{m\alpha}(q) + a_{m\alpha}^\dagger(-q) \right], \quad (1.6.9)
\]

where \(a_{m\alpha}(q)\) and \(a_{m\alpha}^\dagger(-q)\) are, respectively, annihilation and creation operators of phonons. \(\alpha\) represents the even (-) and odd (+) confined phonon modes. \(m\) represents the number of half
wavelengths contained in the QW layer and \( u_{m\alpha}(z) \) is the component of displacement vector in the direction of confinement. In equation (1.6.9) function \( t_{m\alpha} \) is given by

\[
t_{m\alpha}(q) = \frac{L}{2} \left( \frac{2}{L} \int_{-L/2}^{L/2} dz \left[ q^2 u_{m\alpha}^2 + \left( \frac{du_{m\alpha}}{dz} \right)^2 \right] \right)^{-1/2} . \tag{1.6.10}
\]

\( u_{m\alpha} \) is different in different modes and the explicit forms of \( t_{m\alpha} \) for various models can be obtained using the respective \( u_{m\alpha} \) in equation (1.6.10). \( \omega_{LO} \) is assumed to be dispersionless.

**Huang and Zhu model**

In this model both electric potential and polarization of phonon modes have nodes at the interfaces. The optical vibrations between oppositely charged ions are given by a simple cubic lattice of charged oscillators. The two materials that form a SL differ only in their bulk LO and TO phonon frequencies. The resulting dynamical matrix is then diagonalized numerically [1.36]. For a QW of width \( L \) centered at \( z = 0 \) the function \( u_{m\alpha}(z) \), in HZ model, is defined as
\[ u_{m+}(z) = \sin\left(\frac{\pi m z}{L}\right) + \frac{C_m z}{L} \quad (1.6.11) \]

for odd modes, \( m = 3, 5, 7, \ldots \), and

\[ u_{m-}(z) = \cos\left(\frac{\pi m z}{L}\right) - (-1)^{m/2} \quad (1.6.12) \]

for even modes, \( m = 2, 4, 6, \ldots \), and \( \mu_m \) being solutions of

\[ \tan(\mu_m \pi/2) = \frac{\mu_m \pi/2}{m - 1 < \mu_m < m}, \quad (1.6.13) \]

with the smallest one \( (\mu_1) \) being omitted. \( C_m \) are given by

\[ C_m = -2 \sin (\frac{\mu_m \pi}{2}). \quad (1.6.14) \]

The odd modes in equation (1.6.11) start from \( m = 3 \). The \( m = 1 \) mode is associated with the interface mode [1.36]. Using equations (1.6.11) and (1.6.12) in (1.6.10) we obtain

\[ t_{m+}(q) = \left\{ \left[ 1 + \left( \frac{1}{C_m^2} - \frac{\mu_m^2 - \pi^2}{\mu_m^2} \right) q^2 + \left( \frac{\mu_m^2 \pi^2 - C_m^2}{\mu_m^2} \right) L^{-2} \right]^{-1/2} \right\} \quad (1.6.15) \]

for odd modes and
1/2
for even modes.

Slab modes

In this model the different semiconductor layers are approximated by uniform slabs of material with each slab assumed to have dielectric properties of the same material in bulk \([1.33]\) and phonons are treated without any dispersion. Fuchs-Kliewer slab modes or simply slab modes are obtained by imposing boundary conditions on electrostatic field without regard to the atomic displacements at the interfaces. The labeling of the modes is different from the modes obtained by microscopic calculation i.e., the \(m\)th mode has an opposite parity to the \(m\)th mode in microscopic model. The displacement associated with \(m\)th phonon mode is given by \([1.34]\)

\[
\begin{align*}
\quad u_{m^+} &= \cos(m\pi z/L), & m &= 1, 3, 5, \ldots & (1.6.17) \\
\quad u_{m^-} &= \sin(m\pi z/L), & m &= 2, 4, 6, \ldots & (1.6.18)
\end{align*}
\]

for odd modes and
for even modes. The function $t_{\text{max}}$ for slab modes is

$$t_{\text{max}}(q) = \left[q^2 + \left(m\pi/L\right)^2\right]^{-1/2}, \quad m = 1, 2, 3, \ldots$$  \hspace{1cm} (1.6.19)

**Guided modes**

Ridley's guided mode model [1.35] or simply guided modes is based on the use of hydrodynamic boundary conditions proposed by Babiker [1.41] for LO phonons. Electrostatic boundary conditions are neglected in favour of the approximate boundary conditions on the atomic displacements at the interfaces. The parity of the phonon modes of the guided modes matches with those obtained in the microscopic calculations.

The displacement of the $m$th phonon mode is

$$u_{m^+} = \sin(m\pi z/L), \quad m = 1, 3, 5, \ldots$$  \hspace{1cm} (1.6.20)

for odd modes and

$$u_{m^-} = \cos(m\pi z/L), \quad m = 2, 4, 6, \ldots$$  \hspace{1cm} (1.6.21)

for even modes. The function $t_{\text{max}}$ in the case of guided modes is same as that obtained for slab modes [equation (1.6.19)].
1.6.3 Electron-Interface Optical Phonon Interaction

Using the dielectric continuum model, Fuchs and Kliewer [1.33] showed that the spectrum of phonons of polar layer consists of interface phonons with fields mainly localized at the interfaces of the system and decaying exponentially from them, in addition to the confined LO modes. The interface modes of different parity are identified as symmetric and antisymmetric modes, and for each of these modes there are two modes of different frequency for an interface such as formed between GaAs and AlAs.

A Fröhlich type Hamiltonian describing electron optical phonon interaction in a double heterostructure of polar semiconductor was derived by Lassnig [1.42] using electron energy loss method. It is given by

\[
H_\nu = \sum_{q \mu} \left( \frac{2\pi e^2 f_{\nu\mu}}{\hbar a q \omega_{\nu\mu}} \right)^{1/2} \exp(i q \cdot r) \left( \frac{\gamma}{1 \pm \gamma} \right)^{1/2}
\]

\[
\times \left[ \exp(qz) \pm \exp(-qz) \right] \left\{ a_{\nu\mu}(q) + a^\dagger_{\nu\mu}(-q) \right\}, \quad (1.6.22)
\]

where \( a_{\nu\mu} \), \( a^\dagger_{\nu\mu} \) are, respectively, the phonon annihilation and
creation operators and $A$ the normalization area. The subscript $\nu$ represents the symmetric (s) or antisymmetric (a) forms of the interface phonon modes and $\mu = \pm$ distinguishes the two interface phonon modes corresponding to the well (−) and the barrier (+) materials. In equation (1.6.22) the other quantities are

$$f_{\nu \mu} = \left| \frac{h^2 (\omega_{\nu \mu}^2 - \omega_{\nu \mu}^{TO1}) (\omega_{\nu \mu}^2 - \omega_{\nu \mu}^{TO2})}{(\omega_{\nu \mu}^2 - \omega_{\nu \mu}^{TO1})(\varepsilon_{1\nu} + \varepsilon_{2\nu})} \right|, \quad (1.6.23)$$

$$\varepsilon_{1s} = \varepsilon_{1\infty}(1 - \gamma), \quad \varepsilon_{1a} = \varepsilon_{1\infty}(1 + \gamma), \quad (1.6.24)$$

$$\varepsilon_{2s} = \varepsilon_{2\infty}(1 + \gamma), \quad \varepsilon_{2a} = \varepsilon_{2\infty}(1 - \gamma), \quad (1.6.25)$$

$$\gamma = \exp(-qL).$$

The index 1 refers to the well material (GaAs) and 2 to the barrier material (AlAs). $\omega_{TO1}$ and $\omega_{TO2}$ are the bulk TO phonon frequencies, assumed to be dispersionless. $\varepsilon_{1\infty}$ and $\varepsilon_{2\infty}$ are the high frequency dielectric constants of the well and barrier materials, respectively. The interface optical phonon
frequencies are given by

\[ \omega_{\nu \mu}^2 = \frac{\zeta \pm \sqrt{\left( \zeta^2 - \frac{\hbar^4}{\epsilon_{1\nu}^2 + \epsilon_{2\nu}^2} \left( \epsilon_{1\nu} \omega_{LO1}^2 \omega_{TO2}^2 - \epsilon_{2\nu} \omega_{LO2}^2 \omega_{TO1}^2 \right) \right)^2}}{\left( \epsilon_{1\nu}^2 + \epsilon_{2\nu}^2 \right) \hbar^2} \]

(1.6.26)

with

\[ \zeta = \frac{\hbar^2}{2} \left[ \epsilon_{1\nu} (\omega_{TO2}^2 + \omega_{LO1}^2) + \epsilon_{2\nu} (\omega_{TO1}^2 + \omega_{LO2}^2) \right], \]  

(1.6.27)

where \( \omega_{LO1} \) and \( \omega_{LO2} \) are the frequencies of the bulk LO phonons.

In chapter 4 we will use the above mentioned models to study the effects of electron interaction with confined and interface optical phonons on hot electron energy loss rates in GaAs/AlAs QW.