3.1 Introduction

In this chapter we shall study the DMR under size quantization in tetragonal semiconductors, II-VI semiconductors and Bi in section 3.2, 3.3 and 3.4 respectively. The well-known expressions of parabolic energy bands have also been obtained in all the cases. In section 3.4 we shall discuss the above cases under magnetic quantization.

3.2 Formulation of DMR in tetragonal semiconductors under size quantization:

The modified 2D electron energy spectrum in tetragonal semiconductors in the presence of an infinitely deep potential well of depth $d_0$ can be written following equation (2.19)

$$C(E) = A(E)k_s^2 + B(E)\left(\frac{l\pi}{d_0}\right)^2$$

where $l (=1,2,3,...)$ is the size quantum number. The use of equation (3.1) leads to the expression of the 2D density-of-states function as

$$N(E) = \frac{1}{2\pi} \sum_l \left[ \frac{1}{A(E)} \left\{ C_l(E) - B_l(E) \left(\frac{l\pi}{d_0}\right)^2 \right\} - \frac{A_l(E)}{(A(E))^2} \left\{ C(E) - B(E) \left(\frac{l\pi}{d_0}\right)^2 \right\} \right] H(E - E_l)$$

where $A_l(E), B_l(E)$ and $C_l(E)$ are defined in connection with equation (3.3), $H$ is the Heaviside step function and $E_l$ is obtained from equation (3.1) by putting $E = E_l$ and $k_s = 0$ in equation (3.1). Combining equation (3.2) with the Fermi-Dirac occupation probability factor and
using the generalized Sommerfeld's lemma we get an expression of the surface electron concentration per unit area as

\[ n_0 = \frac{1}{2\pi} \sum_{l=1}^{\infty} [I_{11}(E_F^l) + I_{12}(E_F^l)] \]  
(3.3)

where \( I_{11}(E_F^l) = \frac{1}{A(E_F^l)} \left[ C(E_F^l) - B(E_F^l) \left( \frac{l\pi}{d_0} \right)^2 \right] \).

\( I_{13}(E_F^l) = \sum_{r=1}^{\infty} L(r,0)[I_{11}(E_F^l)] \) and \( E_F \) is the Fermi energy in the present case.

Using equations (2.11) and (3.3), the DMR in tetragonal semiconductors under size quantization can be written as

\[ \frac{D}{\mu} = \frac{1}{|\varepsilon|} \sum_{l=1}^{\infty} \frac{I_{11}(E_F^l) + I_{12}(E_F^l)}{I_1^l(E_F^l) + I_2^l(E_F^l)} \]  
(3.4)

**Special cases**

(a) Under the conditions \( \Delta_\| = \Delta_\perp = \Delta, m_\|=m_\|=m^* \) and \( \delta = 0 \), from equation (3.1) we can write

\[ \gamma(E) = \frac{\hbar^2 k_F^2}{2m^*} + \frac{\hbar^2 \pi^2}{2m^*} \left( \frac{l}{d_0} \right)^2 \]  
(3.5)

where the function \( \gamma(E) \) has been defined in equation (2.22). The equation (3.5) is the 2D electron energy spectrum in ultrathin semiconductors whose energy band spectra is defined by three-band Kane model. The surface electron concentration and the DMR can, respectively, be expressed as

\[ n_0 = \frac{m^*}{\hbar^2} \sum_{l=1}^{\infty} [I_{13}(E_F^l) + I_{14}(E_F^l)] \]  
(3.6)

\[ \frac{D}{\mu} = \frac{1}{|\varepsilon|} \sum_{l=1}^{\infty} \frac{I_{13}(E_F^l) + I_{14}(E_F^l)}{I_1^l(E_F^l) + I_2^l(E_F^l)} \]  
(3.7)
where \( I_{13}(E_F) = \left[ \gamma(E_F) - \left( \frac{\hbar^2 \pi^2}{2m^*} \left( \frac{1}{d_0} \right) \right)^2 \right] \) and \( I_{14}(E_F) = \sum_{r=1}^{s} L(r,0)[I_{13}(E_F)] \)

(b) For \( \Delta \gg E_g \) and \( \Delta \ll E_g \), equation (3.5) gets simplified as

\[
E(1 + \alpha E) = \frac{\hbar^2 k_y^2}{2m^*} + \left( \frac{\hbar^2}{2m^*} \left( \frac{l\pi}{d_0} \right) \right)^2
\]

(3.8)

which is two dimensional electron energy spectrum in ultrathin semiconductors whose energy band structures are defined by two-band Kane model. Therefore the surface electron concentration and the DMR in size quantized semiconductors whose energy band structures are defined by two-band Kane model can, respectively, be expressed as

\[
n_0 = \frac{m^* k_BT}{\pi \hbar^2} \sum_{l=1}^{l_b} \left[ (1 + 2\alpha E_l) F_0(\eta_l) + 2\alpha k_BT F_1(\eta_l) \right]
\]

(3.9)

and

\[
\frac{D}{\mu} = \frac{k_BT}{\pi \hbar^2} \sum_{l=1}^{l_b} \left[ (1 + 2\alpha E_l) F_0(\eta_l) + 2\alpha k_BT F_1(\eta_l) \right]
\]

(3.10)

where

\[
E_l = \frac{1}{2\alpha} \left[ -1 + \sqrt{1 + \frac{2\alpha}{m^*} \left( \frac{\pi \hbar l}{d_0} \right)^2} \right] \quad \text{and} \quad \eta_l = \frac{1}{k_BT} [E_F - E_l]
\]

(c) For relatively wide-gap materials \( \alpha \to 0 \) and the equations (3.8) to (3.10) get simplified as

\[
E = \frac{\hbar^2 k_y^2}{2m^*} + \left( \frac{\hbar^2}{2m^*} \left( \frac{l\pi}{d_0} \right) \right)^2
\]

(3.11)

\[
n_0 = \frac{m^* k_BT}{\pi \hbar^2} \sum_{l=1}^{l_b} F_0(\eta_l)
\]

(3.12)
$$D = \frac{k_B T}{\mu} \sum_{l=1}^{\infty} \frac{F_0(\eta_l)}{e^{\frac{F_{-1}(\eta_l)}{k_B T}}}$$  

(3.13)

where  

$$E_l = \left( \frac{\hbar^2 \pi^2}{2m^*} \right) \left( \frac{l}{d_0} \right)^2$$

3.3 **Formulation of DMR in II-VI semiconductors under size quantization**

In this case the modified 2D carrier energy spectrum can be written following equation (2.38) as

$$E = a_0 k^2 + c_0 \lambda k + b_0 \left( \frac{l \pi}{d_0} \right)^2$$  

(3.14)

Using equation (3.14), the surface carrier concentration per unit area is given by

$$n_o = \frac{1}{na_0^2} \sum_{l=1}^{\infty} \left[ I_{15}(E_P) + I_{16}(E_P) \right]$$  

(3.15)

where  

$$I_{15}(E_P) = \left[ -C_0 + \left[ C^2 + 4a_0 \left( E_P - b_0 \left( \frac{l \pi}{d_0} \right)^2 \right) \right]^{1/2} \right]$$

and  

$$I_{16}(E_P) = \sum_{r=1}^{\infty} L(r,0) \left[ I_{15}(E_P) \right]$$

Using equations (3.15) and (2.11), the DMR in ultrathin films of II-VI semiconductors can be expressed as

$$\frac{D}{\mu} = \frac{1}{\rho} \sum_{l=1}^{\infty} \left[ I_{15}(E_P) + I_{16}(E_P) \right]$$  

(3.16)

Under the limiting conditions $C \to 0$ and $a_0 = b_0$, the equation (3.16) gets simplified to equation (3.13).
3.4 Formulation of DMR in ultrathin films of Bi in accordance with various band models

(a) McClure and Choi model

The dispersion relation of the carriers in ultrathin films of Bi in the presence of size quantization among bisectrix axis can be written following equation (St-izjas

\[ \alpha_4(E,n) = k_4^2\alpha_4(n) + k_6^2\alpha_6(n) \] (3.17)

where

\[ \alpha_4(E,n) = \left[ E(1 + \alpha E) - \frac{\hbar^2\pi^2}{2m_2} \left( \frac{n_y}{d_y} \right)^2 - \frac{\alpha\hbar^4\pi^4}{4m_3m_2} \left( \frac{n_y}{d_y} \right)^4 \right] \]

\[ \alpha_6(n) = \left[ \frac{\hbar^2}{2m_3} - \frac{\alpha\hbar^4}{4m_3m_2} \left( \frac{n_y}{d_y} \right)^2 \right] \]

\[ \alpha_6(n) = \left[ \frac{\hbar^2}{2m_3} - \frac{\alpha\hbar^4}{4m_3m_2} \left( \frac{n_y}{d_y} \right)^2 \right] \]

\[ n_y \text{ and } d_y \text{ are the size quantum numbers and thickness along y-direction respectively.} \]

The use of equation (3.17) leads to the expression of the density-of-states function as

\[ N_{2D}(E) = \frac{g \sum_{n=1}^{n_{max}} (1 + 2\alpha E)(\alpha_4(n)\alpha_6(n))^{1/2}H(E - E_0)}{2\pi} \] (3.18)

where

\[ E_0 = \frac{1}{2\alpha} \left[ \left\{ \frac{\alpha}{2m_2} \left( \frac{\hbar m y}{d_y} \right)^2 \left( 1 - \frac{m_2}{m_3} \right) \right\}^{1/2} + \left\{ \frac{1 - \alpha}{2m_3} \left( \frac{\hbar m y}{d_y} \right)^2 \left( 1 - \frac{m_3}{m_2} \right) \right\}^{1/2} \right] \]

\[ + 4\alpha \left\{ \frac{\hbar^2\pi^2}{2m_2} \left( \frac{n_y}{d_y} \right)^2 + \frac{\alpha\hbar^4}{4m_3m_2} \left( \frac{n_y}{d_y} \right)^2 \right\}^{1/2} \]

Thus combining equation (3.18) with the Fermi-Dirac occupation probability factor, the surface electron concentration per unit area can be written as
\[ n_0 = \frac{g_0 k_B T}{\pi^2} \sum_{\eta_y=1}^{N_{\text{max}}} \left[ F_0(\eta_y) + 2\alpha k_B T F_1(\eta_y) + 2\alpha F_0 F_0(\eta_y) \left[ a_3(n) a_6(n) \right] \right] \frac{1}{2} \] (3.19)

where \( \eta_y = \frac{1}{k_B T} (E_F - E_0) \)

Thus using equations (2.11) and (3.19), the DMR in ultrathin films of Bi in accordance with McClure and Choi model can be expressed as

\[
\frac{D}{\mu e} = \frac{k_B T}{\sum_{\eta_y=1}^{N_{\text{max}}} a_7(n) \left[ (1 + 2\alpha E_0) F_0(\eta_y) + 2\alpha k_B T F_1(\eta_y) \right]} \left[ \sum_{\eta_y=1}^{N_{\text{max}}} a_7(n) \left[ (1 + 2\alpha E_0) F_0(\eta_y) + 2\alpha k_B T F_1(\eta_y) \right] \right] \]

(3.20)

where \( a_7(n) = \left[ a_3(n) a_6(n) \right]^{1/2} \)

\((b)\) **Hybrid model**

The 2D carrier energy spectrum for this model can be expressed following equation (2.49) as

\[ E(1 + \alpha E) = \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_y^2}{2m_3} + \beta(E) \left( \frac{\hbar m_n}{d_y} \right)^2 + \alpha \hbar^4 \pi^4 \left( \frac{n_y}{d_y} \right)^2 \] (3.21)

The density-of-states function can be written as

\[ N_{2D}(E) = \frac{g_0 \sqrt{m_1 m_3}}{\pi \hbar^2} \sum_{\eta_y=1}^{N_{\text{max}}} \left[ 1 + 2\alpha E - \frac{\alpha (1 - \gamma_0) \left( \hbar m_n \right)^2}{2M_2} \right] H(E - E_0) \] (3.22)

where

\[
E_7 = \frac{1}{2\alpha} \left\{ \frac{\alpha (1 - \gamma_0) \left( \hbar m_n \right)^2}{2M_2} \left( \frac{d_y}{d_y} \right) - 1 \right\} + \left[ \frac{\hbar m_n}{2M_2} \left( \frac{d_y}{d_y} \right)^2 \right]^2 + 4\alpha \left[ \frac{\alpha \hbar^2 \pi^2}{2M_2^2} \left( \frac{n_y}{d_y} \right)^2 + \frac{\delta_y \left( \hbar m_n \right)^4}{2M_2^2} \left( \frac{d_y}{d_y} \right)^2 \right] \]

(3.23)

The surface electron concentration is given by

\[ n_0 = \frac{g_0 \sqrt{m_1 m_3} k_B T}{\pi \hbar^2} \sum_{\eta_y=1}^{N_{\text{max}}} \left[ a_3(n) F_0(\eta_y) + 2\alpha k_B T F_1(\eta_y) \right] \]
where
\[ \alpha_y(n) = \left[ 1 + 2\alpha E_y - \frac{\alpha(1-\gamma_y)}{2M_2} \left( \frac{\hbar m_{n_y}}{d_y} \right)^2 \right] \] and \[ \eta_y = \frac{1}{k_BT} (E_y - E_\gamma) \]

Using equations (3.23) and (2.11), the DMR in ultrathin films of Bi in accordance with hybrid model can be written as
\[
\frac{D}{\mu} = \frac{k_BT}{e} \sum_{n_y=1}^{n_y=2} \alpha_y(n) F_y(\eta_y) + 2ak_{BT}F_y(\eta_y) + \frac{\alpha h^4 \pi^4}{4m_1 m_2} (n_y^4) - \frac{\alpha h^2 k^2}{2m_1} + \frac{\alpha h^2 k^2}{2m_2} + \frac{\alpha(E) \left( \frac{\hbar m_{n_y}}{d_y} \right)^2}{2m_2} + (1 + \alpha E) \left( \frac{n_y}{d_y} \right)^2 + \frac{\alpha h^4 \pi^4}{4m_1 m_2} (n_y^4) \quad (3.24)
\]

(c) Cohen model

The 2D carrier energy spectrum for this model can be expressed following equation (2.4) as
\[
E(1 + \alpha E) = \frac{h^2 k_1^2}{2m_1} + \frac{h^2 k_2^2}{2m_3} - \frac{\alpha(E) \left( \frac{\hbar m_{n_y}}{d_y} \right)^2}{2m_2} + \frac{h^2 \pi^2}{2m_2} (1 + \alpha E) \left( \frac{n_y}{d_y} \right)^2 + \frac{\alpha h^4 \pi^4}{4m_1 m_2} (n_y^4) - \frac{\alpha h^2 k^2}{2m_1} + \frac{\alpha h^2 k^2}{2m_2} + \frac{\alpha(E) \left( \frac{\hbar m_{n_y}}{d_y} \right)^2}{2m_2} + (1 + \alpha E) \left( \frac{n_y}{d_y} \right)^2 + \frac{\alpha h^4 \pi^4}{4m_1 m_2} (n_y^4) \quad (3.25)
\]

The basic forms of the expressions for carrier statistics and DMR in the present case will respectively be given by equations (3.23) and (3.24) where
\[
E_\gamma = \frac{1}{2\alpha} \left[ \left( \frac{\alpha \left( \frac{\hbar m_{n_y}}{d_y} \right)^2}{2m_1} - \frac{\alpha \left( \frac{\hbar m_{n_y}}{d_y} \right)^2}{2m_2} \right) + \left( \frac{\alpha h^2 \pi^2}{2m_2} (n_y^2) \right)^2 + 4\alpha \left( \frac{h^2 \pi^2}{2m_2} (n_y^2) + \frac{\alpha h^4 \pi^4}{4m_1 m_2} (n_y^4) \right) \right]^{1/2}
\]

and \[ \eta_y = \frac{1}{k_BT} (E_y - E_\gamma) \]
(d) Lax model

For this model following equation (2.48) the modified carrier dispersion law, density-of-states function, the electron concentration and the DMR for ultrathin films of Bi can, respectively, be expressed as

\[
E(1 + aE) = \frac{\hbar^2 k^2}{2m_1} + \frac{\hbar^2 k^2}{2m_3} + \frac{\hbar^2 \pi^2}{2m_2} \left( \frac{n_y}{d_y} \right)^2
\]  

\[
N_{2D}(E) = \frac{g_v}{\pi \hbar^2} \sum_{n_y=1}^{n_{\text{max}}} \left[ 1 + 2aE \right] H(E - E_6)
\]

\[
n_0 = \frac{g_v k_B T}{\pi \hbar^2} \sum_{n_y=1}^{n_{\text{max}}} \left[ (1 + 2aE_0) F_0(\eta_y) + 2ak_B TF_1(\eta_y) \right]
\]

and

\[
D = \frac{k_B T}{\mu} \frac{\sum_{n_y=1}^{n_{\text{max}}} \left[ (1 + 2aE_0) F_0(\eta_y) + 2ak_B TF_1(\eta_y) \right]}{e \sum_{n_y=1}^{n_{\text{max}}} \left[ (1 + 2aE_0) F_0(\eta_y) + 2ak_B TF_1(\eta_y) \right]}
\]

where \( E_0 = \frac{1}{2a} \left[ -1 + \left[ 1 + \frac{2a \hbar^2 \pi^2}{m_2} \left( \frac{n_y}{d_y} \right)^2 \right]^{1/2} \right] \)

and \( \eta_y = \frac{1}{k_B T} \left( E - E_0 \right) \)

(e) Ellipsoidal model

For ellipsoidal model, the carrier energy spectrum can be written as

\[
E = \frac{\hbar^2 k^2}{2m_1} + \frac{\hbar^2 k^2}{2m_3} + \frac{\hbar^2 \pi^2}{2m_2} \left( \frac{n_y}{d_y} \right)^2
\]

\[
E = \frac{\hbar^2 k^2}{2m_1} + \frac{\hbar^2 k^2}{2m_3} + \frac{\hbar^2 \pi^2}{2m_2} \left( \frac{n_y}{d_y} \right)^2
\]

The expressions for the surface electron concentration and the DMR for ellipsoidal model can, respectively, be written as
\[ n_0 = \frac{g_e B}{\hbar} \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} \left[ \frac{1 + \exp(-\eta) \cos(\lambda_0)}{1 + \exp(-2\eta) + 2 \cos(\lambda_0) \exp(-\eta)} \right] \]  

(3.31)

and

\[ D = \frac{k_B T}{\mu} \frac{\sum_{l=0}^{\infty} \sum_{n=0}^{\infty} \left[ \frac{1 + \exp(-\eta) \cos(\lambda_0)}{1 + \exp(-2\eta) + 2 \cos(\lambda_0) \exp(-\eta)} \right]}{\exp \left( \exp(-\eta) \cos(\lambda_0) + (\cos(\lambda_0) \exp(-2\eta) + 2 \exp(-\eta)) \right)} \]  

(3.32)

where \( \eta = \frac{1}{k_B T} \left( E_F - E_0 \right) \), \( E_0 \) is the magneto sized energy and \( \lambda_0 = \frac{\Gamma}{k_B T} \). Using equations (2.11) and (3.33), the DMR can be expressed as

3.5 Formulation of magneto DMR in ultrathin films of tetragonal semiconductors, II-VI semiconductors and Bi

In ultrathin films the motion of the carriers along the direction of size quantization is not allowed. In the presence of a direct quantizing magnetic field \( B \) along the direction of quantization, the three dimensional quantization occurs. The DMR exists only due to the motion of the carriers in the broadened Landau subbnds. The carrier concentration per unit area in magneto-sized films can be written in presence of spin and broadening as

\[ n_0 = \frac{g_e B}{\hbar} \sum_{l=0}^{\infty} \sum_{n=0}^{\infty} \left[ 1 + \exp(-\eta) \cos(\lambda_0) \right] \]  

(3.33)

It appears from equations (3.32) and (3.34) that the basic forms of these equations will be unaltered of any dimension law. For tetragonal semiconductors \( E_0 \) can be expressed as
\[
C(E_0) = \frac{2|eB|}{\hbar} \left( n + \frac{1}{2} \right) A(E_0) + B(E_0) \left( \frac{1}{d_o} \right)^2 + \frac{|eBhE_s\Delta_\mu|}{6m^*} \left( E_s + \frac{2E_0}{3} \Delta_1 \right) \left[ E + E_s + \delta + \frac{\Delta_2 - \Delta_1^2}{3\Delta_\mu} \right]
\]

(3.35)

For three-band Kane model, two-band Kane model and that of parabolic energy band, the \( E_0 \) can, respectively, be expressed as

\[
\gamma(E_0) = \left( n + \frac{1}{2} \right) \hbar \omega_0 + \frac{\hbar^2}{2m^*} \left( \frac{n\ell}{d_o} \right)^2 \pm \frac{eBh\Delta}{6m^* \left( E_0 + E_s + \frac{2\Delta}{3} \right)}
\]

(3.36)

\[
E_0(1 + \alpha E_0) = \left( n + \frac{1}{2} \right) \hbar \omega_0 + \frac{\hbar^2}{2m^*} \left( \frac{n\ell}{d_o} \right)^2 \pm \frac{1}{2} \gamma^* \mu_0 B
\]

(3.37)

and

\[
E_0 = \left( n + \frac{1}{2} \right) \hbar \omega_0 + \frac{\hbar^2}{2m^*} \left( \frac{n\ell}{d_o} \right)^2 \pm \frac{1}{2} \gamma^* \mu_0 B
\]

(3.38)

For II-VI semiconductors \( E_0 \) can be expressed as

\[
E_0 = \overline{\Psi}(n) + \bar{b}_0 \left( \frac{n\ell}{d_o} \right)^2
\]

(3.39)

For Bi, the basic forms of equations (3.33) and (3.34) will be unaltered where the sum over \( l \) should be replaced by sum over \( n_y \). The form of \( E_0 \) for the McClure and Choi model, the hybrid model, the Cohen model, the Lax model and the ellipsoidal parabolic model, can, respectively, be expressed as

\[
E_0(1 + \alpha E_0) = \left( n + \frac{1}{2} \right) \hbar \omega_0 + \frac{\hbar^2\pi^2}{2m_z^*} \left( \frac{n\ell}{d_y} \right)^2 + \frac{\hbar^2\pi^2}{2m_z^*} \alpha E_0 \left( \frac{1}{m_z^2} \right) \left( \frac{n\ell}{d_y} \right)^2
\]

\[
+ \frac{\alpha \hbar^4 \pi^4}{4m_z m_{z^*}} d_y \left( \frac{n\ell}{d_y} \right)^4 - \frac{\hbar^2\pi^2}{2m_z^*} \left( \frac{n\ell}{d_y} \right)^2 \left( n + \frac{1}{2} \right) \hbar \omega_0 \pm \frac{1}{2} \gamma^* \mu_0 B
\]

(3.40)

\[
E_0(1 + \alpha E_0) = \left( n + \frac{1}{2} \right) \hbar \omega_0 + \frac{\beta(E_s)}{2M_z} \left( \frac{\hbar m_{l_\alpha}}{d_y} \right)^2 + \frac{\alpha \gamma^*}{4M_z^*} \left( \frac{\hbar m_{l_\alpha}}{d_y} \right)^4 \pm \frac{1}{2} \gamma^* \mu_0 B
\]

(3.41)
\[
E'_0(1 + \alpha E'_0) = \left( n + \frac{1}{2} \right) \hbar \omega_0 \pm \frac{1}{2} g^* \mu_0 B - \frac{\alpha E}{2m_2} \left( \frac{\hbar m_y}{d_y} \right)^2 + \frac{\hbar^2 \pi^2}{2m_2} \left( 1 + \alpha E \right) \left( \frac{n_y}{d_y} \right)^2
\]
\[
+ \frac{\alpha \hbar^4 \pi^4}{4m_2 m_2} \left( \frac{n_y}{d_y} \right)^4
\]
(3.42)

\[
E'_0(1 + \alpha E'_0) = \left( n + \frac{1}{2} \right) \hbar \omega_0 + \frac{\hbar^2 \pi^2}{2m_2} \left( \frac{n_y}{d_y} \right)^2 \pm \frac{1}{2} g^* \mu_0 B
\]
(3.48)

and

\[
E'_0 = \left( n + \frac{1}{2} \right) \hbar \omega_0 \pm \frac{1}{2} g^* \mu_0 B + \frac{\hbar^2 \pi^2}{2m_2} \left( \frac{n_y}{d_y} \right)^2
\]
(3.44)