

CHAPTER 6

Results on the Density of States for ZnS_xSe_{1-x} in the Presence of Quantizing Magnetic Field

6.1 INTRODUCTION

Physical properties e.g. optical transitions, charge transport etc., require information about the density of states (DOS) [Pankove, 1971]. The density of states depends on dimensionality of the system and energy-wave vector dispersion relation [Böer, 1990]. When a semiconductor absorbs light for example, electrons can be promoted from occupied valence states to empty conduction states. The energy of the photons must match the energy difference between the occupied and the empty states. Without the empty states, the transitions cannot occur. More occupied valence states and more unoccupied conduction states means that the possibility of greater transition rates and therefore higher levels of absorption. The same reasoning applies to thermal transitions. In other words, DOS determines the basic characteristics of semiconductors and reflects important information regarding the transport properties under different physical conditions [Shum, 1984]. The importance of DOS was pointed out by Landsberg [1986].

The analytical formulations of various quantum processes in semiconductors having different band structures are based on the DOS of such materials. The DOS has been investigated extensively [Nag, 1980; Ghatak *et al.*, 2005; Mitra and K.P. Ghatak, 1989; Biswas and K.P. Ghatak, 1992].

The definition of density of states uses “per unit crystal volume” in order to remove geometrical considerations from the measure of the type of state. If each unit volume has N_v traps given by

$$N_v = \int_0^{\infty} dE g(E) = \int d(\text{energy}) \frac{\text{states}}{\text{energy} * \text{vol}} = \frac{\text{states}}{\text{vol}} \quad (6.1)$$

then the volume V must have $N = N_v V$ traps.

The band structure may be altered by applying a magnetic field. The effect of the magnetic field on the band structure is easily observed in experiments [Uhlenbeck and Young, 1930]. A number of transport phenomena arise when the band structure is altered by magnetic fields. These have been extensively studied and serve as diagnostic tools for characterizing the materials. The basic theory developed by Landau [1930] explains the diamagnetic behavior of quasi-free electrons in a solid, which cannot be explained by classical theory.

In the presence of magnetic field, the electrons experience the transverse Lorentz force and curl around the magnetic field and are expected to contribute to the magnetic moment of the system. However, for confined electron systems, the total sum when worked out classically turns out to be zero. Landau’s theory, which is based on the solution of Schrödinger equation, shows that the energy of the electrons corresponding to the transverse components of the wave vector is quantized. These quantized levels are called the Landau levels.

Chakrabortya *et al.* [2007] studied the DOS function in the case of external electric field for the III-V, ternary and quaternary semiconductors whose unperturbed energy band structures are defined by the non-parabolic bands. We shall derive the DOS

for the ZnS_xSe_{1-x} materials with unperturbed energy band structure as defined by the parabolic band in the presence of a quantizing magnetic field. Finally we calculate the results for ZnS_xSe_{1-x} materials.

6.2 THE FORMULATION OF THE DOS FOR THE ZnS_xSe_{1-x} ALLOYS IN THE PRESENCE OF A QUANTIZING MAGNETIC FIELD

The Schrödinger equation, in the presence of a magnetic field has the form [Nag, 1980],

$$(2m^*)^{-1} (-i\hbar\nabla + eA)^2 \psi - E\psi = 0 \quad (6.2)$$

where $-i\hbar\nabla$ is the momentum operator, A is the vector potential due to the magnetic field, and m^* is the effective mass of the electrons at the edge of the conduction band, which takes into account the effect of the periodic crystal potential.

The magnetic vector potential A is related to the magnetic induction by the equation

$$\vec{B} = \nabla \times \vec{A} \quad (6.3)$$

In the problem under consideration B is specified and assumed it to be in the z direction. A cannot be uniquely expressed in terms of B ,

$$\nabla \cdot B = 0 \quad (6.4)$$

so we may take for A , (see Appendix B)

$$A = \hat{y}Bx \quad (6.5)$$

Replacing A in Eqn. (6.2) by Eqn. (6.5) and try the solution by the form

$$\psi = \psi_1(x) \exp[i(k_y y + k_z z)] \quad (6.6)$$

then upon rearranging the terms we get

$$\left[\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + \left(\frac{\partial}{\partial x} + \frac{i}{\hbar} eBx \right)^2 + \frac{2m^*}{\hbar^2} E \right] \psi = 0 \quad (6.7)$$

It is seen that the magnetic field introduces only an additional x-dependent term, so that y and z dependence of the ψ function is unaltered. Eqn. (6.7) can be written as

$$\left(\frac{d\psi_1}{dx} + \frac{i}{\hbar} eBx \right)^2 + \left[\frac{2m^*}{\hbar^2} E - (k_y^2 + k_z^2) \right] \psi_1 = 0 \quad (6.8)$$

Putting $x_1 = x - \hbar k_y (eB)^{-1}$, we can write

$$\left(-\frac{\hbar^2}{2m^*} \frac{d^2}{dx_1^2} + \frac{e^2 B^2}{2m^*} x_1^2 \right) \psi_1(x_1) = \left(E - \frac{\hbar^2 k_z^2}{2m^*} \right) \psi_1(x_1) \quad (6.9)$$

The energy eigenvalue is given by [Nag, 1972] as

$$E_l = (l + 1/2) \hbar eB / m^* \quad (6.10)$$

where l is an integer. From Eqn. (6.9) it can be conclude that the energy is independent of k_y but varies continuously with k_z .

The energy eigenvalues of quasi-free electrons in the presence of a magnetic field can be expressed as [Nag, 1980]

$$E_{l,k_z} = \frac{\hbar^2 k_z^2}{2m^*} + (l+1/2) \left(\frac{\hbar e B}{m^*} \right). \quad (6.11)$$

In the case of parabolic bands we may use $m^* = m_c$ [Ghatak *et al.*, 2007]. Hence Eqn. (6.11) can be expressed as

$$E = \frac{\hbar^2 k^2}{2m_c} + (l+1/2) \left(\frac{\hbar e B}{m_c} \right). \quad (6.12)$$

From Eqn. (6.12) we get

$$\begin{aligned} dk &= \left(\frac{m_c}{\hbar^2} \right) \frac{dE}{k} = \frac{m_c}{\hbar^2} \frac{dE}{\left(\frac{2m_c}{\hbar^2} \right)^{1/2} \left[E - \left(l + \frac{1}{2} \right) \frac{\hbar e B}{m_c} \right]^{1/2}} \\ &= \left(\frac{m_c}{2\hbar^2} \right)^{1/2} \left[E - \left(l + \frac{1}{2} \right) \frac{\hbar e B}{m_c} \right]^{-1/2} dE \end{aligned} \quad (6.13)$$

From Eqn. (6.6) it can be seen that the wave function is not periodic in the x direction; so that the periodic boundary condition cannot be applied. The wave function is periodic in the direction of the applied magnetic field, the y-direction, and in the z-direction. The number of states in these two directions are $L_2/2\pi$ and $L_3/2\pi$ per unit lengths of k_y and k_z where L_2, L_3 are the dimensions of the crystal in these two directions.

From the assumption $x_1 = x - \hbar k_y (eB)^{-1}$, the wave function is localized around $x = \hbar k_y / eB$, the extent being of the order $(2l\hbar/eB)^{1/2}$ [McKelvey, 1966]. The boundary condition that may apply for the x-direction is that $\hbar k_y / eB$ should lie within 0 and L_1 , where L_1 is the dimension of the crystal in the x-direction. The maximum length of k_y is thus $L_1 eB / \hbar$ and the degeneracy of the level $(L_2/2\pi) \times (L_1 eB / \hbar)$. The number of values of k_y per unit length of k-space along the y-direction is $(L_2/2\pi)$.

The number of states per unit volume of the crystal surface associated with each cylindrical surface of length dk_z , lying between k_z and $k_z + dk_z$ is given as [Nag, 1980],

$$dg(k_z) = eB (4\pi^2 \hbar)^{-1} dk_z \quad (6.14)$$

which means that Eqn. (6.13) should be represented in terms of k_z , and it should be noted that the magnetic field does not affect the total number of states but only alters the distribution of the states. Substituting Eqn. (6.13) into Eqn. (6.14) we get

$$g(E)dE = \frac{1}{4\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{3/2} \frac{\hbar eB}{2m_c} \sum_{l=0}^{l_{\max}} \left(E - \left(l + \frac{1}{2} \right) \frac{\hbar eB}{m_c} \right)^{-1/2} dE \quad (6.15)$$

where $g(E)dE$ gives the number of states lying between E and $E+dE$, and l_{\max} is defined by [Nag, 1980],

$$\left(l_{\max} + \frac{3}{2} \right) \frac{\hbar eB}{m_c} > E > \left(l_{\max} + \frac{1}{2} \right) \frac{\hbar eB}{m_c} \quad (6.16)$$

Inserting the maximum value of l into Eqn. (6.15) we get

$$g(E)dE = \frac{1}{4\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{3/2} \frac{\hbar eB}{2m_c} \left(E - \left(l + \frac{1}{2} \right) \frac{\hbar eB}{m_c} \right)^{-1/2} dE. \quad (6.17)$$

This gives the expression of DOS for the II-VI materials in the presence of a quantizing magnetic field.

After integrating Eqn. (6.17) can be written as

$$\begin{aligned} N(E) &= \frac{1}{4\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{3/2} \frac{\hbar eB}{m_c} \left[E - \left(l + \frac{1}{2} \right) \frac{\hbar eB}{m_c} \right]^{1/2} \\ &= \frac{1}{4\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{3/2} \frac{\hbar eB}{m_c} \left[E - \left(\frac{\mu^*}{m_c} \right) \left(l + \frac{1}{2} \right) \frac{\hbar eB}{\mu^*} \right]^{1/2} \end{aligned} \quad (6.18)$$

after using the assumption

$$\frac{\mu^*}{m_c} = (0.124Eg_0)^{1.76} \quad (6.19)$$

we can write the DOS for the ZnS_xSe_{1-x} alloys in the presence of quantizing magnetic field as

$$N(E) = \frac{1}{4\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{3/2} \frac{\hbar eB}{m_c} \left[E - \left((0.124Eg_0)^{1.76} \right) \left(l + \frac{1}{2} \right) \frac{\hbar eB}{\mu^*} \right]^{1/2} \quad (6.20)$$

Eqn. (6.20) written in terms of Eg_0 .

6.3 THE EFFECT OF MAGNETIC FIELD ON THE FERMI LEVEL IN THE CASE OF PARABOLIC BANDS

The function giving the occupancy of the level, which is called the Fermi function, is [Fermi, 1926]

$$n/g = 1/\{1 + \exp[(E - E_F)/k_B T]\} \quad (6.21)$$

where n is the number of electrons occupying levels of energy E ; k_B is the Boltzman constant, T is the lattice temperature, E_F is the Fermi energy. Now, the relation between carrier concentration and Fermi level is obtained from Eqn. (6.15) and Eqn. (6.21) as

$$\begin{aligned} n &= \frac{1}{4\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{3/2} \frac{\hbar e B}{m_c} \times \int_0^\infty \{1 + \exp[(E - E_F)/k_B T]\}^{-1} \left(E - (l + \frac{1}{2}) \frac{\hbar e B}{m_c} \right)^{-1/2} dE \\ &= \frac{1}{4\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{3/2} \frac{\hbar e B}{m_c} \times \int_0^\infty \{1 + \exp[(E - E_F)/k_B T]\}^{-1} \left(E - ((0.124 E g_0)^{1.76}) (l + \frac{1}{2}) \frac{\hbar e B}{\mu^*} \right)^{-1/2} dE. \end{aligned} \quad (6.22)$$

If we express Eqn. (6.22) in terms of Fermi integral by changing the order of integration and summation, we introduce

$$\begin{aligned} n &= N_c \phi \sum_{l=0}^\infty \int_0^\infty M_l^{-1/2} \left\{ 1 + \exp \left[M_l + (l + \frac{1}{2}) \phi - \eta \right] \right\}^{-1} dM_l \\ &= N_c \phi \sum_{l=0}^\infty F_{-\frac{1}{2}} \left[\eta - (l + \frac{1}{2}) \phi \right] \end{aligned} \quad (6.24)$$

where $N_c = \frac{1}{4\pi^2} \left(\frac{2m_c k_B T}{\hbar^2} \right)^{3/2}$, $\phi = ((0.124 E g_0)^{1.76}) \frac{\hbar e B}{\mu^* k_B T}$, $\eta = \frac{E_F}{k_B T}$, $M_l = \frac{E}{k_B T} - (l + \frac{1}{2}) \phi$,

and the Fermi integral has the form [Sommerfeld, 1928; McDougall and Stoner, 1938]

$$F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{W^j dW}{1 + \exp(W - \eta)} \quad (6.25)$$

and $\Gamma(j+1)$ is a complete gamma function for all j .

Since only one band is occupied so we got only one term on the right hand side of Eqn. (6.24) and the relation can be simplified as

$$n = N_c \phi F_{-\frac{1}{2}} \left[\eta - \frac{\phi}{2} \right] \quad (6.26)$$

and with the unperturbed state $l=0$.

6.4 RESULTS

Figures 6.1 to 6.3 illustrate the DOS as a function of electron energy for ZnS_xSe_{1-x} ($x=0, 0.9, \text{ and } 1$) in the B -field of 0.1, 0.5, 0.75 and 1 Tesla for angular momentum state $l=1$. The DOS increases with electron energy, and is higher for $ZnSe$ compared to ZnS . This may be attributed to the difference in the mass of electron at the edge of conduction band (m_c) for the three different alloys. $m_c = m^*$ [Ghatak *et al.*, 2007].

It is clear from the curve of ZnS that the DOS is gradually increasing with the electron energy. This is also true for $ZnSe$ and ZnS_xSe_{1-x} for $x=0.9$.

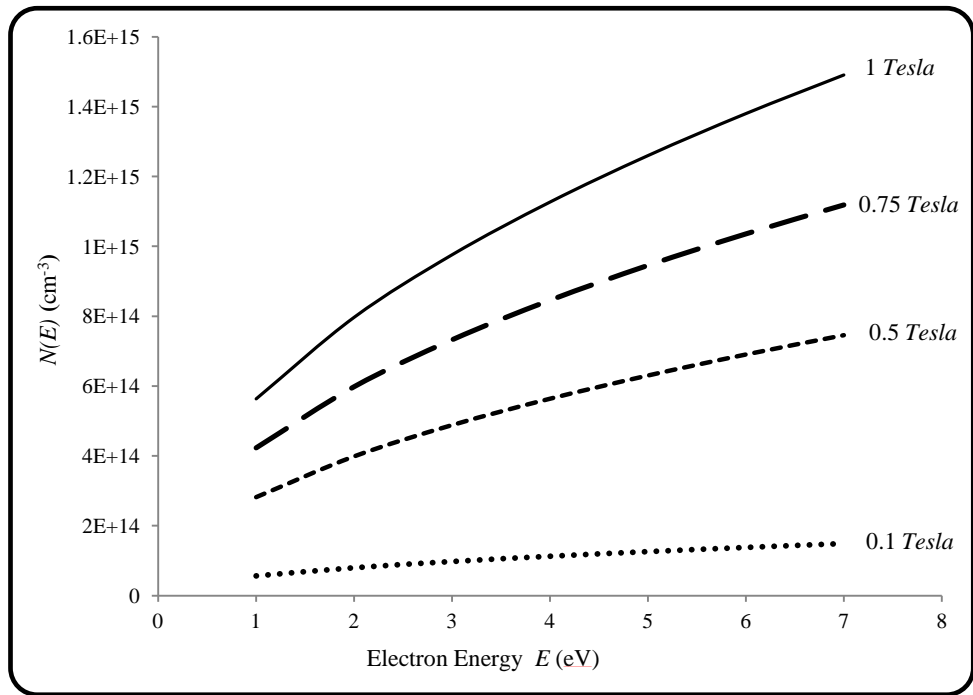


FIGURE 6.1: Density of states as a function of electron energy for ZnS ($B=0.1, 0.5, 0.75, 1$ Tesla and $l=1$).

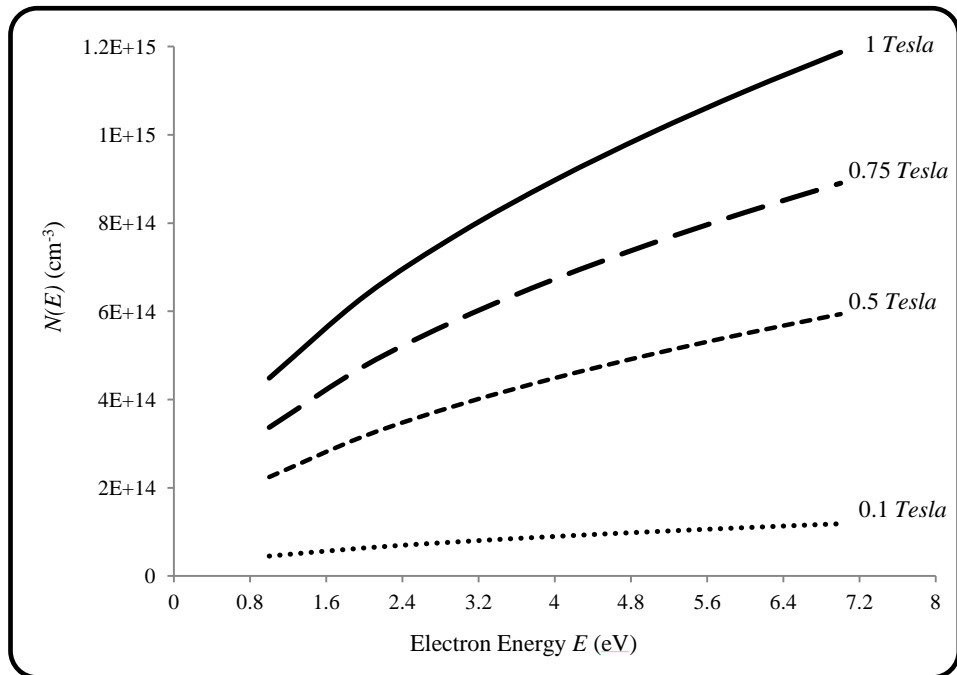


FIGURE 6.2: Density of states as a function of electron energy for $ZnSe$ ($B=0.1, 0.5, 0.75, 1$ Tesla and $l=1$).

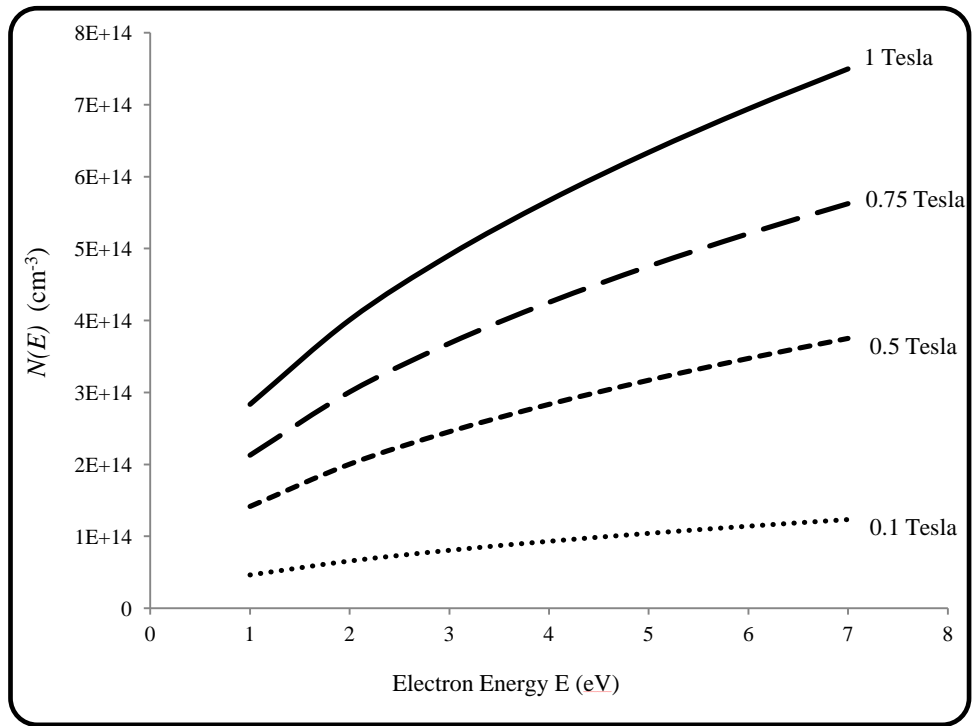


FIGURE 6.3: Density of states as a function of electron energy for $ZnS_xSe_{1-x}(x=0.9)$ ($B=0.1, 0.5, 0.75, 1$ Tesla and $l=1$).

In Figure 6.4 we have plotted DOS as a function of x . DOS is increasing with increasing x and is higher with increase in magnetic field for a particular x .

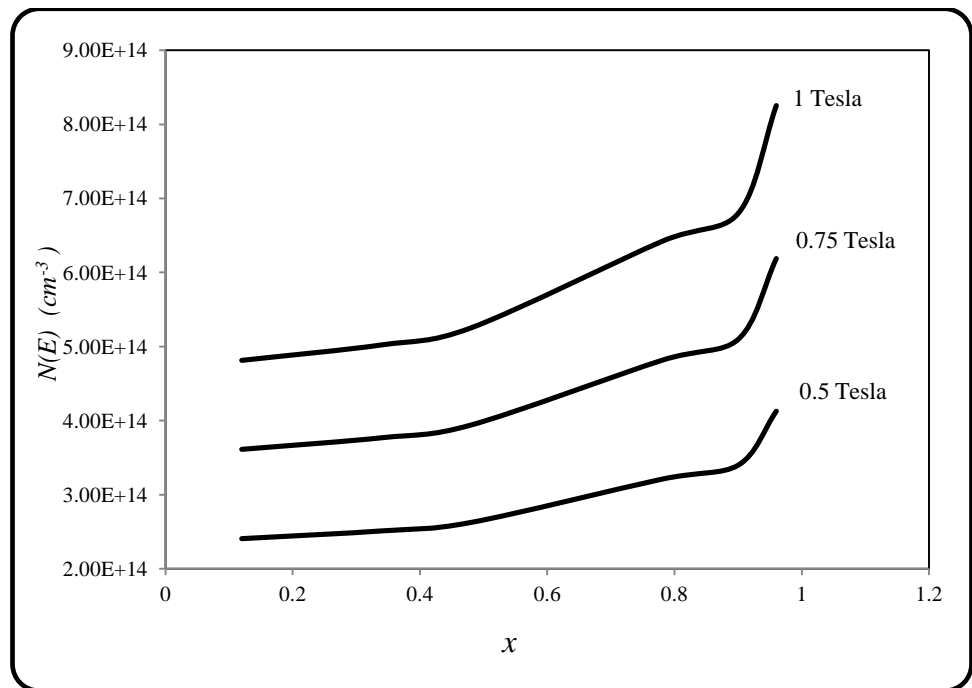


FIGURE 6.4: Density of status as a function of x . ($0 < x < 1$) for $B= 0.5, 0.75,$ and 1 Tesla and $E=1eV$.

In Figure 6.5 we have plotted n/N_c as a function of $\eta-\phi/2$ for $l=0$. The values for $F_{-\frac{1}{2}}\left[\eta-\frac{\phi}{2}\right]$ was taken from Cloutman [1989]. Plugging in the values of ϕ , k_B as taking $T=300$ k (room temperature), we get $E_F = 0.07$ to 0.28 eV when $(\eta-\phi/2)$ varies from 2 to 10. E_F varies from 0.09 to 0.30 eV and E_F varies from 0.11 to 0.32 eV when $(\eta-\phi/2)$ varies from 2 to 10. Hence it may be inferred that the carries concentration increases in Fermi level.

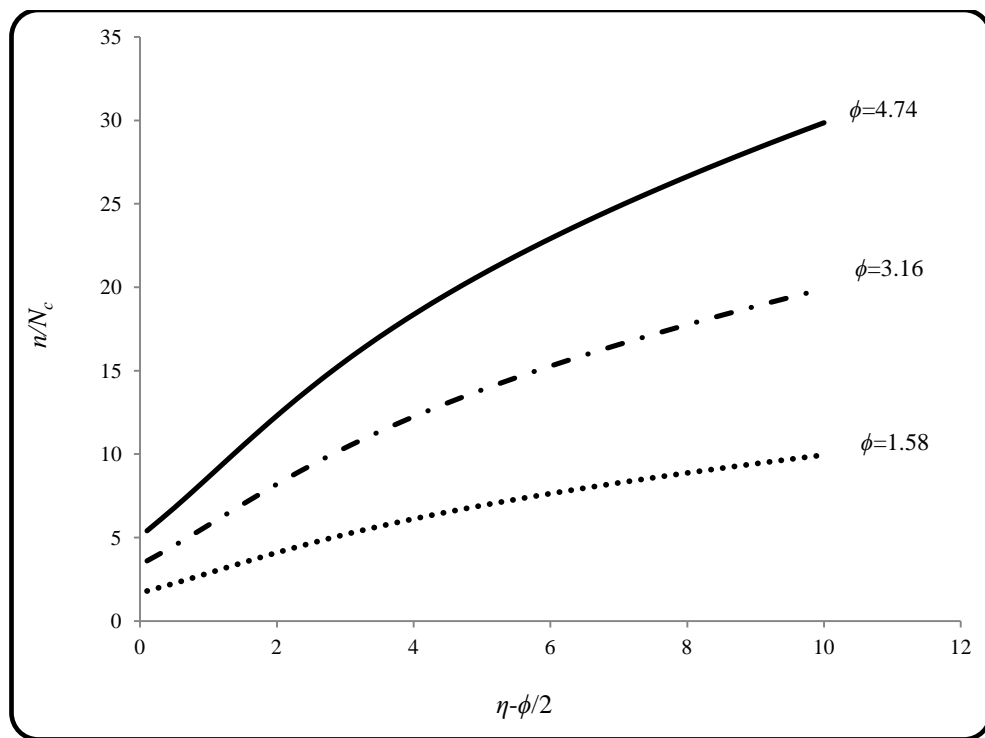


FIGURE 6.5: n/N_c as a function of $\eta-\phi/2$, showing the effect of magnetic field on the Fermi level for a constant electron concentration.

6.5 SUMMARY

The theoretical results on the Density of States for ZnS_xSe_{1-x} in the presence of quantizing magnetic field were presented in Eq. (6.18)

$$\begin{aligned}
N(E) &= \frac{1}{4\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{3/2} \frac{\hbar eB}{m_c} \left[E - l \frac{\hbar eB}{m_c} \right]^{1/2} \\
&= \frac{1}{4\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{3/2} \frac{\hbar eB}{m_c} \left[E - \left(\frac{\mu^*}{m_c} \right) \frac{l\hbar eB}{\mu^*} \right]^{1/2}
\end{aligned}$$

and Eq. (6.20)

$$N(E) = \frac{1}{4\pi^2} \left(\frac{2m_c}{\hbar^2} \right)^{3/2} \frac{\hbar eB}{m_c} \left[E - \left((0.124Eg_0)^{1.76} \right) \frac{l\hbar eB}{\mu^*} \right]^{1/2}$$

after using the empirical relationship given in Eqn. (6.20)

$$\frac{\mu^*}{m_c} = (0.124Eg_0)^{1.76}$$

The effect of magnetic field on the Fermi level in the case of parabolic bands was represented in Eqn. (6.24)

$$\begin{aligned}
n &= N_c \phi \sum_{l=0}^{\infty} \int_0^{\infty} M_l^{-1/2} \{1 + \exp[M_l + l\phi - \eta]\}^{-1} dM_l \\
&= N_c \phi \sum_{l=0}^{\infty} F_{-\frac{1}{2}} \left[\eta - l\phi \right]
\end{aligned}$$

and because only one band is occupied hence Eqn. (6.24) can be simplified as Eqn. (6.26)

$$n = N_c \phi F_{-\frac{1}{2}} \left[\eta - \frac{\phi}{2} \right]$$