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Intro to Spintronics - Chapter 15

15.5 Some elements of semiconductor physics: particular applications in nanostructures

15.5.1 Density of states: bulk (3-D) to quantum dot (0-D)

Consider the quantum confined geometries shown in Fig. 15.3 (2D: two-dimensional electron gas, 1D: one-dimensional electron gas, 0D: three-dimensional quantum box). Calculate the energy dependence of the *density of states* in these structures and compare them to that of the 3D bulk sample shown in the upper left corner in Fig. 15.3.

Solution

3D: Consider a uniform homogeneous bulk piece of semiconductor whose conduction band has a parabolic $E - \vec{k}$ relationship with the bottom at E_{co}, as shown in Figure 15.4:

$$E(\vec{k}) = E_{co} + \frac{\hbar^2 k^2}{2m^*}. \quad (15.99)$$

The solutions of the 3D effective mass Schrödinger equation are of the form of plane waves

$$\phi_k(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\vec{r}}, \quad (15.100)$$

normalized over a volume $\Omega = L^3$, where L is the length of the side of a cube large compared to the lattice unit cell. Assuming periodic boundary conditions for $\phi_k(\vec{r})$, i.e.,

$$\phi_k(x+L, y+L, z+L) = \phi_k(x,y,z), \quad (15.101)$$

the allowed values of $\vec{k} = (k_x, k_y, k_z)$ are given by

$$k_x = n_x \frac{\pi}{L}, \quad (15.102)$$

$$k_y = n_y \frac{\pi}{L}, \quad (15.103)$$

and

$$k_z = n_z \frac{\pi}{L}, \quad (15.104)$$

where n_x, n_y, n_z are integers.

The density of electrons at location $\vec{r}$ can then be calculated as follows

$$\rho(\vec{r}) = \frac{N}{\Omega} = \sum_{\vec{k}} f(E_k)|\phi_k(\vec{r})|^2, \quad (15.105)$$

where $f(E_k)$ is the Fermi-Dirac distribution function. We can assume that the carrier statistics is governed by the Fermi-Dirac distribution as long as the system is in *equilibrium* (e.g., no current flows and no light is shining on it generating electron-hole pairs).

Each electron eigenstate occupies a volume $\frac{(2\pi)^3}{\Omega}$ in $\vec{k}$-space. Therefore, in a volume of size $d^3\vec{k}$, we have a number of electron eigenstates equal to

$$2\frac{\Omega}{(2\pi)^3} d^3\vec{k}, \quad (15.106)$$

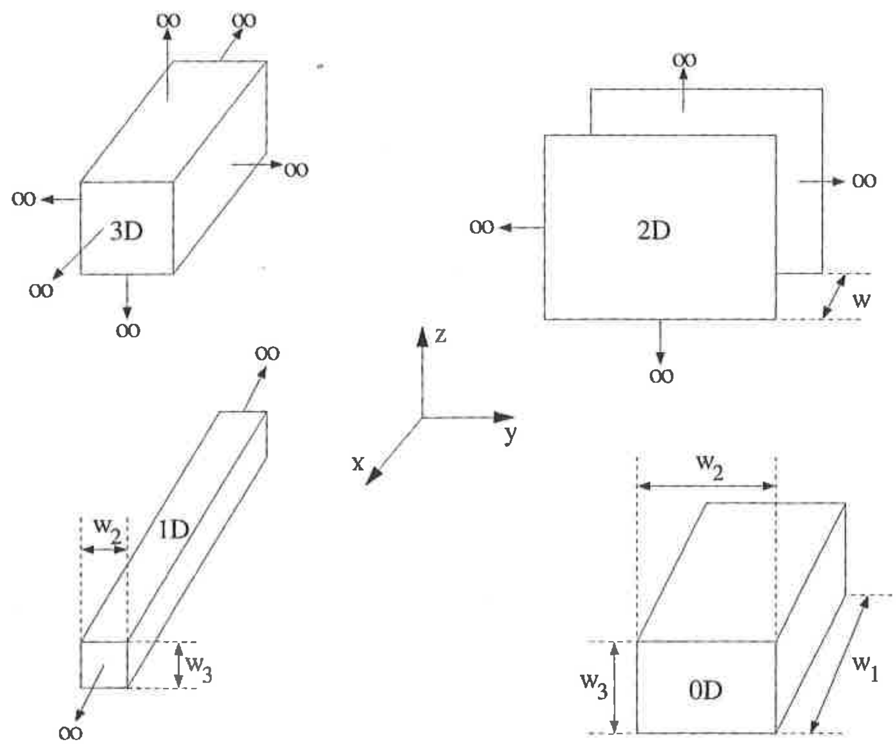

FIGURE 15.3
Illustration of the formation of a quantum dot (bottom right figure) through the gradual squeezing of a bulk piece of semiconductor (upper left). When the dimension of the bulk structure is reduced in one direction to a size comparable to the de Broglie wavelength, the resulting electron gas is referred to as a two-dimensional electron gas (2 DEG) because the carriers are free to move in the y and z directions only. If quantum confinement occurs in two directions, as illustrated in the bottom left figure, the resulting electron gas is referred to as a one-dimensional electron gas (1 DEG) since an electron in this structure is free to move in the x direction only. If confinement is imposed in all three directions, we get a quantum dot (0 DEG).

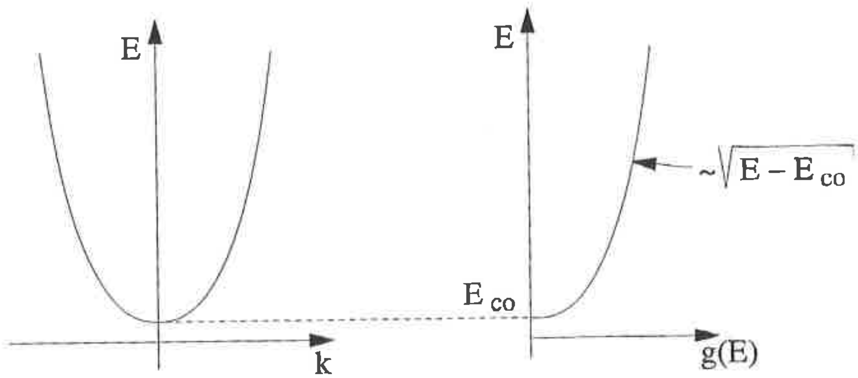

FIGURE 15.4
(Left) Parabolic energy dispersion relation close to the bottom of the conduction band (E_{c0}) of a typical semiconductor. (Right) Corresponding energy dependence of the three-dimensional density of states in a bulk semiconductor.

where the extra factor 2 has been added to take into account the spin degeneracy of each eigenstate in $\vec{k}$-space, as required by the Pauli Exclusion principle. For a large value of Ω, the $\sum_{\vec{k}}$ in Equation (15.105) can be replaced by an integral and we obtain

$$\rho(\vec{r}) = \frac{1}{4\pi^3} \int d^3\vec{k} f(E_k), \tag{15.107}$$

which is spatially invariant.

Since $f(E_k)$ is spherically symmetric in $\vec{k}$-space, the last integration can be easily performed using spherical coordinates leading to

$$\rho = \int_{E_{co}}^{+\infty} dE g_{3D}(E) f(E), \tag{15.108}$$

where $g_{3D}(E)$ is by definition the three-dimensional density of states and is given by

$$g_{3D}(E) = \frac{k^2}{\pi^2 (\frac{dE}{dk})} = \frac{m^* k}{\pi^2 \hbar^2}, \tag{15.109}$$

where we have used the dispersion relation in Equation (15.99) to arrive at the last equality.

Using the E-k relationship (15.99) once again to express k in terms of E, we get the well-known result for the 3-D density of states:

$$g_{3D}(E) = \frac{m^*}{\pi^2 \hbar^3} \sqrt{2m^*(E - E_{co})}, \tag{15.110}$$

whose energy dependence is illustrated in Figure 15.4.

Using the above equation in Equation (15.107), the electron density in a bulk sample is given by

$$\rho = \frac{2}{\pi} N_c F_{\frac{1}{2}}(\xi), \tag{15.111}$$

where

$$N_c = \frac{1}{4\hbar^3}\left(\frac{2m^* k_B T}{\pi}\right)^{\frac{3}{2}}, \tag{15.112}$$

and

$$\xi = \frac{(E_F - E_{co})}{k_B T}. \tag{15.113}$$

In equation (15.111), $F_{\frac{1}{2}}$ is the Fermi-Dirac integral of index $\frac{1}{2}$:

$$F_{\frac{1}{2}}(\xi) = \int_{E_{co}}^{+\infty} \frac{dE\sqrt{E - E_{co}}}{[1 + e^{\frac{E-E_F}{kT}}]}. \tag{15.114}$$

2D: Next, we generalize the derivation above to determine the two-dimensional density of states in a 2 DEG. In this case, the electron density is calculated as follows

$$\rho(\vec{r}) = \sum_m \sum_{k_y,k_z} f_o(E_m)|\phi_{m,k_y,k_z}(\vec{r})|^2. \tag{15.115}$$

The eigenfunctions and corresponding eigenvalues of the Schrödinger equation are given by:

$$\phi_{m,k_y,k_z}(\vec{r}) = \frac{1}{\sqrt{A}} e^{ik_y y} e^{ik_z z} \xi_m(x), \tag{15.116}$$

where

$$E_{m,k_y,k_z} = E_m + \frac{\hbar}{2m^*}(k_y^2 + k_z^2), \tag{15.117}$$

and

$$A = L_y L_z \tag{15.118}$$

is a normalization area to describe the in-plane free motion of carriers in the (y, z) directions, x being the direction of quantum confinement of the well. The wavefunctions $\xi_m(x)$ are solutions of the one-dimensional Schrödinger equation and depend on the potential confinement $E_c(x)$ in the x-direction

$$-\frac{\hbar^2}{2m^*}\frac{d^2\xi_m(x)}{dx^2} + E_c(x)\xi_m(x) = E_m \xi_m(x). \tag{15.119}$$

Each $\xi_m(x)$ is assumed to be normalized and has a corresponding eigenvalue E_m.

Therefore,

$$\rho(\vec{r}) = \sum_m \sigma_m |\xi_m(x)|^2, \tag{15.120}$$

where

$$\sigma_m = \sum_{k_y,k_z} \frac{1}{A} f_o(E_{m,k_y,k_z}). \tag{15.121}$$

Converting the $\sum_{k_y,k_z}$ to an integral following the 3-D case, we get

$$\sum_{k_y,k_z} = 2\left(\frac{A}{4\pi^2}\right)\int d^2\vec{k}. \tag{15.122}$$

Using polar coordinates in the (k_y, k_z) plane

$$\sigma_m = \int_0^{2\pi} \frac{d\phi}{2\pi^2} \int_0^{+\infty} dkk f_o(E_{m,k_y,k_z}), \tag{15.123}$$

and since $f_o(E_{m,k_y,k_z})$ is independent of ϕ,

$$\sigma_m = \int_0^{+\infty} \frac{kdk}{\pi} f_o(E_{m,k_y,k_z}). \tag{15.124}$$

Using the dispersion relationship of the subbands in the well, we get

$$dE_{m,k_y,k_z} = \frac{\hbar}{n^*} kdk, \tag{15.125}$$

and σ_m becomes

$$\sigma_m = \int_{E_m}^{+\infty} dE g_{2D}(E) f_o(E), \tag{15.126}$$

where

$$g_{2D}(E) = \frac{m^*}{\pi\hbar^2} \tag{15.127}$$

is *independent of energy* and is the density of states in each subband in the well.

Substituting the expression for the Fermi-Dirac factor $f_o(E)$, σ_m can be calculated exactly,

$$\sigma_m = \frac{m^*}{\pi\hbar^2} k_B T ln(1 + e^{\frac{E_m - E_F}{k_B T}}). \tag{15.128}$$

This analytical expression for σ_m is valid for any shape of the confining potential in the x direction. This quantity determines the sheet electron concentration in a 2-DEG.

1D:

If we have confinement in the y-z plane and free motion of carriers is allowed in the x-direction, then

$$\rho(\vec{r}) = \sum_{k_x}\sum_{n}\sum_{m} f_o(E_{n,m})|\phi_{k_x,n,m}(\vec{r})|^2 \tag{15.129}$$

where

$$\phi_{k_x,n,m}(\vec{r}) = \frac{1}{\sqrt{L}} e^{ik_x x} \xi_{n,m}(y,z), \tag{15.130}$$

where L is a normalization factor of the plane wave moving along the x-direction and $\xi_{n,m}(y,z)$ are the solutions of the two-dimensional Schrödinger equation

$$-\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dy^2} + \frac{d^2}{dz^2}\right)\xi_{n,m}(y,z) + E_c(y,z)\xi_{n,m}(y,z) = E_{n,m}\xi_{n,m}(x,y). \tag{15.131}$$

Here, n, m are quantum numbers characterizing the quantization in the y and z directions. They are also called *transverse subband indices.*

The energy dispersion relationship in each subband characterized by the two quantum numbers (n, m) is given by

$$E_{k_x,n,m} = E_{n,m} + \frac{\hbar^2}{2m^*} k_x^2. \tag{15.132}$$

Therefore, in this 1-DEG, the electron density is invariant in the x-direction

$$\rho(y,z) = \sum_{n,m} \sigma_{n,m} |\xi_{n,m}(y,z)|^2, \tag{15.133}$$

where

$$\sigma_{n,m} = \sum_{k_x} \frac{1}{L} f_o(E_{k_x,n,m}). \tag{15.134}$$

Converting the sum over k_x into an integral, i.e.,

$$\sum_{k_x} = 2\left(\frac{L}{2\pi}\right) \int dk_x, \tag{15.135}$$

we get

$$\sigma_{n,m} = \frac{1}{\pi} \int_{-\infty}^{+\infty} dk_x f_o(E_{k_x,n,m}) = \frac{2}{\pi} \int_0^{+\infty} dk_x f_o(E_{k_x,n,m}). \tag{15.136}$$

$$\tag{15.137}$$

Using the dispersion relation ($E - k_x$ relation), we get

$$dE_{k_x,n,m} = \frac{\hbar}{m^*} k_x dk_x; \tag{15.138}$$

hence

$$\sigma_{n,m} = \int_{E_{n,m}}^{+\infty} dE g_{1D}(E) f_o(E), \tag{15.139}$$

where

$$g_{1D}(E) = \frac{1}{\pi}\sqrt{\frac{2m^*}{\hbar^2}}\frac{1}{\sqrt{E - E_{n,m}}}, \tag{15.140}$$

which is the expression for the one-dimensional density of states in each sub-band in the quantum wire. It diverges at $E = E_{n,m}$, the threshold energy for free propagation in that subband.

0D: In that case, we are dealing with a quantum box with quantum confinement in all three directions.

$$\rho(\vec{r}) = \sum_{n,m,l} f_o(E_{n,m,l})|\phi_{n,m,l}(\vec{r})|^2, \tag{15.141}$$

where $\phi_{n,m,l}$ are the solutions of the three-dimensional Schrödinger equation for the $E_c(x, y, z)$ representing the quantum confinement in all three directions. The indices (n, m, l) are three quantum numbers characterizing the eigenstates of the Schrödinger equation.

We can write

$$\rho(\vec{r}) = \sum_{n,m,l} \sigma_{n,m,l}|\phi_{n,m,l}(\vec{r})|^2, \tag{15.142}$$

with

$$\sigma_{n,m,l} = \int_0^{+\infty} dE g_{0D}(E) f_o(E). \tag{15.143}$$

Therefore the 0-dimensional density of states is simply

$$g_{0D}(E) = 2\sum_{n,m,l} \delta(E - E_{n,m,l}) \tag{15.144}$$

where δ is the Dirac delta function and the factor 2 has been included since each $E_{n,m,l}$ state can be occupied by two electrons with opposite spin.

Example 1: Electron sheet concentration in a quantum well

(a) Show that the sheet carrier concentration in a HEMT device (which has a 2-DEG in the channel) is given by

$$n_s = \frac{m^*}{\pi\hbar^2}k_B T ln\left[(1 + e^{\frac{E_F - E_1}{k_B T}})(1 + e^{\frac{E_F - E_2}{k_B T}})\right], \tag{15.145}$$

when only two subbands are occupied. Here, E_1 and E_2 are the bottom energies of the first two subbands.

(b) Starting with the result of the part (a), show that at low temperature

$$n_s = \frac{m^*}{\pi\hbar^2}(E_F - E_1), \tag{15.146}$$

when the second subband is unoccupied and

$$n_s = \frac{m^*}{\pi\hbar^2}(E_2 - E_1) + 2\frac{m^*}{\pi\hbar^2}(E_F - E_2), \tag{15.147}$$

when both subbands are occupied.

Solution

The electron concentration in the 2 DEG formed at the heterointerface between the high and low bandgap materials in a HEMT structure (see Fig. 12.6) is given by

$$\rho(x) = \sum_m \sigma_m |\xi_m(x)|^2, \tag{15.148}$$

where

$$\sigma_m = \frac{m^*(k_BT)}{\pi\hbar^2} ln(1 + e^{-\frac{(E_m - E_F)}{k_BT}}). \tag{15.149}$$

The sheet carrier concentration in the 2 DEG is given by

$$n_s = \int_{-\infty}^{+\infty} \rho(x)dx. \tag{15.150}$$

If the wavefunctions $\xi_m(x)$ are normalized, i.e.,

$$\int_{-\infty}^{+\infty} |\xi_m(x)|^2 dx = 1, \tag{15.151}$$

the sheet carrier concentration is given by the simple formula

$$n_s = \sum_m \sigma_m. \tag{15.152}$$

If only one subband in the 2 DEG is occupied,

$$n_s = k_BTln(1 + e^{\frac{E_F - E_1}{k_BT}}). \tag{15.153}$$

If $k_BT << E_F - E_o$,

$$n_s = \frac{m^*}{\pi\hbar^2}(E_F - E_1). \tag{15.154}$$

When the second subband is occupied (but the third one unoccupied),

$$n_s = \frac{m^*}{\pi\hbar^2}k_BT\left[ln(1 + e^{\frac{E_F - E_1}{k_BT}}) + ln(1 + e^{\frac{E_F - E_1}{k_BT}})\right], \tag{15.155}$$

which can also be written as follows

$$n_s = \frac{m^*}{\pi\hbar^2}k_BTln\left[(1 + e^{\frac{E_F - E_1}{k_BT}})(1 + e^{\frac{E_F - E_2}{k_BT}})\right]. \tag{15.156}$$

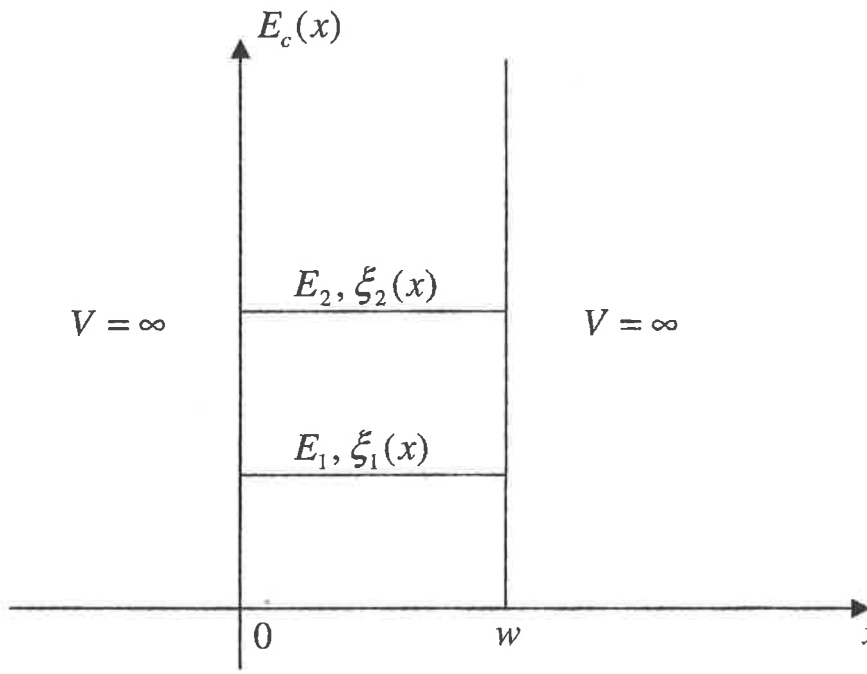

FIGURE 15.5
Confined states in a quantum well (2 DEG) of width w.

If $k_BT << E_F - E_1$, $E_F - E_2$, (i.e., at low temperature), then

$$ln\left(1 + e^{\frac{E_F - E_1}{k_BT}}\right) = \frac{E_F - E_1}{k_BT}, \tag{15.157}$$

and

$$ln\left(1 + e^{\frac{E_F - E_2}{k_BT}}\right) = \frac{E_F - E_2}{k_BT}. \tag{15.158}$$

Hence

$$n_s = \frac{m^*}{\pi\hbar^2}(E_F - E_o) + \frac{m^*}{\pi\hbar^2}(E_F - E_1) = \frac{m^*}{\pi\hbar^2}(2E_F - E_1 - E_2). \tag{15.159}$$

Example 2: Fermi level location in a Quantum Well

Consider a 100$\AA$ wide potential well (quantum well or 2-DEG) with infinite walls at $T = 0K$. Assume all impurities are ionized (i.e., neglect carrier freeze out). Assume $m^* = 0.067m_0$ and calculate the location of the Fermi level for

- $N_D = 10^{17}cm^{-3}$,
- $N_D = 10^{19}cm^{-3}$.

Solution

Assuming that all impurities are ionized, the sheet carrier concentration in the well is given by

$$n_s = N_D W. \tag{15.160}$$

Therefore, for $N_D = 10^{17}$ and $10^{19} cm^{-3}$, n_s is equal to 10^{11} and $10^{13} cm^{-2}$, respectively.

At zero temperature, if the Fermi level E_F is between the N^{th} and $(N+1)^{th}$ subbands in the well, then

$$n_s = \frac{m^*}{\pi\hbar^2} \sum_{i=1}^{N} (E_F - E_i). \tag{15.161}$$

Hence

$$n_s = \frac{m^*}{\pi\hbar^2} \left(N E_F - \sum_{i=1}^{N} E_i \right), \tag{15.162}$$

which is a generalization of the results found in the previous example. Solving for E_F we get

$$E_F = \frac{1}{N} \left[\frac{N_D W}{(\frac{m^*}{\pi\hbar^2})} + \sum_{i=1}^{N} E_i \right]. \tag{15.163}$$

For a well surrounded by a infinite wall (particle in a box problem), the different eigenstates energies are given by

$$E_i = \frac{\hbar^2}{2m^*} (\frac{i\pi}{W})^2, \tag{15.164}$$

where i is an integer.

For $m^* = 0.067 m_o$ and $W = 100 \AA$, we find

$$E_i \simeq i^2 56 meV. \tag{15.165}$$

Therefore, the subband energy bottoms due to the particle-in-a-box confinement in two dimensions are given by the above equation.

For $N_D = 10^{17} cm^{-3}$, if we assume E_F is between E_1 and E_2, and $N = 1$ in Equation (15.163) above, we get

$$E_F = 59.78 meV, \tag{15.166}$$

which tells us that only one subband is occupied, as assumed.

For $N_D = 10^{19} cm^{-3}$, assuming E_F is between E_2 and E_3, the Fermi level is found to be

$$E_F = 329.4 meV, \tag{15.167}$$

which is below E_3. In this case, only two subbands are occupied. The number of subbands that are occupied is usually found by trial and error.

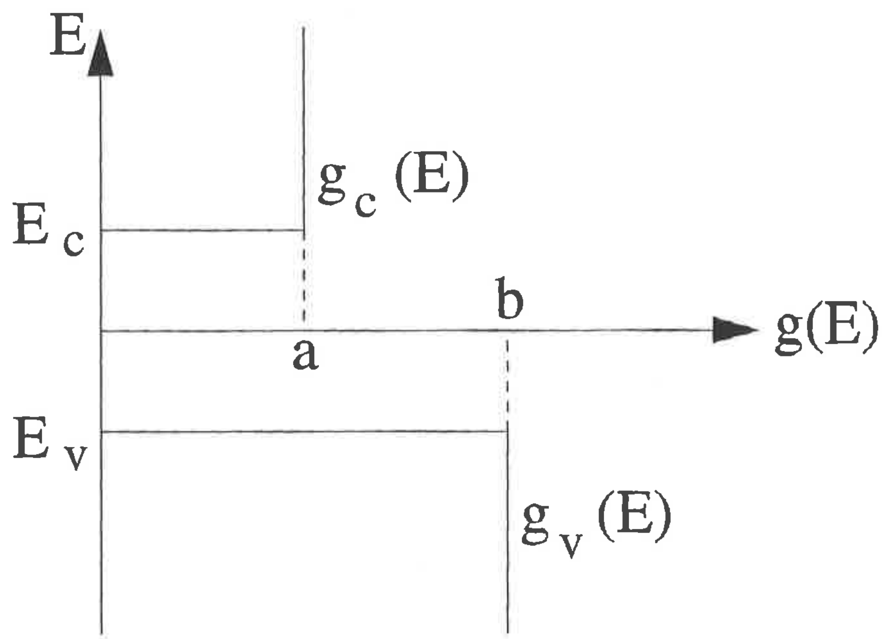

FIGURE 15.6
Density of states of electrons or holes in a two dimensional electron or hole gas (2-DEG or 2-DHG).

Example 3: Intrinsic carrier concentration in a 2DEG

Consider the density of states as shown in the Fig. 15.6 representing the two-dimensional density of states of electrons and holes in a quantum well.

(a) Assuming the well is undoped, obtain an expression for the Fermi level E_F at room temperature in terms of a, b and temperature T. Assume Boltzmann statistics to be valid. When is E_F exactly equal to the midgap energy, $\frac{(E_c+E_v)}{2}$?

(b) Obtain the expression for n_i, the intrinsic carrier concentration.

Hint: Start with the approximate expressions for the electron (n) and hole (p) concentrations in terms of $g_c(E)$ and $g_v(E)$ [subscripts c and v denote conduction and valence bands], and assume Boltzmann statistics of carriers:

$$f(E) = e^{\frac{E_F - E}{k_B T}}, \tag{15.168}$$

where k_B is Boltzmann's constant.

Solution

(a) The electron and hole concentrations are given by

$$n = \int_{E_c}^{\infty} g_c(E) f(E) dE, \tag{15.169}$$

$$p = \int_{-\infty}^{E_v} g_v(E)[1 - f(E)] dE. \tag{15.170}$$

Use the Boltzmann approximation, $f(E) = e^{\frac{(E_F - E)}{k_B T}}$ and $g_c(E) = a\theta(E - E_c)$ and $g_v(E) = b\theta(E_v - E)$ where $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ for $x \leq 0$ (Heaviside function). We get

$$n = \int_{E_c}^{\infty} a e^{\frac{(E_F - E)}{k_B T}} dE = a k_B T e^{\frac{E_F - E_c}{k_B T}}. \tag{15.171}$$

Similarly,

$$p = \int_{-\infty}^{E_v} b e^{\frac{(E - E_F)}{k_B T}} dE = b k_B T e^{\frac{E_v - E_F}{k_B T}}. \tag{15.172}$$

If the sample is intrinsic, then $n = p = n_i$. Therefore,

$$a k_B T e^{(\frac{E_F - E_c}{k_B T})} = b k_B T e^{(\frac{E_v - E_F}{k_B T})}, \tag{15.173}$$

from which we derive

$$E_F = \frac{E_v - E_c}{2} + \frac{k_B T}{2} ln(\frac{b}{a}). \tag{15.174}$$

Hence, $E_F = \frac{E_v + E_c}{2}$ whenever $a = b$.

(b) The intrinsic carrier concentration is given by $n_i = \sqrt{np}$. Hence, using Equations (15.171) and (15.172) above, we obtain

$$n_i = k_B T \sqrt{ab} e^{\frac{(E_c - E_v)}{2k_B T}} = k_B T \sqrt{ab} e^{-\frac{E_g}{2k_B T}}. \tag{15.175}$$

Example 4: Connection between 2D and 3D density of states

The density of states in the conduction band of a bulk sample is given by Equation (15.110).

If a 2D quantum well (of width W) is formed with infinite barriers on both sides, show that

$$g_{3D}(E_{c0} + E_n) = \frac{n}{W} g_{2D}(E_{c0} + E_n), \tag{15.176}$$

where $g_{2D}(E)$ is the two-dimensional density of states in each subband of the 2 DEG, given by Equation (15.127).

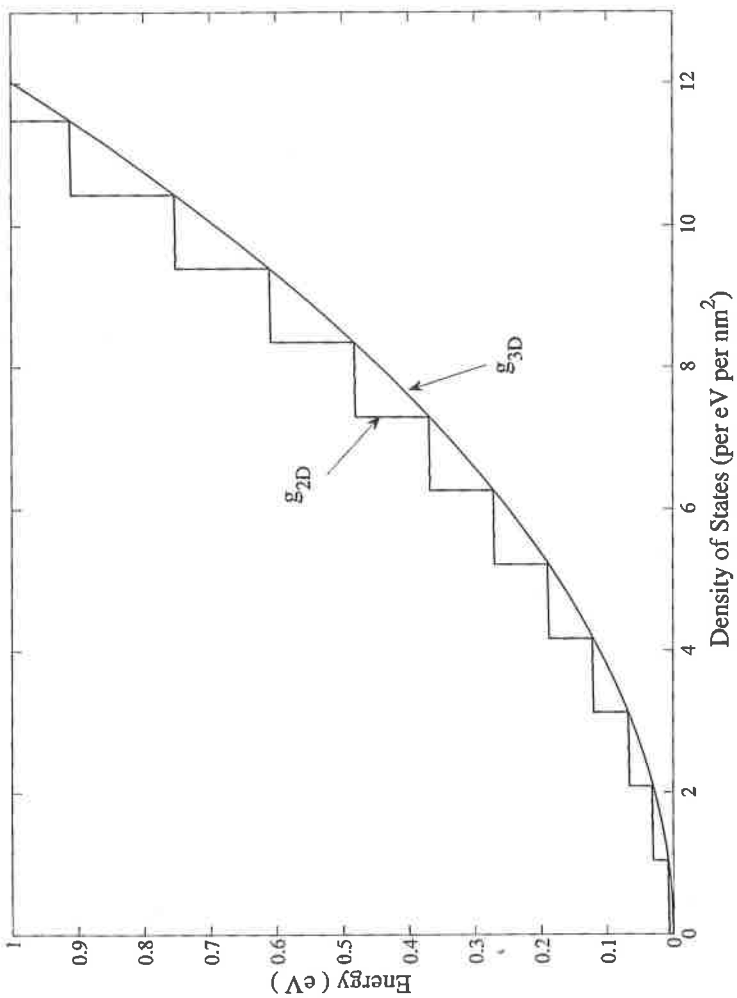

FIGURE 15.7
Illustration of the 2D density-of-states staircase touching the 3D density of states curve. For this illustration, the effective mass of electrons was assumed to be $m^* = 0.5m_o$ and the quantum well width was assumed equal to $100\mathring{A}$.

Solution

For a particle in a box with a constant potential energy E_{co}, the eigenenergies are given by

$$E_n = E_{co} + \frac{n^2\hbar^2\pi^2}{2m^*W^2}. \tag{15.177}$$

Hence, using Equation (15.110) we get

$$g_{3D}(E_n) = \frac{m^*}{\pi^2\hbar^3}\sqrt{2m^*(\frac{n^2\hbar^2\pi^2}{2m^*w^2})}, \tag{15.178}$$

i.e.,

$$g_{3D}(E_n) = \frac{m^*}{\pi^2\hbar^2}\frac{n}{w} = \frac{n}{w}g_{2D}(E_{co} + E_n). \tag{15.179}$$

A plot of $Wg_{3D}(E_n)$ and $g_{2D}(E_{co} + E_n)$ is shown in Fig. 15.7. This figure shows that the corners of the staircase representing the $\frac{m^*}{\pi\hbar^2}$ jump for each appearance of a new subband in the 2DEG touches the curve $Wg_{3D}(E_n)$. As the well width is increased, the energy levels for the particle-in-a-box are more closely spaced and the staircase becomes closer and closer to the Wg_{3D} curve, i.e.,

$$g_{3D}(E) = \lim_{W\to\infty} \frac{1}{W}g_{2D}(E). \tag{15.180}$$