2.4   Quantum confined electrons

We will now focus our attention on the electron charge densities in case of one, two and three-dimensional confinement. All the relations will be then used in the self-consistent solution of the Poisson/Schrödinger equation.

2.4.1   Integration over the k space

Consider a function f defined in the k-space. The sum of f over $\mathbf{k}$ is

$$I = \sum_{\mathbf{k}} f(\mathbf{k}) \tag{2.70}$$

(2.70) can be written as

$$\sum_{\mathbf{k}} f(\mathbf{k}) = \frac{L^3}{(2\pi)^3} \sum_{\mathbf{k}} f(\mathbf{k}) \frac{(2\pi)^3}{L^3}, \tag{2.71}$$

where L is the sample size along each direction, and $\frac{(2\pi)^3}{L^3}$ is the volume occupied by one state in the k-space. If the available states are continuous rather than discrete, the quantity $\frac{(2\pi)^3}{L^3}$ can be seen as an infinitesimal volume $(\Delta k)^3$. As a consequence, the sum becomes an integral, and (2.70) can be expressed as

$$\sum_{\mathbf{k}} f(\mathbf{k}) = \frac{L^3}{(2\pi)^3} \sum_{\mathbf{k}} f(\mathbf{k})(\Delta k)^3 \approx \frac{L^3}{(2\pi)^3} \int f(\mathbf{k}) d\mathbf{k}. \tag{2.72}$$

In general, we can generalize to a generic dimensionality d and make the following substitution

$$\sum_{k} f(k) \rightarrow 2 \times \frac{L^d}{(2\pi)^d} \int f(k)(dk)^d \tag{2.73}$$

where we have also considered the spin degeneracy. This relation will result to be very useful in the derivation of the electron density whose general expression at the equilibrium is [11]

$$n(\mathbf{r}) = \sum_{i} f_0(E_i) |\Psi_i(\mathbf{r})|^2 \tag{2.74}$$

where the sum is performed over the single energy levels E_i, and f_0 is the Fermi-Dirac distribution function.

Quantum confinement in one direction

The eigenfunction Ψ can be then expressed as

$$\Psi_{i,k_y,k_z}(x,y,z) = \frac{e^{jk_y y}e^{jk_z z}}{\sqrt{L_y L_z}}\psi_i(x,y,z) \qquad (2.86)$$

where L_y and L_z are the system size in the y and z direction, respectively, while $\psi_i(x,y,z)$ is the $i-th$ eigenfunction. Using (2.74), we obtain

$$n(x,y,z) = \sum_i \sigma_i |\psi_i(x,y,z)|^2 \qquad (2.87)$$

where

$$\sigma_i \overset{\text{def}}{=} \sum_{k_y,k_z} \frac{f_0(E_{i,k_y,k_z})}{L_y L_z} \qquad (2.88)$$

$$E_{i,k_y,k_z} = \epsilon_i + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 k_z^2}{2m_z} \qquad (2.89)$$

and ϵ_i is the i-th energy level in the x-direction Making the following variable transformation

$$k'_y = \frac{k_y}{\sqrt{2m_y}} \; ; \; k'_z = \frac{k_z}{\sqrt{2m_z}} \tag{2.90}$$

we obtain

$$dk^2 = dk_y dk_z = 2\sqrt{m_y m_z}\, dk'_y dk'_z \tag{2.91}$$

while (2.89) becomes

$$E_{i,k'_y,k'_z} = \epsilon_i + \hbar^2 k'^2_y + \hbar^2 k'^2_z = \epsilon_i + \hbar^2 k'^2 \tag{2.92}$$

By means of eqs. (2.73),and (2.91), and using cylindrical coordinates [13]

$$\sum_{k_y,k_z} \to 2 \times \frac{L_y L_z}{4\pi^2} 2\sqrt{m_y m_z} \int_0^{2\pi} d\theta \int_0^\infty k' dk' \tag{2.93}$$

we can evaluate σ_i

$$\begin{aligned} \sigma_i &= \int_0^{2\pi} d\theta \int_0^\infty \frac{\sqrt{m_y m_z}}{\pi^2} k' dk' f_0(E_{i,k'_y,k'_z}) \\ &= \int_0^\infty \frac{2\sqrt{m_y m_z}}{\pi} k' dk' f_0(E_{i,k'_y,k'_z}) \end{aligned} \tag{2.94}$$

From (2.92), we can replace dk' in terms of dE_{i,k'_y,k'_z},

$$dE_{i,k'_y,k'_z} = 2\hbar^2 k' dk' \tag{2.95}$$

and obtain

$$\sigma_i = \int_{\epsilon_i}^\infty \frac{\sqrt{m_y m_z}}{\pi \hbar^2} f_0(E_{i,k'_y,k'_z}) dE_{i,k'_y,k'_z} \tag{2.96}$$

and finally

$$\sigma_i = \frac{\sqrt{m_y m_z} K_B T}{\pi \hbar^2} \ln\left[1 + \exp\left(\frac{\epsilon_i - E_F}{K_B T}\right)\right] \tag{2.97}$$

where K_B is the Boltzmann constant, T is the temperature and E_F is the Fermi level.

The electron concentration can be then expressed as

$$n(x,y,z) = \sum_i |\psi_i(x,y,z)|^2 \frac{\sqrt{m_y m_z} K_B T}{\pi \hbar^2} \ln\left[1 + \exp\left(\frac{\epsilon_i(y,z) - E_F}{K_B T}\right)\right] \tag{2.98}$$

2.4.3   Two-dimensional quantum confinement

The considerations in the previous section, similarly apply when quantum confinement is predominant in the $y-z$ plane. The two-dimensional Schrödinger equation reads,

$$-\left[\frac{\hbar^2}{2}\frac{\partial}{\partial y}\frac{1}{m_y}\frac{\partial}{\partial y} + \frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m_z}\frac{\partial}{\partial z}\right]\chi_i$$
$$= E_{i,k_x}\chi_i. \tag{2.99}$$

while the three-dimensional eigenfunctions can be expressed as

$$\Psi_{k_x,i} = \frac{e^{jk_xx}}{\sqrt{L_x}}\chi_i(y,z) \tag{2.100}$$

where $\chi_i(y,z)$ are the eigenfunctions associated to the energy level $\epsilon_i(x)$ and the total energy reads

$$E_{i,k_x} = \epsilon_i(x) + \frac{\hbar^2 k_x^2}{2m_x} \tag{2.101}$$

The electron concentration is

$$n(x,y,z) = \sum_i |\chi_i(x,y,z)|^2\alpha_i \tag{2.102}$$

where

$$\alpha_i = \sum_{k_x}\frac{f_0(E_{i,k_x})}{L_x} \tag{2.103}$$

Using (2.73),

$$\alpha_i = 2\frac{L_x}{2\pi}\int_{-\infty}^{+\infty}\frac{f_0(E_{i,k_x})}{L_x}dk_x = \frac{2}{\pi}\int_0^{+\infty}\frac{f_0(E_{i,k_x})}{L_x}dk_x \tag{2.104}$$

Expressing k_x as

$$k_x = \frac{\sqrt{2m_x(E-\epsilon_i)}}{\hbar} \tag{2.105}$$

and deriving with respect to E we obtain

$$dk_x = \frac{\sqrt{2m_x}}{2\hbar\sqrt{E-\epsilon_i}}dE \tag{2.106}$$

Substituting (2.106) in (2.104), we obtain

$$\alpha_i = \frac{2m_x}{\pi\hbar} \int_{\epsilon_i}^{\infty} \frac{1}{\sqrt{(E-\epsilon_i)}} \frac{1}{1+e^{\frac{E-E_F}{K_B T}}} dE \qquad (2.107)$$

and multiplying and dividing by $\sqrt{K_B T}$, we obtain the final expression for the electron density

$$n(y,z) = \frac{1}{\pi} \left(\frac{2m_x K_B T}{\hbar^2}\right)^{\frac{1}{2}} \sum_i |\chi_i(x,y,z)|^2 \mathcal{F}_{-\frac{1}{2}}\left(\frac{E_F - \epsilon_i(x)}{K_B T}\right) \qquad (2.108)$$

where $\mathcal{F}_{-\frac{1}{2}}$ is the Fermi integral of order $-\frac{1}{2}$:.

$$\mathcal{F}_{-\frac{1}{2}}(y) = \int_0^{\infty} \frac{x^{-\frac{1}{2}}}{1+e^{x-y}} dx \qquad (2.109)$$

2.4.4 Three-dimensional quantum confinement

For what concerns three-dimensional quantum confinement, (2.74) reduces to

$$n(\mathbf{r}) = \sum_i |\Psi_i(\mathbf{r})|^2 \frac{1}{1+e^{\frac{E_i - E_F}{K_B T}}} \qquad (2.110)$$

where Ψ_i is the orbital associated to the i-th eigenvalue, with energy E_i. However for a system with very few electrons, we cannot define a Fermi level, thence it is improper to fix the Fermi energy.

A more proper approach is then represented by fixing the number of electrons in the system and using in (2.74) the Gibbs statistic. However the Gibbs statistics in the grand canonical ensemble is rather complicated, so it is worth following a simpler approach represented by considering the ground-state of the confined region and filling the energy levels starting from the lowest.

The electron density, can then be expressed as

$$n(\mathbf{r}) = 2 \sum_{i=1}^{m} |\Psi_i(\mathbf{r})|^2 + (N-2m)|\Psi_{m+1}(\mathbf{r})|^2 \,, \qquad (2.111)$$

where $m = \lfloor \frac{N}{2} \rfloor$ is the number of fully occupied single electron levels.

2.5   3D Poisson/Schrödinger equation

As introduced at the beginning of this chapter, as dimensions becomes smaller and smaller, quantum confinement effects becomes relevant. A proper simulation approach requires thence solving the Schrödinger equation together with the Poisson equation, in a self-consistent iterative scheme. However, at nanoscale dimensions, not only quantum confinement affects device behavior, but also other effects whose nature is purely electrostatic, limit the performance of the device. We refer for example to the charge sharing effects that lower the threshold voltage in MOSFET devices, or to the random distribution of dopants that can affect the conductivity in the channel.

In order to take into account this wide variety of effects, a three-dimensional simulation approach has to be followed.

In particular the Poisson equation in the three-dimensional simulation domain reads

$$
\begin{aligned}
&\nabla\left[\varepsilon(\mathbf{r})\nabla\phi(\mathbf{r})\right] \\
&= -q\left[p(\mathbf{r}) - n(\mathbf{r}) + N_D^+(\mathbf{r}) - N_A^-(\mathbf{r}) + \rho_{fix}(\mathbf{r})\right], \quad (2.112)
\end{aligned}
$$

where ϕ is the electrostatic potential, ε is the dielectric constant, p and n are the hole and electron densities, respectively, N_D^+ is the concentration of ionized donors, N_A^- is the concentration of ionized acceptors, and ρ_{fix} is the fixed charge concentration.

In all the simulations that we have performed (which will be shown in the following chapters), we have considered quantum confinement of the electrons, while a semiclassical expression has been assumed for the other densities.

For what concern the exchange term V_{exc}, we have considered the expression in [4]

$$
V_{exc} = -\frac{q^2}{4\pi^2\varepsilon_0\varepsilon_r}\left[3\pi^2 n(\mathbf{r})\right]^{\frac{1}{3}}, \qquad (2.113)
$$

which differ by the exchange potential found by Slater by a factor of $\frac{2}{3}$. We have found that the above expression, valid for a 3D system, has an impact on the results only inside the confined regions, while it turns out that exchange corrections to the potential are negligible in the other regions of the analyzed structures.

From a numerical point of view, the coupled Poisson and Schroedinger equations are solved by means of a Newton-Raphson method with a predictor-corrector scheme [14], that we have verified to be faster and