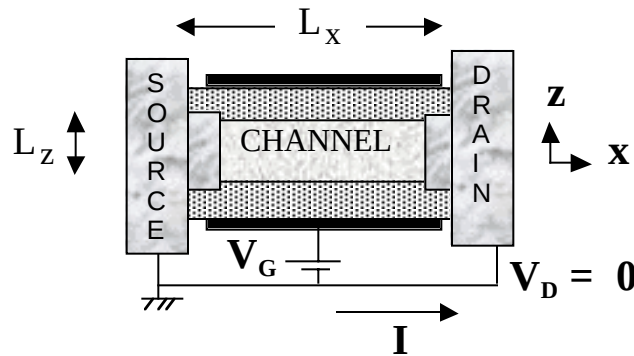


7 / Capacitance

- 7.1. Model Hamiltonian
- 7.2. Electron density / Density matrix
- 7.3. Quantum vs. electrostatic capacitance
- 7.4. Supplementary notes: Multiband effective mass equation

In Chapter one I stated that the full quantum transport model required us to generalize each of the parameters from the one-level model into its corresponding matrix version. Foremost among these parameters is the Hamiltonian matrix $[H]$ representing the energy levels and we are almost done with this aspect. This chapter could be viewed as a transitional one where we discuss an **equilibrium** problem that can be handled using $[H]$ alone, without a knowledge of other parameters like broadening that we will discuss in the next Chapter.

Fig.7.1. An MOS capacitor. The problem is to find the charge induced in the channel in response to an applied gate voltage V_G .



The problem we will discuss is the following: How does the electron density inside the device change as a function of the gate voltage, V_G assuming that the source and the drain are held at the same potential (drain voltage $V_D = 0$, see Fig.7.1)? Strictly speaking this too is a non-equilibrium problem since the gate contact is not in equilibrium with the source and drain contacts (which are in equilibrium with each other). However, the insulator isolates the channel from the gate and lets it remain essentially in equilibrium with the source and drain contacts which have the same electrochemical potential $\mu_1 = \mu_2 \equiv \mu$. The density matrix (whose diagonal elements in a real space representation give us the electron density $n(\vec{r})$) is given by

$$[\rho] = f_0 ([H] - \mu[I]) \quad (7.1)$$

and can be evaluated simply from $[H]$ without a detailed knowledge of the coupling to the source and drain. I am assuming that the channel is large enough that its energy levels are nearly continuous so that the broadening due to the source and drain coupling makes no significant difference.

The matrix $[H]$ includes two parts (cf. Section 1.4)

$$H = H_0 + U([\delta\rho]) \quad (7.2)$$

where H_0 represents just the isolated materials deduced from a knowledge of their bandstructure, while U represents the potential due to the applied gate voltage and any **change** in the density matrix from the reference condition described by H_0 . Neglecting any corrections for correlation effects (see Section 3.2), we can calculate U from the Poisson equation describing Coulomb interactions (ϵ_r is the relative permittivity which could vary spatially):

$$\vec{\nabla} \cdot (\epsilon_r \vec{\nabla} U) = -\frac{q^2}{\epsilon_0} (n(\vec{r}) - n_0) \quad (7.3)$$

subject to the boundary conditions: $[U]_{\text{source}} = [U]_{\text{drain}} = 0$

$$[U]_{\text{gate}} = -qV_G$$

In this chapter I will use this problem to illustrate how we choose the Hamiltonian $[H_0]$ to describe an inhomogeneous structure like a transistor (Section 7.1), how we evaluate the density matrix $[\rho]$ (Section 7.2) and finally (Section 7.3) how the capacitance, C obtained from a self-consistent solution of Eqs.(7.1)-(7.3) can be viewed as a series combination of an electrostatic capacitance, C_E that depends on the dielectric constant and a quantum capacitance, C_Q that depends on the density of eigenstates in the channel.

7.1. Model Hamiltonian

Atomistic Hamiltonian: Let us start with the question of how we write down $[H_0]$ to represent the inhomogeneous collection of isolated materials that comprise the device, from a knowledge of their individual bandstructures. For example, we could model the channel material with a $[H_0]$ that can be represented schematically as a network of unit cells $[H_{nn}]$ interconnected by ‘bonds’ $[H_{nm}]$ of the same size (bxb). Each of these matrices is of size bxb, ‘b’ being the number of basis functions per unit cell.

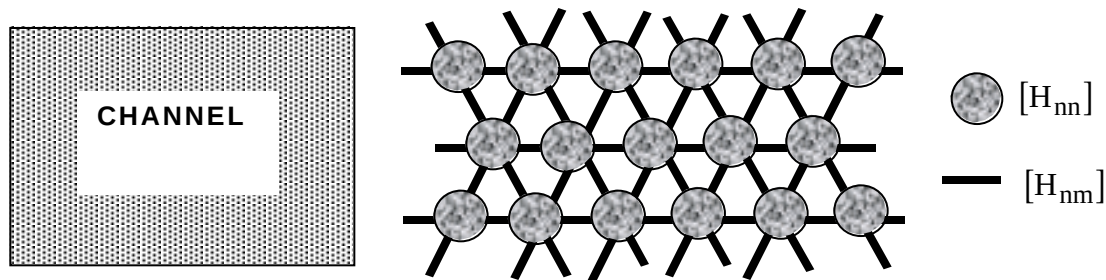


Fig.7.1.1. Any part of the device like the channel can be represented by an atomistic Hamiltonian matrix which can be depicted schematically as a 3-D network of unit cells described by matrices $[H_{nn}]$ and bonds described by matrices $[H_{nm}]$, $n \neq m$. We have arranged the unit cells in an FCC-like network since that is the arrangement for most common semiconductors. Note that the matrices $[H_{nm}]$ for different neighbors ‘m’ are in general different though we have represented them all with the same symbol.

We have seen in Chapter 4 that knowing all the $[H_{nm}]$ the full bandstructure can be calculated from the eigenvalues of the (bxb) matrix

$$[h(\vec{k})] = \sum_m [H_{nm}] e^{i\vec{k} \cdot (\vec{d}_m - \vec{d}_n)} \quad (7.1.1)$$

(which is independent of ‘n’) for each value of ‘ $\vec{k}$ ’. Conversely, we can write down the matrices $[H_{nm}]$ from a knowledge of the bandstructure and thereby write down the matrix $[H_0]$ representing a periodic solid which is of size $(N_b \times N_b)$, N being the total number of unit cells.

The insulator material would obviously be described by a different set of matrices which can be deduced from its bandstructure. The difficult part to model is the **interface**. This is partly due to our ignorance of the actual atomistic structure of the actual interface. But assuming that we know the microstructure exactly, it is still not straightforward to figure out the appropriate bond matrix $[H_{nm}]$ between two unit cells 'n' and 'm' belonging to different materials A and B. Clearly this information is not contained in the individual bandstructures of either A or B and it requires a more careful treatment. We will not get into this question and simply represent an A-B bond using the average of the individual $[H_{nm}]$'s for A-A bonds and B-B bonds.

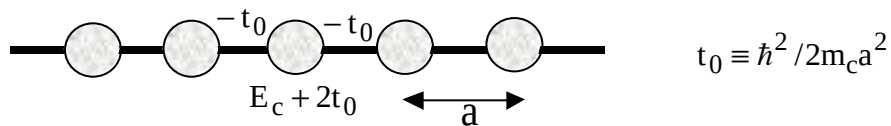
Effective mass Hamiltonian: We have seen before (see Fig.5.1.2) that the energy levels around the conduction band minimum can often be described by a simple relation like

$$h(\vec{k}) = E_c + \frac{\hbar^2 k^2}{2m_c} \quad (7.1.2)$$

where E_c and m_c are constants that can be determined to obtain the best fit. We could easily write down a differential equation that will yield energy eigenvalues that match Eq.(7.1.2). We simply have to replace $\vec{k}$ with $-i\vec{\nabla}$ in the expression for $h(\vec{k})$:

$$\left[E_c - \frac{\hbar^2}{2m_c} \nabla^2 \right] f(\vec{r}) = E f(\vec{r}) \quad (7.1.3)$$

It is easy to check that the plane wave solutions, $f(\vec{r}) = \exp(i\vec{k} \cdot \vec{r})$ with any $\vec{k}$ are eigenfunctions of this differential equation with eigenvalues $E(\vec{k}) = E_c + (\hbar^2 k^2 / 2m_c)$. We could use the finite difference method (Section 1.2) to convert Eq.(7.1.3) into a Hamiltonian matrix, that is much simpler than the original atomistic Hamiltonian. For example in 1-D we could write a tridiagonal matrix with $E_c + 2t_0$ on the diagonal and $-t_0$ on the upper and lower diagonals (see Eq.(1.3.1)) that can be represented in the form



We can use the basic bandstructure equation in Eq.(7.1.1) to write down the corresponding dispersion relation:

$$h(k_x) = (E_c + 2t_0) - t_0 e^{ik_x a} - t_0 e^{-ik_x a} = E_c + 2t_0(1 - \cos k_x a)$$

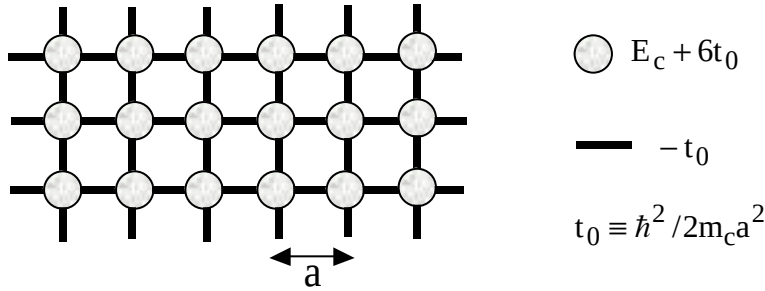


Fig.7.1.2. The effective mass Hamiltonian matrix can be depicted schematically as a 3-D network of unit cells (unrelated to the actual crystal structure) with energy $E_c + 6t_0$ bonded to its nearest neighbors by $-t_0$.

For a general 3-D structure the effective mass Hamiltonian has the form shown in Fig.7.1.2 leading to the dispersion relation

$$h(\vec{k}) = E_c + 2t_0(1 - \cos k_x a) + 2t_0(1 - \cos k_y a) + 2t_0(1 - \cos k_z a) \quad (7.1.4a)$$

which reduces to the parabolic relation in Eq.(7.1.2) if $k_x a$ is small enough that $(1 - \cos k_x a)$ can be approximated with $(k_x a)^2 / 2$ (and the same with $k_y a$ and $k_z a$):

$$h(\vec{k}) = E_c + \frac{\hbar^2}{2m_c} (k_x^2 + k_y^2 + k_z^2) \quad (7.1.4b)$$

This Hamiltonian only describes the eigenstates around the bottom of the conduction band where Eq.(7.1.2) provides an adequate approximation, unlike an atomistic Hamiltonian that describes the full bandstructure (see Eq.(7.1.1)). What we gain, however, is simplicity. The resulting Hamiltonian matrix $[H_0]$ is much smaller than the atomistic counterpart for two reasons. Firstly, the matrices $[H_{nm}]$ representing a unit cell or a bond are scalar numbers rather than (bxb) matrices. Secondly the unit cells in

Fig.7.1.2 do not have to correspond to atomic unit cells as in atomistic Hamiltonians (see Fig.7.1.1). The lattice can be simple cubic rather than face-centered cubic (FCC) and the lattice constant ‘a’ can be fairly large depending on the energy range over which we want the results to be accurate. A simple rule of thumb is that ‘a’ should be small enough that the corresponding t_0 is larger than the energy range (above E_c) we are interested in. Since $t_0 \equiv \hbar^2 / 2m_c a^2$, this means that for a given energy range, we can use a larger ‘a’ if the effective mass m_c is small. But it is important to remember that the wavefunction does not provide information on an atomic scale. It only provides information on a coarse spatial scale and is sometimes referred to as an “envelope function”.

Spatially varying effective mass: Effective mass equations are often used to model “heterostructures” consisting of different materials such that the conduction band edge E_c and/or the effective mass m_c appearing in

$$\left[E_c - \frac{\hbar^2}{2m_c} \nabla^2 \right] f(\vec{r}) = E f(\vec{r}) \quad (\text{same as Eq.(7.1.3)})$$

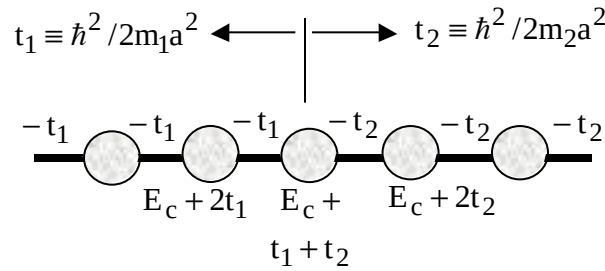
vary spatially. The variation of E_c leads to no special problems, but the variation of m_c cannot be incorporated simply by writing

$$\left[E_c(\vec{r}) - \frac{\hbar^2}{2m_c(\vec{r})} \nabla^2 \right] f(\vec{r}) = E f(\vec{r})$$

The correct version is

$$\left[E_c(\vec{r}) - \frac{\hbar^2}{2m_c} \vec{\nabla} \cdot \left(\frac{1}{m_c(\vec{r})} \vec{\nabla} \right) \right] f(\vec{r}) = E f(\vec{r}) \quad (7.1.5)$$

and it can be shown that if we apply the finite difference method to this version at an interface where the effective mass changes from m_1 to m_2 then we obtain a Hamiltonian matrix that can be represented as



The point to note is that the resulting Hamiltonian matrix

$$\begin{bmatrix} -t_1 & E_c + 2t_1 & -t_1 & 0 & 0 \\ 0 & -t_1 & E_c + t_1 + t_2 & -t_2 & 0 \\ 0 & 0 & -t_2 & E_c + 2t_2 & -t_2 \end{bmatrix}$$

is Hermitian as needed to ensure that the energy eigenvalues are real and current is conserved. By contrast if we start from one of the other possibilities like

$$\left[E_c - \frac{\hbar^2}{2m_c(\vec{r})} \nabla^2 \right] f(\vec{r}) = E f(\vec{r})$$

and use the finite difference method we will end up with a Hamiltonian matrix of the form ($t_0 \equiv (t_1 + t_2)/2$)

$$\begin{bmatrix} -t_1 & E_c + 2t_1 & -t_1 & 0 & 0 \\ 0 & -t_0 & E_c + 2t_0 & -t_0 & 0 \\ 0 & 0 & -t_2 & E_c + 2t_2 & -t_2 \end{bmatrix}$$

which is clearly **non-Hermitian**.

As we have mentioned before, writing down the appropriate Hamiltonian for the interface region requires a knowledge of the interfacial microstructure and simple approximations are often used. But the important point to note is that whatever approximation we use, a fundamental zero-order requirement is that the Hamiltonian matrix should be **Hermitian**. Otherwise we can run into serious inconsistencies due to the non-conservation of probability density and the resulting lack of continuity in electron flow.

An example: One-band effective mass models are widely used to model heterostructures of materials that are not too different. Consider for example, a GaAs quantum well sandwiched between $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ barriers. For GaAs we use $E_c = 0$ eV, $m_c = 0.07m$, while for AlAs , $E_c = 1.25$ eV, $m_c = .15m$ and interpolate linearly to obtain E_c and m_c for the AlAs -GaAs alloy. Fig.7.1.3 shows the energies of the two lowest levels in the GaAs quantum well as a function of the well width, while Fig.7.1.4 shows the dispersion relation $E(\vec{k})$ as a function of the magnitude of the in-plane wavevector $\vec{k} = \{k_x, k_y\}$ for the two lowest subbands of a quantum well with $W = 69\text{\AA}$.

Fig.7.1.3. Energy of the two lowest energy levels of a GaAs quantum well sandwiched between $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ barriers (shown in inset) as a function of the well width (W) calculated from a one-band effective mass model.

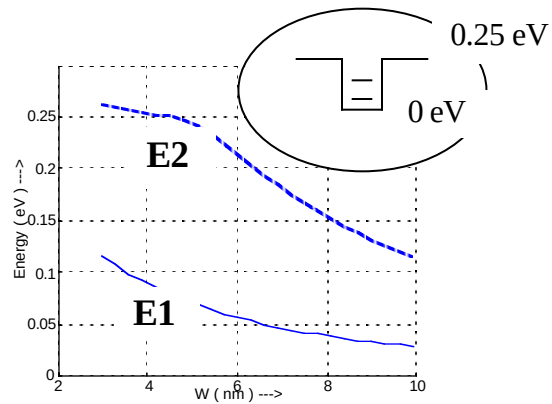
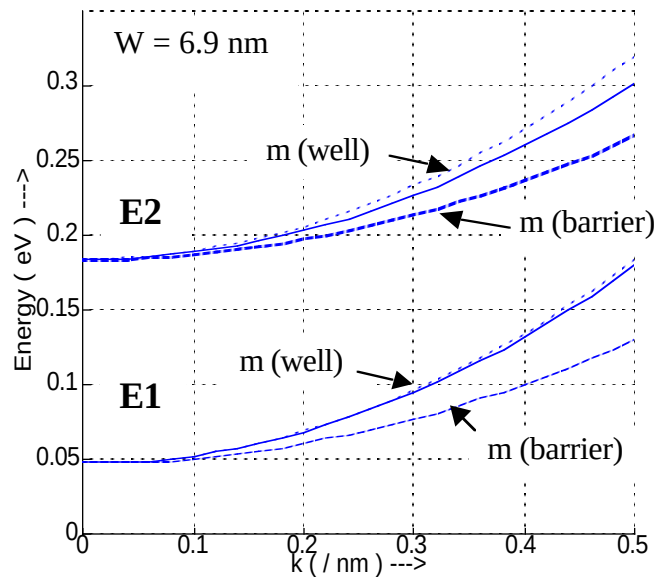


Fig.7.1.4. Solid lines show the dispersion relation $E(\vec{k})$ as a function of the magnitude of the in-plane wavevector $\vec{k} = \{k_x, k_y\}$ for the two lowest subbands of a quantum well with $W = 6.9$ nm, calculated from the one-band effective mass model. The dotted lines show the dispersion expected for an effective mass equal to that in the well and in the barrier.



Problems like this are essentially one-dimensional and easy to solve numerically. The basic idea is that our usual prescription for obtaining the effective mass equation is to replace $\vec{k}$ with $-i\vec{\nabla}$ which consists of three simultaneous replacements:

$$k_x \rightarrow -i\partial/\partial x, \quad k_y \rightarrow -i\partial/\partial y, \quad k_z \rightarrow -i\partial/\partial z$$

To obtain a 1-D effective mass equation while retaining the periodic boundary condition in the x-y plane, we replace k_z with $-i\partial/\partial z$ in $h(\vec{k})$, while leaving k_x, k_y intact:

$$\left[h(k_x, k_y; k_z \Rightarrow -i\partial/\partial z) + U(z) \right] \phi_m(z) = E f(z) \quad (7.1.6)$$

For example, if we start from the one-band effective mass relation,

$$h(\vec{k}) = E_c + \frac{\hbar^2 k^2}{2m_c} \quad (\text{same as Eq.(7.1.2)})$$

we obtain

$$\left[E_c - \frac{\hbar^2}{2} \frac{\partial}{\partial z} \left(\frac{1}{m_c} \frac{\partial}{\partial z} \right) + U(z) + \frac{\hbar^2}{2m_c(z)} (k_x^2 + k_y^2) \right] \phi_m(z) = \epsilon_\alpha \phi_m(z) \quad (7.1.7)$$

which is a 1-D equation that can be numerically solved for any given value of k_x, k_y .

The one-band effective mass model works very well when we have an isotropic parabolic band that is well separated from the other bands. This is usually true of the conduction band in wide bandgap semiconductors. But the valence band involves multiple closely spaced bands which are strongly anisotropic and non-parabolic and a multi-band effective mass model is needed for a proper treatment of the valence band (“p-type” devices) or even the conduction band in narrow-gap semiconductors. General device models based on multi-band models (see supplementary notes in Section 6.4) and atomistic models are topics of current research and I will not discuss them in any depth in this book. I will largely use the one-band model to illustrate the essential concepts underlying the treatment of equilibrium and non-equilibrium problems. However, I will try to describe the approach in a general form that readers can adapt to more sophisticated Hamiltonians in the future as the need arises.

7.2. Electron density / Density matrix

Once we have identified the basic Hamiltonian matrix H_0 representing the isolated materials comprising a device, the next step is to evaluate the density matrix (specially the diagonal elements in a real space representation which give us the electron density)

$$n(\vec{r}) = 2 \rho(\vec{r}, \vec{r}) = 2 \sum_{\alpha} |\phi_{\alpha}(\vec{r})|^2 f_0(\epsilon_{\alpha} - \mu) \quad (7.2.1)$$

where $\phi_{\alpha}(\vec{r})$ are the eigenfunctions of $[H]$ with eigenvalues ϵ_{α} , with $[H]$ given by

$$H = H_0 + U([\delta\rho]) \quad (7.2.2)$$

where U represents the potential due to the applied gate voltage and due to any **change** in the density matrix from the reference condition described by H_0 . In general the matrix representation $[U]$ of the function $U(\vec{r})$ requires a knowledge of the basis functions, but if the potential varies slowly from one unit cell to the next, then we can simply assume the potential to have a constant value $U(\vec{r} = \vec{d}_n)$ throughout a unit cell 'n' so that

$$[U_{nn}] = U(\vec{r} = \vec{d}_n)[I] \quad \text{and} \quad [U_{nm}] = [0] \quad \text{for } m \neq n \quad (7.2.3)$$

where $[I]$ and $[0]$ are the identity matrix and the null matrix of the appropriate size.

How do we calculate $U(\vec{r})$? Neglecting any corrections for correlation effects (see Section 2.2), we can use the Poisson equation describing Coulomb interactions (ϵ_r is the relative permittivity which could vary spatially):

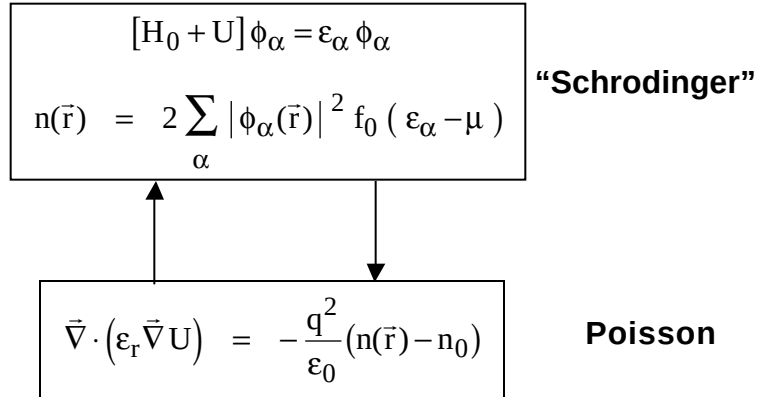
$$\vec{\nabla} \cdot (\epsilon_r \vec{\nabla} U) = -\frac{q^2}{\epsilon_0} (n(\vec{r}) - n_0) \quad (7.2.4)$$

subject to the boundary conditions: $[U]_{\text{source}} = [U]_{\text{drain}} = 0$

$$[U]_{\text{gate}} = -qV_G$$

What we need is a “Schrodinger-Poisson solver” that solves the two aspects of the problem self-consistently as shown schematically in Fig.7.2.1. In general, 3-D solutions are needed but this is numerically difficult and we will use an essentially 1-D example to illustrate the “physics”.

Fig.7.2.1. Modeling a device in equilibrium generally requires a self-consistent solution of a “Schrodinger” equation with the Poisson equation.



1-D Schrodinger-Poisson solver: There are many problems that can be modeled with a 1-D Schrodinger Poisson solver: the MOS capacitor (Fig.7.2.2) we mentioned at the beginning of this chapter represents such an example if we neglect any boundary effects in the x-y plane. What do the 1-D version of the equations in Fig.7.2.1 look like? Let us assume we are using the one-band effective mass Hamiltonian. We might guess that we should first solve a 1-D version of Eq.(7.1.3)

$$\left[E_c - \frac{\hbar^2}{2m_c} \frac{\partial^2}{\partial z^2} + U(z) \right] \phi_m(z) = \epsilon_m \phi_m(z) \quad (7.2.5)$$

then evaluate the electron density from the 1-D version of Eq.(7.2.1)

$$n(z) = 2 \sum_m |\phi_m(z)|^2 f_0(\epsilon_m - \mu) \quad (\text{WRONG}) \quad (7.2.6)$$

and do all this self-consistently with a 1-D version of Eq.(7.2.4):

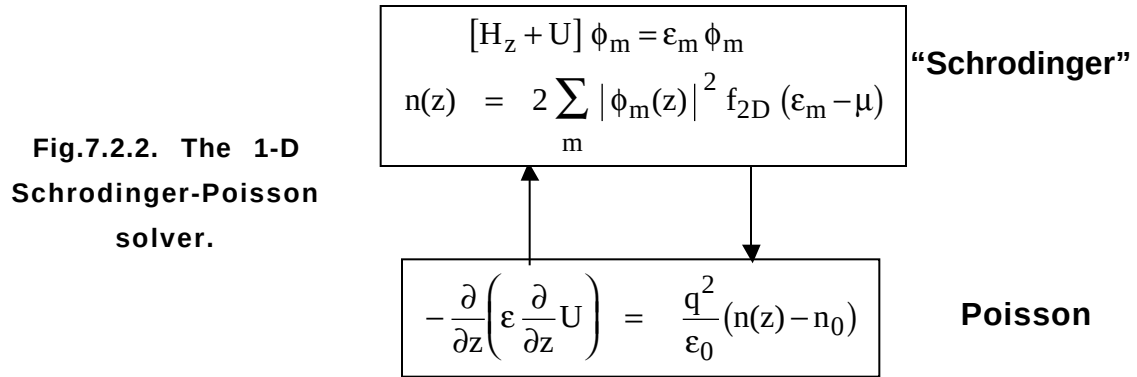
$$-\frac{d}{dz}(\epsilon_r \frac{dU}{dz}) = \frac{q^2}{\epsilon_0} n(z) \quad (7.2.7)$$

All the 1-D versions listed above are correct except for Eq.(7.2.6). The Fermi function f_0 appearing in this equation should be replaced by a new function f_{2D} defined as

$$f_{2D}(E) = N_0 \ln(1 + \exp[-E/k_B T]) \quad \text{with} \quad N_0 \equiv \frac{m_c k_B T}{2\pi\hbar^2} \quad (7.2.8)$$

$$\text{cf.} \quad f_0(E) = \frac{1}{1 + \exp[E/k_B T]}$$

The correct 1-D version of the Schrodinger-Poisson solver is shown below in Fig.7.2.2.



Where does this new function f_{2D} come from? As long as the structure can be assumed to be uniformly periodic in the x-y plane and we can neglect all boundary effects, the eigenfunctions can still be written in the form of plane waves in the x- and y-directions:

$$\phi_\alpha(\vec{r}) = \frac{\exp[ik_x x]}{\sqrt{L_x}} \frac{\exp[ik_y y]}{\sqrt{L_y}} \phi_m(z) \quad (7.2.9)$$

and the electron density is obtained from Eq.(7.2.1) after summing over all three indices $\{m, k_x, k_y\} \equiv \alpha$:

$$n(z) = 2 \sum_m \sum_{k_x, k_y} |\phi_m(z)|^2 f_0(\epsilon_\alpha - \mu) \quad (7.2.10)$$

Eq.(7.2.6) is wrong because it simply ignores the summations over k_x, k_y . The correct version is obtained by noting that

$$\epsilon_\alpha = \epsilon_m + \frac{\hbar^2}{2m_c} (k_x^2 + k_y^2) \quad (7.2.11)$$

which follows from Eq.(7.1.7) with a constant (z-independent) effective mass. Note that, things could get more complicated if the mass itself varies with z since the extra term

$$\frac{\hbar^2}{2m_c(z)} (k_x^2 + k_y^2)$$

would no longer be a constant that can just be added on to obtain the total energy. Under some conditions, this may still be effectively true since the wavefunction is largely confined to a region with a constant effective mass (see for example Problem 6.1c), but it is not generally true. Also, the simple parabolic relation in Eq.(7.2.11) usually does not hold for the multiband effective mass equation (see Fig.7.4.4).

Using Eq.(7.2.11), the summation over k_x, k_y can now be performed analytically to show that

$$\begin{aligned} \sum_{k_x, k_y} f_0(\epsilon_\alpha - \mu) &= \sum_{k_x, k_y} f_0 \left(\epsilon_m - \mu + \frac{\hbar^2}{2m_c} [k_x^2 + k_y^2] \right) \\ &= f_{2D}(\epsilon_m - \mu) \end{aligned} \quad (7.2.12)$$

This is shown as follows:

$$\begin{aligned} \frac{1}{S} \sum_{k_x, k_y} f_0 \left(E + \frac{\hbar^2}{2m_c} [k_x^2 + k_y^2] \right) \\ &= \int_0^\infty \frac{2\pi k dk}{4\pi^2} \frac{1}{1 + A \exp[\hbar^2 k^2 / 2m_c k_B T]} \quad \text{where } A \equiv \exp[E / k_B T] \\ &= \frac{m_c k_B T}{2\pi \hbar^2} \int_0^\infty \frac{dy}{1 + A \exp[y]} \end{aligned}$$

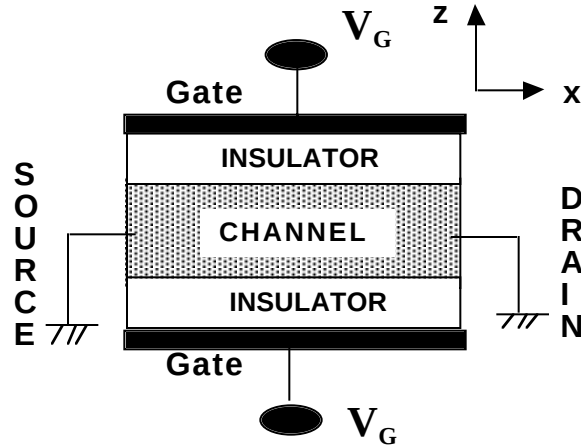
$$\begin{aligned}
&= \frac{m_c k_B T}{2\pi\hbar^2} \left\{ \ln \left[A + e^{-y} \right] \right\}_{-\infty}^0 \\
&= \frac{m_c k_B T}{2\pi\hbar^2} \ln \left[1 + \exp \left[-E / k_B T \right] \right] \equiv f_{2D}(E)
\end{aligned}$$

This relation (Eq.(7.2.12)) allows us to simplify Eq.(7.2.10) to obtain the equation listed in Fig.7.2.2:

$$n(z) = 2 \sum_m |\phi_m(z)|^2 f_{2D}(\epsilon_m - \mu) \quad (7.2.13)$$

A numerical example:

Fig.7.2.3. The MOS capacitor can be modeled with a 1-D Schrodinger equation if we neglect any boundary effects in the x-y plane.



We can model the MOS capacitor shown above by setting up a 1-D Schrodinger-Poisson solver assuming the cross-section to be uniform in the x-y plane with periodic boundary conditions.

We set up a lattice along the z-direction with a 1-D Hamiltonian, H_z that looks like

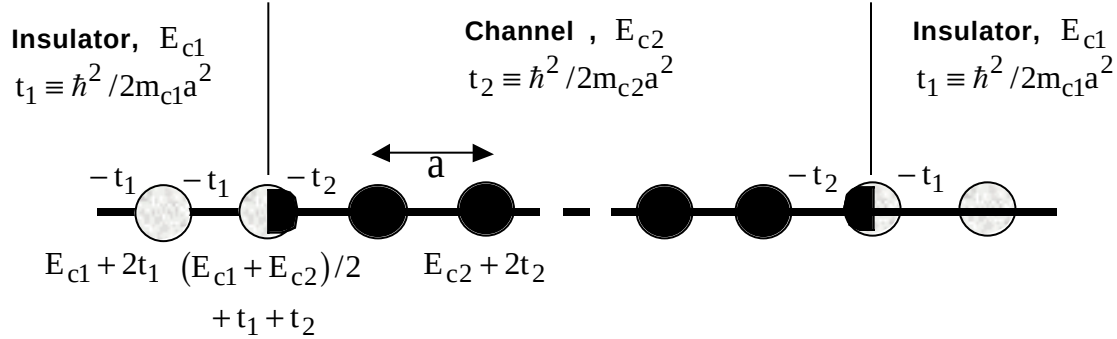


Fig.7.2.4. 1-D one-band effective mass Hamiltonian used to model a channel sandwiched between two insulators.

where we have assumed that both the conduction band edge E_c and the effective mass m_c could be different for the insulator and the channel. However, we will use Eq.(7.2.13) with N_0 (see Eq.(7.2.8)) given by the channel effective mass, since the wavefunctions are strongly excluded from the insulator region.

Once we have set up this Hamiltonian H_z it is straightforward to evaluate the electron density $n(z)$ which can be viewed as the diagonal elements of the 1-D density matrix given by

$$\rho(z, z') = \sum_m \phi_m(z) f_{2D}(\epsilon_m - \mu) \phi_m^*(z') \quad (7.2.15a)$$

As we have discussed before (see discussion following Eq.(3.3.8)) we could view Eq.(7.2.15a) as the real space representation of a more general matrix relation

$$\rho = f_{2D}(H_z - \mu I) \quad (7.2.15b)$$

As before, the function of a matrix $[H_z]$ is evaluated by (1) first diagonalizing $[H_z]$, (2) calculating the density matrix in the eigenrepresentation and then (3) transforming it back to the real space lattice. This can be achieved in MATLAB using the set of commands

1. $[V, D] = \text{eig}(Hz); D = \text{diag}(D);$
2. $\rho = \log(1 + (\exp(\mu - D) / kT));$
3. $\rho = V * \text{diag}(\rho) * V'; N = \text{diag}(\rho);$

The electron density $n(z)$ is obtained from N by multiplying with $2 N_0$ (see Eq.(7.2.8), with an extra factor of two for spin) and dividing by the size of a unit cell 'a': $n(z) = N * 2 N_0 / a$.

We can use the same lattice to solve the Poisson equation

$$-\frac{d}{dz}(\epsilon_r \frac{dU}{dz}) = \frac{q^2}{\epsilon_0} n(z)$$

which looks just like the Schrodinger equation and can be solved by the method of finite differences in exactly the same way:

$$[D2] \{U\} = \frac{q^2}{\epsilon_0 a} (2N_0 a^2) \{N\} + \{U_{\text{bdy}}\} \quad (7.2.16)$$

where $[D2]$ is the matrix operator representing the second derivative. For a constant ϵ_r ,

$$[D2] \equiv \epsilon_r \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & \dots \\ -1 & 2 & -1 & 0 & 0 & \dots \\ 0 & -1 & 2 & -1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix} \quad (7.2.17)$$

Spatial variations in ϵ_r can be handled in the same way that we handled spatially varying effective masses. The boundary term comes from the non-zero values of U at the two boundaries:

$$\{U_{\text{bdy}}\}^T = \epsilon_r \{-qV_G \quad 0 \quad \dots \quad \dots \quad 0 \quad -qV_G\} \quad (7.2.18)$$

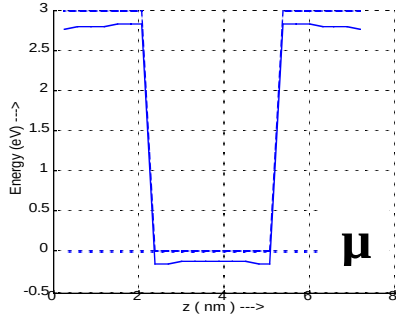
Knowing N , we can calculate the potential U from Eq.(7.2.16):

$$\{U\} = \frac{q^2}{\epsilon_0 a} (2N_0 a^2) [D2]^{-1} \{N\} + [D2]^{-1} \{U_{\text{bdy}}\} \quad (7.2.19)$$

Fig.7.2.5a,b show the equilibrium band diagram and electron density for a 3 nm wide channel and a 9 nm wide channel respectively. We have assumed that the conduction band edge E_c is zero in the channel and at 3 eV in the insulator. We use a relative dielectric constant $\epsilon_r = 4$ and an effective mass $m_c = 0.25m$ everywhere. Also, we have assumed that the electrochemical potential μ is equal to E_c . In real structures the proper location of μ is set by the work function of the metal. The thickness of the oxide is assumed to be 2.1 nm and the calculation was done using a discrete lattice with $a = 0.3$ nm. The gate voltage V_G is assumed to be 0.25V.

For the 3 nm channel, the charge density is peaked near the middle of the channel as we might expect for the wavefunction corresponding to the lowest energy level of a "particle in a box" problem. By contrast the semiclassical charge density piles up near the edges of the channel as we might expect from purely electrostatic considerations. This is an example of what is referred to as *size quantization*. It disappears as we make the channel wider, since the "particle in a box" levels get closer together and many of them are occupied at low temperatures. Consequently the electron distribution looks more classical for the 9 nm channel. Also shown in dotted lines is the electron density if the gate voltage is applied asymmetrically: 0V on one gate and 0.25V on the other gate. Note that for the 9 nm channel there is a significant skewing of the distribution when the bias is applied asymmetrically, as we would expect intuitively. But for the 3 nm channel the electron distribution is only slightly changed from the symmetric to the asymmetric bias. The wavefunction remains relatively unaffected by the applied bias, because the eigenstates are further separated in energy.

(a) 3 nm wide channel



(b) 9 nm wide channel

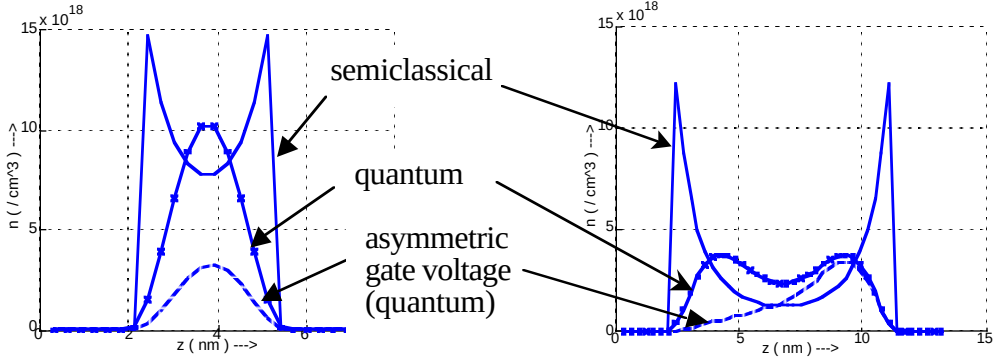
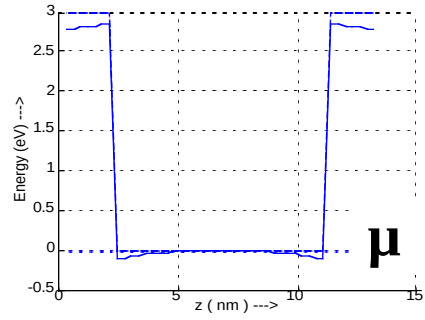


Fig.7.2.5. An MOS Capacitor (see Fig.7.2.2) with a channel thickness of (a) 3 nm and (b) 9 nm. We assume $\mu = 0$, $E_C = 0$ in the silicon and $E_C = 3$ eV in the oxide. Top figure shows the equilibrium band diagram: the solid curve includes both the conduction band profile (dashed) and the self-consistent potential. The lower figure shows the electron density. The thickness of the oxide is assumed to be 2.1 nm and the calculation was done using a discrete lattice with $a = 0.3$ nm. The gate voltage V_G is assumed to be 0.25V. The dashed lines show the electron density when the voltage is applied asymmetrically: 0.25 V on one gate, 0V on another.

Semiclassical method: Also shown in Fig.7.2.5 is a comparison of the electron density with that obtained from a semiclassical approach which works like this. In a homogeneous structure the eigenfunctions are given by

$$\phi_{\alpha}(\vec{r}) = \frac{\exp[ik_x x]}{\sqrt{L_x}} \frac{\exp[ik_y y]}{\sqrt{L_y}} \frac{\exp[ik_z z]}{\sqrt{L_z}} \quad (7.2.20)$$

so that the electron density obtained from Eq.(7.2.1) after summing over all three indices $\{k_x, k_y, k_z\} \equiv \alpha$ is uniform in space ($\Omega = L_x L_y L_z$):

$$n = 2 \text{ (for spin)} \times \frac{1}{\Omega} \sum_{k_x, k_y, k_z} f_0(\epsilon_{\alpha} - \mu)$$

$$\text{with } \epsilon_{\alpha} = E_c + \frac{\hbar^2}{2m_c} (k_x^2 + k_y^2 + k_z^2) \quad (7.2.21)$$

This summation can be performed following the same procedure as described in connection with the 2-D version in Eq.(7.2.12):

$$\begin{aligned} & \frac{1}{\Omega} \sum_{k_x, k_y, k_z} f_0 \left(E_c - \mu + \frac{\hbar^2}{2m_c} [k_x^2 + k_y^2 + k_z^2] \right) \\ &= \int_0^{\infty} \frac{4\pi k^2 dk}{8\pi^3} \frac{1}{1 + A \exp[\hbar^2 k^2 / 2m_c k_B T]} \quad \text{where } A \equiv \exp[(E_c - \mu)/k_B T] \\ &= \left(\frac{m_c k_B T}{2\pi \hbar^2} \right)^{3/2} \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{dy \sqrt{y}}{1 + A \exp[y]} \end{aligned}$$

so that we can write $n = 2 f_{3D}(E_c - \mu)$ (7.2.22)

$$\text{where } f_{3D}(E) \equiv \left(\frac{m_c k_B T}{2\pi \hbar^2} \right)^{3/2} \mathfrak{S}_{1/2} \left(-\frac{E}{k_B T} \right) \quad (7.2.23)$$

$$\mathfrak{S}_{1/2}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{d\xi \sqrt{\xi}}{1 + \exp[\xi - x]}$$

This expression for the (uniform) electron density, n is only correct for a homogeneous medium with no external potential. The semiclassical method consists of calculating the

spatially varying electron density $n(z)$ in the presence of a potential $U(z)$ from a simple extension of Eq.(7.2.22):

$$n = 2 f_{3D} (E_c + U(z) - \mu) \quad (7.2.24)$$

as if each point ‘ z ’ behaves like a homogeneous medium with a conduction band edge located at $E_c + U(z)$. Replacing the upper block in Fig.7.2.2 (labeled “Schrodinger”) with this equation we obtain the semiclassical Schrodinger-Poisson solver widely used in device simulation programs.

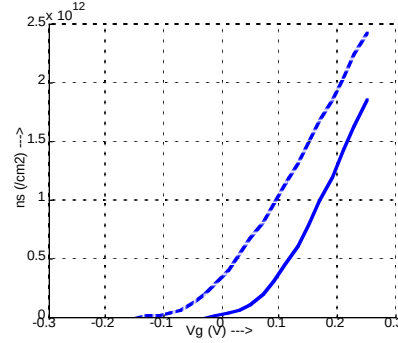
7.3. Quantum vs. electrostatic capacitance

The electron density in the channel per unit area is obtained by integrating $n(z)$ in Eq.(7.2.13) and noting that the wavefunctions are normalized: $\int dz |\phi_m(z)|^2 = 1$:

$$n_s = \int dz n(z) = 2 \sum_m f_{2D}(\epsilon_m - \mu) \quad (7.3.1)$$

Fig.7.3.1 shows the electron density n_s as a function of the gate voltage V_g applied symmetrically to both gates.

Fig.7.3.1. Electron density per unit area, n_s in a 3 nm (solid) and a 9 nm (dashed) channel as a function of the gate voltage V_g applied symmetrically to both gates calculated numerically using the model described in Section 7.2.



The basic physics is illustrated in Fig.7.3.2. A positive gate voltage lowers the overall density of states (DOS) and increases the electron density n_s . As long as the electrochemical potential μ is located below the lowest energy level, the device is in the **off-state**. Once μ moves into the energy range with a non-zero DOS the device is in the **on-state**. Fig.7.3.1 shows that it takes a higher threshold voltage to turn on the device with the 3 nm channel relative to the one with the 9 nm channel. This is because of the increase in the lowest energy level due to size quantization.

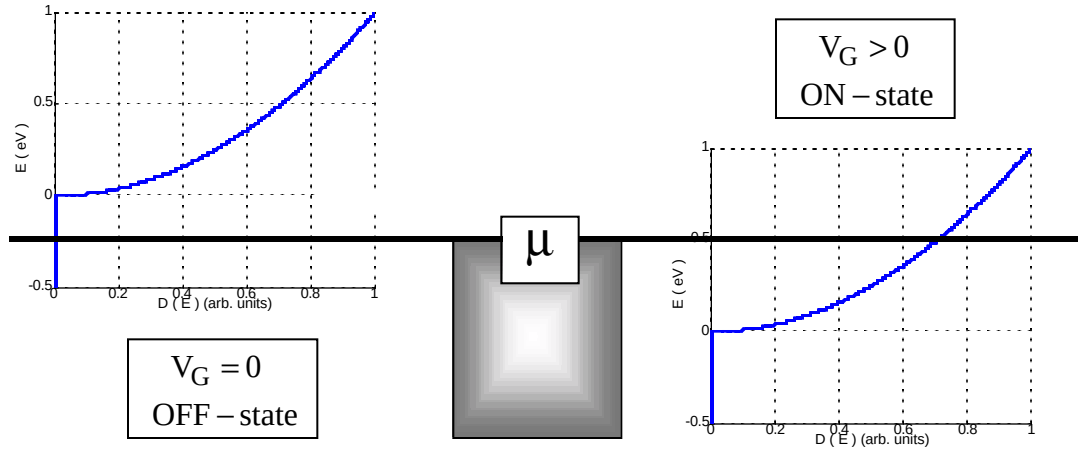


Fig.7.3.2. A positive voltage V_G applied to the gate moves the density of states, $D(E)$, downwards. Since the electrochemical potential μ remains fixed, this increases the number of occupied states and hence the number of electrons, N .

Equivalent circuit: An interesting question to ask is the following: how does the potential V_C in the channel change as the gate voltage V_G is changed. It is easy to answer this question in two extreme situations. If the channel is in the off-state, then it behaves basically like an insulator, and the channel potential V_C is equal to V_G . But if the channel is in the on-state then it behaves like the negative plate of a parallel plate capacitor, so that the channel potential V_C is equal to the source (or drain) potential which we have assumed to be the ground. What is not obvious is the answer in intermediate situations when the channel is neither an insulator or a conductor. The approximate equivalent circuit shown in Fig.7.3.3 can be used to answer this question. Let me explain where it comes from.

The channel is connected to the two gate electrodes by the familiar parallel plate capacitors (per unit area) proportional to the effective dielectric constant ϵ and inversely proportional to the distance 'd' between the center of the channel and the gate electrode.

$$C_{\text{ins}} \equiv \epsilon/d \quad (7.3.2)$$

Of course this is just an approximate expression since the electrons in the channel are not all located at the center as we have idealized. Also, one could raise questions about the exact dielectric constant ϵ to use, since it should represent an appropriate average over the channel and the insulator. One could take such “details” into account and try to come up with a more accurate expression, but that would obscure the purpose of this discussion which is to gain “insight”. To get the quantitative details right, we can always use the numerical model described at the end of the last section. The point is that the capacitors labeled C_{ins} are essentially the same capacitors that we learnt about in freshman physics.

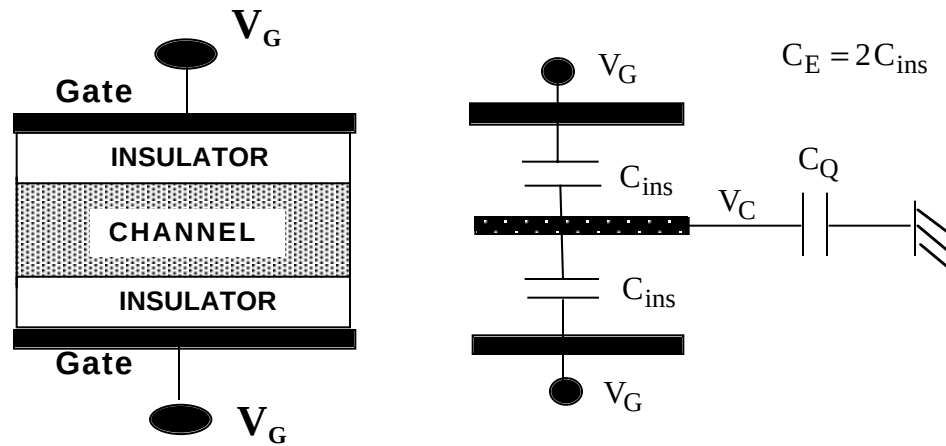


Fig.7.3.3. Approximate equivalent circuit representation of the MOS capacitor.

But where does the quantum capacitance C_Q come from? We have seen in the last Section that we have to perform a simultaneous solution of two relations connecting the electron density to the potential (see Fig.7.2.2): An electrostatic relation (Poisson), and a quantum relation (Schrodinger). The electrostatic relation can be written as

$$U = U_L + (q^2(N - N_0)/C_E) \quad (7.3.3)$$

where U_L is the channel potential obtained from a solution to the **Laplace** equation assuming zero charge, while $(N - N_0)$ tells us the extra electron density relative to the number n_0 required to keep it neutral. The quantum relation can be written as

$$N = \int_{-\infty}^{+\infty} dE \, D(E-U) f_0(E-\mu) \quad (7.3.4)$$

where $D(E-U)$ is the density of states (per unit area) shifted by the potential U . This is a non-linear relation and we could get some insight by linearizing it around an appropriate point. For example, we could define a **“neutral potential”** $U = U_N$, for which makes $N = N_0$ and keeps the channel exactly neutral:

$$N_0 = \int_{-\infty}^{+\infty} dE \, D(E-U_N) f_0(E-\mu)$$

Any increase in U will raise the energy levels and reduce N , while a decrease in U will lower the levels and increase N . So, for small deviations from the neutral condition, we could write

$$N - N_0 \approx C_Q [U_N - U]/q^2 \quad (7.3.5)$$

$$\text{where } C_Q \equiv -q^2 [dN/dU]_{U=U_N} \quad (7.3.6)$$

is called the quantum capacitance and depends on the density of states. We can substitute this linearized relation into Eq.(7.3.3) to obtain

$$\begin{aligned} U &= U_L + \frac{C_Q}{C_E} [U_N - U] \\ \rightarrow U &= \frac{C_E U_L + C_Q U_N}{C_E + C_Q} \end{aligned} \quad (7.3.7)$$

Eq.(7.3.7) is easily visualized in terms of the capacitive network shown in Fig.7.3.3. The actual channel potential U is intermediate between the Laplace potential, U_L and the neutral potential, U_N . How close it is to one or the other depends on the relative magnitudes of the electrostatic capacitance, C_E and the quantum capacitance, C_Q .

From Eqs.(7.3.4) and (7.3.6) it is straightforward to show that the quantum capacitance C_Q is proportional to the density of states averaged over a few $k_B T$ around μ :

$$C_Q \equiv q^2 D_0 \quad (7.3.8)$$

$$D_0 \equiv \int_{-\infty}^{+\infty} dE D(E - U_N) F_T(E - \mu) \quad (7.3.9)$$

where $F_T(E)$ is the thermal broadening function defined as

$$F_T(E) \equiv -\frac{df_0}{dE} = \frac{1}{4k_B T} \operatorname{sech}^2\left(\frac{E}{2k_B T}\right) \quad (7.3.10)$$

Fig.7.3.4. Plot of the thermal broadening function $F_T(E)$ (Eq.(7.3.10)) with $k_B T = 0.025$ eV.

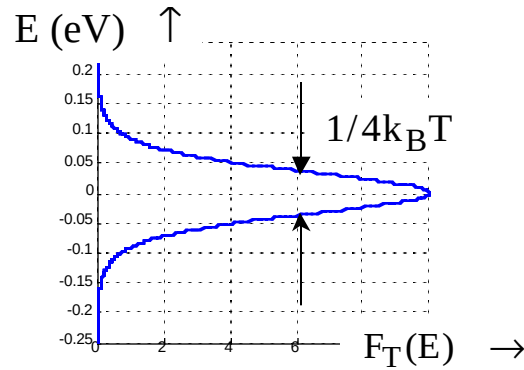


Fig.7.3.4 shows a sketch of the thermal function; its maximum value is $(1/4k_B T)$ while its width is proportional to $k_B T$; it is straight forward to show that the area obtained by

integrating this function is equal to one, independent of $k_B T$: $\int_{-\infty}^{+\infty} dE F_T(E) = 1$. This

means that at low temperatures $F_T(E)$ becomes very large but very narrow while maintaining a constant area of 1: Such a function can be idealized as a delta function: $F_T(E) \rightarrow \delta(E)$, which allows us to simplify the expression for the quantum capacitance at low temperatures

$$C_Q \approx q^2 D(E = \mu + U_N) \quad (7.3.11)$$

showing that it is proportional to the density of states around the electrochemical potential μ after shifting by the neutral potential U_N .

It is easy to see from the equivalent circuit in Fig.7.3.3 that

$$V_C = V_G \frac{C_E}{C_E + C_Q} \quad \text{where} \quad C_E = 2C_{\text{ins}} \quad (7.3.12)$$

Devices in the off-state have zero C_Q , so that $V_C = V_G$. But in the on-state, C_Q is non-zero and V_C is smaller than V_G . The measured capacitance C is the series combination of the electrostatic and quantum capacitances

$$C = \frac{C_E C_Q}{C_E + C_Q} \quad (7.3.13)$$

and is dominated by the smaller of the two.

We can get an approximate feeling for the magnitude of the quantum capacitance C_Q in the on-state, by noting that a 2-D conductor described by a parabolic dispersion relation has a constant density of states (Table 5.2.1) : $D(E) = m_c S / \pi \hbar^2$, so that we can write the quantum capacitance approximately as

$$C_Q = \frac{q^2 m_c S}{\pi \hbar^2} = \frac{\epsilon S}{a_0^* / 4} \quad (7.3.14)$$

where a_0^* is given by an expression similar to that for the Bohr radius that we defined in Chapter one (see Eq.(1.1.5)). But it is larger than the Bohr radius ($= 0.053 \text{ nm}$) because the effective mass (m_c) is smaller than the free electron mass (m) and the dielectric constant (ϵ) is larger than that for free space (ϵ_0):

$$a_0^* \equiv \frac{4\pi \epsilon \hbar^2}{m_c q^2} = (0.053 \text{ nm}) \frac{m}{m_c} \frac{\epsilon}{\epsilon_0} \quad (7.3.15)$$

The quantum capacitance is thus equal to that of a parallel plate capacitor whose plates are separated by $a_0^*/4$. Since this is usually a very small number, the quantum capacitance in the on-state is typically well in excess of the electrostatic capacitance C_E and the measured capacitance is dominated by the latter (see Eq.(7.3.13)). But in materials with a small effective mass, the quantum capacitance can be small enough to have a significant effect, especially if the insulator is very thin making C_E large.

Off Regime: In the off-regime, the density of states close to $E = \mu$ is negligible, and so is the quantum capacitance C_Q . Consequently the channel potential V_C is essentially equal to the gate voltage V_G , so that we can write

$$\begin{aligned} N &= \int_{-\infty}^{+\infty} dE f_0(E - \mu - qV_G) D(E) \\ &\approx \int_{-\infty}^{+\infty} dE \exp\left(-\frac{E - \mu - qV_G}{k_B T}\right) D(E) \end{aligned}$$

since $E - \mu - qV_G \gg k_B T$ in the energy range where $D(E)$ is non-zero. In this regime, the number of electrons changes exponentially with gate voltage:

$$\begin{aligned} N &\sim N_0 \exp\left(\frac{qV_G}{k_B T}\right) \\ \text{so that} \quad \log_{10}\left(\frac{N}{N_0}\right) &\approx \left(\frac{qV_G}{2.3 k_B T}\right) \end{aligned} \quad (7.3.16)$$

This is basically the well-known result that in the off-regime, the number of electrons increases by a decade (a factor of 10) for every $2.3 k_B T$ (~ 60 meV at room temperature) increase in the gate voltage. This relation can be verified by re-plotting Fig.7.3.1 on a logarithmic scale and looking at the slope in the off-regime.

On-regime: In the on-regime, the electrochemical potential μ lies well inside the band of states where $D(E)$, and hence the quantum capacitance C_Q is significant. The actual capacitance is a series combination of the quantum and electrostatic capacitances as

explained above. From the slope of the n_s vs. V_g curve in the on-region (see Fig.7.3.1), we deduce a capacitance of approximately $1.8 \times 10^{-6} \text{ F/cm}^2$ for the 3 nm channel. If we equate this to $2\epsilon/d$, we obtain $d = 3.9 \text{ nm}$ which compares well with the number obtained by adding half the channel width (1.5 nm) to the oxide thickness (2.1 nm), showing that the effective capacitance is largely electrostatic (rather than quantum) in origin.

7.4. Supplementary notes: Multiband effective mass Hamiltonian

The one-band effective mass model works very well when we have an isotropic parabolic band that is well separated from the other bands. This is usually true of the conduction band in wide bandgap semiconductors. But the valence band involves multiple closely spaced bands which are strongly anisotropic and non-parabolic. Close to the Γ point the energy dispersion can usually be expressed in the form (A, B and C being constants)

$$E(\vec{k}) = E_v - Ak^2 \pm \sqrt{B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2)} \quad (7.4.1)$$

This dispersion relation can be described by a 4x4 matrix of the form (I: 4x4 identity matrix)

$$\begin{aligned} [\tilde{h}(\vec{k})] &= -PI - T \\ \text{where } [T] &\equiv \begin{bmatrix} Q & 0 & -S & R \\ 0 & Q & R^+ & S^+ \\ -S^+ & R & -Q & 0 \\ R^+ & S & 0 & -Q \end{bmatrix} \end{aligned} \quad (7.4.2)$$

$$P \equiv E_v + \frac{\hbar^2 \gamma_1}{2m} (k_x^2 + k_y^2 + k_z^2)$$

$$Q \equiv \frac{\hbar^2 \gamma_2}{2m} (k_x^2 + k_y^2 - 2k_z^2)$$

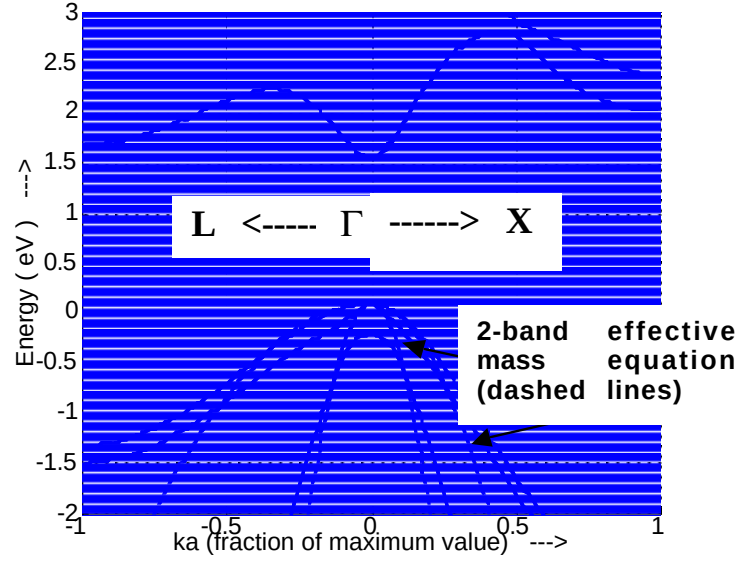
$$R \equiv \frac{\hbar^2}{2m} \left(-\sqrt{3} \gamma_2 [k_x^2 - k_y^2] + i 2\sqrt{3} \gamma_3 k_x k_y \right)$$

$$S \equiv \frac{\hbar^2 \gamma_3}{2m} 2\sqrt{3} (k_x - i k_y) k_z$$

The Luttinger parameters γ_1 , γ_2 and γ_3 are available in the literature for all common semiconductors (see, for example, P. Lawaetz, “Valence Band Parameters in Cubic Semiconductors”, Phys. Rev. **B4**, 3460 (1971)). One can argue that Eqs.(7.4.1) and (7.4.2) are equivalent, since it can be shown using straightforward algebra that

$$[T]^2 = (Q^2 + R^2 + S^2) I = \left(B^2 k^4 + C^2 (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2) \right) I$$

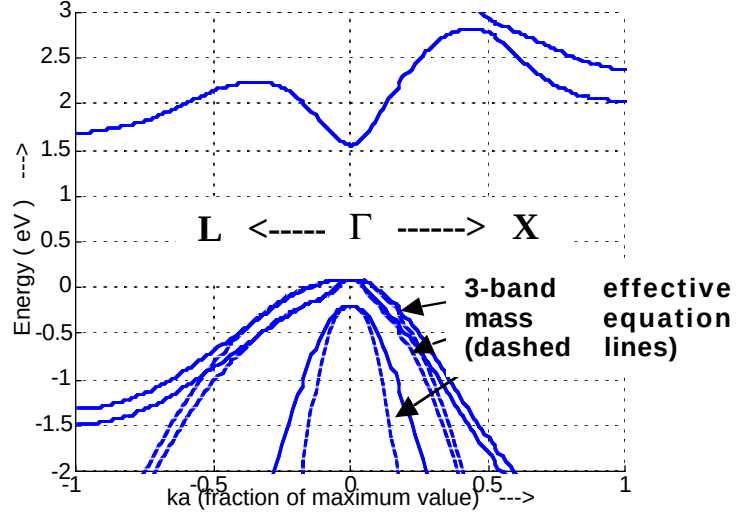
Fig.7.4.1. Solid lines show the full bandstructure obtained from the sp^3s^* model described in Chapter 4. Dashed line shows the dispersion obtained from a two-band effective mass model (Eq.(7.4.2)) with parameters adjusted for best fit.



It can be seen from Fig.7.4.1 that the eigenvalues of $[h(\vec{k})]$ describe the two highest valence bands (light hole and heavy hole) well very close to the Γ point. To get better agreement over a wider range of k -values and to include the split-off band (see Fig.7.4.2), one often uses a three-band $[h(\vec{k})]$ of the form

$$[h(\vec{k})] = - \begin{bmatrix} P+Q & 0 & -S & R & -S/\sqrt{2} & \sqrt{2} R \\ 0 & P+Q & R^+ & S^+ & -\sqrt{2} R^+ & -S^+/\sqrt{2} \\ R^+ & 0 & P-Q & 0 & -\sqrt{2} Q & \sqrt{3/2} S \\ 0 & R^+ & 0 & P-Q & \sqrt{3/2} S^+ & \sqrt{2} Q^+ \\ -S^+/\sqrt{2} & -\sqrt{2} R & -\sqrt{2} Q^+ & \sqrt{3/2} S & P+\Delta & 0 \\ \sqrt{2} R^+ & -S/\sqrt{2} & \sqrt{3/2} S^+ & \sqrt{2} Q & 0 & P+\Delta \end{bmatrix} \quad (7.4.3)$$

Fig.7.4.2. Solid lines show the full bandstructure obtained from the sp^3s^* model described in Chapter 4. Dashed line shows the dispersion obtained from a three-band effective mass model (Eq.(7.4.3)) with parameters adjusted for best fit.



We can use either the 2-band $[h(\vec{k})]$ in Eq.(7.4.1) or the three-band $[h(\vec{k})]$ in Eq.(7.4.2) to construct an effective mass equation for the valence band using the same principle that we used for the conduction band (cf. Eq.(7.1.2), (7.1.3)). We simply replace $\vec{k}$ with $-i\vec{\nabla}$ in the expression for $h(\vec{k})$ to obtain a coupled differential equation of the form

$$[h(\vec{k} \rightarrow -i\vec{\nabla})]\{f(\vec{r})\} = E\{f(\vec{r})\} \quad (7.4.3)$$

where the “wavefunction” $\{f(\vec{r})\}$ now has four (or six) components. It is easy to check that plane wave solutions of the form, $\{f(\vec{r})\} = \{f_0\} \exp(i\vec{k} \cdot \vec{r})$ with any $\vec{k}$ will satisfy Eq.(7.4.2) provided $\{f_0\}$ is an eigenfunction of $[h(\vec{k})]$

$$[h(\vec{k})]\{f_0\} = E\{f_0\} \quad (7.4.4)$$

This means that the effective mass equation in Eq.(7.4.3) will generate a bandstructure identical to that obtained from the original $[h(\vec{k})]$.

We could use the finite difference method to convert Eq.(7.4.3) into a Hamiltonian matrix, the same way we went from Eq.(7.1.3) to the matrix depicted in Fig.7.1.2. In Fig.7.1.5, the unit cell matrices $[H_{nn}]$ and the bond matrices $[H_{nm}, n \neq m]$ will all be (4x4) or (6x6) matrices depending on whether we start from the 2-band (Eq.(7.4.2)) or the 3-band (Eq.(7.4.3)) model. For example, the 2-band model leads to matrices $[H_{nm}]$ of the form

$$[H_{nm}] \equiv \begin{bmatrix} -P_{nm} - Q_{nm} & 0 & S_{nm} & -R_{nm} \\ 0 & -P_{nm} - Q_{nm} & -R_{mn}^* & -S_{mn}^* \\ S_{mn}^* & -R_{nm} & -P_{nm} + Q_{nm} & 0 \\ -R_{mn}^* & -S_{nm} & 0 & -P_{nm} + Q_{nm} \end{bmatrix}$$

where the individual terms P_{nm} , Q_{nm} etc. are obtained from the corresponding functions $P(\vec{k})$, $Q(\vec{k})$ using the same procedure that we use to obtain a one-band effective mass Hamiltonian (see Fig.7.1.2) from the one-band $\hbar(\vec{k})$ (see Eq.(7.1.2)).

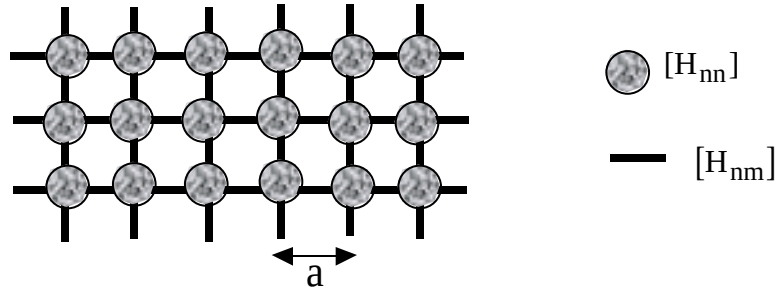


Fig.7.4.3. The multiband effective mass Hamiltonian matrix can be depicted schematically as a 3-D network of unit cells (unrelated to the actual crystal structure) described by $[H_{nn}]$ bonded to its nearest neighbors by $[H_{nm}]$.

These matrices will be (4x4) or (6x6) depending on whether we start from the 2-band (Eq.(7.4.1)) or the 3-band (Eq.(7.4.2)) model.

The same approach is used to write down the $[H_{nm}]$ matrices for the 3-band model (Eq.(7.4.2)). For narrow-gap semiconductors, it is common to use a 4-band model where the matrices $[H_{nm}]$ are (8x8) in size. Multiband effective mass models may not appear to represent much of a simplification relative to an atomistic model like the sp^3s^* model. However, the simplification (numerical and even conceptual) can be considerable for two reasons:

- (a) the matrices $[H_{nm}]$ are somewhat smaller (cf. (20x20) for the sp^3s^* model),
- (b) the lattice can be much coarser and have a simpler structure (simple cubic rather than FCC) than the real atomic lattice, resulting in a smaller overall Hamiltonian that is also easier to visualize.

A short example to illustrate the basic approach is given below, but as I have said earlier, I will not discuss multiband models (or any model other than the one-band effective mass model) any further in this book.

An example: Fig.7.4.4 shows the energies of the four highest valence band levels of a GaAs quantum well sandwiched between $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ barriers calculated as a function of the well width using the two-band model assuming

$$\text{for GaAs: } E_v = 0 \text{ eV}, \gamma_1 = 6.85, \gamma_2 = 2.1, \gamma_3 = 2.9$$

$$\text{and for AlAs: } E_v = 0.75 \text{ eV}, \gamma_1 = 3.45, \gamma_2 = 0.68, \gamma_3 = 1.29$$

and interpolating linearly for the AlAs - GaAs alloy. Fig.7.4.5 shows the dispersion relation $E(\vec{k})$ as a function of k_y with $k_x = 0$ for the four highest valence subbands of a quantum well with $W = 51\text{\AA}$.

Fig.7.4.4. Energy of the four highest energy levels of a GaAs quantum well sandwiched between $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ barriers (shown in inset) as a function of the well width (W) calculated from a two-band effective mass model.

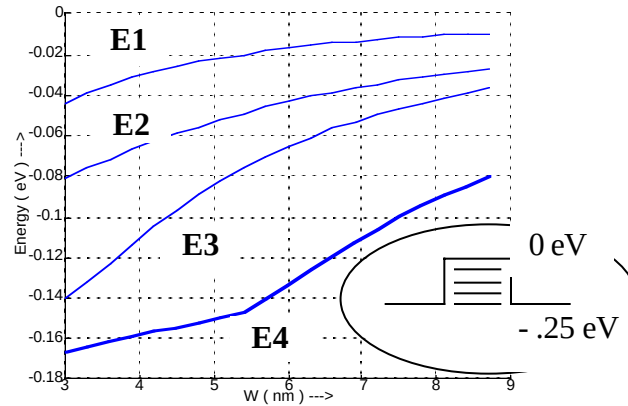
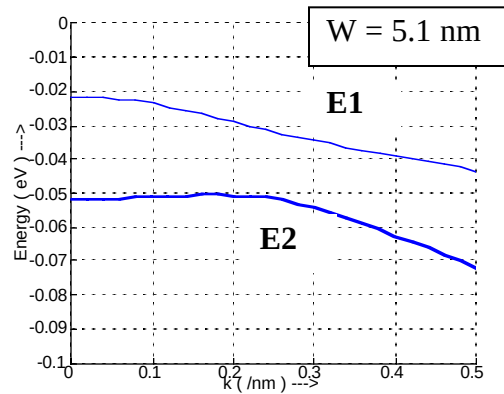


Fig.7.4.5. Solid lines show the dispersion relation $E(\vec{k})$ as a function of k_y with $k_x = 0$ for the two highest subbands of a quantum well with $W = 5.1 \text{ nm}$, calculated from the two-band effective mass model.



Exercises

E.7.1. (a) Plot $E(k)$ along Γ -X and Γ -L from

$$h(\vec{k}) = E_c + \frac{\hbar^2 k^2}{2m_c}$$

and compare with the plot from the sp^3s^* model (see Problem 4.2) over the appropriate energy and wavevector range (cf. **Fig. 5.1.2**). What values of E_c and m_c give the best fit?

(b) Use a one-band effective mass model to calculate the energies of the two lowest levels of a GaAs quantum well sandwiched between $Al_{0.3}Ga_{0.7}As$ barriers as a function of the well width. Assume that for GaAs: $E_c = 0$ eV, $m_c = 0.07 m$

and for $AlAs$: $E_c = 1.25$ eV, $m_c = .15 m$

and interpolate linearly to obtain E_c and m_c for the $AlAs$ - GaAs alloy (cf. **Fig.5.1.3**).

(c) Use a one-band model to calculate the dispersion relation $E(\vec{k})$ as a function of the magnitude of the in-plane wavevector $\vec{k} = \{k_x, k_y\}$ for the two lowest subbands of a quantum well with $W = 69A$, using the same parameters as in part (b) (cf. **Fig.5.1.4**).

E.7.2. (a) Consider the MOS capacitor shown in Fig.7.2.3 and calculate the self-consistent conduction band profile and the electron density using a discrete lattice with $a = 0.3$ nm. Assume that (1) the thickness of the oxide is 2.1 nm and the channel thickness is 3 nm, (2) $\mu = 0$, $E_c = 0$ in the silicon and $E_c = 3$ eV in the oxide, (3) dielectric constant $\epsilon = 4 \epsilon_0$ and $m_c = 0.25m$ everywhere, and (3) the gate voltage $V_G = 0.25V$. Repeat with a channel thickness of 9nm and also with the gate voltage applied asymmetrically with 0V on one gate and 0.25V on the other gate. Compare with **Fig.7.2.5**.

(b) Calculate the electron density per unit area as a function of the gate voltage (applied symmetrically to both gates) for the structure with a 3nm channel and with a 9 nm channel. Compare with **Fig.7.3.1**. Calculate the effective capacitance from the slope of the curve in the ON-state and deduce an effective plate separation 'd' by equating the capacitance to $2\epsilon/d$.