# Series 5 - Basic notions on the physics of semiconductor heterostructures: case of superlattices

## I - Superlattice dispersion relations

1. From the properties of the translation operator $T_d$ we deduce that:

$T_{nd}\,\chi_q(z) = \chi_q(z+nd) = \exp(iqnd)\,\chi_q(z)$

As a result $\chi_q(z)$ functions can be written as:

$$\boxed{\chi_q(z) = U_q(z)\exp(iqz) \quad \text{with } U_q(z+d) = U_q(z)}$$

The $\chi_q(z)$ functions are the products of a plane wave and a periodic function in $z$. Previous equations correspond to those satisfying the Bloch-Floquet theorem. $\chi_q$ is the Bloch function and $U_q$ the associated periodic part.

2. $\chi_q(z)$ must be such that $\chi_q(z+Nd) = \chi_q(z)$ which means that: $qNd = 2p\pi$ with $p \in \mathbb{Z}$. Consequently $q$ must be a real. $N$ values of $q$ are available, each of them being separated by $\frac{2\pi}{Nd}$

3. At interface (I) we can write:

$$\alpha\exp\left(ik_w\frac{L}{2}\right) + \beta\exp\left(-ik_w\frac{L}{2}\right) = \gamma\exp\left(-ik_b\frac{b}{2}\right) + \delta\exp\left(ik_b\frac{b}{2}\right)$$

$$ik_w\left[\alpha\exp\left(ik_w\frac{L}{2}\right) - \beta\exp\left(-ik_w\frac{L}{2}\right)\right] = ik_b\left[\gamma\exp\left(-ik_b\frac{b}{2}\right) - \delta\exp\left(ik_b\frac{b}{2}\right)\right]$$

At interface (II), $\chi_q\left[z=(n+1)d-\frac{L}{2}+0\right] = \gamma\exp\left(ik_b\frac{b}{2}\right) + \delta\exp\left(-ik_b\frac{b}{2}\right)$

In addition the Bloch theorem is such that

$$\chi_q\left[z=(n+1)d-\frac{L}{2}+0\right] = e^{iqd}\,\chi_q\left[z=nd-\frac{L}{2}+0\right]$$

The same type of operation can be performed with the first derivative of $\chi_q(z)$.

From previous equations, one can establish a $4\times 4$ homogeneous system in $\alpha$, $\beta$, $\gamma$ and $\delta$. Solutions to this system are solutions to the $4\times4$ determinant which is derived after some algebraic transformations. Non trivial solutions (i.e. $\neq 0$) exist if and only if the following equation is verified:

$$\boxed{\cos(qd) = \cos(k_w L)\cos(k_b h) - \frac{1}{2}\left(\xi + \frac{1}{\xi}\right)\sin(k_w L)\sin(k_b h) \quad \text{with } \xi = \frac{k_b}{k_w}}$$

Such an equation is a transcendental equation linking the energy $\mathcal{E}$ of the system to the wavevector $q$. In other words, it corresponds to the dispersion relation $\mathcal{E}(q)$ of Bloch waves.

4- For large $\mathcal{E}$ values (i.e. $\mathcal{E} \gg V_b$), $k_b \sim k_w$ and thus $\xi \sim 1$ so that:

$$\cos(qd) = \cos(k_w L)\cos(k_w h) - \sin(k_w L)\sin(k_w h)$$

i.e. $\cos(qd) = \cos(k_w(L+h))$ which means that $qd = k_w(L+h) + 2j\pi$ $(j\in\mathbb{Z})$

and thus $\boxed{k_w = q + 2j'\frac{\pi}{d} \quad (j'\in\mathbb{Z})}$ The potential of the superlattice is almost not felt by highly energetic electrons, i.e the electron wavelength $(2\pi/k_w) \ll$ characteristic length of the obstacle $(d)$ and corresponding diffraction effects $\to 0$. Superlattice states corresponding to the continuum of states of isolated quantum wells can be seen as the result of the hybridization of virtual bound states of isolated wells.

5. By analogy with question (3), it can be shown in this case that:

$$\boxed{\cos(qd) = \underbrace{\cos(k_w L)\cosh(\mathcal{K}_b h) - \frac{1}{2}\left[-\xi + \frac{1}{\xi}\right]\sin(k_w L)\sinh(\mathcal{K}_b h)}_{=F(\mathcal{E})}}$$

For a system with infinitely thick barriers, the right-hand side of previous equation will diverge as $\exp(\mathcal{K}_b\, h)$ unless $\cos(k_w L) - \frac{1}{2}\left[-\xi + \frac{1}{\xi}\right]\sin(k_w L) = 0$

This transcendental equation accepts for solutions the bound states of isolated quantum wells of thickness $L$.

The subbands of the superlattice of negative energies appear as the hybridization of bound states of isolated quantum wells due to the tunnel coupling between the wells across the barriers.

$F(\varepsilon)$ exhibits large variations with $\varepsilon$ and regions where $|F(\varepsilon)| < 1$ are fairly narrow ones. To obtain the dispersion relations of the subbands (called $E_1, E_2, \ldots E_n$) which are simplified ones, we make use of the previous equation.

In addition when expanding $F(\varepsilon)$ near $E_j$ values, we get to the first order in $\varepsilon - E_j$ for the $j^{th}$ subband:

$$F(\varepsilon) = F(E_j) + (\varepsilon - E_j) F'(\varepsilon)\Big|_{\varepsilon = E_j} + O(2)$$

Thus $\cos qd = F(E_j) + (\varepsilon - E_j) F'(\varepsilon)\Big|_{\varepsilon = E_j}$

i.e. $$(\varepsilon(q) - E_j) = \underbrace{-\frac{F(E_j)}{F'(\varepsilon)\big|_{\varepsilon = E_j}}}_{s_j} + \underbrace{\frac{1}{F'(\varepsilon)\big|_{\varepsilon = E_j}}}_{2t_j} \cos qd$$

so that $$\boxed{\varepsilon(q) = E_j + s_j + 2 t_j \cos qd}$$

The previous equation is a tight-binding description of the subbands. In addition, if we consider that $\chi_{jq}(z) = \frac{1}{\sqrt{N}} \sum_n \exp(iqnd) \underbrace{\varphi_{loc}^{(j)}(z - nd)}$

$\hookrightarrow$ $j^{th}$ wavefunction of the bound state of wells centered in $z_n = nd$

and by keeping only terms corresponding to interactions at the nearest neighbor level.

$$t_j = \int \varphi_{loc}^{(j)}(z)\, V_b(z)\, \varphi_{loc}^{(j)}(z - d)$$

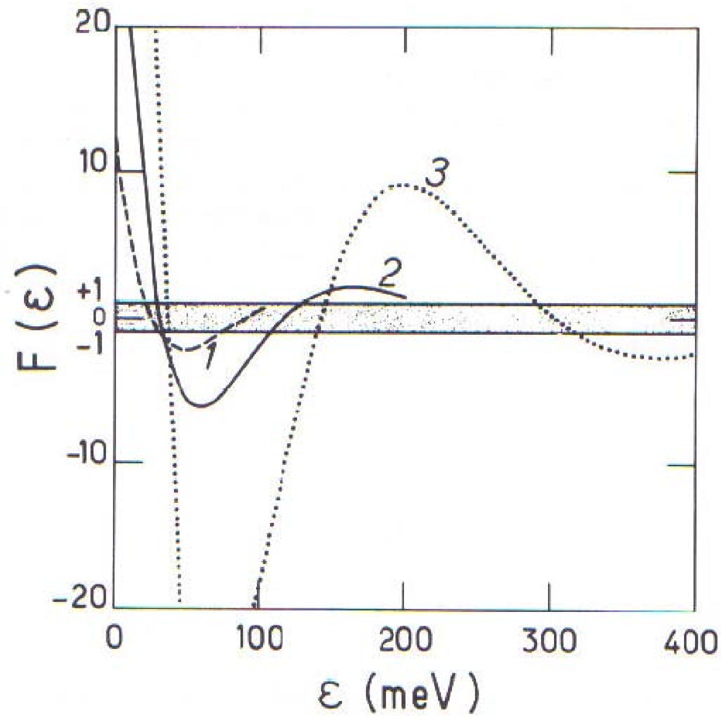



Fig. 10. — The right-hand side of equation (89) is plotted *versus* the energy $\varepsilon$. Three barrier heights are considered : curve (1) : $V_b = 0.1$ eV ; curve (2) : $V_b = 0.2$ eV ; curve (3) : $V_b = 0.4$ eV. $m^* = 0.067\, m_0$, $L = 100$ Å, $h = 50$ Å. In all three curves the energy zero is taken at the bottom of the well. Each curve is interrupted at the top of the well. The shaded area corresponds to the allowed superlattice states : $|F(\varepsilon)| < 1$.

$$s_j = \sum_{n\neq 0} \int \varphi_{loc}^{(j)}(z)\, V_b(z-nd)\, \varphi_{loc}^{(j)}(z)$$

Note that it is essential to keep in mind that "$q$" is the wavevector associated with the superlattice, "$k_w$" is the wavevector associated with electrons inside the wells and "$k_b$" is the wavevector corresponding to electrons propagating in the barriers.

## II - Density of states of a superlattice

1- $\mathcal{E}(n, q, \vec{k}_\perp, \sigma_z) = \mathcal{E}_n(q) + \dfrac{\hbar^2 k_\perp^2}{2m^*}$

By definition $\rho(\mathcal{E}) = \sum_{n q, \vec{k}_\perp, \sigma_z} \delta\left[\mathcal{E} - \mathcal{E}_n(q) - \dfrac{\hbar^2 k_\perp^2}{2m^*}\right]$

and since $\sum_{q \in 1^{st} BZ} g(q) \underset{N\to+\infty}{\longrightarrow} \dfrac{Nd}{2\pi}\displaystyle\int_{-\pi/d}^{+\pi/d} g(q)\, dq$ we get

$$\rho(\mathcal{E}) = 2 \frac{Nd}{2\pi} \int_{-\pi/d}^{+\pi/d} dq \sum_{n, \vec{k}_\perp} \delta\left[\mathcal{E} - \mathcal{E}_n(q) - \frac{\hbar^2 k_\perp^2}{2m^*}\right]$$

spin

In addition, $\sum_{\vec{k}_\perp} = \sum_{k_x k_y} \underset{L_x, L_y \to +\infty}{\longrightarrow} \dfrac{L_x L_y}{(2\pi)^2} \displaystyle\int dk_x\, dk_y$

so that $\sum_{\vec{k}_\perp} \longrightarrow \dfrac{S}{(2\pi)^2} \displaystyle\int d\vec{k}_\perp$ (as $\vec{k}_\perp^2 = k_x^2 + k_y^2$)

and as $\displaystyle\int_{-\pi/d}^{+\pi/d} dq = 2 \int_0^{+\pi/d} dq$ we therefore obtain:

$$\rho(\mathcal{E}) = 2 \times 2 \frac{Nd}{2\pi} \times \frac{S}{(2\pi)^2} \sum_n \int_0^{+\pi/d} dq \int d\vec{k}_\perp\, \delta(\mathcal{E}_{/\!/} - \mathcal{E}_n(q))\, \delta\left(\mathcal{E}_\perp - \frac{\hbar^2 k_\perp^2}{2m^*}\right)$$

The term $2 \displaystyle\int \frac{d\vec{k}_\perp}{(2\pi)^2} \delta\left(\mathcal{E}_\perp - \frac{\hbar^2 k_\perp^2}{2m^*}\right)$ is directly connected to the 2D-DoS of a free particle $\Rightarrow \dfrac{m^*}{\pi\hbar^2}$.

In the end, we get $\boxed{\rho(\varepsilon) = \sum_n \rho_n(\varepsilon) = \frac{SNd}{\pi^2} \frac{m^*}{\hbar^2} \sum_n \int_0^{+\pi/d} dq \, \Theta(\varepsilon_{/\!/} - \varepsilon_n(q))}$

where $\Theta(\varepsilon_{/\!/} - \varepsilon_n(q))$ is the Heaviside/step function.

It is thus seen that as soon as the energy exceeds the minimum allowed energy by the system, the accessible DOS will be non-zero and constant between two bound states of the quantum well (eigenvalues which do not encompass the kinetic energy term). The DOS evolution is a succession of steps in the 2D case (as a first approximation for the superlattice, see next questions).

2- On a general basis, the subband $\varepsilon_{nq}$ has a finite energy width when $q$ explores the 1st BZ: $\varepsilon_{min} \leq \varepsilon_{nq} \leq \varepsilon_{max}$. For $\varepsilon < \varepsilon_{min}$, $\rho_n(\varepsilon) = 0$ whereas for $\varepsilon > \varepsilon_{max}$, $\rho_n(\varepsilon)$ is a constant: $\boxed{\rho_n(\varepsilon) = \frac{Nm^*S}{\pi\hbar^2}}$

This value of the DOS is precisely $N$ times that associated with a single quantum well. When $\varepsilon$ lies within the forbidden bands of dispersion relations of the superlattice, the DOS is quantized in units of $\rho_0 = \frac{Nm^*S}{\pi\hbar^2}$.

3- In the vicinity of $q = 0$ (center of the 1st BZ), we obtain:

$$\varepsilon_{nq} \approx E_n + s_n - 2|t_n| + |t_n| q^2 d^2$$

Close to the edge of the 1st BZ, $q = \frac{\pi}{d}$ and we get:

$$\varepsilon_{nq} = E_n + s_n - 2|t_n| \cos(qd)$$

i.e. $\varepsilon_{nq} = E_n + s_n + 2|t_n| \cos(\pi - qd)$ and $\pi - qd \to 0$

thus $\varepsilon_{nq} \approx E_n + s_n + 2|t_n| - |t_n| (\pi - qd)^2$

which leads to $\varepsilon_{nq} \approx E_n + s_n + 2|t_n| - |t_n| \left(q - \frac{\pi}{d}\right)^2 d^2$

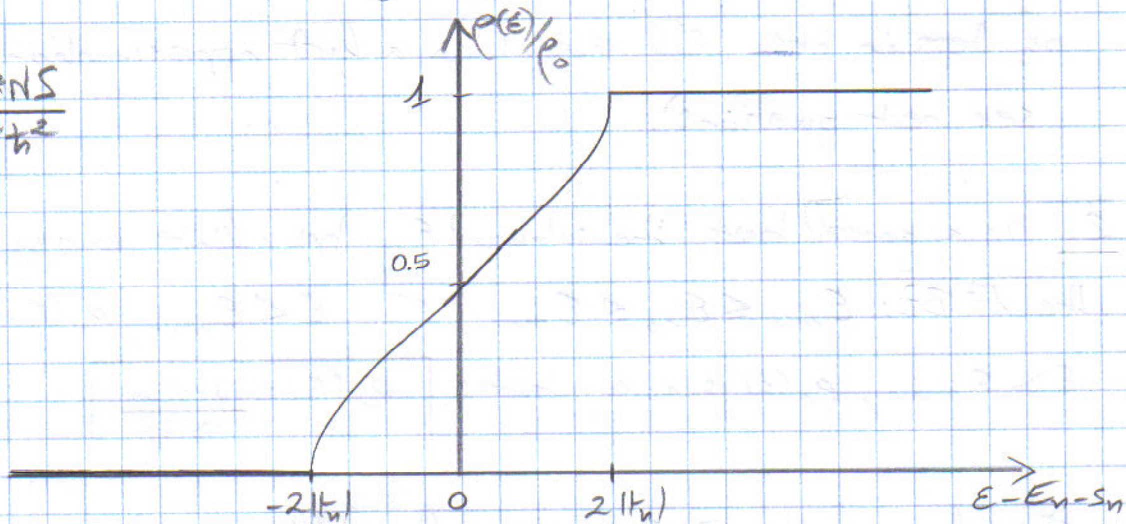
It is seen that a quadratic dependence in $q^2$ is present around $q = 0$ and $q = \frac{\pi}{d}$.

4- From the tight-binding description we can derive the expression:

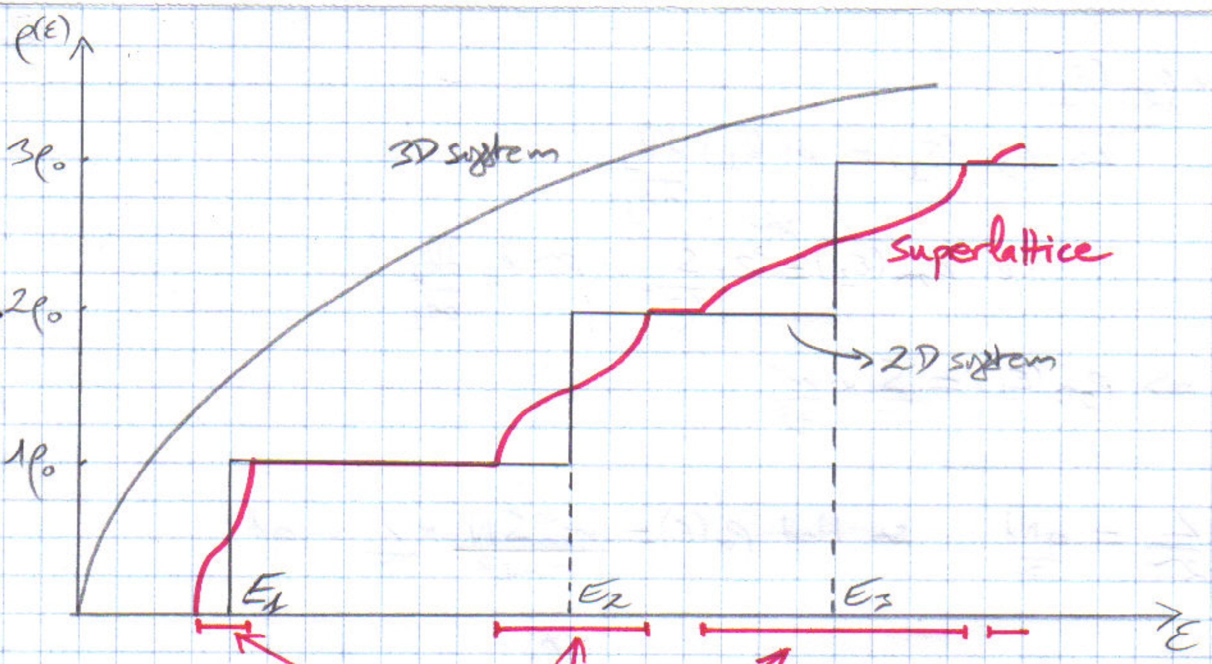
$qd = \mathrm{Arccos}\left(\frac{-\varepsilon + E_n + s_n}{2|t_n|}\right)$. As a result the dependence of the DOS will be:

$$\rho_n(\varepsilon) = \begin{cases} 0 & \text{if } \varepsilon < E_n + s_n - 2|t_n| \\ \frac{\rho_0}{\pi} \mathrm{Arccos}\left(\frac{-\varepsilon + E_n + s_n}{2|t_n|}\right) & \text{if } |\varepsilon - E_n - s_n| < 2|t_n| \\ \rho_0 & \text{if } \varepsilon > E_n + s_n + 2|t_n| \end{cases}$$

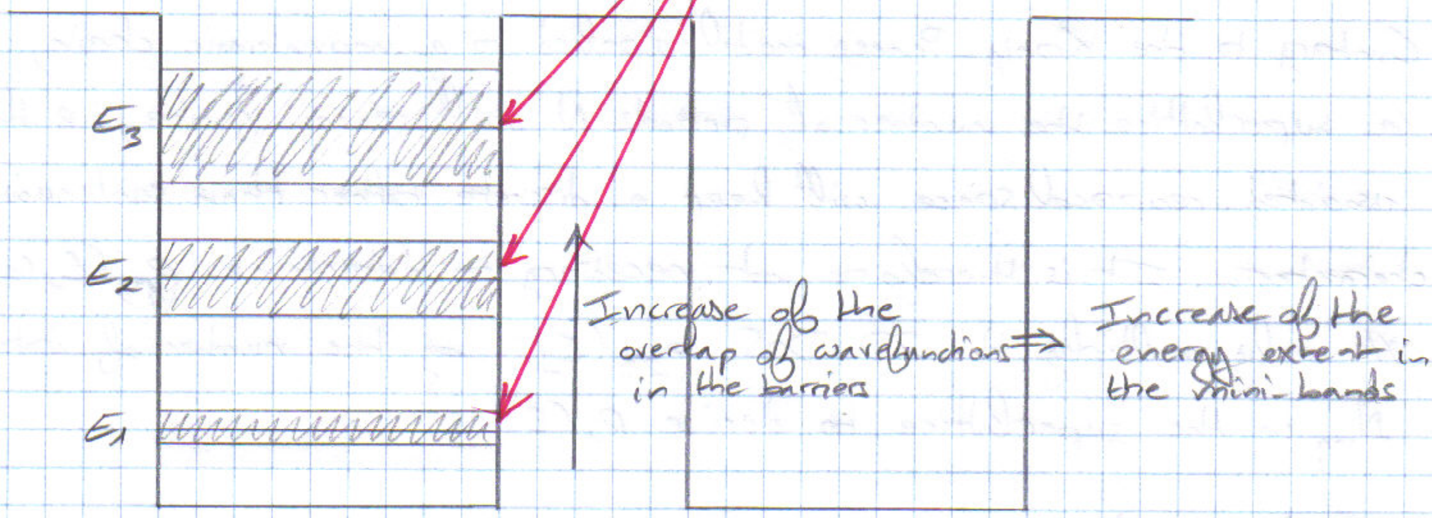
where $\rho_0 = \frac{m^* NS}{\pi \hbar^2}$




It is essential to understand that the deeper the characteristic potential well of the system of interest, the narrower the extent of the superlattice mini-bands (see next figures). Indeed, the penetration of the wave functions in the barriers will be weaker so that the overlap between adjacent wavefunctions will be reduced.




Energy extent of the mini-bands




## Remark on the evolution of the DOS close to energies $E_n$

The total energy of the system can be written as:

$$\varepsilon = \varepsilon_\perp + \underbrace{\varepsilon_n(q)}_{\text{contribution only in the region of mini-bands}} = \underbrace{\frac{\hbar^2 k_\perp^2}{2m^*}}_{\text{continuous term}} + E_n + s_n - 2|t_n| \cos qd$$

continuous term → parabolic dispersion of $e^-$ in the plane of the wells

contribution only in the region of mini-bands

↳ miniband extent

$$\rho_n(\mathcal{E}) = N_{nq} \times \underbrace{\rho_{2D}(\mathcal{E}_\perp)}$$

$$\hookrightarrow \rho_{2D}(\mathcal{E}_\perp) = \rho(k_\perp)\frac{dk_\perp}{d\mathcal{E}_\perp}$$

$$\text{i.e. } \rho_{2D}(\mathcal{E}_\perp) = \overset{\text{spin}}{2} \times \frac{S}{4\pi^2} \times 2\pi k_\perp \frac{dk_\perp}{d\mathcal{E}_\perp}$$

$$\frac{d\mathcal{E}_\perp}{dk_\perp} = \frac{\hbar^2 k_\perp}{m^*} \Rightarrow \rho_{2D}(\mathcal{E}_\perp) = \frac{S}{\pi} \times \frac{m^*}{\hbar^2}$$

$$N_{nq} = 2q \times \frac{L}{2\pi} = \frac{qNd}{\pi} \quad \text{so that } \rho_n(\mathcal{E}) = \underbrace{\frac{m^* S N}{\pi \hbar^2}}_{\rho_0} \times \frac{1}{\pi} \times qd$$

$$\text{i.e. } \boxed{\rho_n(\mathcal{E}) = \frac{\rho_0}{\pi} \operatorname{Arccos}\left(\frac{-\mathcal{E} + E_n + s_n}{2|t_n|}\right)}$$

Contrary to the Kronig-Penney model applied to a monatomic chain, in a superlattice the number of periods $N$ will remain finite, i.e the associated reciprocal space will keep a discrete rather than continuous character. It is therefore not necessary to determine $\rho_{1D}(\mathcal{E}_n(q))$. We only multiply the 2D-DOS $\rho_{2D}(\mathcal{E}_\perp)$ by the number of states $N_{nq}$ in the superlattice to derive $\rho_n(\mathcal{E})$.

## Further readings


① G. Bastard, Phys. Rev. B 24, 5693 (1981).

② G. Bastard, Phys. Rev. B 25, 7584 (1982).


In these two articles, the difference of the effective masses between the barriers and the wells is fully taken into account!