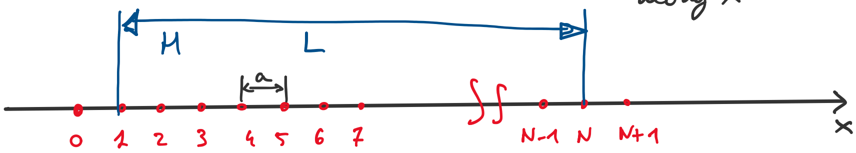
PERIODIC BOUNDARY CONDITIONS

Friday, 30 November 2018 09:05

BLOCH THEOREM

$$\psi(\underline{r}+\underline{T}) = \psi(\underline{r})\, e^{j\underline{k}\cdot\underline{T}}$$

Let's consider a 1D case, with a domain L-long, which is periodically repeated along x



In this domain, you can define the Hamiltonian H

In the generic i-th point:

$t_0 = -\frac{\hbar^2}{2 m a^2}$

$$+t_0\,\psi_{i-1} + (E_{ci} - 2t_0)\,\psi_i + t_0\,\psi_{i+1} = E\,\psi_i$$

Let's focus on point 1

$$+t_0\,\psi_0 + (E_{c1} - 2t_0)\,\psi_1 + t_0\,\psi_2 = E\psi_1$$

In principle, I don't know ψ_0, since I have discretized the domain (long L) from point 1 to point N.

But I can exploit the Bloch theorem:

$$\psi_N = \psi_0\, e^{jk_x \cdot L} \Rightarrow \psi_0 = \psi_N\, e^{-jk_x\cdot L} \Rightarrow (E_{c1} - 2t_0)\,\psi_1 + t_0\,\psi_2 + t_0\, e^{-jk_xL}\,\psi_N = E\psi_1$$

$$H = \begin{bmatrix} E_{c1}-2t_0 & t_0 & & t_0 e^{-jkL} \\ t_0 & E_{c2}-t_0 & \ddots & \\ & \ddots & E_{c3}-t_0 \ \ddots & t_0 \\ +t_0 e^{jkL} & & t_0 & E_{cN}-t_0 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix} = E \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix}$$

we can can apply the same consideration for the other end of the domain and we have another term here

So the Hamiltonian H, can be expressed as the sum of the "Hard wall" Hamiltonian (HW) + another matrix including the exponential terms just obtained

$$H = \underbrace{\begin{bmatrix} E_{c1}-2t_0 & t_0 & & \\ t_0 & E_{c2}-t_0 & \ddots & \\ & \ddots & E_{c3}-t_0 \ \ddots & t_0 \\ & & t_0 & E_{cN}-t_0 \end{bmatrix}}_{H_W} + \begin{bmatrix} & & & t_0 e^{-jkL} \\ & & 0 & \\ & & & \\ t_0 e^{jkL} & & & \end{bmatrix}$$

OPEN BOUNDARY CONDITIONS (OBC)

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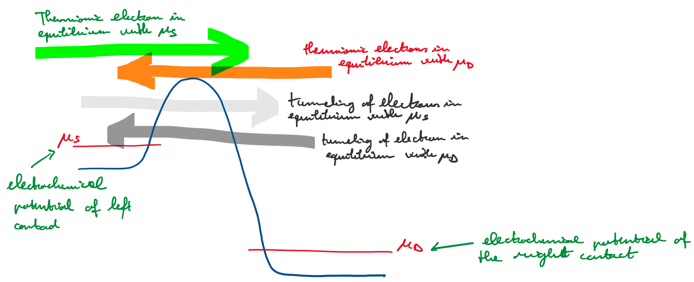
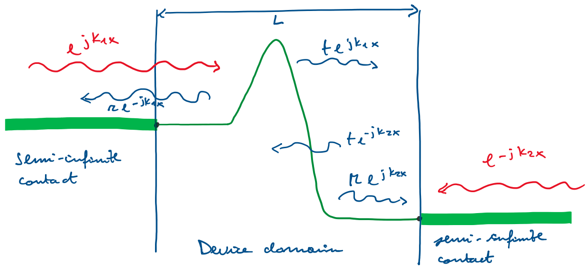
If you want to study transport in a device, we apply OBC.

In a device the transport mechanism is ruled by the modulation of the barrier.



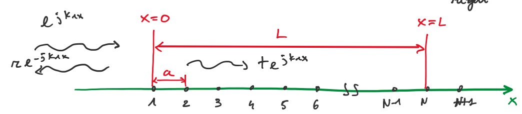
We have two population of free charges, one in equilibrium with μ_S and one with μ_D. The current is due to electrons flowing on top of the barrier (thermionic transport) + charges flowing through the barrier (tunneling transport)

Let's solve this problem, and consider a domain L-long + 2 semi-infinite contacts



I have 2 waves travelling from the left and from the right, which will be transmitted and reflected.

Let's discretize the problem, and let's consider only the electron travelling from the left to the right



for $x \leq 0 \Rightarrow \varphi(x) = 1 \cdot e^{jk_1x} + r\, e^{-jk_1x}$

$$\varphi(x=0) = \boxed{\varphi_1 = 1 + r}$$

$$\varphi(x=-a) = \varphi_0 = e^{-jk_1a} + r\,e^{jk_1a} = e^{-jk_1a} + r\,e^{jk_1a} + e^{jk_1a} - e^{+jk_1a} =$$

$$= e^{-jk_1a} - e^{jk_1a} + e^{jk_1a}\boxed{[r+1]} =$$

$$= e^{-jk_1a} - e^{jk_1a} + \varphi_1 e^{jk_1a} = \varphi_0$$

For $i=1$, the Schrödinger equation is:

$$t_0\varphi_0 + (E_{c1} - 2t_0)\varphi_1 + t_0\varphi_2 = E\varphi_1 \Rightarrow$$

$$\Rightarrow \boxed{+t_0 e^{jk_1a}\varphi_1} + (E_{c1} - 2t_0)\varphi_1 + t_0\varphi_2 = E\varphi_1 + \boxed{t_0\left[e^{jk_1a} - e^{-jk_1a}\right]}$$

With respect to the H_W, we have the two terms highlighted in yellow.

Same considerations holds for the electrons flowing from the right.

So, the discretized problem become:

$$\underbrace{\begin{bmatrix} E_{c1}-2t_0 & t_0 & & \\ t_0 & E_{c2}-2t_0 & \ddots & \\ & \ddots & \ddots & t_0 \\ & & t_0 & E_{cN}-2t_0 \end{bmatrix}}_{H_W}\begin{bmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \varphi_N\end{bmatrix} + \underbrace{\begin{bmatrix} t_0 e^{jk_1a} & & \\ & 0 & \\ & & t_0 e^{jk_2a}\end{bmatrix}}_{\text{SELF-ENERGY MATRIX}}\begin{bmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \varphi_N\end{bmatrix} = E\begin{bmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \varphi_N\end{bmatrix} + \underbrace{\begin{bmatrix} t_0\left[e^{jk_1a} - e^{-jk_1a}\right] \\ 0 \\ t_0\left[e^{jk_2a} - e^{-jk_2a}\right]\end{bmatrix}}_{S}$$

In the end we can write the problem as:

$$(E \cdot I - H_W - \Sigma)\varphi = S \qquad \Sigma = \Sigma_1 + \Sigma_2$$

$$\Sigma_1 = \begin{bmatrix} t_0 e^{jk_1a} & \\ & 0 \end{bmatrix} \qquad \Sigma_2 = \begin{bmatrix} 0 & \\ & t_0 e^{jk_2a} \end{bmatrix}$$

$$\varphi = \underbrace{\left[EI - H_W - \Sigma\right]^{-1}}_{G(E)} S$$

Green's Function