Université de Bourgogne
M1-QT-PPN
Numerical Methods
Final exam
Deadline : February 6th, 2024 at 12 :00 by e-mail to alain.dereux@u-bourgogne.fr

This assignment relies on the conventions introduced during the lectures and applied in the lecture notes.

This project shall exploit the suite of Matlab/Octave/Python scripts developped by the student during the practical sessions in order to solve the one-dimensional time independent Schrödinger equation by the localized Green's function method in configurations (chapter 4 and Appendix A of the lecture notes) that are relevant to model an electron scattered by a quantum junction.

1 Constant background as reference system

Items

1. Consider a reference system featuring a constant potential background $U_0 = 0 \quad \forall x$. The Green's function $G_0(x, x'; k)$ associated with this sytem is given by eq. (4.34). As a first approach to the orders of magnitude or resonant tunneling devices in GaAs-AlGaAs heterostructures, consider the following potential profile featuring two barriers of same height defined relatively to this constant potential background by :

$$\begin{aligned} U(x') &= 0.2\text{eV} \ ; \ \forall x' \in \left[0\mathring{\text{A}}, 15\mathring{\text{A}}\right] \\ U(x') &= 0.2\text{eV} \ ; \ \forall x' \in \left[65\mathring{\text{A}}, 80\mathring{\text{A}}\right] \\ U(x') &= 0 \quad \text{elsewhere} \end{aligned} \tag{1}$$

   Set the step of the grid used for discretizing $U(x)$ to $0.5\mathring{\text{A}}$. What are the lower (E_a) and upper (E_b) bounds of the interval of energy $[E_a, E_b]$ that are not affected by aliasing ?

2. Let E_0 by the incident energy associated to electron incident as a plane wave from $x' = -\infty$. On a same graph, produce curves of the reflection, $R(E_0)$, transmission $T(E_0)$ and absorption coefficients $A(E_0)$ for $E_0 \in [0\text{eV}, 0.3 \ \text{eV}]$ by steps as fine as 0.0005 eV and using a 1 nanosecond recombination time (lifetime) parameter.

3. How do you define a resonance in this context ? Are they all reliable results in the sense that they are inside $[E_a, E_b]$?

4. On the same graph featuring $x \in [-20, 100]\mathring{\text{A}}$ as abscissae, provide graphical representations of the potential profile, of the scattering eigenstate wavefunction and of the scattering eigenstate probability density for each of the resonances found in $[E_a, E_b]$. Compare these wavefunctions to the wave function of an eigenstate that is clearly not resonant and featuring an energy between the second and the third resonance. When preparing your graph, remember that the potential profile and the wavefunction are not expressed in the same unit.

5. As a crude approach to an applied bias, modify the potential profile so that the two barrier have different heights as follows :

$$\begin{aligned} U(x') &= 0.2\text{eV} \ ; \ \forall x' \in \left[0\mathring{\text{A}}, 15\mathring{\text{A}}\right] \\ U(x') &= 0.1\text{eV} \ ; \ \forall x' \in \left[65\mathring{\text{A}}, 80\mathring{\text{A}}\right] \\ U(x') &= 0 \quad \text{elsewhere} \end{aligned} \tag{2}$$

Keeping the other computation parameters as above, on a same graph, produce curves of the reflection, $R(E_0)$, transmission $T(E_0)$ and absorption coefficients $A(E_0)$. How do they compare to the previous case of two barriers featuring the same height?

2 Step function as reference system

Items

1. Consider a reference system featuring a step function $U_0(x < 0) = 0$ and $U_0(x > 0) = U_1 = -0.1$ eV as potential background. The Green's function $G_1(x, x'; k)$ associated with this sytem is given by equations (A.76) and (A.77). For this reference system, the incident wave from $x = -\infty$ and the wave transmitted towards $+\infty$ are then given by eq. (A.65). The step function means that a potential bias is applied to the junction. Across the heterostructure, the electric field associated to this bias is thus given by :

$$|\mathbf{E}| = -\frac{U_1}{x'_{max} - x'_{min}} \tag{3}$$

where $x'_{max} - x'_{min}$ is the width of the heterostructure (domain where $U(x') \neq 0$). Therefore, the potential defined by (1) must be modified as follows :

$$W(x') = U(x') - |\mathbf{E}|x' \quad \text{only if} \quad x'_{min} < x' < x'_{max} \tag{4}$$

Provide a plot of the profile of the final potential experienced by an electron for $x \in [-20, 100]\mathring{\text{A}}$.

2. For the potential defined by (4), keeping the other computational parameters of the previous section, what are the lower (E_a) and upper (E_b) bounds of the interval of energy $[E_a, E_b]$ that are not affected by aliasing?

3. Let E_0 by the incident energy associated to electron incident as a plane wave from $x' = -\infty$. On a same graph, produce curves of the reflection, $R(E_0)$, transmission $T(E_0)$ and absorption coefficients $A(E_0)$ for $E_0 \in [0\text{eV}, 0.3 \text{ eV}]$ by steps as fine as 0.0005 eV and using a 1 nanosecond recombination time (lifetime) parameter.

4. To model an electron at the Fermi level, we now set $E_0 = 0.01$ eV and explore the effect of tuning the bias, thereby meaning that $U_1 \in [-0.2, 0.2]$ eV. For $U_1 = -0.2$ eV and $U_1 = +0.2$ eV , provide the plots of the profiles of the potential experienced by an electron for $x \in [-20, 100]\mathring{\text{A}}$.

5. On a same graph, produce curves of the reflection, $R(U_1)$, transmission $T(U_1)$ and absorption coefficients $A(U_1)$ by varying U_1 by steps as fine as 0.0005 eV (all other parameters are unchanged). From this spectrum, what do you expect as I-V (current-bias) curve for this junction in this range of bias? Do you expect the I-V curve to be similar to the one an electrical resistance? Do you expect the I-V curve to be similar to the one of a diode?

Deliverables :

(a) Matlab/Octave/Python scripts where the comments refer to the equation numbers of the lecture notes, specifically to equations in chapter 4 and appendix A.

(b) Readable pdf file providing a clear and focuses answer to each item.

(c) Showing all requested plots in appropriate units.

Grading

2 points for each item.