

**PART 1 : Constant background as reference system**

**Problem 1.**

*Solution.*  $E_a = 0$  eV and  $E_b = 0.4$  eV 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.  $\square$

**Problem 2.**

*Solution.* The reflection coefficient  $R(E_0)$ , transmission coefficient  $T(E_0)$ , and absorption coefficient  $A(E_0)$  for incident energies  $E_0$  ranging from 0 eV to 0.3 eV have been plotted on the same graph. The energy steps were set at 0.0005 eV intervals, and a 1 nanosecond recombination time (lifetime) parameter was used.

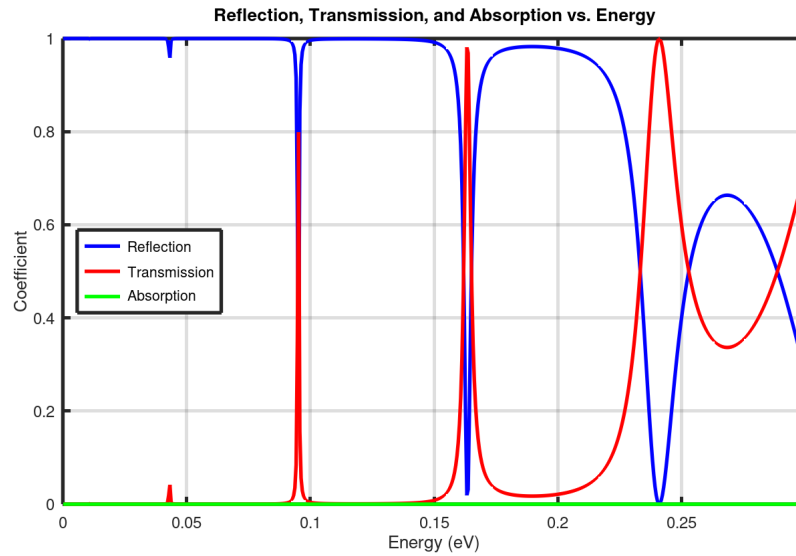


Figure 1: Unbiased junction behaviour

The graph shows how the reflection, transmission, and absorption coefficients vary with incident energy  $E_0$  across the specified energy range.

$\square$

**Problem 3.**

*Solution.* In the context of electronic systems, resonance occurs when the incident energy  $E_0$  matches the energy levels of the system's bound states or resonant states. This alignment of energy levels leads to a significant enhancement in the transmission probability through the system. Resonances can manifest as sharp peaks or dips in the transmission coefficient  $T(E_0)$  or as pronounced changes in the reflection coefficient  $R(E_0)$  and absorption coefficient

$A(E_0)$  as a function of incident energy  $E_0$ . Reliability depends on whether the results fall within the interval  $[E_a, E_b]$ , to avoid aliasing effects. If the results fall within this interval, they are considered reliable because they are accurately sampled without aliasing distortions. This ensures that the observed resonances and their characteristics are accurately captured and not artefacts of the sampling process.

□

#### Problem 4.

*Solution.* The graph illustrates the potential profile, scattering eigenstate wavefunctions, and probability densities for resonances within the energy interval  $[E_a, E_b]$ , where  $x$  ranges from -20 Å to 100 Å. It also contrasts these resonant wavefunctions with those of a non-resonant eigenstate, situated between the second and third resonances (shown by the red line).

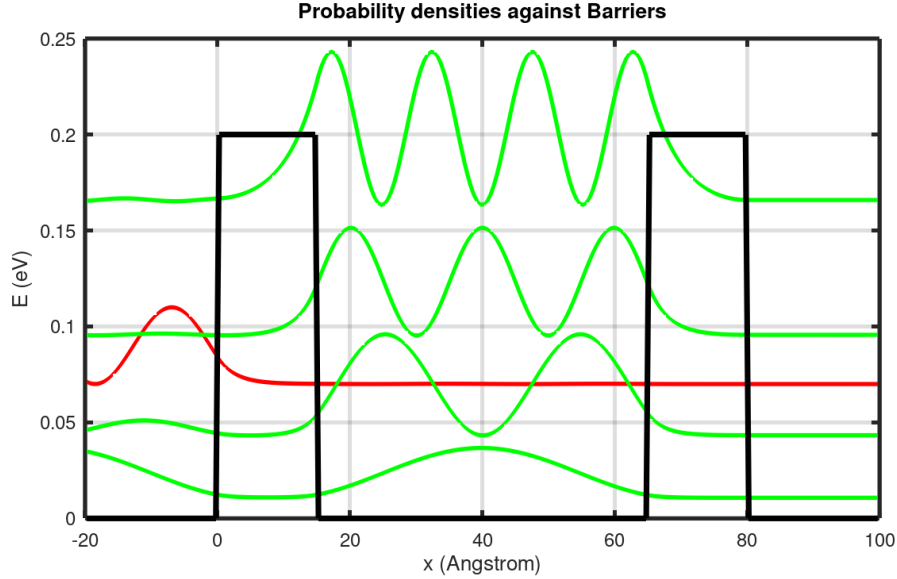


Figure 2: Resonant and non-resonant scattering eigenstates alongside the potential profile and probability densities within the energy interval  $[E_a, E_b]$ .

This comparative analysis provides insights into the behavior of resonant wavefunctions compared to non-resonant ones, offering valuable observations about the system's response to various energy levels and potential configurations. □

### Problem 5.

*Solution.* Curves representing the reflection  $R(E_0)$ , transmission  $T(E_0)$ , and absorption coefficients  $A(E_0)$  have been plotted using the same computation parameters as before.

- When barriers have equal heights, the transmission coefficient tends to be higher for specific energy values. This behaviour is consistent with quantum mechanical principles such as tunnelling. It allows particles to pass through barriers that would be classically impenetrable, and there are certain energy levels where tunnelling is more probable.
- With different barrier heights, transmission can be seen to increase beyond a certain energy threshold. This increase in transmission can occur because the higher barrier presents a greater impedance to particle transmission, effectively blocking particles with lower energies. However, once the energy of the particles exceeds a threshold determined by the higher barrier, transmission can increase significantly due to quantum mechanical effects like resonant tunneling.

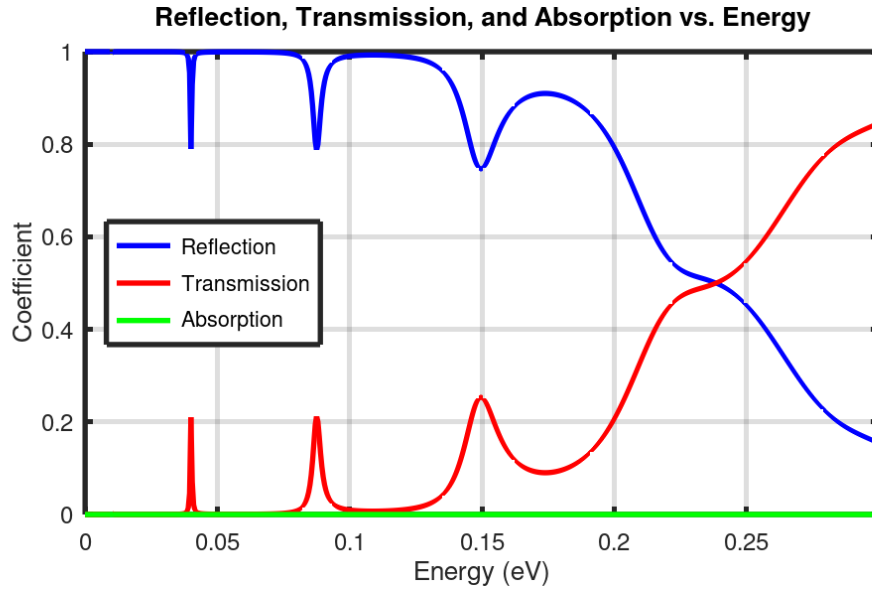


Figure 3: Roughly biased (0.1 eV)

□

## PART 2: Step function as reference system

### Problem 6.

*Solution.* The plot illustrates the final potential experienced by an electron across the range  $x \in [-20, 100]$  Å.

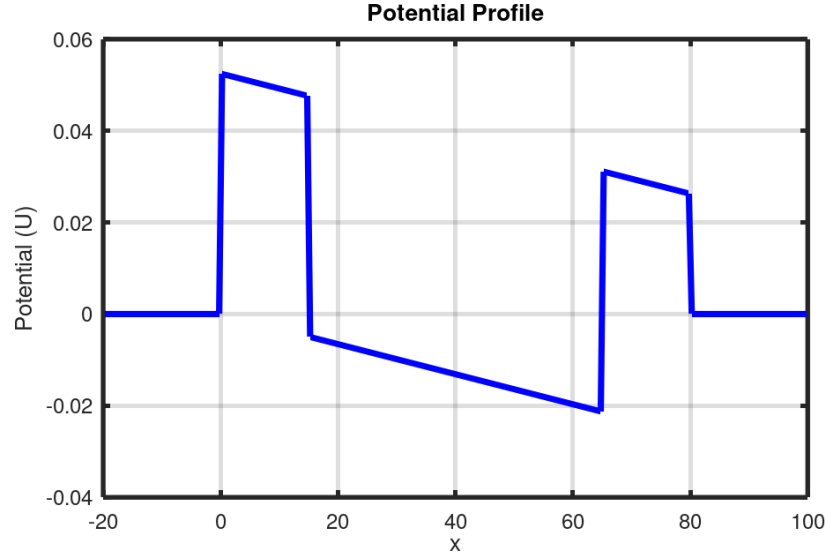


Figure 4: Final potential profile experienced by an electron.

□

### Problem 7.

*Solution.*  $E_a = 0$  eV and  $E_b = 0.8$  eV 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. □

### Problem 8.

*Solution.* The graph illustrates curves representing the reflection coefficient  $R(E_0)$ , transmission coefficient  $T(E_0)$ , and absorption coefficient  $A(E_0)$  for incident energies  $E_0$  ranging from 0 eV to 0.3 eV. The energy intervals are set at 0.0005 eV increments. □

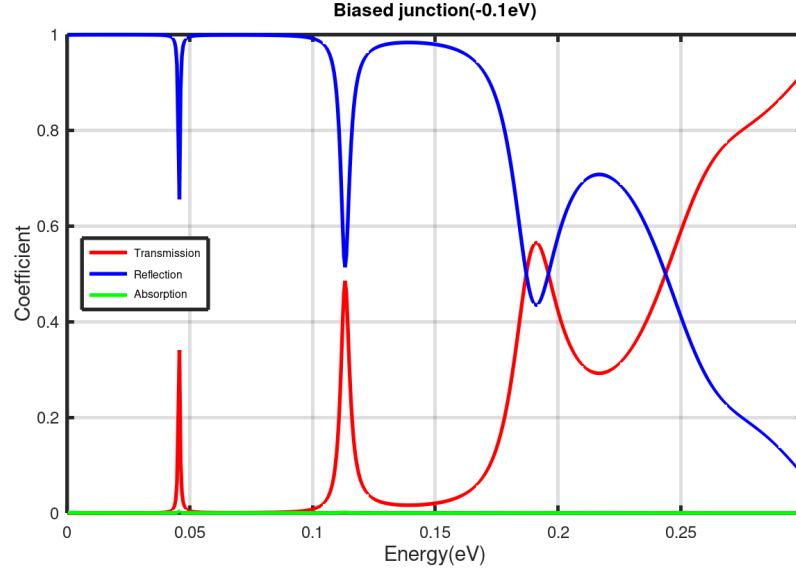


Figure 5: Biased junction (-0.1eV)

### Problem 9.

*Solution.* The plots illustrate the profiles of the potential experienced by an electron across the range  $x \in [-20, 100]$  Å for different bias voltages. Specifically, the plots depict the potential profiles when  $U_1 = -0.2$  eV and  $U_1 = +0.2$  eV.  $\square$

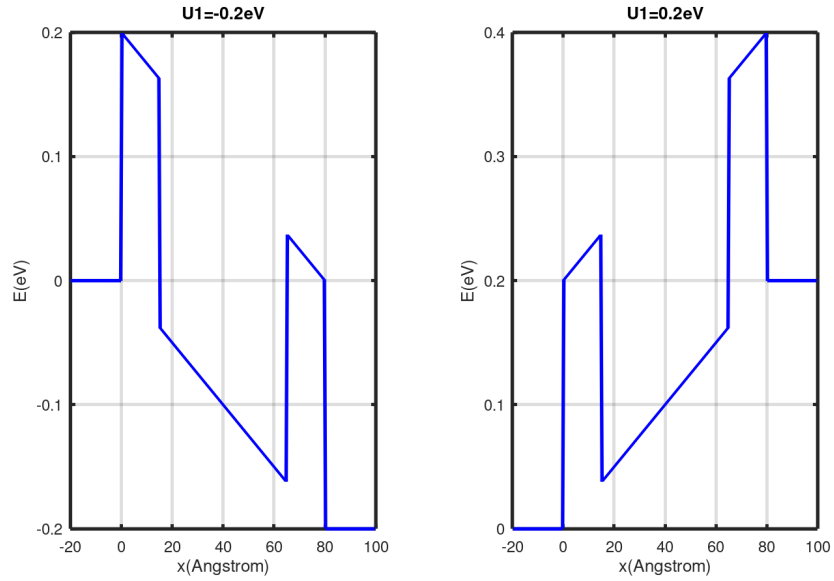


Figure 6: Potential profiles experienced by an electron

### Problem 10.

*Solution.* The junction's current-voltage (I-V) curve, is expected to be non-linear due to varying bias. Transmission peaks around biases near 0.06 eV and 0.17 eV, indicating increased current due to resonant tunnelling. Beyond these peaks, transmission levels stay low, accompanied by high reflection, signifying minimal current passage and resulting in flat segments on the I-V curve. These attributes diverge from the linear behaviour of an ohmic resistor and the exponential I-V trait of a diode. The spectrum suggests diode-like behaviour, with rectifying characteristics resembling semiconductor junctions. As bias voltage increases, a non-linear current response is expected, analogous to diode behaviour (more specifically rectifying diode) rather than linear resistance.

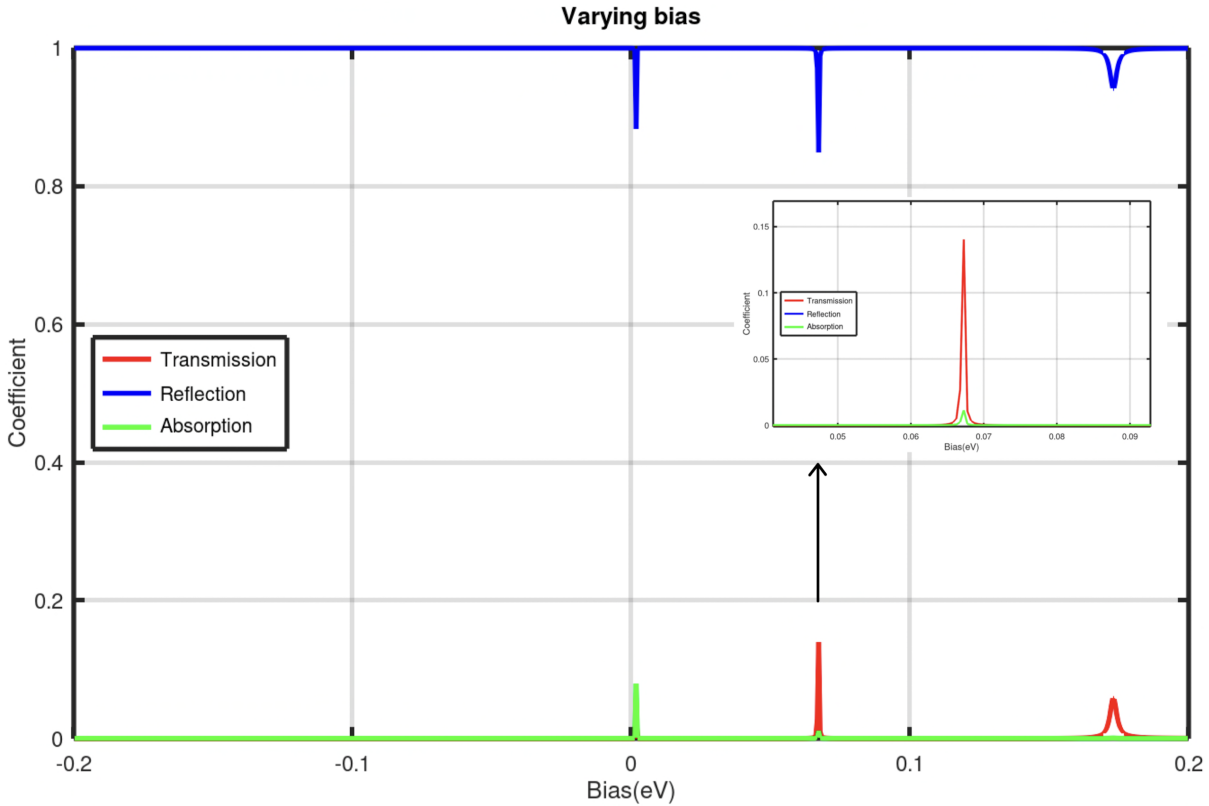


Figure 7: Varying bias by steps as fine as 0.0005 eV.

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