Practice 2: Quantum Monte Carlo Simulation of a Resonant Tunneling Diode

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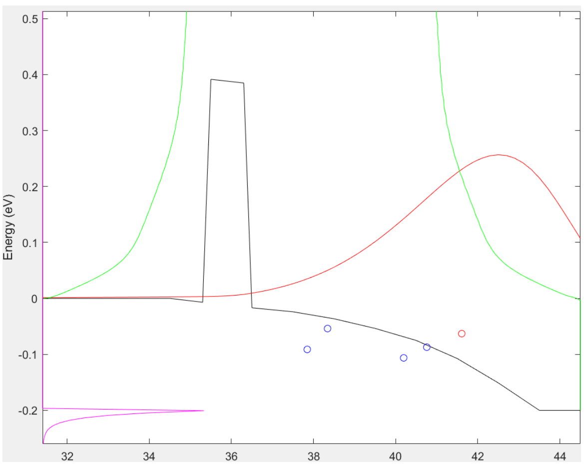
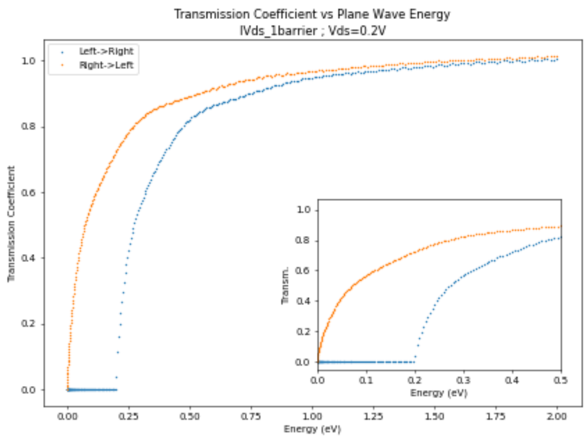
In the present report we summarize some of the results of interest obtained after manipulating the *RTD.txt* scenario offered under the *examples* directory by the Bitlles software, following the practice guide. This time, we simulate the scenario using Bitlles [1] and employing a full quantum treatment based on Bohmian mechanics [2], where each electron is mathematically represented with a (conditional) wavefunction in addition to its position-space trajectory as in classical mechanics. This wavefunction obeys a Schrödinger-like equation [3] that will pilot the trajectories in a non-classical manner, introducing all the relevant quantum mechanical features into the problem. It turns out that either the single barrier or the double barrier require a full quantum treatment in terms of waves in order to match the experimental results. This is because both "devices" exploit intrinsically quantum/wave-like properties: the former relays on the quantum tunneling while the latter relays as well on the resonant quantized energy states within the barriers.

1 Single Tunneling Barrier

By changing one of the AlGaAs barriers of the *RTD.txt* setting to GaAs, we obtain a channel with a conduction band shaping a single quantum barrier. We can forget about the strict band-structure below the conduction band of these epitaxial semiconductor layers, because we place the chemical potential of the source contact over the conduction band of the GaAs bulk, which makes only the electron wave-packets formed by the Bloch states over the conduction band relevant for the transport discussion. Since AlGaAs has a conduction band that ends up 0.4 eV over GaAs, the barrier has an effective height of 0.4 eV.



(a)



(b)

Figure 1: Setting $V_{DS} = 0.2V$, in (a) we see for a certain simulation time, the single tunneling barrier potential profile in black, a conditional wavefunction and its Bohmian trajectory in red, some additional trajectories in blue and the transmission profiles in green. In (b) we see the transmission coefficient profiles (for drain to source and source to drain, respectively left to right and right to left).

We apply a $V_{DS} = 0.2V$ voltage difference between the two contacts and run the simulator. We obtain a potential energy profile as shown in Figure 1, clearly showing a single barrier. In the same plot an example conditional wavefunction can be appreciated (in red), pertaining to the electron whose position is drawn with a red dot. We can see that the (conditional) wavefunction of that electron is extended also in the region before, inside and after the barrier, even if the electron's position itself is after. That is, the trajectory of the electron will be affected by all the setting at once, and not only its locality. This readily indicates that the electron will evolve following a non-local non-classical trajectory, which in this context is known as the Quantum-Wholeness.

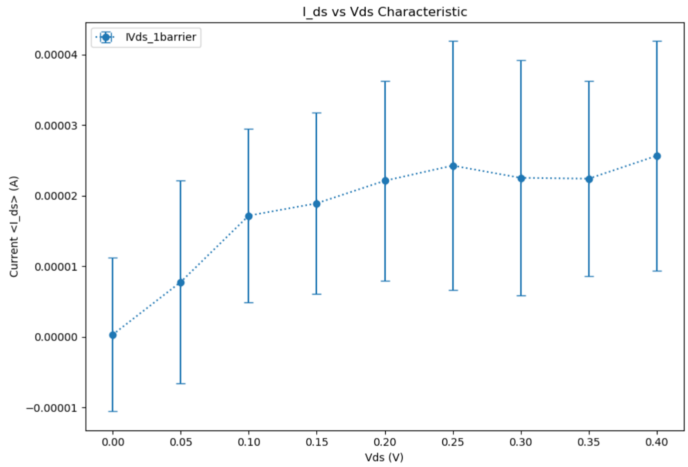
In Figure 1 we can also see the raw transmission probability profile for single-particle plane-waves, given the potential energy computed with the Poisson equation and the boundary conditions that take into account as well the rest of the electrons. We find a transmission probability profile that shows non-zero transmission even for electrons with less energy than the barrier. This increases till unity while the energy of the electron approaches the barrier top. This is what is called quantum tunneling.

1.1 I_{DS} vs V_{DS} Characteristic

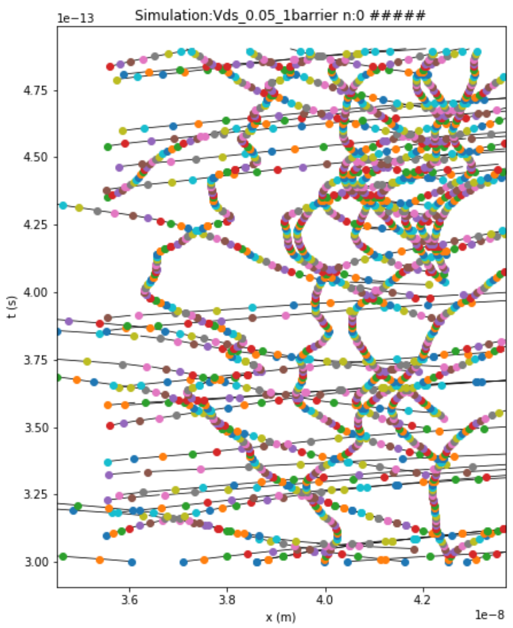
We sweep a range of $V_{DS} \in [0, 0.4]V$ voltages and compute the instantaneous I_{DS} current employing the Bohmian particles crossing the drain, just as done in the previous (classical particle) practice. Then, in each V_{DS} case, we compute the average current in the simulation window of $t = 10^{-12}s$, which would be a phenomenologically accessible measurable information (not as trivially computable if we did not have the Bohmian trajectories). With these time average currents we plot the I_{DS} vs V_{DS} characteristic of Figure 2, where we can also see the standard deviation (or "noise") of the (Bohmian) instantaneous currents used to compute each point. On the one hand, regarding the means, we see that even if we expected an ever increasing current for increasing voltage (following what the transmission coefficients tell us), we find the current saturates around $2.5e-6A$. This is due to the fact that the Fermi level of the source is not capable of giving more carriers above a certain voltage.

On the other hand, regarding the noise, one would expect that the noise in the instantaneous current is bigger when the transmission probability is smaller (lower V_{DS}). However, we find quite the opposite. This could be due to the current saturation, that impedes us to correctly see what would happen in the linear regime. Nonetheless, what is true is that the relative standard deviation, normalized by the current value in each time, is indeed smaller as the voltage increases. We can easily explain this noise and both rationales thanks to Bohmian mechanics. Because particles are still particles in this view, even when the system is closed, the current in each time as measured in a certain surface of the device (like the drain) will fluctuate as they cross or not the channel. This is known typically as partition noise. The point is that if more electrons are allowed to cross, the more likely will be to have bigger fluctuations in this (bigger) number of electrons in each time crossing a surface (thus the absolute increase). However, if the transmission coefficient is further from 1, such that "most plane waves above this energy may cross", the current will need to increase monotonously but having each time less electrons that do not cross or cross in the opposed direction, implying the bounds of the standard deviation centered on the mean will also need to increase monotonously (except when saturated). This implies the reduction of the standard deviation to mean ratio.

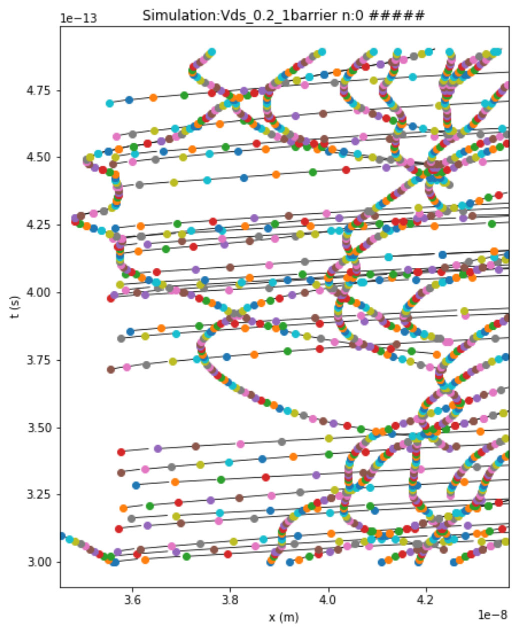
As a clear intuition on how this noise is due to the discrete nature of the charge carriers (in Bohmian mechanics), in Figure 2, we can see the Bohmian trajecotries for one example case $V_{DS} = 0.2V$, where in each time, a different number of electrons crosses the channel. Without the ontologically persistent Bohmian view of the electrons, such an intuitive understanding of the (quantum) paritition noise would be essentially impossible and would rather be a pathological phenomenon for the quantum explanation.



(a)



(b) $V_{DS} = 0.05V$

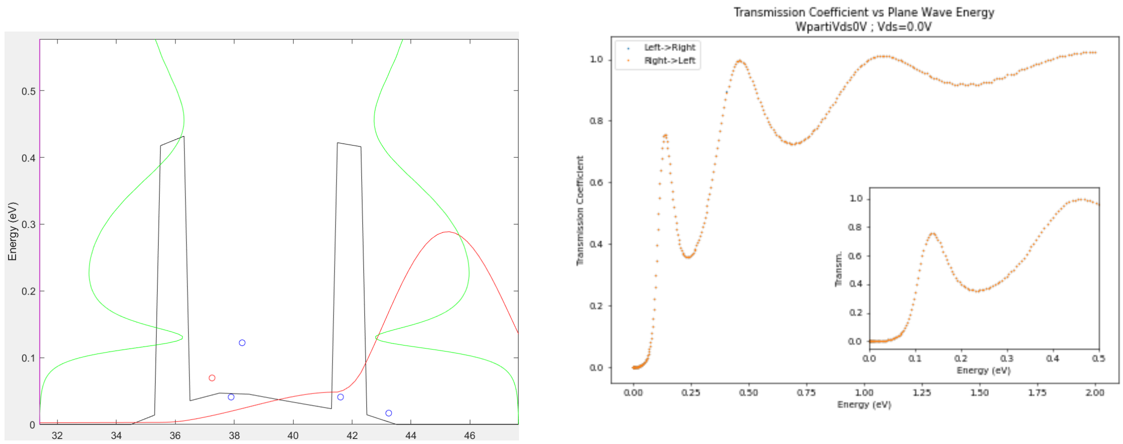


(c) $V_{DS} = 0.2V$

Figure 2: In (a) we see the average I_{DS} vs V_{DS} characteristic for the single barrier scenario. The bars represent the standard deviation of the instantaneous currents. The averages were computed over a 10^{-12}s time window. In (b) and (c) we see the Bohmian trajectories of the electrons, for $V_{DS} \in \{0.05, 0.2\}V$ respectively, along the channel position (in the horizontal axis, in $1e-8m$ units), in time (the vertical axis, in $1e-13s$ units). The different colours represent consecutive time frames. Trajectories are joined by their velocity vectors. Note that for the higher voltage, almost all electrons flow in from source to drain (left to right) at a high velocity.

2 Resonant Tunneling Diode

We now resort back to the original *RTD.txt* setting, with some minor modifications, but leaving both 0.4 eV AlGaAs barriers instead of erasing one. We apply a voltage difference $V_{DS} = 0V$ between the two ends of the device and compute the single-particle plane-wave transmission coefficients across the double well. See in Figure 3 the result. We clearly distinguish two transmission maxima, at about 0.13 and 0.45 eV.[1] This phenomenon by which a free electron can cross a multiple barrier with almost no reflection probability when it matches the energy of one of the energy eigenstates within the barriers is called the "resonant tunneling". Otherwise, the transmission coefficient follows a simple-tunneling-like law, such that the higher the energy of the electron, the higher the transmission probability.



(a) (b)

Figure 3: Setting $V_{DS} = 0V$, in (a) we see for a certain simulation time, the double tunneling barrier potential profile in black, a conditional wavefunction and its Bohmian trajectory in red, the norm in pink and some additional trajectories in blue and the transmission profiles in green. In (b) we see the transmission coefficient profiles (for drain to source and source to drain, respectively left to right and right to left).

2.1 I_{DS} vs V_{DS} Characteristic

We now sweep a range of V_{DS} drain to source voltages such that four different cases of the band-bending are captured, while the barrier-well is pushed to lower and lower potentials relative to the source. For each case, an instantaneous single-particle conditional potential energy profile and some representative Bohmian trajectories are plotted in Figure 5. These trajectories allow the computation of the current, to plot an I_{DS} vs V_{DS} plot (Figure 4) just as done in the previous section. The four mentioned cases are the following ones:

1. At the lower V_{DS} regime ($V_{DS} < 0.15V$), the Fermi level of the source is below the first resonant mode of the well. As V_{DS} increases, the resonant mode is pushed downwards, closer to the Fermi level of the source and thus the amount of charge carriers that access the resonant channel increases. This results in an increase of the resulting current with V_{DS}. The RTD behaves as a traditional resistance.

2. As V_{DS} continues increasing, for $V_{DS} \in (0.15, 0.3)V$, the (first) resonant energy goes below the Fermi level of the source until it goes below the conduction band of the source GaAs. At that point, even if by the Fermi-Dirac distribution the current should increase monotonously, there is no more possible states in the source aligned with the resonant energy (the density of states

[1]These turn out to match the energies of the two energy eigenstates inside the quantum well between the barriers, which can be estimated typically with the infinite quantum potential well analytical solution $E_n = n^2\hbar^2\pi^2/(2mL^2)$, with L the width of the well, $n \in \mathbb{Z}$ and m the electron mass.

drops to zero). The resonant level gets aligned with the band-gap of the source. This will drastically reduce the current flow through the barrier. As V_{DS} increases, the current through the device will now decrease. This is called the "negative differential conductance regime", since if we had set the origin of currents at the maximum current point, the device would look like it had negative resistence.

3. However, as the drop of V_{DS} continues to pull the well, eventually, at $V_{DS} = 0.3V$, the second resonant energy level of the well will start to align with the Fermi level of the source, which will allow current-flow again, with an increase in I_{DS} with V_{DS}.

4. This continues to happen until at $V_{DS} \sim 0.55V$ the $2.5e-6$A saturation current is achieved as in the single barrier scenario. At this point, the source cannot inject more carriers and the current saturates.

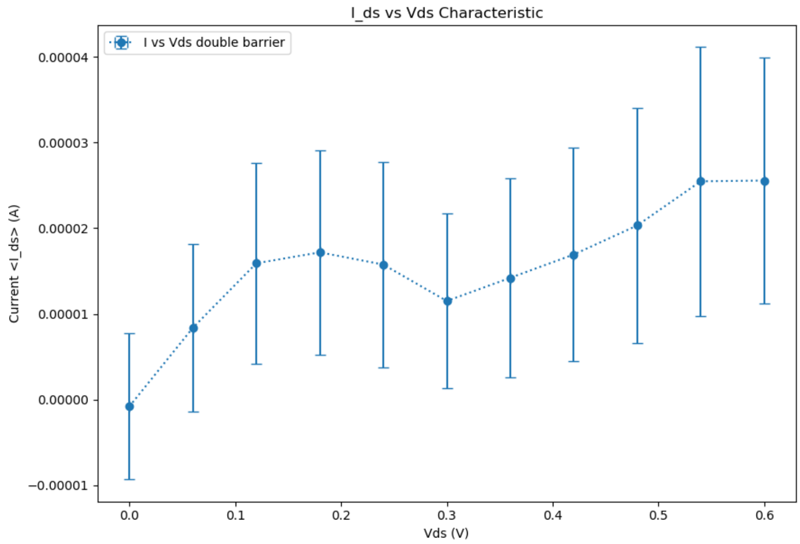
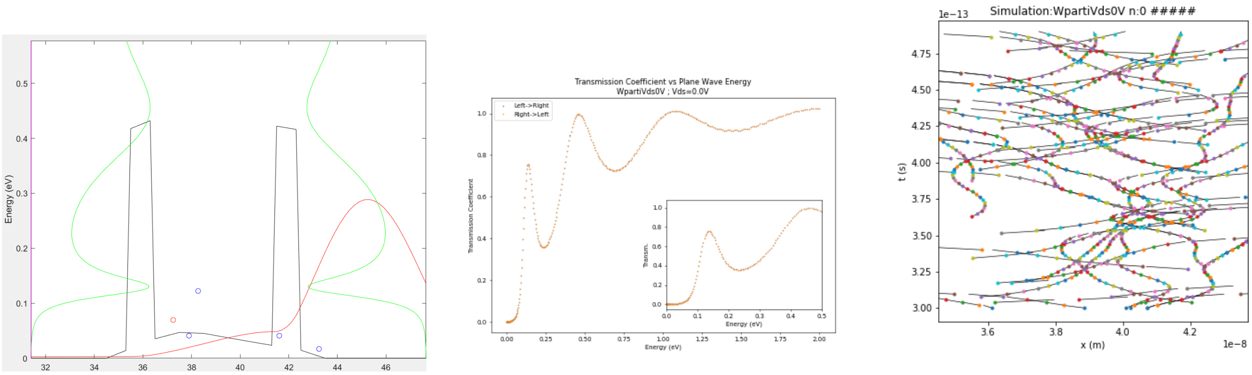


Figure 4: Average I_{DS} vs V_{Ds} characteristic for the double barrier scenario (the resonant tunneling diode. The bars represent the standard deviation of the instantaneous currents employed to compute the averages (takem over $1e-12s$).

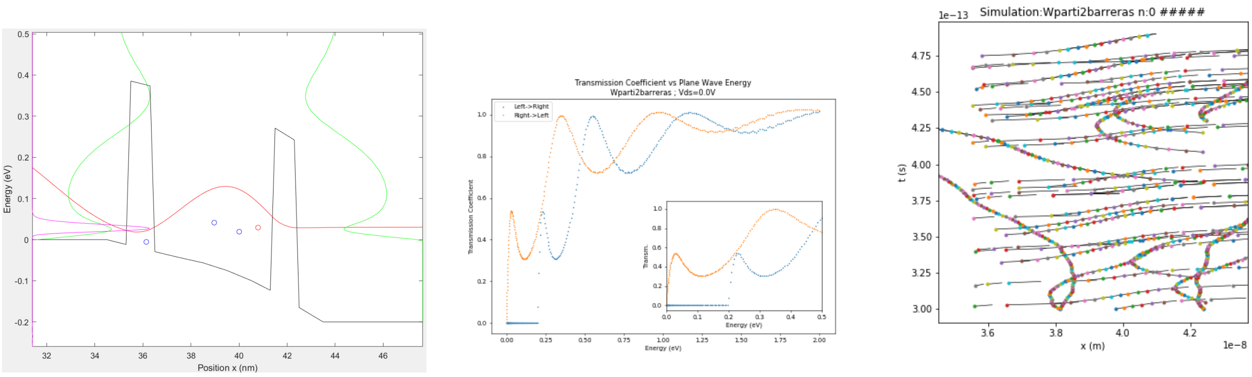
Note the standard deviation (fluctuation) of the instantaneous currents measured with the Bohmian trajectories, plotted as well in Figure 4. The behaviour and conceptual explanation of this partition noise follows exactly the same rationale as the one described in the previous section. See now the trajectories giving its intuition in Figure 5.

2.2 About the Negative Differential Conductance Regime

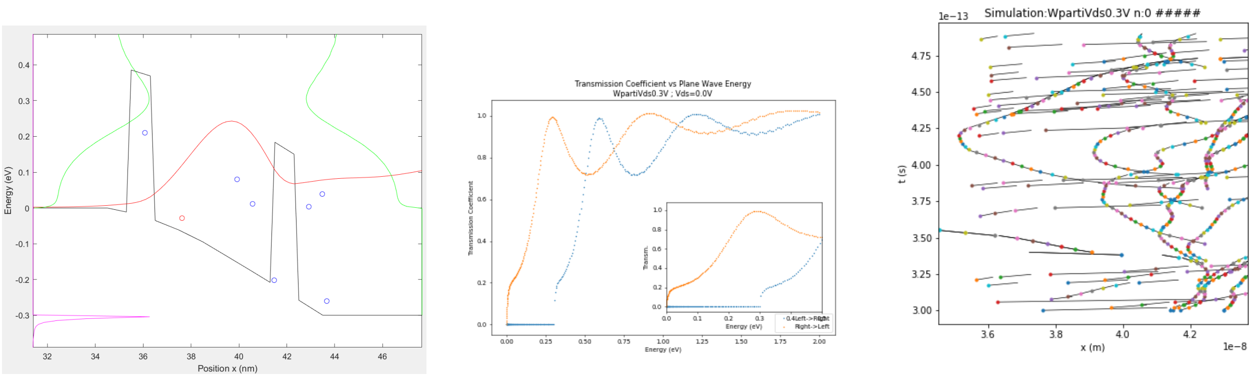
Two theoretical inquiries must be answered at this point. As a first question, one could ask how it is that the electrons cannot make use of the first eigenstate of the well when this lies below the conduction band of the source. One could say that if the laws of thermodynamics tend to populate primarily the states of lowest energy, it should not happen that the eigenstate of the well is not populated at all (and thus there is a decrease in conduction), when there are plenty of electrons in the colindant conduction band states, at a higher energy. An incomplete answer could be that this is due to the fact that electronic devices are only possible out of equilibrium, while there is still dynamics that can carry information from one point to the other. And thus, the question appears to be irrelevant. Yet, the complete answer requires to consider that most electronic devices, if not equilibrium systems, are still quasi-equilibrium systems, in the sense that there are "decohering" collision processes in the electron flow across its elements that dissipate its energy and let the electrons loose energy to tend towards



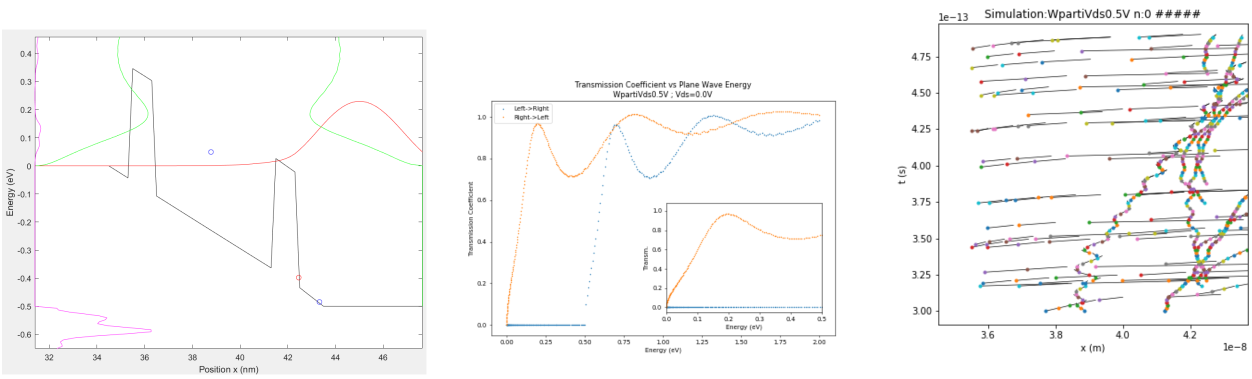
(a) $V_{DS} = 0V$ (b) $V_{DS} = 0V$ (c) $V_{DS} = 0V$



(d) $V_{DS} = 0.2V$ (e) $V_{DS} = 0.2V$ (f) $V_{DS} = 0.2V$



(g) $V_{DS} = 0.3V$ (h) $V_{DS} = 0.3V$ (i) $V_{DS} = 0.3V$



(j) $V_{DS} = 0.5V$ (k) $V_{DS} = 0.5V$ (l) $V_{DS} = 0.5V$

Figure 5: In the first column, the same as Figure 3.a but for different V_{DS}, capturing all the scenarios of the text. In the second column the transmission profiles relative to the source conduction band. In the third column the trajectories as in Figure 2.b and c, but for the present scenario and V_{DS}.

the lowest energy states, recovering a “lowest energy preference” out of equilibrium. Then, the key is to notice that the channel of an RTD is small enough and the materials are adequate enough to allow a ballistic transport of the electrons along the channel and in particular within the barrier, such that by conservation of energy, the electrons cross the channel with the same energy they had in the entrance, which had to be above the conduction band.

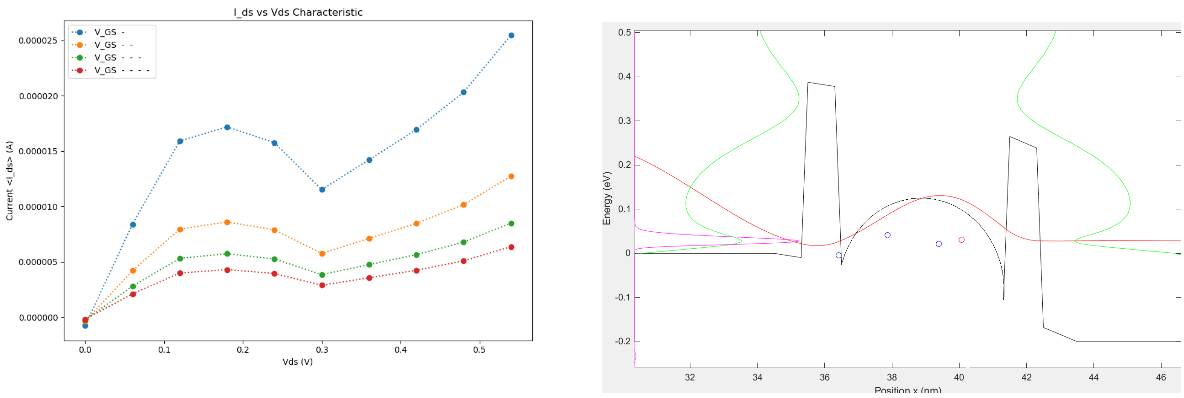
The second question would be about how the dissipated power behaves for this apparent “negative conductance/resistance”. Since the formula for the power consumption is $P = I_{DS}^2 R$, with R the resistance of the channel, one could think that the negative resistance acts as a counter-intuitive power source or the like. However, nothing further than this, the power dissipation is actually the same classical one, because in reality both the current and the voltage are positive in the forward direction, and the negative conductance is only negative in the “differential” sense. This however, does not avoid the usage of an RTD in this regime to effectively “damp” the “positive resistence” of other (more conventional) circuit elements.

All in all, the decrease in current with increasing voltage contradicts no fundamental principle.

2.3 An RTD Transistor?

If we set a metal-oxide gate in one of the sides of the RTD device, this would allow a control of the potential energy height at which the well between the barriers lays, independently of the drain to source voltage. This is the fundamental idea of a transistor. This would allow us to switch-off the electron transport bewteen source and drain by just decreasing the voltage on the gate relative to the source, because the resonant energy level is defined relative to the bottom of the well.

After we tried to simulate such a scenario for hours, solving consecutive errors given by the software like the one shown in Figure 8, we ended giving up in the attempt to study it. However, we expected that the output would be something like what we emulated in Figure 6, where the expected I_{DS} vs V_{DS} characteristic for several gate to source voltages are plotted. Clearly, we would be able to switch off the current by just decreasing the voltage of the gate.



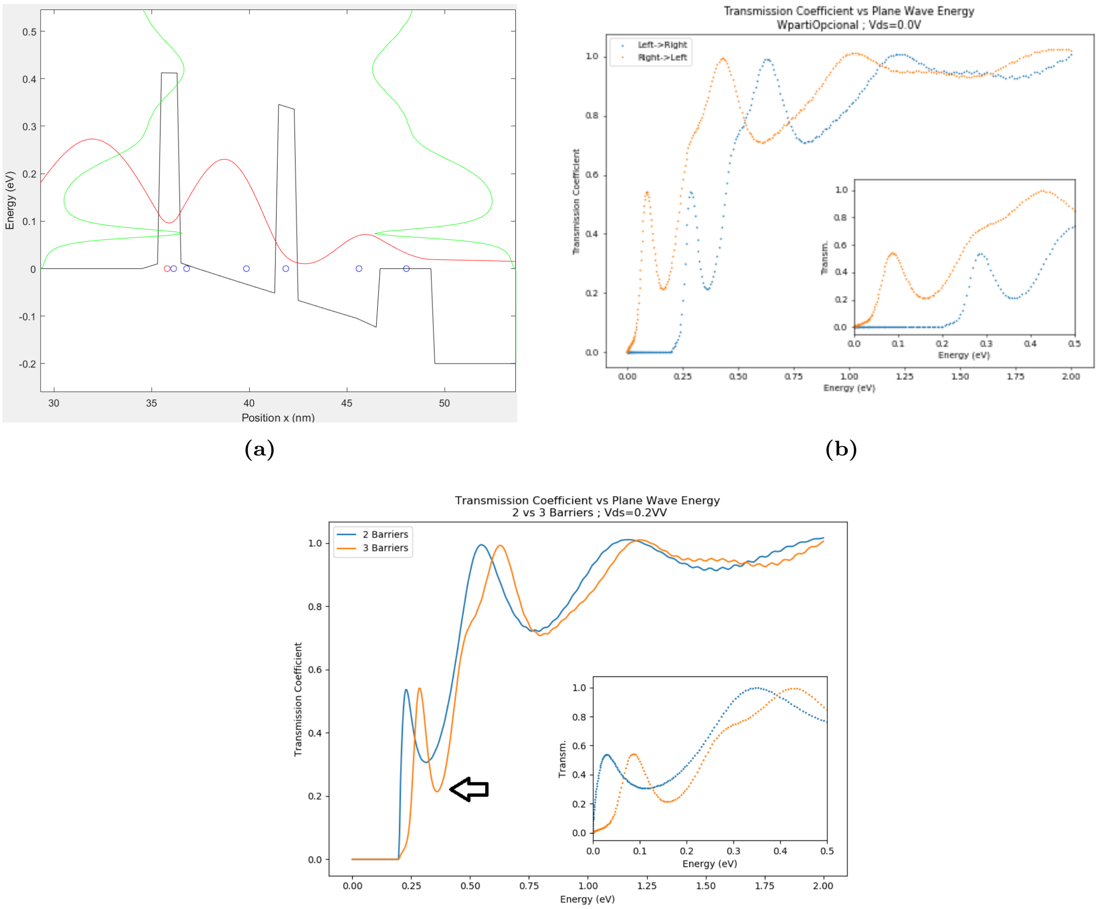
(a) (b)

Figure 6: What we expected to obtain by setting a gate in the channel. In (a) the expected I_{DS} vs V_{DS} characteristic for several decreasing gate voltages (increasing the potential energy bump in the well). In (b) the expected potential energy profile for a gate barrier that closes the current through the channel.

In Figure 6, we also plot the expected potential energy profile when the gate closes the channel. The resulting profile is similar to the Coulomb blockage happening in a single electron RTD, when the area of the device decreases as well, in addition to the channel length.

2.4 A Resonant Band Diode?

What we did achieve in the simulation was to look what happens when we add an additional barrier. In Figure 7 (a), we can see the scenario with an additional barrier with an approximately same width as the previous one[2]. After simulating it with a $V_{DS} = 0.2V$, we find the transmission coefficients of Figure 7 (b), where we compare them with the single well case in Figure 7 (c). We can see that the energy regions outside the peaks get less transmission (as indicated by the arrow in Figure 7 (c)), while the peaks of resonance start to get broadened. This is an indicator that a band structure has started to form. That is, the consecutive wells can be seen as a periodic potential profile, which is reminiscent of a 1D crystal lattice. As such, as we add more barriers (if we could) around where the resonant energies lied, now continuous bands would start to appear, while the regions in between would start to get more strictly banned. This is a very interesting feature, since what really supports all the scenario is actually another crystal lattice with its own band structure, so we would achieve a crystal defined over another crystal. Somewhat a cool feature.



(a) (b)

(c)

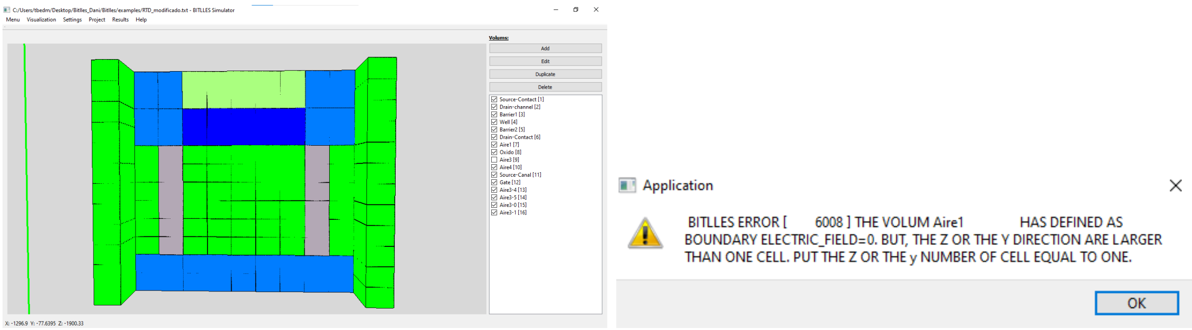
Figure 7: In (a) the scenario with $V_{DS} = 0.2V$ and three barriers, following the same notation and color code as in Figure 5. In (b) the transmission coefficient for this case. In (c) a comparison of the transmission coefficents in this case with the two barriers (and $V_{DS} = 0.2V$.

[2]We could not introduce additional volumes without having software troubles, as can be seen in Figure 9. We either tried to introduce the additional barriers within the same scenario, or extending volumes, but both cases failed after some wasted hours.

2.5 Problems during the design

After constructing the designs that can be seen in Figure 8 (a) and 9 (b) and checking them, the software warned us about different problems. With some of the warning messages we were able to figure out what was happening so we could fixe them. For example, we figured out that the grid of the different volumes had to match between them and also that there were some boundary conditions or configurations that were not trivial to see and change if one did not know about their existence.

In the case of the transistor, after acknowledging that the design of a whole new device was not going to be easy, we decided that the way to go was to mimic as much as possible the transistor design that we used in the first practice. Thus, we added the Polysilicon material for the Gate, copying all the characteristics from the *transistor.txt* example and made sure that all the pieces of air matched the boundary conditions from that example. Even thought we did this, we still encountered a new warning message when checking the design that we could not solve as easily. It was then that we gave up and went for resonant band idea.



(a) **(b)**

Figure 8: In (a) the scenario built for the RTD transistor, in (b) the respective last error at which we gave up..

When designing the "resonant band diode" we first tried to add 3 more barriers to the original design in order to have 5 (9 (a)), but the software warned us with a message that can be seen in Figure 9 (b). We initially thought that this error was due to the device being too large (because by only adding one barrier we did not face any warning message), so we decided to add barriers in the middle of the wells, in order to shorten the design as a whole. And yet, we still faced the same warning message as before. This design and the error can be seen in Figurs 9 (c) and (d) respectively. It is then that we decided to go for the final 3 barrier design.

We find it relevant to underline that the documentation of the software was not at all helpful when trying to debug our problems, not either when we were looking for specific data in the output files. For example, it appeared that some of the descriptions in the manual about the structuring of the data columns was incomplete or slightly misleading. Yet, being an open source software for research and educational purposes, we are still happy with the powerful tool it has been for us, and the results we have been able to obtain.

References

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[2] X. O. Pladevall and J. Mompart, *Applied Bohmian mechanics: From nanoscale systems to cosmology*. CRC Press, 2019.

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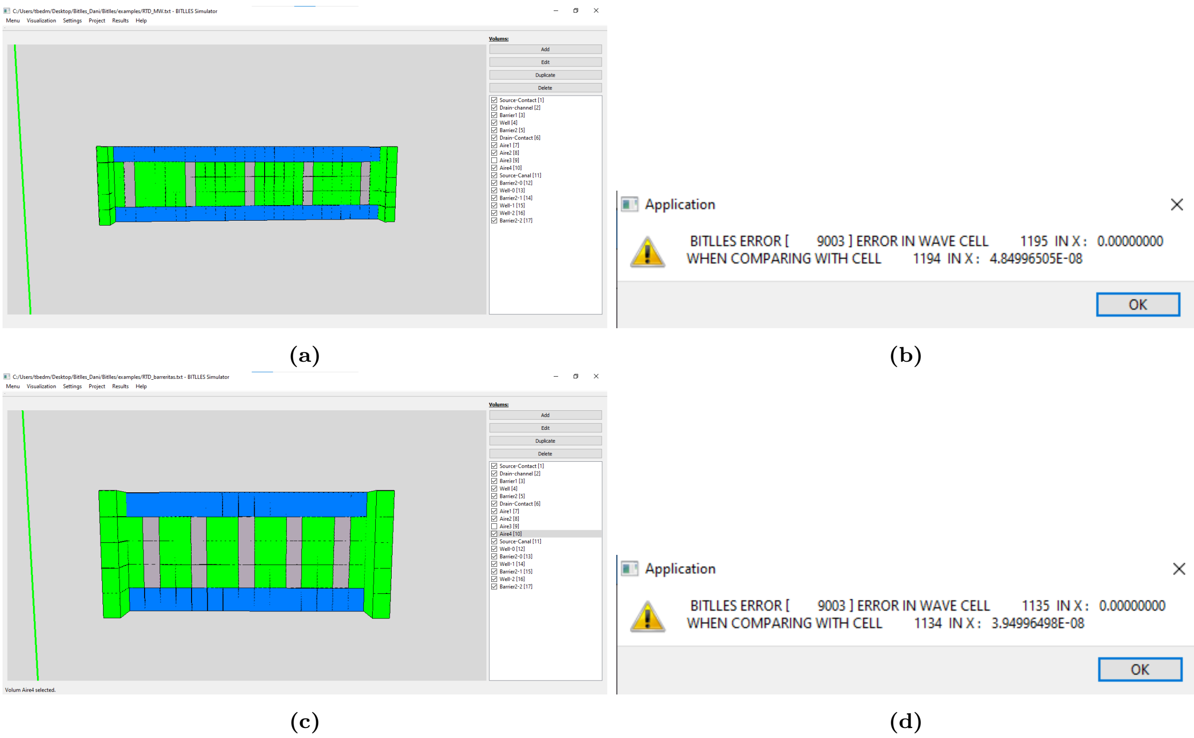

Figure 9: In (a), (c) the scenarios built for the resonant band diode and in (b), (d) the respective last errors at which we gave up. In (a), we tried preserving the same simulation overall volume in case it was the fault. In (c) we tried extending additional volumes, in case it was the problem. Eventually we achieved the simulation of three barriers of the (c) kind, but no more.