TFYA17 Project

Transmission properties in a short biased quantum wire

Patrik Hallsjö, Felix Faber

Abstract

This project is dedicated to study an electron transport in a biased quantum wire. The potential used is similar to the potential in [1], but with an added bias voltage. The goals were to construct a solver for the potential and to calculate the transmission and reflection for an electron sent towards the potential. All the goals that was set up where solved.

1 Introduction

The physics of low-dimensional semiconductor structures such as quantum wires and quantum point contacts has developed into an important part of nanotechnology, especially in connection with spintronics and quantum informatics. Conductance in quantum wires quantum and quantum point contacts made from split gate semiconductor heterostructures is quantized in steps of $2e^2/h$ [2]. This phenomenon may be explained in terms of non-interacting electrons and the stepwise occupation of higher sub-bands as the electron density is increased. Each occupied sub-band contributes a fixed amount $2e^2/h$ to the conductance where the factor of 2 comes from spin degeneracy. Experiments have also revealed other conductance features, which may not be explained by a single-particle model. The most well-know example is the 0.7 conductance anomaly for which different explanations have been proposed [3]. In addition to 0.7 anomaly there are 0.25 and 0.85 non-linear conductance features that have been observed in the biased quantum wires [4]. In paper [5] the model of spontaneous spin polarization was proposed to explain these anomalies. This project deals with study of an electron transport in a short biased quantum wire. To model the quantum constriction in a quantum wire for this project it has been proposed to introduce a model potential that has been used in their previous study [1]. By introducing a bias along the wire this potential can be modified to treat the electron transport in the case of biased wire. The following goals have been specified to the project:

1. To set and to solve a problem with boundary conditions when an electron is injected into a wire.
2. To calculate the transmission and reflection coefficients as functions of energy of injected electron and bias.
3. To represent solutions in graphical form.
4. Optional: to calculate a conductance.

2 Experimental Details

The experimental details only concern the coding in MATLAB. The calculation has been done in MATLAB since it suited the purpose well and it is very straightforward and easy. One drawback to using this is that the code can only be used on MATLAB version 2013a or newer. This is the main drawback of this work. One should note that the code can be written using for instance C++. It is also important to note that speed of calculation was not prioritized and that the code is not well optimized.

2.1 Theory

The potential that is used in this report is very similar to the potential used in [1], only that a bias has been added so the potential looks like

$$V(x) = \beta * V_{sd} + V_g * tanh(s * (x - dx_1)) - (V_{sd} + V_g) * tanh(s * (x - dx_2)) \quad (1)$$

where V_{sd} is the source-drain potential, V_g the hight of the barrier and β is a constant that will be set equal to $\frac{1}{2}$ for symmetric bias drop.

2.1.1 Finite difference approximation

A way to approximate a derivative is to use the so-called finite difference $f'(x) = \frac{f(x+h)-f(x+k)}{h-k}$, which is commonly used when the derivative of a function is calculated numerically. h and k are usually small and the limit $h, k- > 0$ is the derivative. There are three variants of the finite difference that are the most commonly used i.e., forward derivation: $\frac{f(x+h)-f(x)}{h}$, backwards derivation: $\frac{f(x)-f(x-h)}{h}$ and central derivation $\frac{f(x+\frac{h}{2})-f(x-\frac{h}{2})}{h}$.

This type of approximation can be applied to higher order derivatives in the same way and if one applies the central derivation two times one will yield an approximation for the second order derivative $\frac{f(x-h)-2f(x)+f(x+h)}{h^2}$.

2.1.2 Finite steps in differential equations

A second order differential equation without any first order terms can be written in the form $y''(x) = g(y(x), x)$ with boundary conditions $y(x_0) = y_0$ and $y(x_N) = y_N$, on the interval $[x_0, x_N]$. The derivative $y''(x)$ can be replaced the with the central finite difference approximation with $h = d$ and $x = n * d$, to yield $d * g(y(n * d), n * d) + 2y(n * d) - (y((n + 1) * d) + y((n - 1) * d)) = 0$. This is a system of $N + 1$ equations with $N + 1$ unknowns so it will have one unique solution which can be found by using linear algebra.

2.1.3 Quantum barrier problem

In the problem at hand, we want to find the transmission and reflection of an electron current through the potential (1). This means that we need to solve the stationary Schrödinger equation with the boundary conditions $y_0 = (I + R)\exp(-ikx_0)$ and $y_N = T\exp(-ikx_N)$ where $|T|^2, |R|^2$ and $|I|^2$ are the probabilities for the transmitted, reflected and incoming particle. We have put $I = 1$, which gives $y_0 = (1 + R)\exp(-ikx_0)$ to make the equations easier to solve.

We can use the finite difference approximation to solve the stationary Schrödinger equation as a second order ordinary differential equation (ODE). However, with R and T we have $N+3$ unknowns but only $N+1$ equations. Two more equations will be needed in order to fully solve the problem.

The solution to Schrödinger equation is continuous everywhere in the interval because it is a second order ODE, however it also needs to be continuous at the two boundaries. The finite difference approximation of the derivative yields: $y'_0 = y'_1$ and $y'_{N-1} = y'_N$. There are now $N + 3$ unknowns and $N + 3$ equations which will have a unique solution.

2.2 Code

We have developed the code based on the theory outlined above which calculates the conductance for a certain potential. It also plots both the potential and the wave-function that are calculated by solving the Schrödinger equation. The code can be used for calculating any potential. However, in this project a specific potential, (1), was of interest.

In the code, by default, V_{sd} and V_g are specified as 0.3, x_2 and x_1 are equal to 6, 4 respectively. For the user, the energy of the incoming electron E, the

size of steps to divide the interval in, the value of s in (1) for the potential and also the colour of the plot should be specified. Detail can be found in the code description in the appendix.

3 Results

Running the code for certain values of E, β, x_1, x_2, V_{sd}, V_g results in the following images, where the code has been run three times with different s parameters for each plot.

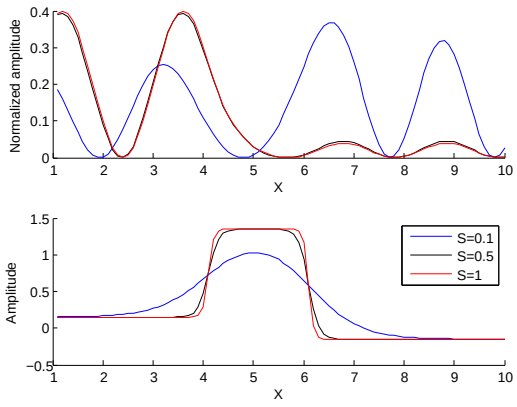

Figure 1: E=1, $\beta = 0.5$, $x_1 = 4$, $x_2 = 6$, $V_{sd} = 0.3$, $V_g = 0.6$

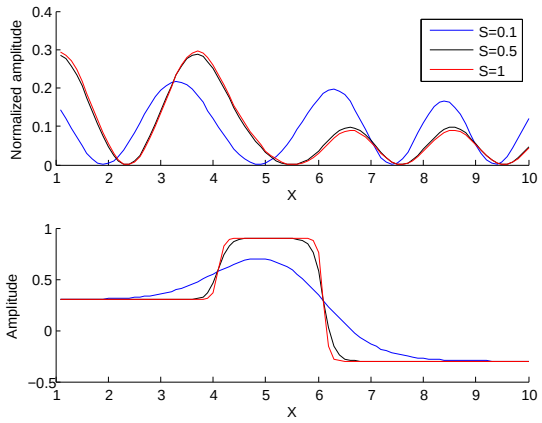

Figure 2: E=1, $\beta = 0.5$, $x_1 = 4$, $x_2 = 6$, $V_{sd} = 0.6$, $V_g = 0.3$

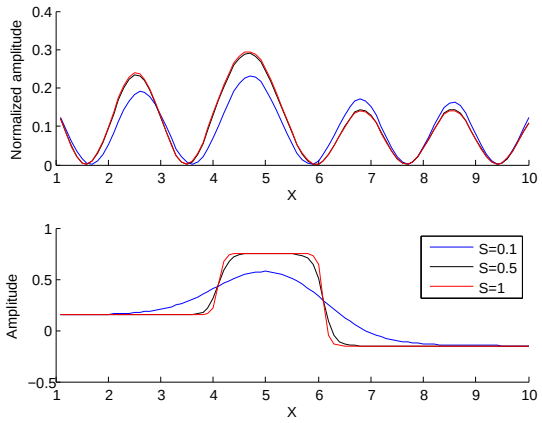

Figure 3: E=1.5, $\beta = 0.5$, $x_1 = 4$, $x_2 = 6$, $V_{sd} = V_g = 0.3$

The code also calculate the conductance for each run, by calculating the reflection and transmission coefficients and using the following relation:

$$R = |R|^2/(|R|^2 + |T|^2)$$
$$T = |T|^2/(|R|^2 + |T|^2)$$
$$C = T/(R + T)$$

4 Discussion

The code can most likely be optimized to run faster if one has enough time, but we prioritised get a working code. The main reason for the long computing time is that several different MATLAB packages were used. In a longer project a good idea would be to create a code using in C++ or any other usual programming language.

Computing power was a problem in the beginning. The reason where that we only had access to sun-ray computers with minimal computing power in the school, however we got access to research computers with a lot more computing power at the end of the course. The research computers were very helpful to produce a lot of graphs and they also had newer versions of MATLAB that ran better with the code. One thing that needs to be improved is the routines that are in place for students to gain access to the research computers.

For the potential given in this report there were no references of what results that were expected. However for known solutions, (radial potential, harmonic oscillator, etc.) the code has been tested and the results given were exactly as predicted.

4.1 Analysis of the figures

The figures show the potentials and wave-functions for different input parameters. As discussed above, calculations give the expected results for well-known potentials.

The solutions are similar to those of an electron sent through a square potential, especially in the limit $s \to \infty$ as can be seen in Figure[1]. The conductance increases as V_g becomes smaller. Resonances can occur for certain parameters inside potential (no pictures are shown of this though), especially when s is large. The probability for seeing the particle is greatly increased in these resonances.

5 Conclusion

The goals are listed below and it is commented the results achieved:

- To set and to solve a problem with boundary conditions when an electron is injected into a wire.

Done through the code by solving the Schrödinger equation and with that solution imposing boundary conditions.

- To calculate the transmission and reflection coefficients as functions of energy of injected electron and bias.

The code where able to calculate the transmission and reflection of from the solution. There are however, no specific examples of the calculated transmission or reflection shown in this article.

- To represent solutions in graphical form.

Done through the graphs plotted under Results.

- Optional: to calculate a conductance.

This was also discussed under Results.

In conclusion, we have achieved all the goals that were set up for the project, even the optional part. The code could have been optimized to improve speed, but we judged that the speed is sufficient.

References

[1] V. S. Tsykunov I. I. Yakimenko and K.-F. Berggren. Bound states, electron localization and spin correlations in low-dimensional gaas/algaas quantum constrictions. *J. Phys. Condens. Matter*, 25(072201), 2013.

[2] S. M. Goodnick D. K. Ferry and J. P. Bird. *Transport in Nanostructures.* Cambridge, 2nd edition, 2010.

[3] M. Pepper and J. Bird. The 0.7 feature and interactions in one-dimentional systems. *J. Phys.: Cond. Matter 20*, (16), 2008. Special section and references therein.

[4] M. Pepper I. Farrer D. A. Ritchie T.-M. Chen, A.C. Graham and M. Y. Simmons. Bias-controlled spin polarization in quantum wires. *Appl. Phys. Lett.*, 93(032102), 2008.

[5] I. I. Yakimenko H. Lind and K.-F. Berggren. Electric-field control of magnetization in biased semiconductor quantum wires and point contacts. *Phys. Rev. B*, 83(075308), 2011.

Appendix

```
function conductance =Schrodinger(E,step,s,color)
%Schrodinger(E,steps,s,color) plots the solution to the
%Schrodinger equation, the input potential and also calculates the
%conductance of the system. The program
%also requires Matlab 2013a or newer.
%Input the following:
%Energy that the incoming particle has in CGS units.
%The size of steps to divide the interval in, default interval is 1:10
%steps is recomended to be 0.1-0.01 any larger will increase the
%calculation time without improving the calculations significantly.
%The value of s in the potential, since the default potential is
%v=(beta-1/2)*Vsd+
%Vg*tanh(s*((intervalstart/step:intervallength/step-1)-x1/step))-
%(Vsd/2+Vg)*tanh(s*((intervalstart/step:intervallength/step-1)-x2/step));
%Vsd and Vg are set internaly to 0.3, also beta is set to 1/2.
%The colour of the plot, given as e.g. 'k' for black, 'r' for red.
%
hold on
%Solving the equationsystem.
intervallength=10;
intervalstart=1;
syms R T;
h_bar=1;
m=1;
k=sqrt(2*E*m/h_bar^2);
acc=5;
boundryconditions=
[vpa(exp(1i*intervalstart*k),acc)-R*vpa(exp(-1i*intervalstart*k),acc),
    T*vpa(exp(1i*intervallength*k),acc)];
derivativeconditions=
[1i*k*exp(1i*intervalstart*k)+R*1i*k*exp(-1i*intervalstart*k),
    1i*k*T*exp(1i*intervallength*k)];
size=intervallength-intervalstart;
size=size/step;
interval=[intervalstart+step:step:intervallength];
v=zeros(1,size);
H=zeros(size,size);
b=zeros(size,1);
phi=zeros(size,1);
%Input boundry derivative data into b vector
b=[boundryconditions(1);zeros(size-2,1);boundryconditions(2);];
beta=1/2;
Vsd=0.3;
Vg=0.3;
x1=4;
x2=6;
x=intervalstart:step:intervallength-1*step;
%Creating the potential
%v(5/step:15/step)=0.1*sin(0:pi/(5/step):2*pi); Sinus
%v(4/step:6/step)=1; Simple step.
%v=0.5*tanh((intervalstart/step:intervallength/step-1)-4/step)-
%0.3*tanh((intervalstart/step:intervallength/step-1)-6/step);
v=(beta-1/2)*Vsd+
Vg*tanh(s*((intervalstart/step:intervallength/step-1)-x1/step))-
(Vsd/2+Vg)*tanh(s*((intervalstart/step:intervallength/step-1)-x2/step));

H(1,1)=1;
```

```
H(size,size)=1;

%Calculate the H matrix.
for i=2:size-1,
   for j=1:size,
       if j==i-1 || j==i+1,
          H(i,j)=-h_bar^2/(2*m*step^2);
       end
       if j==i
       H(i,j)= h_bar^2/(m*step^2)+v(j)-E;
       end
   end
end
%Get a numerical solution to the problem H*phi =b
answer=linsolve(H,b);

%Now find R,T from this
temp1=solve(answer(2)/step-answer(1)/step == derivativeconditions(1),
answer(size)/step-answer(size-1)/step == derivativeconditions(2),R,T);
temp2=temp1;%[temp1.R temp1.T];
R=temp2.R(1);
T=temp2.T(1);
R=abs(R)^2/(abs(R)^2+abs(T)^2);
T=abs(T)^2/(abs(R)^2+abs(T)^2);
conductance = T/(R+T);
answer=subs(answer);
answer=abs(answer);
answer2=answer.^2;
answer2=answer2/norm(answer);
%conductance=abs(T)/abs(R);

subplot(2,1,1)
hold on
plot(interval',answer2,color)
subplot(2,1,2)
hold on
plot(interval',v,color)

end
```