

Self-Consistent Calculations of Spatial Electron Densities in Quantum Dot's Using a Coupled Recursive Green's Function and Poisson Solver

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ABSTRACT

We are utilizing the Recursive Green's function method to calculate the conductance in quantum dots as a function of Fermi energy, magnetic field and random potentials. We have extended the use of the method to calculate a self-consistent electron charge density and potential profile in the dot. This is accomplished by feeding the imaginary part of the Green's functions into a Poisson solver and feeding the potential obtained from the solver back into the Green's functions solver, until self consistency is better satisfied. Obtaining a more realistic density and potential profiles gives a better physical understanding to what happens in the dot, and provides more accurate results. We demonstrate the process with a $0.3 \times 0.3 \mu\text{m}$ dot formed at a GaAs/AlGaAs 2DEG.

Keywords: Green's Functions, Poisson's Equation, Self-Consistency, Quantum Computations.

1 INTRODUCTION

It is often the case that one approximates the quantum structure problem with a one-electron model. This includes solving the Schrödinger wave equation and obtaining single particle wave functions, or using perturbation theory for the lowest order Green's functions. In most cases, the extracted quantities, i.e., conductance, is close enough to realistic values. But the fact is that there exist electrons *inside* the structure. And according to Poisson's equation, they will create an electric potential inside the structure. This potential is often ignored because of the *complexity* involved if one chooses to include it, and because of the (plausible) *assumption* that ignoring it will not produce large errors. In the following we will touch on one approach to deal with this extra potential.

2 METHODS

First a grid is laid out on the region of concern. The grid is a rectangle n by m points. This is shown in Figure 1. The x direction is represented by the index i which goes from 1 to n . The y direction is represented by the index j

which goes from 1 to m . The mesh size is denoted by a . We use a uniform mesh, although the approach can be easily extended to a non-uniform mesh. Next, the potential V is laid on top of this grid. Also appropriate boundary conditions are set. The (one dimensional) left contact Green's function (GF), which corresponds to $i = 1$, is expanded in terms of the perfect lead transverse and longitudinal wave functions, using the tight-binding energy dispersion relation [1]. The transverse wave functions are simply sinusoids, while the longitudinal ones are complex exponentials. This (mode) GF is then converted to the site representation. We will call this GF $G_{L(old)}$. The isolated GF (in the site representation) corresponding to the next slice ($i = 2$) is simply a matrix with diagonal elements

$$G_0 = \frac{1}{E + V + i\hbar}, \quad (1)$$

where E is the energy, V is the site potential, and \hbar is proportional to the inverse of the phase breaking time [2]. There are two off-diagonal elements of magnitude 1, which correspond to hopping transversely, V_y (all energies are described in units of the hopping energy $\hbar^2 / 2ma^2$). This symmetric GF will be called G_0 . Now one applies Dyson's equation [3-4] to find the total GF corresponding to the system of $G_{L(old)}$ and G_0

$$G_L = G_0 + G_L \Sigma G_0, \quad (2)$$

where the self energy is given by

$$\Sigma = V_x G_{L(old)} V_x^*. \quad (3)$$

This yields

$$G_L = \frac{1}{G_0^{-1} - |V_x|^2 G_{L(old)}}. \quad (4)$$

For simplicity, the x hopping energy, V_x , is assumed to be equal to the y hopping energy, V_y , and therefore is unity. Since all three quantities in the denominator are known, one

can calculate G_L . Now this new G_L becomes the old GF and another G_0 is erected for site $i = 3$. To get the total GF at $i = 3$, the above procedure is repeated. This whole procedure is repeated until $i = n$. Throughout the process other auxiliary GFs are calculated, as they will be used at the end to calculate the conductance. At the end of the recursion ($i = n$), the GFs are converted back to mode representations. Transmission coefficients are calculated via the Landauer formula, and the sum over all propagating modes yields the conductance. To find the electron density \mathbf{r} for each grid point j on slice i , one simply takes the imaginary part of the corresponding point on the diagonal of G_L

$$n(i, j) = -\frac{1}{\mathbf{p}} \int_0^{E_F} \text{Im} G_L^i(j, j) dE. \quad (5)$$

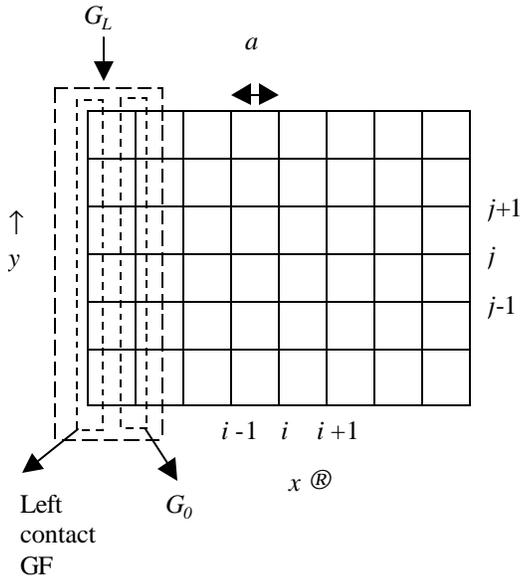


Figure 1: Discretization process and description of Green's functions.

Now that the density is calculated, it is fed into a Poisson solver, which solves

$$\nabla^2 V = -\frac{\mathbf{r}}{\mathbf{e}} \quad (6)$$

for V . This can be solved directly or iteratively, and we choose the latter. The potential is solved for using the simple Gauss-Seidel iteration scheme. The iteration simply states that the potential at any given point is the average of the surrounding four points, plus the density at that given point

$$V_{ij} = \frac{1}{4} (V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1}) + \frac{1}{4} \frac{\mathbf{r}_{ij}}{\mathbf{e}} a^2. \quad (7)$$

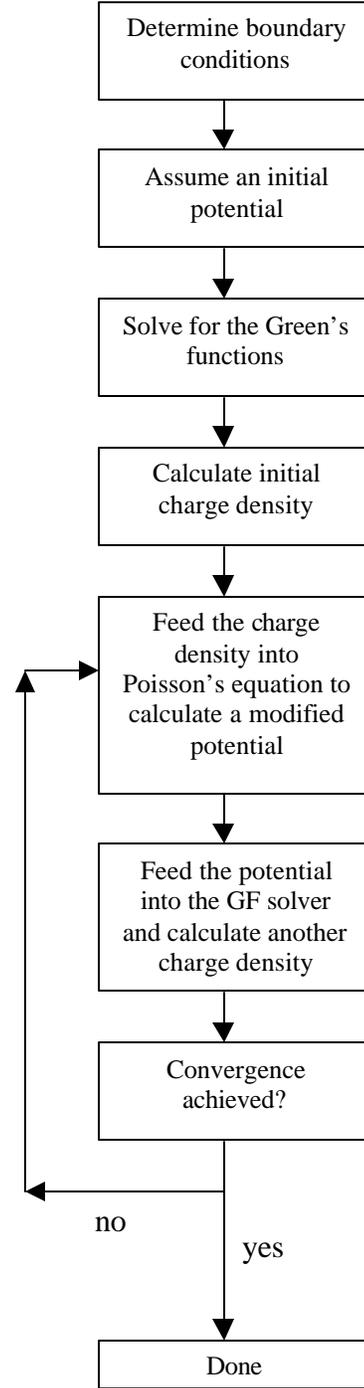


Figure 2: Description of iteration process between the GF solver and the Poisson solver.

Notice that the boundary conditions are always imposed, and that the iteration is done only on the interior points, and not on the boundary regions. This new V is fed back into the GF solver and a new charge density \mathbf{r} is calculated.

The procedure is repeated until convergence is obtained. The above method is illustrated by the block diagram which is shown in Figure 2.

3 RESULTS

We start the simulations assuming the potential shown in Figure 3. It has hard transverse boundary conditions (not shown in the figure) and four rectangular barriers. The plane of the figure corresponds to a 2DEG, and the potential profile (corresponding to the boundary conditions) is imposed by Schottky gates laid on top of the 2DEG. Other potentials could have been used as well. Electrons are restricted to the plane and current flows longitudinally along the indicated arrow. The initial potential is used in the GF solver, which yields, at a given Fermi energy, the charge density shown in Figure 4. Notice that the charge density goes to zero on the upper and lower transverse sides. This is due to the transverse hard wall boundary conditions. Notice also that the four barriers in the potential correspond to lower charge densities. Although the initial potential is symmetric transversely and longitudinally, the charge density is not. It is symmetric only transversely. This is due to the fact that current flows from the left to the right only. Hence the problem is not symmetric. One can visualize the flow of water along such a structure, and one will realize that the resulting water concentration will not be symmetric longitudinally.

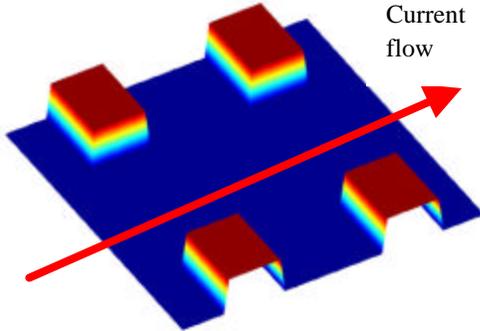


Figure 3: Initial potential assumption. Electrons are restricted to the plane and current flows longitudinally along the arrow. The transverse boundary conditions are set to be hard (not shown in the figure).

At the entrance of the system (left), and at the given energy, the wide opening fits four modes. At higher energies, the opening will fit more modes and vice-versa. The outer two modes get rejected by two of the barriers while the inner ones make it to the second stage (the

quantum dot enclosed by the four barriers). There, the modes spread transversely and longitudinally. They interfere and the net result at the exit is two propagating modes. In fact the conductance calculated at that energy equals two (in units of $2e^2/h$). If one sweeps over energy, one would get a conductance curve shown in Figure 5.

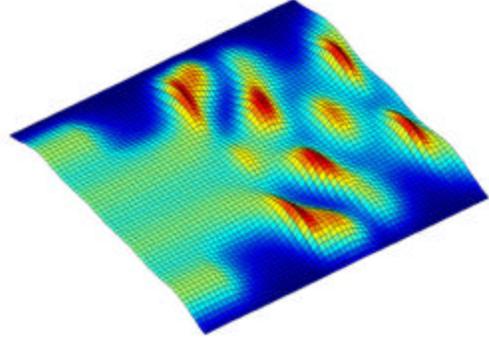


Figure 4: Charge density calculated using the potential profile shown in Figure 3.

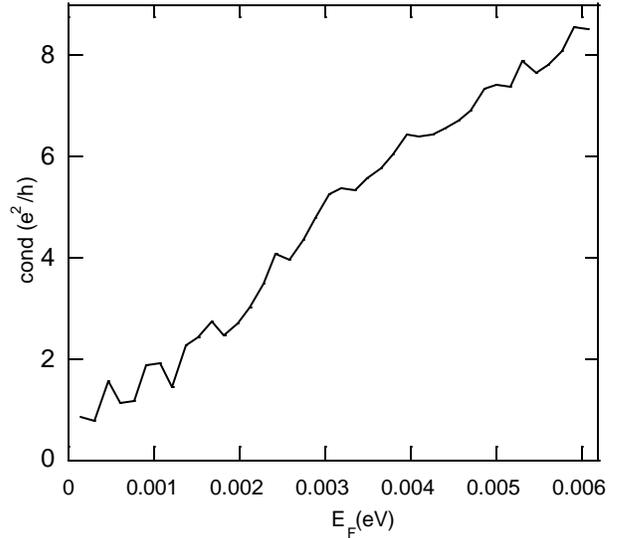


Figure 5: Conductance vs. Fermi energy without the self-consistency.

The next step is to put the computed charge density into the Poisson solver and solve for the new potential. The resulting potential is fed back into the GF solver and the process is repeated. One has to be careful in the iteration scheme, as divergence is very easy to encounter! The final charge density is shown in Figure 6 and the final potential is shown in Figure 7. One can see that the final charge still resembles the initial charge and so is the case for the final potential.

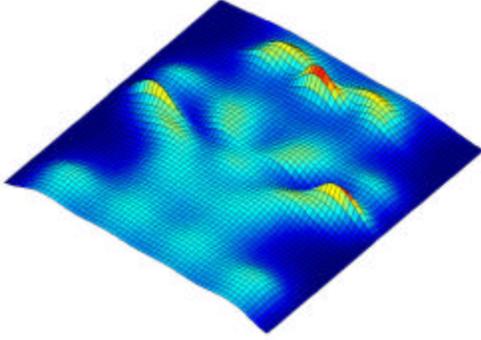


Figure 6: Final charge density calculated using the coupled GF and Poisson solvers.

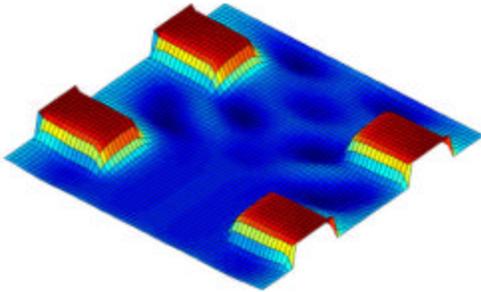


Figure 7: Final potential profile calculated using the coupled GF and Poisson solvers.

To obtain a conductance plot that corresponds to that in Figure 5, but *with* the self-consistency, one would have to do the whole above procedure (the GF recursion, the Poisson solver iteration, and the coupled GF-Poisson solver iteration) at *each* energy level.

4 CONCLUSION

In this paper, we have examined a method for obtaining more realistic charge densities in quantum dots using a coupled recursive Green's function solver and a Poisson solver. We have also sketched out the techniques used in the calculations. The final results are plots of more realistic charge densities and potential profiles. More work can be done to examine the effect of self-consistency on conductance in quantum systems. Future work will address many-body corrections to the potential.

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