EE32 Device Simulation Lab

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Lab 6: Nano-scale Device modelling: the Green's function method

In quantum transport theory, the density matrix is the central quantity from which all quantities of interest can be obtained.

The problem then is to find the density matrix in a chosen representation. For this it is not enough just to know the details of the device through *(H+U);* we also need to know how the device is coupled to the two contacts and the scattering processes that are effective within the device. This information is contained in the self-energy functions.

Given all of this information (*H, U,* Σ_1 Σ_2 Σ_S*,* μ 1 and μ2), the NEGF formalism provides clear well-defined relations that can be used to calculate the density matrix from which the electron density and current can be obtained.

Choice of representation

For simplicity, we would like to assume a uniform conductor as shown in figure which in a way represents a state of MOS too and all parameters are taken to be same as in original paper[1].

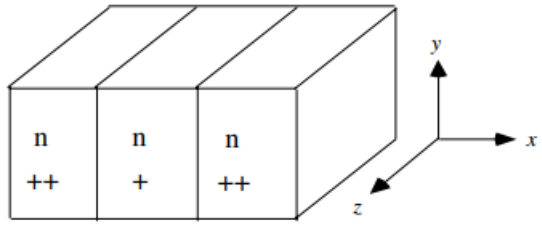
We find it convenient to use the eigenstate representation for the transverse dimensions *(y-z),* but a discrete real space lattice for the longitudinal direction.

We can separate the overall Hamiltonian *H* into a longitudinal part H_L and a transverse part H_T

$$H_L \equiv E_c - \frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)$$

$$H_T \equiv -\frac{\hbar^2}{2m}\left(\frac{d^2}{dy^2} + \frac{d^2}{dz^2}\right) + U_t(y,z).$$

A



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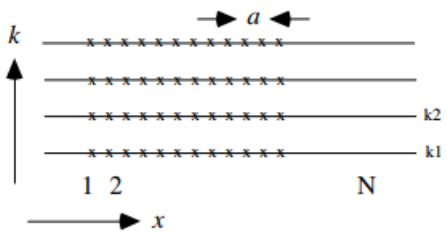


Calculating equilibrium potential profile and electron density

The equilibrium problem can be done in two ways, one that uses the concept of Green's functions and one that does not.

Equilibrium problems can be handled by solving the Poisson equation self consistently with the law of equilibrium statistical mechanics which requires all the eigenstates of the device (that is, $H + U$) to be filled up according to the Fermi function. If we simply truncate the matrix, which makes the calculated electron density go to zero at the ends. This would be an appropriate boundary condition if we had an infinite potential wall at the ends. However, what we actually have is an open boundary and this is better described by periodic boundary conditions which effectively wrap the right end around and connect it to the left end.

However, it is important to note that we are getting rid of end effects by artificially wrapping the device into a ring. We are not really doing justice to the open boundary that we have in the real device. The self-energy method described allows us to do that.

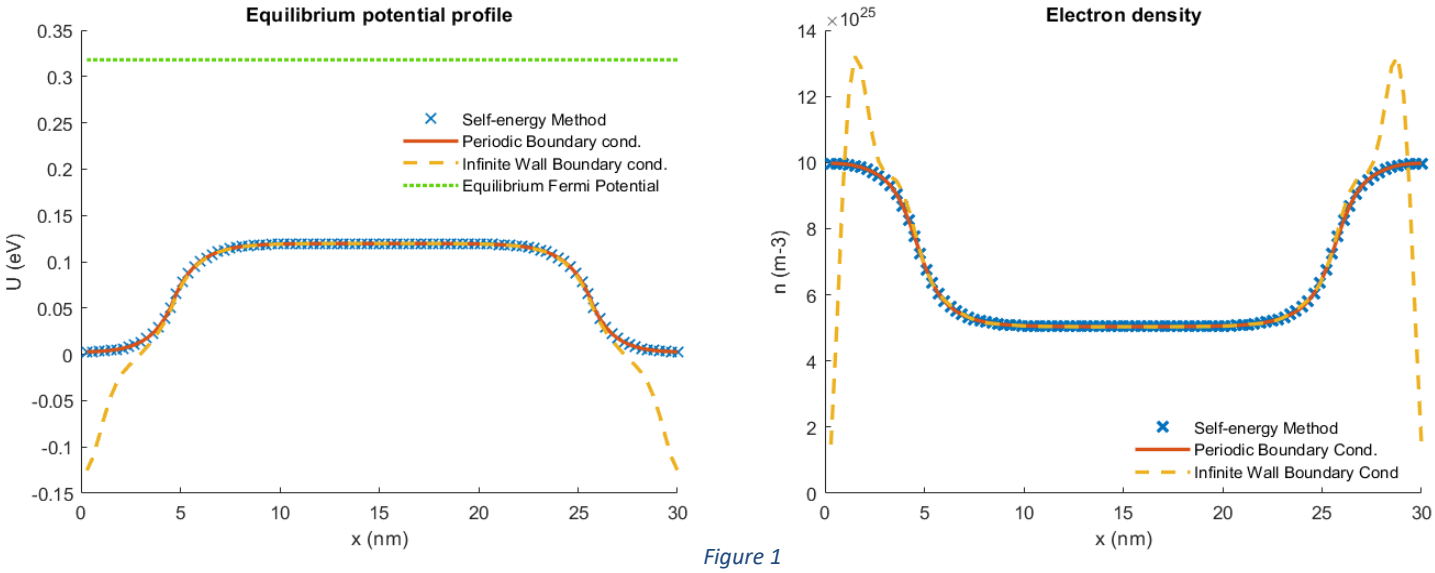


Figure 1

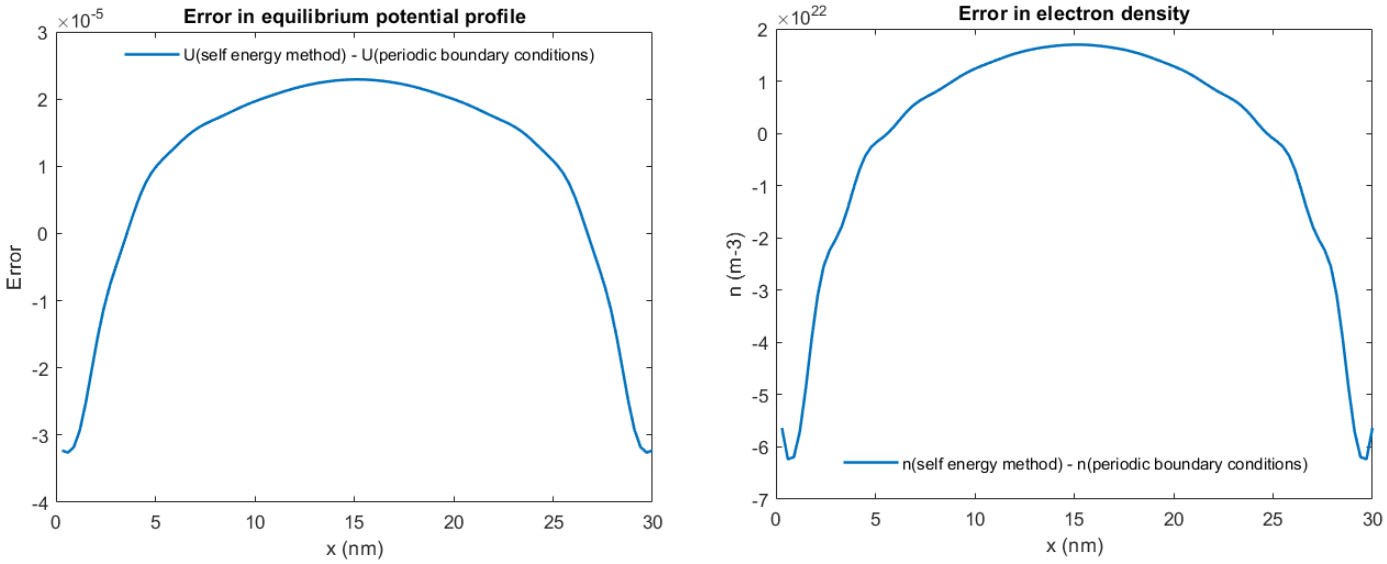


Figure 2

One might wonder what we have gained by introducing an unnecessary integration over the energy coordinate, *E* as required for the Green's function. What makes this extra complication worthwhile is the convenience it affords in the treatment of open systems.

Indeed if our interest was limited to closed systems there would be little reason to use Green's functions. But for open systems the Green's function method allows us to focus on the device of interest and replace the effect of all external contacts and baths with self-energy functions. The full power of the self-energy method becomes apparent when we model a device under bias—a problem that cannot be handled with periodic boundary conditions.

It might also appear that self-energy method is just another method of handling boundary effects. The point we want to make is that the self-energy terms have two effects. One is to change the Hamiltonian, which changes the eigenstates and their energies. But more importantly, it introduces an imaginary part to the energy determined by the 'broadening' functions. They imply how the wavefunction and the associated probability decays with time. A mathematical formulation is provided for that in the paper.

Device driven out of equilibrium by applied bias (neglecting scattering effects)

If the device is connected to two contacts with different Fermi levels $\mu 1$ and $\mu 2$. Using the formulations as provided in the paper, we get the following results. The second graph describes different ways of getting the current in the device (resulting to the same answer)

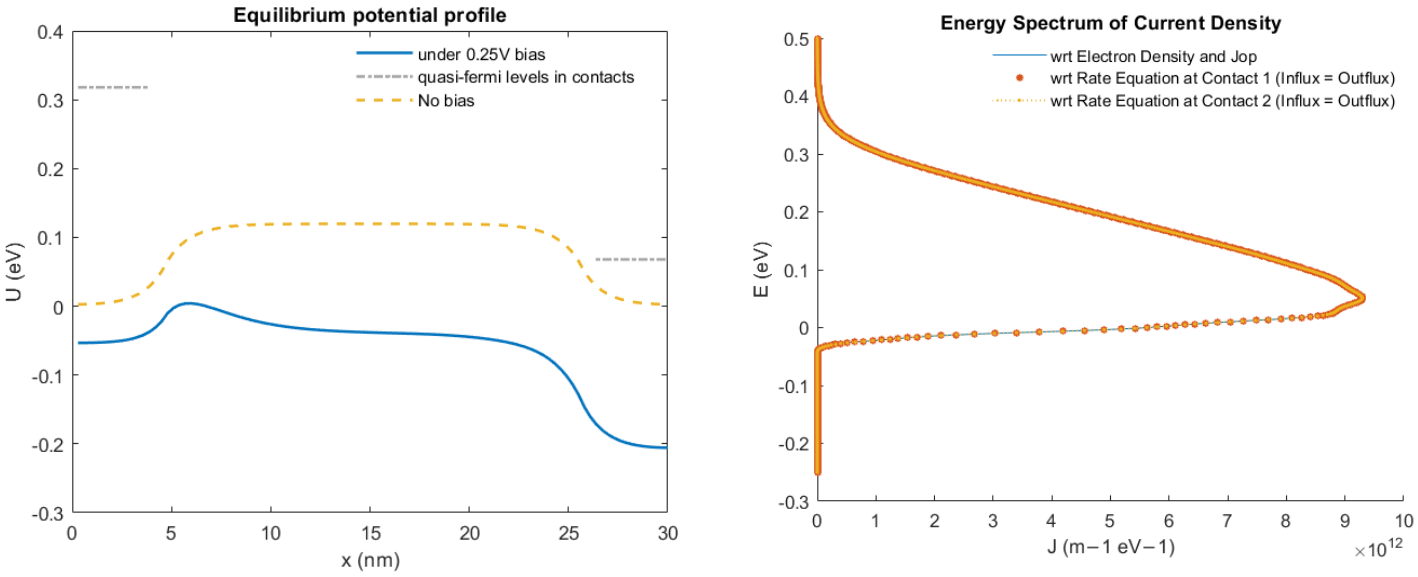
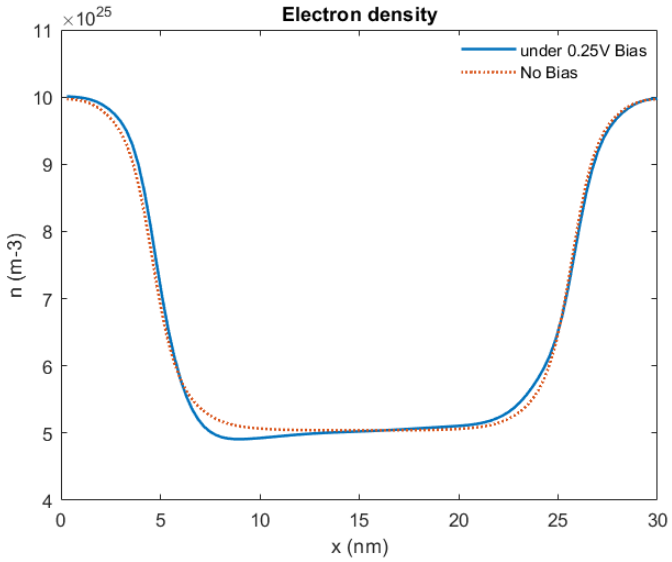


Figure 3

One could associate this external drop with the ideal contact resistance that leads to a non-zero resistance for ballistic conductors. This drop is often obscured in the presence of a large barrier, but is quite apparent in the present example because the barrier is only 100 meV. Such effects are likely to be important for ballistic devices, even with semiclassical models. It is interesting note that *U(x)* under bias is relatively flat inside the middle nC region, unlike what we are used to in MOS transistors.

This unusual profile results from a combination of two factors:

(1) lack of scattering which eliminates any 'voltage drop' inside the device, and
(2) high electron density which screens out the end effects within a short distance making the flat potential profile obvious



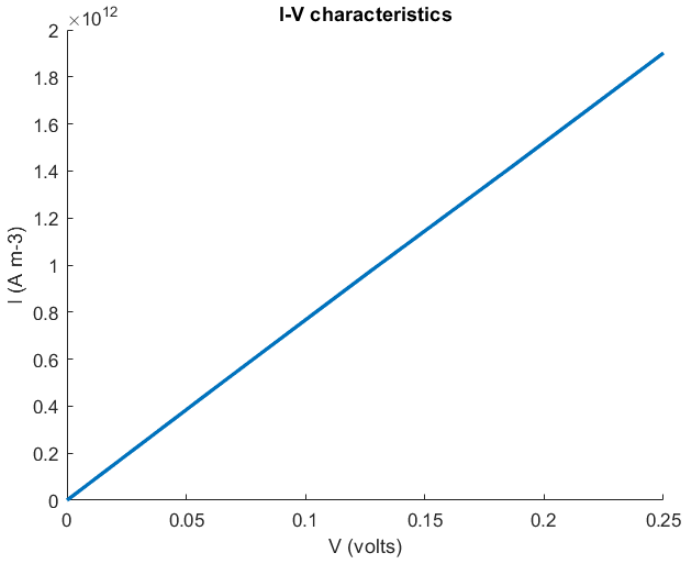
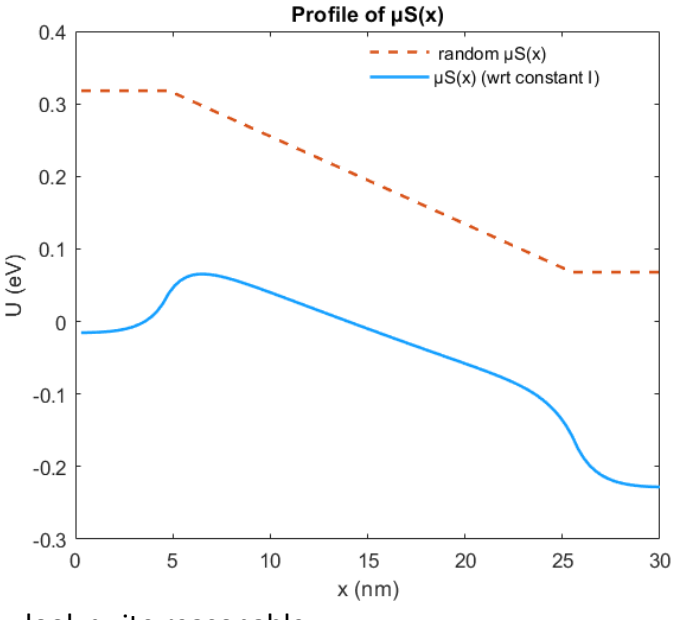


Figure 4

Incorporating scattering effects:

Scattering processes enter the NEGF formalism through the self energy function. The NEGF formalism provides clear prescriptions for calculating $\sum_S$ for every scattering mechanism that we can think of and thus can be used to investigate the effect of different scattering processes from first principles.

We will find that the current will not be the same everywhere inside the device. We could interpret this lack of current conservation as an inflow or outflow of current at the scattering contacts. But scattering processes lead to an exchange of energy without an exchange of particles, so that we need to ensure that the current at the scattering contacts is zero. This can be done by adjusting the μSn self-consistently so as to reduce dI/dx to zero.



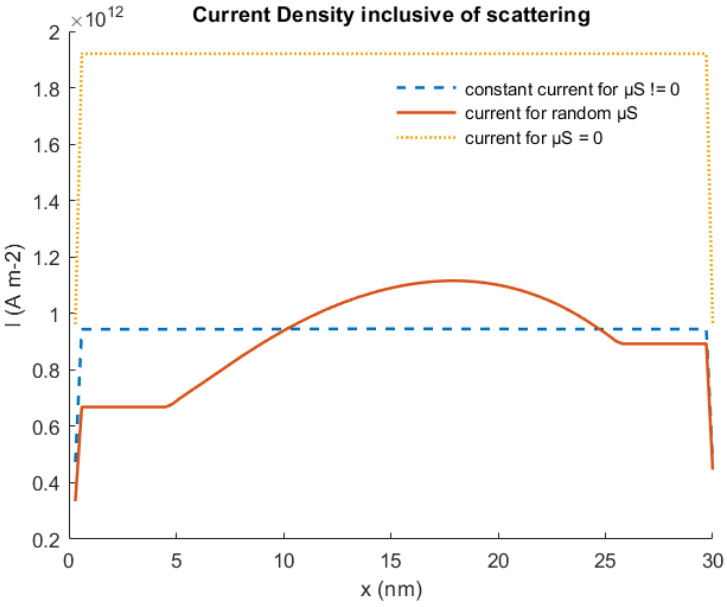


Figure 5

The potential drops linearly across the device instead of remaining flat since we have now effectively introduced a resistance. The fraction of the voltage dropped inside the device is increased relative to the ballistic case. The energy spectrum of the current now moves downwards as we go from contact 1 towards contact 2 as the hot electrons relax their extra energy.

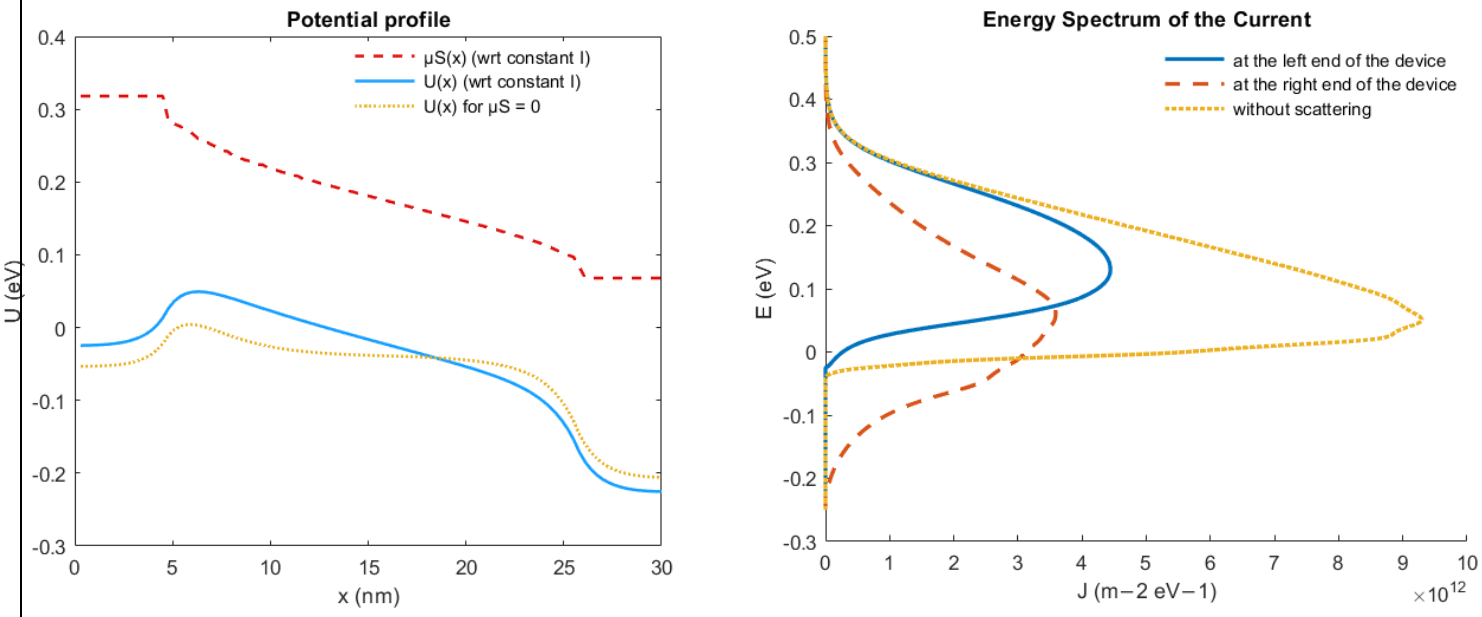


Figure 6

Note:

It is important to remember that the NEGF, with all its impressive sophistication, does not automatically include 'everything'.

For all the mathematical formulations, refer to the original paper[1]

References:

[1] S.Datta, Nanoscale Device Modeling: the Green's Function Method, Superlattices and Microstructures, vol.28, p.253 (2000)