DEPHASING EFFECT IN A*B INITIO* MODELING OF QUANTUM TRANSPORT THROUGH MOLECULAR DEVICES

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In recent years much attention has been directed towards the development of nanometer scale devices. This interest has been mainly fuelled by the advancements in experimental micro/nano-fabrication methods as well as the search for alternative electronic devices that bypass the upcoming miniaturization limits of CMOS technology [1] where certain undesirable quantum effects appear. It is clear that self-organised nanostructures, such as molecules and carbon nanotubes, are excellent candidates for sub-micron electronic systems and will potentially play a crucial role in future technologies. Electron transport in these systems is partially coherent, that is interference effects are present but attenuated due to interactions. Therefore theoretical tools allowing one to accurately design and predict the characteristics of nanodevices from an atomistic viewpoint are of growing importance.

In this work, we study the effect of decoherence on the current-voltage (*I-V)* characteristics of a benzene molecule connected to carbon nanotube leads (see fig. 1) using a self-consistent *ab initio* technique. For calculating nonequilibrium quantum transport (i.e. any external bias potential) properties of atomic/molecular electronic devices, we employ the first principles density functional theory (DFT) approach used in parallel with nonequilibrium Green`s functions (NEGF) [2,3]. DFT allows us to find the energy levels of the system and once this is known we can determine the nonequilibrium density matrix from NEGF. The self-consistent procedure is shown in fig. 2. This DFT-NEGF *ab initio* formalism permits us to study open quantum systems composed of a central region (i.e. the molecule) and the connecting semi-infinite leads, in which the particular atomic structure and effective electron potential are calculated. This powerful technique has been shown to be very useful and accurate, in comparison with experimental data, in many atomic/molecular scale systems [4-7].

A drawback of this method is that transport is entirely coherent. In real devices inelastic collisions result in partial and eventually complete loss of coherence. These processes must be included in the calculations in order to accurately simulate nanoscale devices. It is possible to include *ab initio* electron-phonon interactions, but this becomes impractical for systems larger than several atoms. Using the fictitious voltage probe model proposed by Büttiker [8] in the NEGF formalism, we have worked out a single-parameter analytical method of introducing dephasing in a quantum device of any size. This result is expressed simply as a modified transmission coefficient T given by the sum of a coherent and an incoherent contribution.

In Büttiker`s approach, typically employed in quantum dot or 1D atomic chain systems, the energy levels found in the central region of the device are connected to artificial electron reservoirs via fictitious voltage probes. A certain fraction of electrons, determined by the value of the adjustable parameter, travelling through the central region will scatter into a reservoir losing their phase memory before being reinjected into the device. The conservation of current is imposed by choosing the chemical potential in each reservoir so no net current flows through the fictitious probes. This condition is automatically satisfied in our expression of T. We show that our result is a generalization of Büttiker`s original result for a single scatterer. The effect of decoherence is included into the calculations, by matrix multiplication, once the DFT-NEGF procedure has achieved self-consistence (see fig. 2). The main advantages of this tool are it`s simplicity and the fact that is does not add any computational

time. Eventually, using this method, we hope to analyse complex nanocircuits in which the connecting partially coherent elements would be partitioned.

We shall present the total transmission coefficient T as a function of energy for different values of applied voltage and dephasing constant. We shall also show a plot of the current versus the applied voltage for different values of dephasing constant. Note : We expect to obtain all simulated results before long.

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Figures:

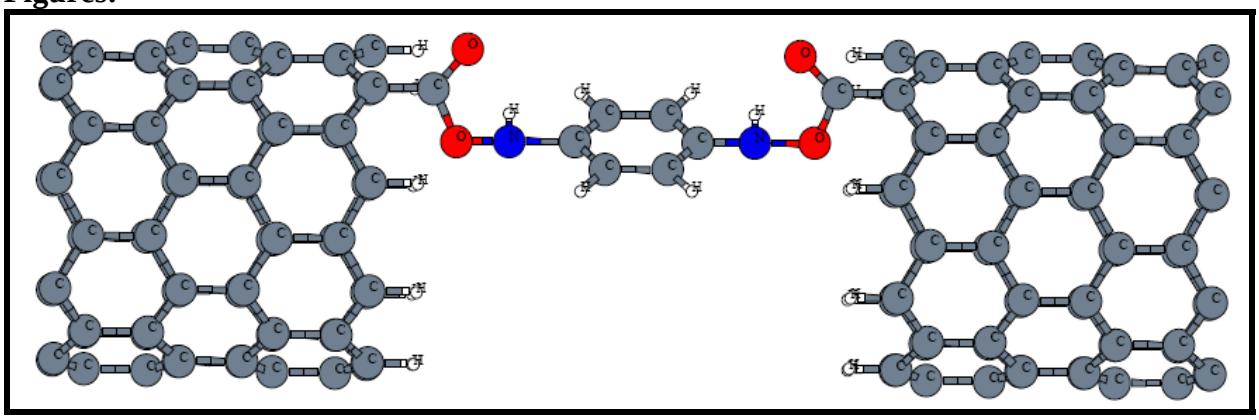

Figure 1 : Benzene molecule coupled to carbon nanotube leads.

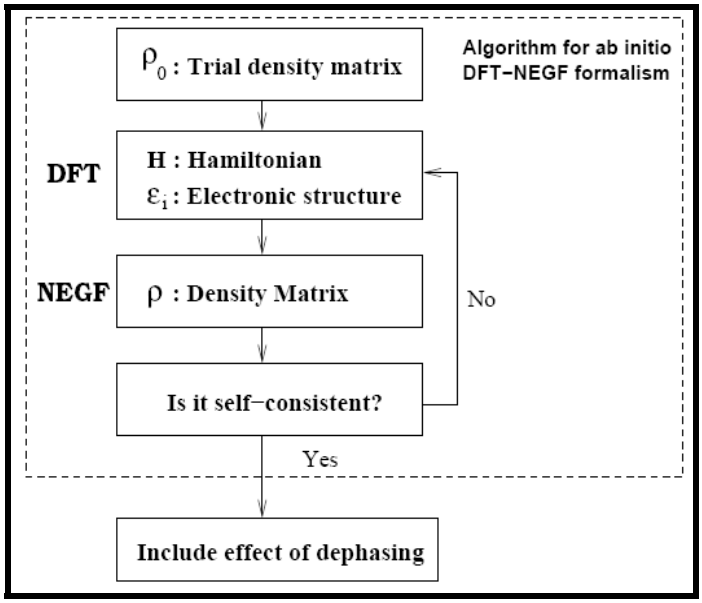

Figure 2 : Algorithm for DFT-NEGF formalism.