# A Frequency-Dependent QM/EM Method: Multi-Scale Simulation of Electronics

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Abstract

Because of fast development of fabricate technique, it is expected that the scale of transistor will go below 10nm in a few years. Under such scale, properties of electrons will be dominated by quantum mechanics effects. In order to handle such a situation, an amount of quantum mechanics methods have been developed. However, the most important defect of all these methods is extremely time-consuming during calculations, especially when more atoms contained. Therefore, when a system consists of a core device under atomic scale and a broader environment outside, a hybrid method which combines quantum mechanics (QM) and electromagnetic (EM) has been proposed, resulting in less accuracy but much faster speed comparing with purely QM solver if this system could still be dealt with by it. For the system mentioned above, its active core device which contributes most properties is simulated by QM solver, while the left environment part containing a large number of atoms which can hardly be solved by QM method, is calculated by EM solver. Moreover, effect on the interface and communications between two solvers should be considered. As a result, this QM/EM method balances the accuracy and efficiency.

The QM/EM method has been successfully developed in time-domain which can now solve steady-state [1] and time-dependent [2] problems. In this work, the application of this method is extended into frequency-domain. Within EM solver, system is treated classically by solving Maxwell's equations directly in frequency domain. Basing on time-dependent density functional method (TDDFT) and non-equilibrium green's function method (NEGF), electronic transport properties are investigated in QM solver. By defining a double-time Fourier transform, its energy spectrum can also be explored [3]. In order to realize an information exchange between QM and EM region, a coupled self-consistent scheme is adopted. Potential distribution V on the interface between two regions is solved by EM solver as the boundary conditions for QM solver. After accomplishment of QM simulation, current density J on the interface calculated by QM solver is fed back to EM solver as its boundary condition. This process is iterated until potential distribution and current density converge.

Basing on this QM/EM method, a carbon nanotube device depicted in Fig. 1 is studied in frequency domain. Result obtained directly from frequency region is compared with that from time-dependent calculation by a numerical Fourier transform $G(\omega) = I(\omega)/V(\omega)$ . A very well agreement can be found in Fig. 2 upon frequency up to 0.6ev (~70THz) by this comparison, which validate this frequency-dependent QM/EM method.

## REFERENCES

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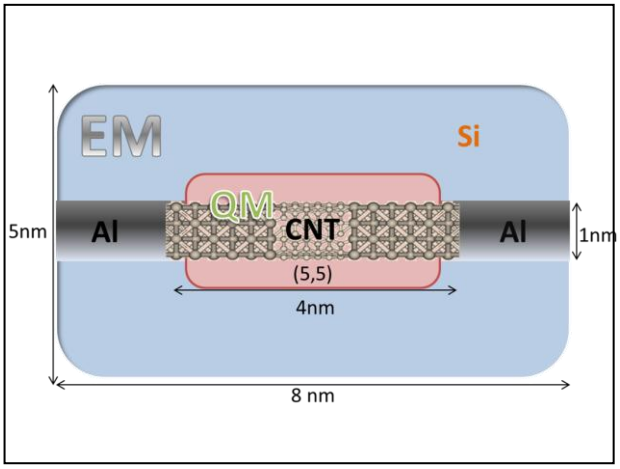


Fig. 1. A (5,5) CNT sandwiched by two aluminum leads in the center of a silicon environment

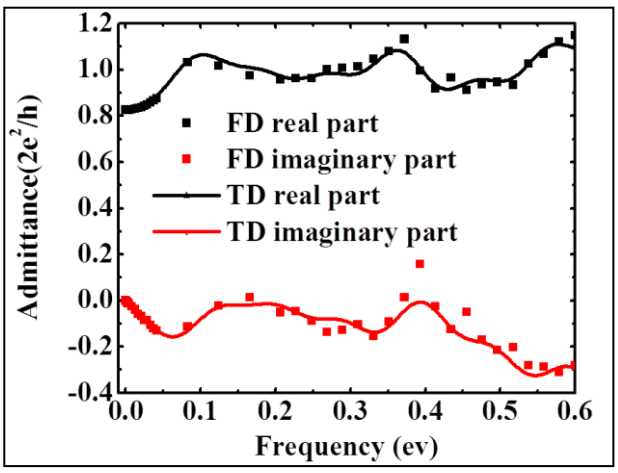


Fig. 2. Solid line: real (imaginary) part of dynamic admittance from time-dependent QM/EM calculation; dashed line: real (imaginary) part of dynamic admittance directly from frequency-dependent QM/EM method. A very well agreement can be found from this picture.