URSI GASS 2021, Rome, Italy, 28 August - 4 September 2021

Combining Electromagnetic and Quantum Simulations at the Nano-Scale

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The progress of nanotechnology allows the design and fabrication of new electromagnetic devices such as nano-antennas and rectifying antennas [1]. The nano-scale size of such devices often leads to the appearance of new quantum effects, which are not found in the classical, larger size devices. Such effects can be used for light harvesting, and other light-matter interactions that can be useful for photovoltaics, sensing, and nano-scale transmission. The modeling of such devices poses several challenges. Firstly, the use of average dielectric properties is no longer correct, and one has to resort to more detailed, atomistic, and quantum simulations of the devices. This poses a formal challenge of combining electromagnetic simulations with quantum modeling and, in particular, with the successful method of time dependent density functional theory (TDDFT). Aside from formal problems, the computational cost, of calculating the quantum properties with the time dependent electromagnetic potentials, can become prohibitively expensive.

In this work, we describe several strategies to achieve this goal. We start by reviewing the formalism of TDDFT and the inclusion of external fields in the quantum Hamiltonian within the semi-classical approach. We then describe the formulation of both the Lorenz and Coulomb gauges within TDDFT in the real-space framework [2]. The time-retarded electromagnetic potentials are calculated via real-space integration, which is also used in classical electromagnetic modeling. To reduce the cost of those integrals, we demonstrate highly efficient methods based on fast Fourier transform (FFT) for the calculation of the time-retarded electromagnetic potentials. Finally, we show how faster propagation techniques and massive parallelization can make the simulation of large systems of practical interest feasible, making it possible to simulate, for example, nano-antennas from first principles. We demonstrate our approach on several carbon based elongated structures.

References

[1] See e.g. G. Moddel and S. Grover, “Rectenna Solar Cells”, Springer Science + Business Media, New York (2013).

[2] D. Gabay, A. Yilmaz, V. Lomakin, A. Boag, and A. Natan, “A Lorenz gauge for TDDFT”, Phys. Rev. B **101**, 235101, (2020)