Simulating Energy Transfer in Collections of Quantum Dots

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In recent years, quantum dots have shown promise as novel semiconductors in a wide array of consumer applications, particularly in areas that require a high degree of control in their optical properties. Modeling the collective response of such many-dot systems due to externally-tuned electromagnetic pulses necessarily requires methodologies that accurately capture both electromagnetic interactions between dots as well as their effects on the time-evolution of each dot.

Conceptually, the simplest approximation of an exciton in a quantum dot consists of a two-level system immersed in a time-harmonic electric field tuned to the transition frequency of the system's energy levels. In the presence of such a field, the semi-classical Maxwell-Bloch equations (MBEs—also called optical Bloch equations) govern the time-evolution of a dipole moment. The variation of this dipole necessarily gives rise to an emitted field, allowing for energy transfer in assemblages of dots. Moreover, the large difference in timescales describing the incident field and exciton lifetime present interesting computational challenges.

In addition to the large disparity in time scales, the loss of accuracy in the field in the vicinity of the dot remains one of the principal challenges when using discrete methods such as DG/FEM (A. Baczewski, "Integral equation and discontinuous Galerkin methods for the analysis of light-matter interaction" 2013). The equivalence principle gives one possible approach to overcoming this bottleneck by covering the dot with a spherical surface and then employing quasi-analytic field computations (J. Li and B. Shanker, arXiv:1412.8171). Our proposed algorithm makes use of an efficient time-domain integral equation (TDIE) method to solve for representations of incident and radiated electromagnetic fields on arbitrary arrangements of such spheres. The TDIE solver makes use of a mesh-free representation of surface fields in terms of spherical harmonics, thereby eliminating singular integrals and dramatically reducing complexity over more conventional volume-based approaches. Further, the resulting Volterra integrals have demonstrated considerable stability and accuracy. A numerical solution of the MBEs subsequently governs the evolution of the dot inside each sphere, thus the resulting method accurately captures the excitonic dynamics in moderate collections of dots in a self-consistent manner. We will present results demonstrating energy transfer between two dots at the conference.