Numerical Challenges in Purcell Factor Evaluation for Nanoscale Light-Matter Interaction

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Project Type: Bachelor, Master Semester project (or a combination or all)

Context: The modification of a quantum emitter's spontaneous emission rate in a structured electromagnetic environment (first discussed by Purcell in 1946) is a hallmark of light–matter interaction, quantified by the Purcell factor, defined as the ratio of the modified emission rate to its free-space value. While spontaneous emission is fundamentally a quantum process described by quantum electrodynamics, the photonic density of states (PDOS) on which it depends is a classical quantity, making the Purcell factor calculable as the ratio of the modified PDOS to that of free space using classical electromagnetic theory [1]. In lossless systems, such as dielectric microcavities, the Purcell factor directly reflects changes in radiative emission; however, in lossy systems like plasmonic nanostructures, the PDOS includes both radiative and non-radiative channels [2]. Computing the PDOS demands the Green's function of the system, which is analytically known only for simple geometries; for more complex structures, numerical solutions to Maxwell's equations are required.

Project overview: The accurate evaluation of the Green's function at small emitter–nanoparticle (Figure 1a) separations is challenging. Numerical results can deviate significantly from analytical predictions (Figure 1c). The most straightforward improvement is to increase the number of degrees of freedom in the simulation (e.g., by refining the mesh), which improves convergence but can still fail at very small distances. The aim of this project is to develop strategies to achieve reliable convergence for geometries lacking analytical solutions, without incurring prohibitive computational cost. We use the Surface Integral Equation (SIE) approach [3], a boundary element method, that is computationally efficient because it solves the electromagnetic problem only on the structure's surface (Figure 1b).

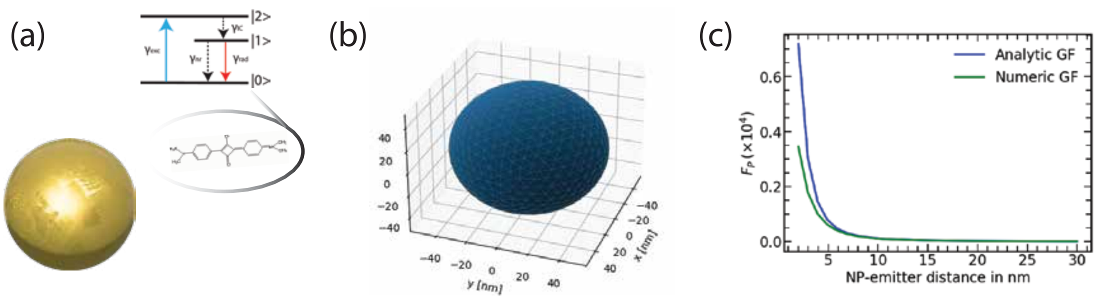

Figure. (a) Schematic of the nanoparticle-emitter system, where the emitter is modeled as a simple three-level system. (b) Discretization of the nanoparticle surfaced used in the SIE method. (c) Deviation of the numerical results from the analytical solution at small nanoparticle-emitter separations.

What the student will do: The student will work in the field of nanophotonics, focusing on the theory and modeling of nanostructure-quantum emitter systems. To begin with, they will be introduced to the physics of nanoscale light–matter interactions through a selection of literature papers, which they will be expected to study early in the project. Their investigation will begin with spherical geometries, where analytical solutions are available for direct comparison. Once this baseline is established, they will aim to bridge the gap between analytical and numerical results and subsequently develop a general strategy to treat non-spherical geometries in a consistent and accurate manner. For the computational work, a good working knowledge of Python is recommended, as the existing simulation framework is implemented in this language.

Benefits: They will work in a highly active research area, gaining valuable insight into current developments and potential future opportunities. The project will provide hands-on experience with a home-built solver for electromagnetic simulations, while exploring computational strategies to improve the estimation of the Purcell factor. Comparisons with analytical solutions will help the student develop both technical expertise and research intuition. They will work closely with a doctoral assistant in the group and have the opportunity to collaborate directly with experimental teams, fostering a strong sense of scientific teamwork.

References:

1. Novotny L. et al., Chapter 8, Principles of Nano-Optics (2012)
2. Pelton M., Naturę Photonics 9, 427-435 (2015)
3. Kern A. et al, J. Opt. Soc. Am. A 26, 732-740 (2009)