OPTICAL TRAPPING OF BIOMOLECULES

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Direct optical trapping of single molecules *in solution* has recently been reported, with a technique based on confocal fluorescence microscopy. We are working to develop a quantitative model for optical trapping of DNA fragments labeled with intercalating dyes, and trapping of dye-labeled polystyrene spheres. In the experiments of Zare and Chiu, biomolecules labeled with fluorescent dye markers are polarized by the electric field of a laser beam within the microscope probe volume; the interaction of the laser with the induced polarization produces an optical "trap." The depth of the trap depends on the polarizabilities and hyperpolarizabilities of the labeled molecules.

The probability that a molecule initially found in the microscope probe volume will return to that volume has been determined as a function of time, by measuring the time interval Δt between photon bursts observed when a labeled molecule enters or re-enters the microscope probe volume. The distribution of intervals Δt between photon bursts deviates from Poissonian statistics at short times (< 600 ms). The observed deviations are too large to be explained by the short-time correlations in molecular positions in the absence of the trapping field. Our goal is to model the distribution of re-entry times and the laser power dependence of the re-entry probabilities.

To analyze the interaction between a laser field and large molecules, it is essential to consider the intramolecular distribution of the induced polarization, rather than using a single, global polarizability. For instance, the elongated DNA fragments studied by confocal fluorescence microscopy are longer than the optical trap, in one direction. We have developed a nonlocal polarizability density theory that automatically accounts for the nonuniformity of the perturbing field on the molecular length scale, and gives the induced polarization as a function of position in the molecule.

Our analysis starts with an interacting site model, taking the dye markers as spatially extended, polarizable sites. As a first approximation, this is useful because the dye molecules are substantially more polarizable than the "host" biomolecule or the solvent, at the laser frequency. The spatial extent of the dye molecules is significant, since they may lie in close proximity: experimental ratios between intercalating dye molecules and DNA base pairs range up to $\sim 1{:}10$. In outline, this project involves:

- determining the configuration of an intercalated dye molecule, to a good approximation,
- constructing approximate polarizability and hyperpolarizability densities for the dye marker molecules in their ground and excited states,
- setting up a distribution of dye sites on the host molecule,
- coupling the site polarizability densities to obtain approximate, overall response tensors for the biomolecule with the dye markers in specified states,
- finding the potential V_{eff} for the interaction of the labeled molecule with the laser field, and
- modeling the molecular motion through the solvent in the presence of V_{eff}.