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An algebraic method to determine the local field of condensed system

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Abstract. An algebraic method is proposed to generate a self-consistent converged complex polarizability of atoms and molecules from limited available data. An iterative method is also suggested to generate the general accurate local field models of condensed systems. The effect of the local fields on the photoabsorption cross sections as the functions of the media density and structures has been studied in the present work. A substantial influence on the photoabsorption cross section has been found when the media density exceeds a critical density in the present unique model.

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Key words: algebraic method, local field effect, photoabsorption cross sections.

1 Introduction

The current understanding of photoabsorption processes has been established from theoretical research assuming the interaction of a laser pulse with gases at low pressures. For the isolated atom or molecule, the main characteristics of the photoabsorption process can be explained by the polarizability of the target. The photoabsorption cross section can usually be represented in terms of linear polarizability [1],

$$\sigma = \frac{4\pi\omega}{c}\zeta \tag{1}$$

where ζ is the imaginary part of the complex dynamic polarizability of an isolated atom or molecule, and is assumed scalar for simplicity. σ is the photoabsorption cross section, ω is the frequency of the laser pulse, and c is the light velocity. This is the fundamental expression for photoabsorption cross sections used for ideal gas in most of theoretical

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studies [2-6] and represents only the properties of isolated atoms or molecules in ideal gas.

However, that at sufficiently high intensities of the laser and high densities of the medium the polarizability of the target will be perturbed by the fields of other ions or atoms in the vicinity [7-10]. This impact of the surrounding medium on the photoabsorption spectrum is interesting in many respects [11-15]. A derivation of photoabsorption cross section for an atom embedded in a dielectric in which the atom and the nearby oscillators of the dielectric mutually interact via the electrodynamic field is needed. It is known from the Beer-Lambert's law that the number density of the medium significantly affects the measured cross-sections [16-21]. The photoabsorption cross section σ at photon energy ω is determined by the Beer-Lambert's law,

$$\sigma(\omega) = \frac{1}{Nl} \ln\left(\frac{I_o}{I}\right) \tag{2}$$

where I_o is the intensity of the incident light, I is the attenuated intensity of the transmitted light, l is the transmitted length of light, and N is the number density of the system. Unless indicated atomic units are used throughout.

The experimental determination of accurate absolute values of photoabsorption cross sections is a difficult procedure using Beer-Lambert's law. One of the most troublesome problems encountered in atomic beam experiments is the accurate determination of the density of the atomic beam. In order to describe the response of a bulk material (high density), the effective permeability is needed. This can be found by averaging the effective dipole field over a large region. The results, known as the Clausius-Mossotti equation, or the Lorentz-Lorenz formula, can be used to relate the bulk effective permeability to the single atomic polarizability [16].

The functions chosen to relate the polarizability of the discrete dipoles to the dielectric properties of the bulk material have been developed in history [19-21]. The Clausius-Mossotti relation provides an exact function for the particular case of an infinite cubic lattice of dipoles in the dc limit, where the size of the dipoles divided by the radiation wavelength approaches zero [19]. Numerous schemes for modifying the Clausius-Mossotti relation have been proposed to improve the accuracy the coupled-dipole method for realistic, finite-sized scattering geometries [20]. Recently, Draine and Goodman developed an expression for polarizability of an infinite array of polarizable points so that the array exhibits the same dispersion relation as a continuum with dielectric constant ϵ. Draine and Flatau claimed in 1994 that this representation yields the best accuracy to date of these expressions for dipole polarizability [21].

A problem is that the electronic structure of these condensed system is not accurately known. Great effort are made to improve this description and the role of the spectroscopies. The data of the photoabsorption cross section is not enough, however, the available data will contain the influence effect model of the state of aggregation. Using the limited available data, in the present work, an algebraic method is developed to study the local field effect on the photoabsorption cross section in any media.