Three-body dispersion coefficients for excited hydrogen atoms

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Abstract. The three-body van der Waals dispersion coefficients $Z(l_1 l_2 l_2)$ (up to $l_i = 5$) for the H(1s)-H(1s)-H(1s) and H(2s)-H(2s)-H(2s) systems are calculated by virtue of the dynamic polarizabilities at imaginary photon frequencies. The expression for the 2^l-pole dynamic polarizabilities of atomic hydrogen is derived by application of the integration properties of the one-dimensional radial Coulomb Green's function. The results for the H(1s)-H(1s)-H(1s) system are consistent with previous calculation in the literature, while the results for the H(2s)-H(2s)-H(2s) systems are reported for the first time, and they are the main contribution of this work.

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1 Introduction

In the last decades, the van der Waals interaction between atoms has received increasing attention due to laser trapping investigations and the realization of Bose-Einstein condensation for some elements such as the hydrogen and a few alkali and alkaline-earth atoms [1,2]. The hydrogen atom has been an important investigation subject, because it is owed to a whole family of atoms and ions, whose properties are described by one-electron potential models for the electrons in the atomic valence shell. Hydrogen and one-electron ions trapped in nanostructures such as fullerene molecules (C_{60}) [3,4], are systems emerging from quantum confinement technology, which may also benefit from efficient calculation procedures for van der Waals dispersion coefficients.

The van der Waals dispersion coefficients are directly related to dynamic polarizabilities [5], which describes the distortion of electronic and charge distribution of an atom in the presence of an oscillating electric field. The problem of evaluating the dynamic polarizabilities and dispersion coefficients for atomic hydrogen have been widely studied by different

methods in various forms [6–15]. The most recent studies have been carried out by Masili and Gentil [16] and Groote *et al.* [17]. They make use of an efficient approach that provides high precision calculation of one electron multipolar dynamic polarizabilities and two- and three-body dispersion coefficients. The method is based on a variationally stable procedure of Gao-Starace [18–20] that has the advantage of fast convergence with respect to the number of terms of a basis set. However, this approach is limited to the ground-state and is not valid for the excited states.

It is known that the dispersion coefficients for excited alkali-metal atoms have been calculated [21]. To our knowledge, however, the dispersion coefficients for excited hydrogen atoms have not been evaluated. The purpose of this paper is to calculate the three-body van der Waals dispersion coefficients for H(1*s*)-H(1*s*)-H(1*s*) and H(2*s*)-H(2*s*)-H(2*s*) systems by virtue of the dynamic polarizabilities at imaginary photon frequencies [5]. The expression for the multipolar polarizabilities of atomic hydrogen is derived analytically by application of the integration properties of the one-dimensional radial Coulomb Green's function [22]. The results for the H(1*s*)-H(1*s*)-H(1*s*) system are compared with that previously calculated by Cebim, Masili and Groote [17], while the results for the H(2*s*)-H(2*s*)-H(2*s*) system are reported for the first time, and they are the main contribution of this work. It is found that the interaction energy is very much stronger for the H(2*s*)-H(2*s*)-H(2*s*) system. This large van der Waals interaction energy and the long lifetime of the metastable 2*s* hydrogen make this work very interesting and might have experimental implications in further quantum confinement investigation. On the other hand, the present approach is also valid for higher interaction orders and can be easily generalized for other excited states and for model potential systems [23–27].

2 Theory

2.1 Dispersion coefficient

A detail description of the van der Waals dispersion coefficients may be found elsewhere [5]. In short, those are the coefficients of the long-range interaction potential of dipole-dipole, dipole-quadrupole, quadrupole-octupole order and so on, between two atoms. The van der Waals interatomic potential is an asymptotic expansion in the internuclear distance R and expressed as

$$V(R) = -\sum_{k=3} \frac{C_{2k}}{R^{2k}}, \tag{1}$$

where C_{2k} are the two-body dispersion coefficients. For two hydrogen atoms, which are in state $\psi_{n_a 00}$ and $\psi_{n_b 00}$ respectively, the two-body dispersion coefficients are given by [28]

$$C_{2k}^{(n_a s, n_b s)} = \frac{(2k-2)!}{2\pi} \sum_{l_a=1}^{k-2} \frac{1}{(2l_a)!\,(2l_b)!} \int_0^\infty \alpha_{l_a}^{n_a 00}(i\omega)\alpha_{l_b}^{n_b 00}(i\omega)\,d\omega,$$

in which l_b is limited by $l_a + l_b + 1 = k$ and $\alpha_{l_a}^{n_a 00}(i\omega)$ is the 2^{l_a}-dipole polarizability of the hydrogen atom in the $\psi_{n_a 00}$ state at imaginary frequency.