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Nuclear Instruments and Methods in Physics Research B 266 (2008) 526–529

NIM B
Beam Interactions with Materials & Atoms

www.elsevier.com/locate/nimb

Dispersion coefficients for interactions between positronium and light atoms with pure Coulomb and screened Coulomb potentials

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Abstract

The Van der Waals two-body dispersion coefficients for interactions between the positronium (Ps) atom and light atoms have been investigated using highly correlated exponential basis functions in the framework of both pure Coulomb and screened Coulomb potentials. The C_6, C_8 and C_{10} coefficients for Ps–Ps and Ps–H interactions, and the C_6 coefficients for Ps–He interactions for both the screened and unscreened cases, are reported.

PACS: 34.20.Cf; 52.20.Hv; 34.85.+x; 36.10.−k; 36.10.Dr; 52.20.−j

Keywords: Debye plasmas; Van der Waals forces; Dispersion coefficient; Ps-atom interactions; Correlated wave functions

1. Introduction

The investigation on the Van der Waals two-body dispersion coefficients in the multipole expansion of second order long-range interaction between a pair of atoms is important for the quantitative interpretation of phenomena, for an example, the phenomena occurring in slow atomic beams [1–3]. The long-range part of the interactions between two atoms in their ground states can be written in the form of a series of inverse powers of the separation R. The Van der Waals force constants, particularly the leading term C_6 arising from the induced dipoles and decreasing as R^{-6}, are of great theoretical and experimental interest in atomic and molecular physics. The coefficients C_8 of the R^{-8} and C_{10} of the R^{-10} term come, respectively, from the instantaneous dipole–quadrupole and dipole–octopole interactions. Due to the Van der Waals interaction, the positronium (Ps)-atom interaction is attractive, and such attractive interaction will impact on the scattering cross sections [2–5]. Few studies have performed so far to calculate the dispersion coefficient C_6 for the positronium-atom interactions [2–4]. In this work, we have investigated the dispersion coefficients C_6, C_8 and C_{10} for the Ps–Ps, Ps–H interactions, and the dispersion coefficient C_6 for the Ps–He interaction, both for pure Coulomb and screened Coulomb potentials. Recently, several studies have been performed on the bound states [6–17], resonance states [12,13,17–19] and other structural properties ([11,15,16], references therein) for plasma-embedded atoms/ions in the framework of Debye concept of plasma modeling. Detail applications of Debye screening on atomic and molecular systems are available from the earlier works ([6–26], references therein).

2. Calculations

The long-range part of the interactions between two atoms a and b in their ground states can be written in the form of a series of inverse powers of the separation R as [27]

$$V_{ab} = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} - \cdots, \tag{1}$$

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doi:10.1016/j.nimb.2007.12.034

with

$$C_6 = \frac{3}{\pi} G_{ab}(1,1), \tag{2}$$

$$C_8 = \frac{15}{2\pi}[G_{ab}(1,2) + G_{ab}(2,1)], \tag{3}$$

$$C_{10} = \frac{14}{\pi}[G_{ab}(1,3) + G_{ab}(3,1)] + \frac{35}{\pi} G_{ab}(2,2), \tag{4}$$

where

$$G_{ab}(l_a, l_b) = \frac{\pi}{2} \sum_{nm} \frac{f_{n0}^{(l_a)} f_{m0}^{(l_b)}}{E_{n0}^a E_{m0}^b (E_{n0}^a + E_{m0}^b)}, \tag{5}$$

$E_{n0}^i = E_n^i - E_0^i$ is the excitation energy for atom i and is positive for the atoms in the ground state, $f_{n0}^{(l)}$ denotes the 2^l-pole oscillator strengths and defined by

$$f_{n0}^{(l)} = \frac{8\pi}{2l+1}(E_n - E_0)\left|\left\langle < \Psi_0 \left| \sum_i r_i^l P_l(\cos\vartheta_i) \right| \Psi_n \right\rangle\right|^2, \tag{6}$$

with $i = 1$ for Ps and H atoms and $i = 2$ for He atom.

For Positronium and hydrogen atoms, we have employed the Slater-type basis set

$$\Psi = \frac{\sqrt{2l+1}}{4\pi} \sum_{i=l}^{N} D_i r^{i+l} e^{-\lambda r} P_l(\cos\theta_1), \tag{7}$$

and for helium atom, we have used the wave functions

$$\Psi = \frac{\sqrt{2l+1}}{4\pi}(1 + \hat{O}_{12}) \sum_{i=1}^{N} D_i r_1^l P_l(\cos\theta_1) \exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}), \tag{8}$$

where λ, α_i, β_i, γ_i are the non-linear variation parameters, $l = 0$, 1 for S, P states, respectively, $D_i (i = 1, \ldots, N)$ are the linear expansion coefficients, $\hat{O}_{12}$ is the permutation operator on the subscripts 1 and 2 representing the two electrons, respectively. Here r_1 and r_2 are the radial coordinates of the two electrons and r_{12} is their relative distance. We use a quasi-random process ([12–19,23,25], references therein) to optimize the non-linear variational parameters α_i, β_i and γ_i. The parameters α_i, β_i and γ_i are chosen from the three positive interval $[a_1, a_2]$, $[b_1, b_2]$ and $[d_1, d_2]$;

$$\begin{aligned} \alpha_i &= \left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{2} \right\rangle\right\rangle (a_2 - a_1) + a_1, \\ \beta_i &= \left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{3} \right\rangle\right\rangle (b_2 - b_1) + b_1, \\ \gamma_i &= \left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{5} \right\rangle\right\rangle (d_2 - d_1) + d_1, \end{aligned} \tag{9}$$

where the symbol $\langle\langle \ldots \rangle\rangle$ designates the fractional part of a real number. The atomic unit (a.u.) has been used throughout the present work.

To investigate the effect on the dispersion coefficients C_6 under Debye screening, we assume that the leading term in the Van der Waals interaction between two atoms a and b in their ground states still has a form of R^{-6}, as

$$V_{ab} = -\frac{C_6(\mu)}{R^6} + O(1/R^8) + \cdots \tag{10}$$

Here the plasma effect on V_{ab} is reflected on the value of C_6, which now depends on the screening parameter μ, and is denoted by $C_6(\mu)$. The parameter $\mu(=1/\lambda_D)$ is called the Debye shielding parameter, and λ_D is called the Debye length. Similarly, to consider the plasma effect on the dispersion coefficients C_8 and C_{10}, we assume the coefficients depend on the screening parameter μ, and are denoted respectively by $C_8(\mu)$ and $C_{10}(\mu)$. To calculate the dispersion coefficients for the interactions among Ps, H and He atoms, one needs to obtain the energy levels for the positronium atom, the hydrogen atom and the helium atom in the different partial wave states with the optimum choices of non-linear parameters. To obtain the energy levels for hydrogen and positronium atoms with different Debye lengths, we diagonalize the Hamiltonian

$$H = -\frac{\rho}{2}\nabla^2 - \frac{\exp(-r/\lambda_D)}{r}, \tag{11}$$

with the wave functions (7). Here $\rho = 1$ is for the hydrogen atom and $\rho = 2$ for the positronium atom. For the helium atom we diagonalize the Hamiltonian

$$\begin{aligned} H = &-\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 \\ &- 2\left[\frac{\exp(-r_1/\lambda_D)}{r_1} + \frac{\exp(-r_2/\lambda_D)}{r_2}\right] \\ &+ \frac{\exp(-r_{12}/\lambda_D)}{r_{12}}, \end{aligned} \tag{12}$$

with wave functions (8).

3. Results and discussions

After calculating the energy levels and eigenfunctions, we use Eqs. (2)–(4) to calculate the dispersion coefficients for interaction between Ps–Ps, Ps–H and Ps–He. We present our results with pure Coulomb and screened Coulomb potentials for different screening parameters λ_D in Tables 1 and 2. In the pure Coulomb case, our results compare well with other values available in the literature [2,3]. The coefficients C_8 and C_{10} for the Ps–Ps systems compare well to the other results by considering the unscreened values of H–H system ([26,27], references therein) using the relation in Eqs. (14) and (15), as explained later in the text. To show the behavior of the dispersion coefficients with the increasing screening parameter μ, we present our calculated dispersion coefficients C_6 for the Ps–He interactions in Fig. 1 for both the screened and unscreened cases. We have not included the plots of the dispersion coefficients C_6, C_8 and C_{10} for the Ps–Ps and Ps–H interactions (shown in Tables 1 and 2) as the coefficients exhibit similar behavior with the increasing μ like that of C_6 coefficients for the Ps–He interactions. For the screened cases, our results show that the C_6 dispersion coefficients for Ps–Ps, Ps–H, and Ps–He interactions increase with increasing plasma strength. Our findings indicate that when the plasma