PHYSICAL REVIEW A **81**, 062506 (2010)

Dispersion coefficients for interactions between helium atoms in Debye plasmas

Sabyasachi Kar[1] and Y. K. Ho[2]
[1]*Center for Theoretical Atomic and Molecular Physics, The Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute of Technology, Harbin 150080, People's Republic of China*
[2]*Institute of Atomic and Molecular Sciences, Academia Sinica, Post Office Box 23–166, Taipei, Taiwan 106, Republic of China*

(Received 31 March 2010; published 11 June 2010)

Effect of Debye plasmas on the dispersion coefficients C_8, C_{10}, and C_{12} for interactions between atoms has been investigated using highly accurate correlated exponential basis functions. In the free-atom case, the dispersion C_{12} coefficient and the hexadecapole polarizability for helium are reported. The dispersion coefficients, hexadecapole polarizability, and $1s5g\ {}^1G^e$ state energy of helium for different screening parameters are also reported.

DOI: 10.1103/PhysRevA.81.062506 PACS number(s): 32.10.Dk, 34.20.Cf, 52.20.Hv, 31.15.ap

I. INTRODUCTION

Despite the fact that van der Waals interactions are often considered to be weak, they dominate the behavior of all neutral physical systems at separations of order appropriate for the system concerned. The investigation of the Van der Waals two-body dispersion coefficients in the multipole expansion of a second-order long-range interaction between a pair of atoms is important for the quantitative interpretation of the equilibrium properties of gases and crystals, of transport phenomena in gases, and of phenomena occurring in slow atomic beams [1]. The leading term of the interaction between two atoms at large separation R is the dipole-dipole interaction decreasing as R^{-6}. This term has a coefficient commonly called the dispersion coefficient C_6. The coefficients C_8, C_{10}, and C_{12} come, respectively, from the instantaneous dipole-quadrupole; dipole-octupole and quadrupole-quadrupole; and dipole-hexadecapole and quadrupole-octupole interactions, respectively.

In the present work, we have investigated the effect of plasmas on the dispersion coefficients C_8, C_{10}, and C_{12} for interactions between helium atoms and the hexadecapole polarizabilities of the helium atom using highly accurate correlated basis functions in the framework of a pseudostate summation method. The pseudostate summation technique, in which mainly the intermediate states of conventional second-order perturbation theory is replaced by a finite set of pesudostates, has been established as being very successful in evaluating a variety of interesting processes, including two-photon transitions and van der Waals dispersion coefficients [2]. The effect of plasmas is to produce an effective screening, characterized by a fundamental length scale determined by the temperature (T) and number density (n) of the charge particles, on the Coulomb potential. In this work, we have considered the Debye-Hückel screening model to represent the interaction between the charged particles. Besides certain limitations (for example, high-temperature and low-density limits), the Debye-Hückel shielding approach of plasma modeling is a very good example for illustrating the ingredients of modeling the ionic potential in weakly coupled hot plasmas [3,4]. The concept of Debye screening has been derived from the effective potential in weakly coupled plasmas. In weakly coupled plasmas, the coupling constant is much less than 1. There are several applications [3] of weakly coupled plasmas, for example, $n \approx 10^{11}$ cm^{-3}, $T \approx 10^4$ K for gaseous-discharge plasma; $n \approx 10^{16}$ cm^{-3}, $T \approx 10^8$ K for plasma in a controlled thermonuclear experiment; and $n \approx 10^6$ cm^{-3}, $T \approx 10^8$ K for plasma in the solar corona. For those plasmas, the coupling constants are 10^{-3}, 10^{-5}, and 10^{-7}, respectively [3,4]. The importance of Debye screening on astrophysical observations, in astrophysical plasma diagnostics, in calculating partition functions in thermodynamics, and in several other applications has been discussed in the literature ([3–6], and references therein).

In the free-atom case, several studies have been performed to calculate the dispersion coefficients C_6, C_8, and C_{10} for the interactions between two He atoms and the dipole, quadrupole, and octupole polarizabilities of the He atom [7–21]. Recently we also reported the effect of Debye screening on the dispersion coefficient C_6 [22], and have calculated the dipole, quadrupole, and octupole polarizabilities of He in its ground state [23,24]. The effect of Debye plasmas on hydrogenlike atoms has also been reported in the literature [25,26]. We have reported the dispersion coefficients for the interaction between two hydrogen atoms in Debye plasmas [22,27]. Details of the atomic process in the Debye plasma environments can be obtained from the recent review [6].

In this investigation, we employ highly accurate correlated exponential wave functions in which the exponent is generated by a quasirandom process to calculate the dispersion coefficients and the hexadecapole polarizability. There are no calculations reported in the literature, to the best of our knowledge, on the hexadecapole polarizability for He ($1\,{}^1S$) and the dispersion coefficient C_{12} for the He-He systems in free-atom cases. In the screening environment, there are no other results on the dispersion coefficient except our earlier work on C_6. In the present work, we have examined the convergence of our calculations with the increasing number of basis terms in the wave functions. The atomic unit (a.u.) has been used throughout the present work. All the calculations were performed on IBM and DEC-ALPHA machines using quadruple precision arithmetic (32 significant figures) in the UNIX, FEDORA, and CENT operating systems.

II. CALCULATIONS

The long-range part of the interaction 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 [1,7,8]

$$V_{ab} = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} - \frac{C_{12}}{R^{12}} - \cdots, \tag{1}$$

where

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

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

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

$$C_{12} = \frac{45}{2\pi}[G_{ab}(1,4) + G_{ab}(4,1)] + \frac{105}{\pi}[G_{ab}(2,3) + G_{ab}(3,2)], \tag{5}$$

with

$$G_{ab}(l_a,l_b) = \frac{\pi}{2} \sum_{nm} \frac{f_{n0}^{(l_a)} f_{m0}^{(l_b)}}{E_{n0}^a E_{m0}^b \left(E_{n0}^a + E_{m0}^b\right)}, \tag{6}$$

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

$$f_{n0}^{(l)} = \frac{8\pi}{2l+1}(E_n - E_0)\left|\langle\Psi_0|\sum_i r_i^l P_l(\cos\vartheta_i)|\Psi_n\rangle\right|^2, \tag{7}$$

where $i = 2$ for the helium atom.

To calculate polarizability, we use the static polarizability relation which can be expressed in terms of a sum over all intermediate states including the continuum [8]:

$$S_l = \sum_n \frac{f_{n0}^{(l)}}{E_{n0}^2}. \tag{8}$$

For the ${}^1S$, ${}^1P$, ${}^1D$, ${}^1F$, and ${}^1G$ states of the helium atom, we employ highly correlated wave functions [24,28–30]

$$\Psi = (1 + \hat{P}_{12}) \sum_{i=1}^{N} \sum_{l_1=\varepsilon}^{L} A_i (-1)^{\varepsilon} \mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2) \times \exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}), \tag{9}$$

with

$$\mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2) = r_1^{l_1} r_2^{l_2} \sum_{m_1,m_2} C_{l_1 m_1, l_2 m_2}^{LM} Y_{l_1 m_1}(\hat{\mathbf{r}}_1) Y_{l_1 m_2}(\hat{\mathbf{r}}_2), \tag{10}$$

where the functions $\mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2)$ are the bipolar harmonics or Schwartz harmonics, $\hat{\mathbf{r}}_j = \mathbf{r}_j / r_j$ $(j = 1, 2)$, $Y_{l_i m_i}(\hat{\mathbf{r}}_j)$ denotes the usual spherical harmonics, $C_{l_1 m_1, l_2 m_2}^{LM}$ are the Clebsch-Gordon coefficients, $\alpha_i, \beta_i, \gamma_i$ are the nonlinear variation parameters, A_i $(i = 1, \ldots, N)$ are the linear expansion coefficients, $l_1 + l_2 = L$ (where $L = 0$ for S states, 1 for P states, 2 for D states, 3 for F states, and 4 for G states), N is the number of basis terms, and the operator $\hat{P}_{12}$ is the permutation of the two identical particles 1 and 2. In Eq. (3), we consider l_1 as the remainder of the integer division $i/(L{+}1)$. The nonlinear variational parameters α_i, β_i, and γ_i are determined using a quasirandom process [5,24,28–33]. The parameters α_i, β_i, and γ_i are chosen from the three positive intervals $[a_1,a_2]$, $[b_1,b_2]$, and $[d_1,d_2]$:

$$\begin{aligned} \alpha_i &= \left\langle\!\left\langle \frac{1}{2} i(i+1)\sqrt{2} \right\rangle\!\right\rangle (a_2 - a_1) + a_1, \\ \beta_i &= \left\langle\!\left\langle \frac{1}{2} i(i+1)\sqrt{3} \right\rangle\!\right\rangle (b_2 - b_1) + b_1, \\ \gamma_i &= \left\langle\!\left\langle \frac{1}{2} i(i+1)\sqrt{5} \right\rangle\!\right\rangle (d_2 - d_1) + d_1, \end{aligned} \tag{11}$$

where the symbol $\langle\langle \cdots \rangle\rangle$ designates the fractional part of a real number.

The nonrelativistic Hamiltonian describing the proposed system characterized by a parameter λ is given by

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

where r_1 and r_2 are the radial coordinates of the two electrons and r_{12} is their relative distance. The parameter λ $(= 1/\mu$, μ is called the Debye screening parameter) is known as the Debye length and is a function of electron density and electron temperature. When the helium atom is placed in vacuum, we have $\mu = 0$. The Debye length can be represented as $\lambda = [k_B T / 4\pi n (Ze)^2]^{1/2}$ [3,4], n denotes plasma density and T its temperature. A set of plasma conditions can be simulated for different choices of $\lambda(n,T)$. For two-component plasmas near thermodynamic equilibrium, the Debye length λ can be represented by [3,4,32]

$$\lambda = \frac{1}{\mu} = \left[\frac{4\pi(1+Z)e^2 n_e}{k_B T_e}\right]^{-1/2}, \tag{13}$$

where k_B is the Boltzmann constant, n_e is the electron density in plasmas, T_e is the electron temperature of the plasma, and Z is the nuclear charge and here its value is unity. For the present problem, the Debye plasma with electron density n_e and with energy of E_λ (in eV) can be written from Eq. (13) in the form [33]

$$n_e = 1.48011 \times 10^{22} \frac{E_\lambda}{\lambda^2}\ \mathrm{cm}^{-3}. \tag{14}$$

The Debye shielding in the present investigation of plasma modeling is a simple and good approximation in weakly coupled hot plasmas and low-density warm plasmas [33,34].

TABLE I. The bound $1s5g\ {}^1G$ state energies of screened helium for different screening parameters, along with the $1S$ threshold energy of He$^+$ ($E_{\mathrm{He}^+(1S)}$).

λ	$1s5g\ {}^1G$	$-E_{\mathrm{He}^+(1S)}$ [28,30]
∞	−2.020 000 710 81 −2.020 000 710 898 58[a]	−2.000 000 000 00
200	−2.005 347 866 26	−1.990 001 871 89
100	−1.991 341 160 08	−1.980 074 751 70
50	−1.965 082 400 10	−1.960 298 026 99
40	−1.952 790 569 76	−1.950 464 909 33

[a] Best result [35].

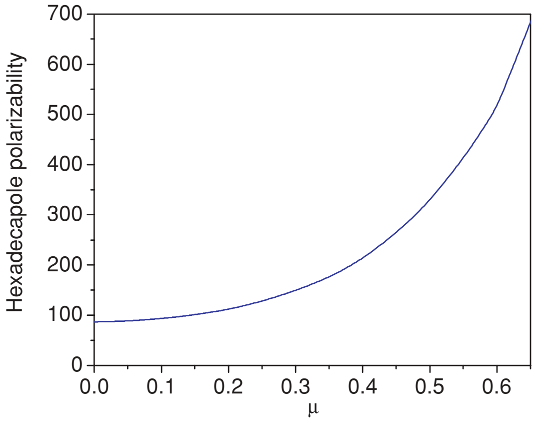

FIG. 1. (Color online) Hexadecapole polarizability of He($1\,^1S$) as a function of the screening parameters.

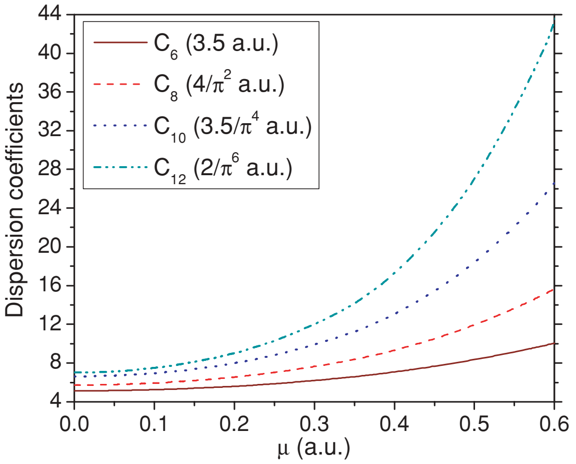

FIG. 2. (Color online) Dispersion coefficients C_6, C_8, C_{10}, and C_{12} as functions of the screening parameters.

III. RESULTS AND DISCUSSIONS

First we optimized the $1\,^1S$, $2\,^1P$, $3\,^1D$, $4\,^1F$, and $5\,^1G$ state energies for different screening parameters using the wave function (9) in the framework of the Ritz variational principle. We have presented $1\,^1S$, $2\,^1P$, $3\,^1D$, and $4\,^1F$ state energy values in our earlier works [24,29,31,33]. The $1s5g\ ^1G$ state energy eigenvalues for different screening parameters obtained from this work are presented in Table I. The $1s5g\ ^1G$ state energy in the unscreened case obtained using 900 term basis functions is well converged with the increasing number of basis terms, and its uncertainty is estimated to be some parts in the order of 10^{-11}, as compared to the best result [35]. It is evident from Table I that the $5\,^1G$ state energy is gradually displaced upward approaching the $\mathrm{He}^+(1S)$ threshold with increasing plasma strength. Next we construct the ground-state eigenfunctions for the best optimized $1s^2\ ^1S$ state eigenenergy. Finally, to calculate polarizabilities and the dispersion coefficients, one needs to obtain the energy levels and wave functions separately for the P, D, F, G states with the optimum choice of nonlinear parameters. To obtain energy levels, we diagonalize the Hamiltonian (12) with the wave functions (9). After calculating the energy levels and eigenfunctions for the final states, we proceed to calculate the hexadecapole polarizability and the dispersion coefficients following the procedure described in Sec. II. We have used a maximum of up to 500, 500, 500, 900, and 900 term wave functions for the S, P, D, F, and G states, respectively. To denote the number of basis terms for S, P, D, F, G state wave functions, we introduce the notation N_s, N_p, N_d, N_f, N_g, respectively, and grouped them as $(N_s, N_p, N_d, N_f, N_g)$.

We calculate the hexadecapole polarizability of the helium atom for different screening parameters using the relation (8), and the results are shown in Fig. 1. Finally, we calculate the dispersion coefficients C_6, C_8, C_{10}, C_{12} for different screening parameters using the relations (2)–(5). From the present computer code, we have reproduced our earlier results of the C_6 coefficients, but we do not repeat the results again in the tables here. Instead, we include them in Fig. 2 for completeness. In Table II, we compare the C_8, C_{10}, and C_{12} results with the available results in the literature for the free-atom case. We present the hexadecapole polarizability and the dispersion coefficient results for different screening parameters in Table III and in Figs. 1 and 2. In Fig. 2, we multiply the C_6, C_8, C_{10}, and C_{12} coefficients by the factors 3.5, $4/\pi^2$, $3.5/\pi^4$, and $2/\pi^6$, respectively, to set them in one figure. To the best of our knowledge, there are no other results in the literature to compare the hexadecapole polarizability and the dispersion coefficient C_{12}. For the unscreened case, our results compare well with other values available in the literature [7–21], especially with the best variational results [8]. For the screened cases, our results

TABLE II. Comparison of C_6, C_8, C_{10}, C_{12} for the He($1\,^1S$)–He($1\,^1S$) in the unscreened case ($\mu = 0$).

Author (year)	Ref.	C_8 (500,500,500)	C_{10} (500,500,500,900)	C_{12} (500,500,500,900,900)
Luyckx *et al.* (1977)	[20]	14.06	183.16	
Bartolotti (1980)	[18]	14.131	183.47	
Thakkar (1981)	[17]	14.111 8	183.600	
Rérat *et al.* (1993)	[16]	13.883		
Bishop and Pipin (1993)	[14]	14.117 855	183.691 25	
Chen (1995)	[11]	14.120	183.74	
Chen and Chung (1996)	[9]	14.1208	183.765	
Yan *et al.* (1996)	[8]	14.117 857 340	183.691 070 5	
Present work		14.117 857 4	183.6910	3364.34

TABLE III. Dispersion coefficients and hexadecapole polarizability for different screening parameters. The numbers within parentheses denote (N_s,N_p,N_d,N_f,N_g).

λ	Hexadecapole polarizability	C_8 (500,500,500)	C_{10} (500,500,500,900)	C_{12} (500,500,500,900,900)
∞	86.905	14.117 857 4	183.6910	3364.34
	86.894[a]	14.117 857 3[b]	183.6898[c]	3364.11[d]
100	86.975	14.123 328 0	183.7929	3366.88
50	87.179	14.139 522 1	184.0942	3374.37
20	88.554	14.249 783 3	186.1426	3425.18
15	89.790	14.349 579 3	187.9966	3471.15
10	93.250	14.629 206 1	193.2036	3600.59
	93.237[a]	14.529 206 0[b]	193.2025[c]	3600.35[d]
8	96.715	14.908 331 3	198.4258	3731.05
6	104.26	15.507 699 2	209.7361	4016.51
5	112.03	16.113 005 5	221.3012	4312.50
	112.01[a]	16.113 005 4[b]	221.3001[c]	4312.24[d]
4	127.08	17.248 613 7	243.3931	4889.59
3	163.96	19.850 640 9	295.9104	6319.20
2.5	208.67	22.735 934 5	357.0511	8075.70
2	317.43	28.946 610 1	497.9173	124 36.4
1.7	485.77	37.204 675 5	702.1183	193 76.9
1.65	532.63	39.311 516 5	756.9426	213 43.7
1.5	739.81	47.944 887	991.882	301 87.9
	739.77[a]	47.944 886[b]	991.881[c]	301 87.3[d]
1.0	6960.34	200.567 35	6775.004	343 018.6
	6960.25[a]	200.567 31[b]	6775.001[c]	343 016.8[d]

[a] Using (500, 800) for (N_s, N_g).
[b] Using (400,400,400).
[c] Using (500,500,500,800).
[d] Using (500,500,500,800,800).

show that the dispersion coefficients for the He($1\,^1S$)–He($1\,^1S$) system and the hexadecapole polarizability for He($1\,^1S$) increase with increasing plasma strength. Our findings indicate that when the plasma screening effect increases, the multipole polarizabilities for the helium atom increase as the ground-state wave functions becoming more diffused. Now when two such diffused atoms come together, the dispersion coefficients will be increased, analogous to the free-atom cases; for example, the C_6 for the H–H case (with dipole polarizability equal to 4.5 for H) is larger than that for the He–He case (with dipole polarizability equal to 1.383192174 for He).

IV. CONCLUSIONS

We have obtained reasonably accurate dispersion C_6, C_8, C_{10}, and C_{12} coefficients for the interactions between helium atoms in their ground states and the hexadecapole polarizability of He($1\,^1S$) for the unscreened case as well as for the screened cases. In the unscreened case, there are no other results to compare the hexadecapole polarizability and the dispersion coefficient C_{12}. In the screened cases, there are no other reported results to compare with our present results. The Van der Walls force constants, particularly the leading term C_6 arising from the induced dipoles, are of great theoretical and experimental interest in atomic and molecular physics [1,2,7–22]. With the recent advancement in laser plasmas [36], we hope our findings will provide new insight and useful information to the communities in atomic, molecular, chemical, and plasma physics.

ACKNOWLEDGMENTS

S.K. thanks the Natural Scientific Research Innovation Foundation in the Harbin Institute of Technology for financial support (Grant No. HIT.NSRIF.2008.01). Y.K.H. is supported by the NSC of Taiwan.

---

[1] A. Dalgarno and W. D. Davison, Adv. At. Mol. Phys. **2**, 1 (1966); A. Dalgarno, Adv. Chem. Phys. **12**, 143 (1967).

[2] D. W. Martin and P. A. Fraser, J. Phys. B **13**, 3383 (1980); G. W. F. Drake, Phys. Rev. A **34**, 2871 (1986); R. J. Drachman, A. K. Bhatia, and A. A. Shabazz, *ibid.* **42**, 6333 (1990); A. K. Bhatia and R. J. Drachman, *ibid.* **45**, 7752 (1992).

[3] S. Ichimaru, *Plasma Physics* (Benjamin/Cummings, Menlo Park, CA, 1986), p. 5.

[4] D. Salzman, in *Atomic Physics in Hot Plasmas* (Oxford University, New York, 1998), p. 19.

[5] S. Kar and Y. K. Ho, J. Phys. B **39**, 2445 (2006); New J. Phys. **7**, 141 (2005).

[6] A. N. Sil, S. Canuto, and P. K. Mukherjee, Adv. Quantum Chem. **58**, 115 (2009).

[7] J.-M. Zhu, B.-L. Zhou, and Z.-C. Yan, Chem. Phys. Lett. **313**, 184 (1999).

[8] Z.-C. Yan, J. F. Babb, A. Dalgarno, and G. W. F. Drake, Phys. Rev. A **54**, 2824 (1996).

[9] M.-K. Chen and K. T. Chung, Phys. Rev. A **53**, 1439 (1996).

[10] V. Magnasco and M. Ottonelli, Chem. Phys. Lett. **259**, 307 (1996).

[11] M.-K. Chen, J. Phys. B **28**, 4189 (1995).

[12] M. J. Jamieson, G. W. F. Drake, and A. Dalgarno, Phys. Rev. A **51**, 3358 (1995).

[13] M.-K. Chen, J. Phys. B **28**, 4189 (1995).

[14] D. M. Bishop and J. Pipin, Int. J. Quantum Chem. **45**, 349 (1993).

[15] M. Rérat, M. Caffarel, and C. Pouchan, Phys. Rev. A **48**, 161 (1993).

[16] M. Rérat, M. Caffarel, and C. Pouchan, Phys. Rev. A **48**, 161 (1993); M. Caffarel, M. Rérat, and C. Pouchan, *ibid.* **47**, 3704 (1993).

[17] A. J. Thakar, J. Chem. Phys. **75**, 4496 (1981).

[18] L. J. Bartolotti, J. Chem. Phys. **73**, 3666 (1980).

[19] D. J. Margoliash and W. J. Meath, J. Chem. Phys. **68**, 1426 (1978).

[20] R. Luyckx, Ph. Coulon, and H. N. W. Lekkerkerker, Chem. Phys. Lett. **48**, 187 (1977).

[21] R. M. Glover and F. Weinhold, J. Chem. Phys. **66**, 191 (1977).

[22] S. Kar and Y. K. Ho, Chem. Phys. Lett. **449**, 246 (2007)

[23] S. Kar and Y. K. Ho, J. Quant. Spectrosc. Radiat. Transfer **107**, 315 (2007).

[24] S. Kar and Y. K. Ho, Phys. Rev. A **80**, 062511 (2009).

[25] B. Saha, P. K. Mukherjee, and G. H. F. Diercksen, Astron. Astrophys. **396**, 337 (2002).

[26] Y. Y. Qi, J. G. Wang, and R. K. Janev, Phys. Rev. A **80**, 032502 (2009).

[27] S. Kar and Y. K. Ho, Nucl. Instrum. Methods Phys. Res. **266**, 526 (2008).

[28] A. M. Frolov and V. H. Smith Jr., Phys. Rev. A **53**, 3853 (1996).

[29] S. Kar and Y. K. Ho, Int. J. Quantum Chem. **110**, 993 (2010).

[30] S. Kar and Y. K. Ho, J. Phys. B **42**, 055001 (2009).

[31] S. Kar and Y. K. Ho, Chem. Phys. Lett. **402**, 544 (2005).

[32] S. Kar and Y. K. Ho, Int. J. Quantum Chem. **106**, 814 (2006); **107**, 353 (2007).

[33] S. Kar and Y. K. Ho, Phys. Lett. A **368**, 476 (2007).

[34] H. Okutsu, T. Sako, K. Yamanouchi, and G. H. F. Diercksen, J. Phys. B **38**, 917 (2005).

[35] G. W. F. Drake, in *Long Range Casimir Forces: Theory and Recent Experiments in Atomic Systems*, edited by F. S. Levin and D. A. Micha (Plenum Press, New York, 1993), p. 129.

[36] S. NaKai and K. Mima, Rep. Prog. Phys. **67**, 321 (2004).