

Polarizabilities of hydrogen molecules calculated without using the Born-Oppenheimer approximation

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The static dipole polarizabilities of the first three lowest states of hydrogen molecules H_2 , HD, and D_2 are calculated using variationally generated wave functions in Hylleraas coordinates without using the Born-Oppenheimer approximation. Our results for H_2 and HD are two orders of magnitude more accurate than the best literature values. We also improve the previous best results for D_2 .

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I. INTRODUCTION

The electric dipole polarizability is an important parameter for measuring the response of an atom or molecule to an electric field. It has close relationships with many physical quantities [1], such as the dielectric constant, refractive index, van der Waals constant, and so on. The polarizabilities of various atoms and molecules have been measured or calculated to some degree of accuracy [2,3]. Among them, the polarizabilities of atomic hydrogen, helium, and lithium, as well as the hydrogen molecular ions have been evaluated to very high precision [4–8]. Taking helium as an example, the nonrelativistic polarizability has been calculated to an accuracy of 10^{-11} or better [9,10] together with relativistic and QED corrections [5,10,11]. The polarizabilities of hydrogen molecular ions have also been calculated to very high precision without using the Born-Oppenheimer (BO) approximation [7,8]. However, for neutral hydrogen molecules, apart from the two sets of inconsistent nonadiabatic values [12,13], there exist only adiabatic results in the literature. After the pioneering work of Ishiguro *et al.*, in 1952 [14], Kolos and Wolniewicz performed the most accurate adiabatic calculations in 1967 [15], which were further refined by Rychlewski in 1980 [16]. Until 2002, the first fully nonadiabatic calculations were carried out by Cafiero and Adamowicz using the finite field method [12]. Nevertheless, their nonadiabatic results deviate significantly from the adiabatic values. Another nonadiabatic calculation was performed for H_2 recently by Tiihonen *et al.*, using the path-integral Monte Carlo method [13]. Their results are consistent with the adiabatic values of Kolos and Wolniewicz [15].

The purpose of this paper is to present a fully nonadiabatic calculation for the electric dipole polarizabilities of the hydrogen molecules H_2 , HD, and D_2 in their three lowest quantum states by treating the four constituent particles of a molecule

on the equal footing. This paper is organized as follows. In Sec. II theoretical formalism is introduced, including the construction of a variational wave function in Hylleraas coordinates. Computational results and comparisons with previous literature values are contained in Sec. III. Finally, Sec. IV is a conclusion. Atomic units (a.u.) are used throughout.

II. THEORETICAL FORMALISM

When an atom or molecule is exposed to a weak external uniform electric-field F , the energy of the system can be expressed as [17]

$$E = E_0 - \sum_{\alpha} \mu_{\alpha} F_{\alpha} - \frac{1}{2} \sum_{\alpha, \beta} \alpha_{\alpha\beta} F_{\alpha} F_{\beta} - \frac{1}{6} \sum_{\alpha, \beta, \gamma} \beta_{\alpha\beta\gamma} F_{\alpha} F_{\beta} F_{\gamma} - \dots, \quad (1)$$

where E_0 is the energy of the state of interest without the external field, μ_{α} ($\alpha = x, y, z$)'s are the Cartesian components of the permanent electric dipole moment of the system, $\alpha_{\alpha\beta}$'s are the polarizability tensor components, and $\beta_{\alpha\beta\gamma}$ is the first hyperpolarizability components. Comparing Eq. (1) with the standard perturbation theory, one obtains

$$\alpha_{\alpha\beta} = 2 \sum_n \frac{\langle 0 | d_{\alpha} | n \rangle \langle n | d_{\beta} | 0 \rangle}{E_n - E_0}, \quad (2)$$

where $|0\rangle$ is the energy eigenstate corresponding to the eigenvalue E_0 , E_n and $|n\rangle$ are for the intermediate states, and d_{α} is the α th component of the dipole moment operator. An alternative expression for the polarizability tensor is

$$\alpha_{\alpha\beta} = - \left. \frac{\partial^2 E}{\partial F_{\alpha} \partial F_{\beta}} \right|_{F=0}, \quad (3)$$

according to Eq. (1). The direct calculation based on the above equation, the so-called finite field method [12,18], involves an extrapolation procedure to the zero field that may introduce

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further errors. In this paper, we perform our calculation of the dipole polarizability using Eq. (2) where the complete set of intermediate states is generated by diagonalizing the Hamiltonian in a fully correlated basis in Hylleraas coordinates. Our molecular wave functions are constructed in a fully nonadiabatic way without using the Born-Oppenheimer approximation; in other words, the two electrons and two protons in H₂, for example, are treated on the same footing.

For a general four-body Coulombic system, the Hamiltonian of the system in the laboratory frame is

$$H = - \sum_{i=0}^3 \frac{1}{2m_i} \nabla_{\mathbf{R}_i}^2 + \sum_{0 \leq i < j}^3 \frac{q_i q_j}{|\mathbf{R}_i - \mathbf{R}_j|}, \quad (4)$$

where m_i , q_i , and \mathbf{R}_i denote the mass, charge, and position vector of the i th particle, respectively. The dipole moment operator of the system is

$$\mathbf{d} = \sum_{i=0}^3 q_i \mathbf{R}_i. \quad (5)$$

By introducing the center-of-mass coordinates and the coordinates relative to one of the nuclei located at \mathbf{R}_0 ,

$$\mathbf{X} = \frac{1}{M_T} \sum_{i=0}^3 m_i \mathbf{R}_i, \quad (6)$$

$$\mathbf{r}_i = \mathbf{R}_i - \mathbf{R}_0, \quad i = 1-3, \quad (7)$$

where $M_T = \sum_{i=0}^3 m_i$ is the total mass of the system, and by separating out the center-of-mass motion, the Hamiltonian describing the internal motion of the system becomes the following quasi-three-body one,

$$H = - \sum_{i=1}^3 \frac{1}{2\mu_i} \nabla_{\mathbf{r}_i}^2 - \frac{1}{m_0} \sum_{1 \leq i < j}^3 \nabla_{\mathbf{r}_i} \cdot \nabla_{\mathbf{r}_j} + \sum_{i=1}^3 \frac{q_0 q_i}{r_i} + \sum_{1 \leq i < j}^3 \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (8)$$

where $\mu_i = m_i m_0 / (m_i + m_0)$. The dipole moment operator of the system in the new coordinates becomes

$$\mathbf{d} = \sum_{i=0}^3 q_i \mathbf{r}_i + \left(\sum_{i=0}^3 q_i \right) \mathbf{R}_0 = \sum_{i=0}^3 q_i \mathbf{r}_i \quad (9)$$

for an electric neutral system.

The wave functions for the states of interest and for the intermediate states are all expanded in terms of the following Hylleraas-type basis functions:

$$r_1^{j_1} r_2^{j_2} r_3^{j_3} r_{12}^{j_{12}} r_{23}^{j_{23}} r_{31}^{j_{31}} e^{-\alpha r_1 - \beta r_2 - \gamma r_3} \times \mathcal{Y}_{(\ell_1 \ell_2) \ell_{12}, \ell_3}^{LM}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \chi(1, 2) - (1 \leftrightarrow 2), \quad (10)$$

where

$$\begin{aligned} \mathcal{Y}_{(\ell_1 \ell_2) \ell_{12}, \ell_3}^{LM}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) &= r_1^{\ell_1} r_2^{\ell_2} r_3^{\ell_3} \sum_{m_i} \langle \ell_1 m_1; \ell_2 m_2 | \ell_{12} \ell_3; \ell_{12} m_{12} \rangle \\ &\times \langle \ell_{12} m_{12}; \ell_3 m_3 | \ell_{12} \ell_3; LM \rangle Y_{\ell_1 m_1}(\mathbf{r}_1) \\ &\times Y_{\ell_2 m_2}(\mathbf{r}_2) Y_{\ell_3 m_3}(\mathbf{r}_3) \end{aligned} \quad (11)$$

is the vector-coupled product of spherical harmonics for the three particles to form a state of total angular momentum L and z -component M , $\chi(1, 2)$ is the two-electron spin-wave function,

$$\chi(1, 2) = \alpha(1)\beta(2) - \beta(1)\alpha(2), \quad (12)$$

and $(1 \leftrightarrow 2)$ denotes the two-electron exchange term. As discussed by Yan *et al.* [8], it is not necessary to impose explicit symmetrization for the two identical nuclei in basis functions, which will be automatically built in progressively as the size of basis set increases due the variational principle. Also see Ref. [19] for a similar discussion.

The Hylleraas basis functions described by Eq. (10) have been recently applied to fully nonadiabatic calculations of energy levels of the hydrogen molecules by Wang and Yan [20,21] where the nonrelativistic energy of the ground state of H₂ has been calculated to an accuracy of 10^{-12} . These calculations laid the foundation for the current paper on the polarizabilities of these systems.

According to Eq. (3), the dipole polarizability of an atom or molecule is generally a second-rank tensor. Following the work of Tang *et al.* [22] and assuming that the external field is along the z direction, we can rewrite the second-order energy correction as

$$\Delta E_2 = -\frac{1}{2} [\alpha_1 + \alpha_1^T g_2(L, M)] F^2, \quad (13)$$

where α_1 and α_1^T are the scalar and tensor polarizabilities, respectively, and

$$g_2(L, M) = \begin{cases} 0, & L = 0, \\ \frac{3M^2 - L(L+1)}{L(2L-1)}, & \text{otherwise,} \end{cases} \quad (14)$$

with L and M being the total angular momentum and its z component, respectively. The scalar and tensor polarizabilities α_1 and α_1^T can further be expressed in terms of the reduced matrix elements of the dipole operator T_1 ,

$$\alpha_1 = \sum_{L_a} \alpha_1(L_a), \quad (15)$$

$$\alpha_1^T = \sum_{L_a} W(L, L_a) \alpha_1(L_a), \quad (16)$$

where L_a denotes the total angular momentum of the intermediate states, and

$$W(L, L_a) = (-1)^{L+L_a} \sqrt{\frac{30(2L+1)L(2L-1)}{(2L+3)(L+1)}} \begin{Bmatrix} 1 & 1 & 2 \\ L & L & L_a \end{Bmatrix}, \quad (17)$$

$$\alpha_1(L_a) = \frac{8\pi}{9(2L+1)} \sum_n \frac{|\langle n_0 L || T_1 || n L_a \rangle|^2}{E_n(L_a) - E_{n_0}(L)}, \quad (18)$$

with

$$T_1 = \sum_{i=1}^3 q_i r_i Y_{10}(\mathbf{r}_i). \quad (19)$$

In particular, for $L = 0$,

$$\alpha_1 = \alpha_1(P), \quad (20)$$

$$\alpha_1^T = 0, \quad (21)$$

TABLE I. Scalar polarizabilities of the ground states ($\nu = 0$, $J = 0$) of H_2 , HD, and D_2 . N denotes the size of the basis set for the intermediate states.

N	H_2	HD	D_2
686	5.401 238 94	5.370 909 61	5.331 430 67
1394	5.415 592 31	5.384 097 49	5.345 702 11
1600	5.417 186 52	5.385 758 19	5.348 203 78
4500	5.417 436 04	5.385 951 63	5.348 409 77
7387	5.417 473 02	5.385 982 25	5.348 502 38
11550	5.417 480 18	5.385 990 71	5.348 532 20
17400	5.417 482 06	5.385 992 56	5.348 543 33
Extrapolation	5.417 483(2)	5.385 993(3)	5.348 550(7)
Sum rule			
686	2.004 293 80	2.003 948 01	2.003 682 3
1394	2.001 397 75	2.001 146 79	2.001 021 7
1600	2.001 232 45	2.000 936 68	2.000 713 7
4500	2.001 111 58	2.000 838 66	2.000 617 7
7387	2.001 096 92	2.000 825 35	2.000 580 2
11550	2.001 091 58	2.000 820 27	2.000 566 4
Extrapolation	2.001 088(3)	2.000 817(3)	2.000 558(8)
Exact	2.001 089 234	2.000 817 060	2.000 544 887

for $L = 1$,

$$\alpha_1 = \alpha_1(S) + \alpha_1(P) + \alpha_1(D), \quad (22)$$

$$\alpha_1^T = -\alpha_1(S) + \frac{1}{2}\alpha_1(P) - \frac{1}{10}\alpha_1(D), \quad (23)$$

and for $L = 2$,

$$\alpha_1 = \alpha_1(P) + \alpha_1(D) + \alpha_1(F), \quad (24)$$

$$\alpha_1^T = -\alpha_1(P) + \alpha_1(D) - \frac{2}{7}\alpha_1(F). \quad (25)$$

The nuclear masses used in this paper are $m_p = 1836.152\,673\,89(17)$ a.u. and $m_d = 3670.482\,967\,85(13)$ a.u. [23].

III. RESULTS AND DISCUSSION

We consider the three lowest molecular states ($\nu = 0$, $J = 1-3$) of H_2 , HD, and D_2 , where ν is the vibrational quantum number, and J is the rotational quantum number that is equal to L . The ground-state wave functions are expanded using 9456 basis functions. Table I shows a convergence study of

TABLE II. Scalar polarizabilities of the lowest P states ($\nu = 0$, $J = 1$) of H_2 , HD, and D_2 . The three numbers in the first column are the sizes of basis sets for the intermediate states of the S , P , and D symmetries, respectively.

N	H_2	HD	D_2
α_1			
560,401,438	5.407 242 60	5.371 663 99	5.336 285 51
1088,874,953	5.424 724 57	5.390 396 58	5.349 510 45
1968,1722,1864	5.426 747 58	5.392 695 20	5.352 883 41
3328,3102,3348	5.427 057 15	5.392 947 02	5.353 163 06
5368,5262,5652	5.427 099 85	5.392 984 91	5.353 272 34
8288,8457,9057	5.427 107 17	5.392 993 78	5.353 303 28
12370,13057,13932	5.427 108 88	5.392 995 71	5.353 314 18
Extrapolation	5.427 110(2)	5.392 997(4)	5.353 32(3)
Sum rule			
560,401,438	2.004 626 74	2.004 622 11	2.004 388 89
1088,874,953	2.001 525 26	2.001 349 11	2.001 240 91
1968,1722,1864	2.001 235 99	2.000 943 07	2.000 721 76
3328,3102,3348	2.001 107 10	2.000 837 93	2.000 619 52
5368,5262,5652	2.001 094 07	2.000 826 85	2.000 578 82
8288,8457,9057	2.001 090 51	2.000 823 66	2.000 568 43
12370,13057,13932	2.001 089 73	2.000 822 81	2.000 561 78
Extrapolation	2.001 089 5(3)	2.000 822(3)	2.000 55(1)
Exact	2.001 089 234	2.000 817 060	2.000 544 887

TABLE III. Scalar polarizabilities of the lowest D states ($\nu = 0$, $J = 2$) of H_2 , HD, and D_2 . The three numbers in the first column are the sizes of basis sets for the intermediate states of the P , D , and F symmetries, respectively.

N	H_2	HD	D_2
α_{\parallel}			
686,251,541	5.420 463 66	5.380 769 78	5.332 201 19
1394,616,1145	5.442 639 51	5.403 419 20	5.357 317 89
2600,1302,2209	5.445 776 20	5.406 843 46	5.362 020 96
4500,2478,3928	5.446 238 86	5.407 252 44	5.362 419 10
7387,4362,6596	5.446 312 93	5.407 328 43	5.362 673 69
11550,7227,10526	5.446 325 42	5.407 341 72	5.362 726 65
17400,11407,16156	5.446 328 02	5.407 345 15	5.362 748 59
Extrapolation	5.446 329(2)	5.407 346(4)	5.362 76(3)
Sum rule			
686,251,541	2.005 293 07	2.005 163 95	2.004 993 93
1394,616,1145	2.001 765 58	2.001 544 17	2.001 517 05
2600,1302,2209	2.001 330 54	2.001 033 42	2.000 961 24
4500,2478,3928	2.001 122 26	2.000 856 22	2.000 858 24
7387,4362,6596	2.001 100 47	2.000 834 66	2.000 792 95
11550,7227,10526	2.001 096 00	2.000 830 91	2.000 794 18
Extrapolation	2.001 094(4)	2.000 830(3)	2.000 79(9)
Exact	2.001 089 234	2.000 817 060	2.000 544 887

the polarizability as the size of basis set of the intermediate states of P symmetry is enlarged progressively from 686 to 17 400. From the table one can see that a convergence to the level of 10^{-6} – 10^{-7} has been achieved.

From Eq. (2) one can see that the accuracy of the polarizability depends not only on the accuracy of the eigenenergy and eigenwave function of the initial state, but also on the degree of completeness of the intermediate states. In fact, the accuracy of the calculated polarizability is usually determined by the latter. Zhou *et al.* derived the generalized Thomas-Reiche-Kuhn (GTRK) sum rule for a general Coulombic system [24], which can be used here to check the completeness of our intermediate states. According to Ref. [24], the GTRK sum rule reads

$$\frac{2}{3} \sum_n \omega_{n0} | \langle 0 | \mathbf{d} | n \rangle |^2 = \sum_{i=0}^3 \frac{q_i^2}{m_i} - \frac{Q_T^2}{M_T}, \quad (26)$$

where $Q_T = \sum_{i=0}^3 q_i$ is the total charge of the system that is zero here and $\omega_{n0} = E_n - E_0$. It is noted that the right-hand side of Eq. (26) only depends on the charges and masses of the system so it can be calculated exactly. Table I also lists a convergence study for the left-hand side of Eq. (26) and compares to the right. One can see that a similar accuracy of 10^{-6} – 10^{-7} has been obtained.

TABLE IV. Tensor polarizabilities for the ($\nu = 0$, $J = 1$) and ($\nu = 0$, $J = 2$) states of H_2 , HD, and D_2 .

System	$\alpha_1^T(0, 1)$	$\alpha_1^T(0, 2)$
H_2	−0.271 425 1(1)	−0.390 740 8(2)
HD	−0.267 167 1(1)	−0.383 926(1)
D_2	−0.262 329(1)	−0.376 187(1)

Next, we consider the two lowest excited states ($\nu = 0$, $J = 1$) and ($\nu = 0$, $J = 2$). For $J = 1$, we should include the contributions from the intermediate states of S , P , and D symmetries, where the P -symmetric configuration has an unnatural parity. For $J = 2$, we should include the P , D , and F symmetries, where the D -symmetric configuration has also an unnatural parity. Tables II and III are the convergence studies for the scalar polarizabilities and the corresponding verifications of the GTRK sum rule, and Table IV lists the tensor polarizabilities. From these tables one can see that a nice convergence has been achieved for these excited states.

Table V is a comparison of our results of the scalar polarizabilities with other theoretical values in the literature. It is seen that our results are consistent with the adiabatic values of Kolos and Wolniewicz [15] and Rychlewski [16] as well as with the nonadiabatic result of Tiihonen *et al.* [13] for the ground state of H_2 using the path-integral Monte Carlo method. However, the first fully nonadiabatic results of the ground-state polarizabilities by Cafiero and Adamowicz [12], using the finite field method, significantly disagree with all the results listed in the table. For example, their ground-state polarizability of H_2 is 6.74, which is close only to the parallel component of the polarizability in the BO model $\alpha_{\parallel} = 6.711 562$ at the internuclear distance $R = 1.45$ by Kolos and Wolniewicz [15].

IV. CONCLUSION

In conclusion, precise values of static dipole polarizabilities of the first three lowest states of hydrogen molecules H_2 , HD, and D_2 have been determined without using the Born-Oppenheimer approximation. Our results can be used as a benchmark for other theoretical methods. It would be interesting to include leading-order relativistic and quantum electrodynamic effects in the calculation of polarizabilities.

TABLE V. Comparison of the scalar polarizabilities (nonrelativistic) for the ($\nu = 0$, $J = 0-2$) states of H_2 , HD, and D_2 . In the table, BO stands for the Born-Oppenheimer approximation.

Reference	Method	$\alpha_1(0, 0)$	$\alpha_1(0, 1)$	$\alpha_1(0, 2)$
H_2				
Kolos and Wolniewicz [15]	BO	5.413 9	5.423 5	5.442 7
Rychlewski [16]	BO	5.417 04	5.426 66	5.445 86
Tiihonen <i>et al.</i> [13]	Non-BO	5.417(37)		
Cafiero and Adamowicz [12]	Non-BO	6.74		
This paper	Non-BO	5.417 483(2)	5.427 110(2)	5.446 329(2)
HD				
Kolos and Wolniewicz [15]	BO	5.382 4	5.389 6	5.403 9
Rychlewski [16]	BO	5.386 71	5.393 88	5.408 20
Cafiero and Adamowicz [12]	Non-BO	6.67		
This paper	Non-BO	5.385 993(3)	5.392 997(4)	5.407 346(4)
D_2				
Kolos and Wolniewicz [15]	BO	5.345 3	5.350 0	5.359 5
Rychlewski [16]	BO	5.348 34	5.353 11	5.362 63
Cafiero and Adamowicz [12]	Non-BO	6.59		
This paper	Non-BO	5.348 550(7)	5.353 32(3)	5.362 76(3)

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