

Complete α^2 relativistic corrections to the pure vibrational non-Born-Oppenheimer energies of HeH⁺

Monika Stanke,^{1,2} Dariusz Kędziera,³ Sergiy Bubin,¹ and Ludwik Adamowicz^{1,4}

¹*Department of Chemistry, University of Arizona, Tucson, Arizona 85721, USA*

²*Institute of Physics, Nicolaus Copernicus University, ul Grudziadzka 5, PL 87-100 Toruń, Poland*

³*Department of Chemistry, Nicolaus Copernicus University, ul Gagarina 7, PL 87-100 Toruń, Poland*

⁴*Department of Physics, University of Arizona, Tucson, Arizona 85721, USA*

(Received 18 October 2007; published 25 February 2008)

We report the implementation of the complete set of the lowest-order relativistic corrections of the order of α^2 (where α is the fine structure constant) for calculating vibrational states of diatomic molecular systems within the framework that does not assume the Born-Oppenheimer approximation. To test the accuracy of the approach we have performed calculations for all rotationless vibrational states (also called pure vibrational states or *S* states) of the HeH⁺ ion in the ground electronic state. For the lowest transitions, where very precise experimental results are available, an excellent agreement with the experimental values has been achieved.

DOI: [10.1103/PhysRevA.77.022506](https://doi.org/10.1103/PhysRevA.77.022506)

PACS number(s): 31.15.xt, 31.15.vn, 31.30.J-, 33.20.Tp

I. INTRODUCTION

The analysis of the relativistic effects in atoms and molecules in bound states can be performed based on the framework of the quantum electrodynamics (QED). Within this framework an effective theory can be derived for light atomic and molecular systems that aims at reproducing the relativistic effects in a nonrelativistic regime. In this effective approach the Hamiltonian representing the relativistic effects is obtained based on the so-called nonrelativistic QED theory (NRQED) [1,2]. The NRQED offers a systematic adaptation of QED to bound states by including all possible local interactions. In the NRQED approach properties of bound states are determined by employing standard computational techniques borrowed from the nonrelativistic quantum mechanics such as the perturbation theory. With that the relativistic and QED effects are determined as perturbation corrections using the nonrelativistic wave function as the zero-order function. In addition, the nonrelativistic energy corrected for the relativistic and QED effects is augmented with the corrections due to the finite mass of the nucleus (nuclei in the molecular case), as well as with the corrections due to the structure of the nucleus and its polarizability. That leads to, what at present is, the most accurate approach for calculating bound states of atomic and molecular systems. We should mention that the perturbation approach to account for the relativistic corrections can also be developed without using the NRQED approach as it was shown by Bethe and Salpeter [3].

In the NRQED framework, there are different ways the effective field theory can be constructed [2,4,5]. From the standpoint of the present calculations the relevant aspect of this theory is the fact that the leading relativistic corrections of the order of α^2 , α^3 , and higher can be derived in an effective way based on NRQED. This shows that the calculations like ours are firmly grounded in a well-defined theoretical framework.

A relative uncertainty of $\sim 10^{-9}$ is now achievable in experimental measurements of rovibrational transitions of small molecular systems. In order for the theory to keep up with these advancements, new computational tools need to

be developed to perform increasingly more precise calculations on atomic and molecular systems. This has been the goal of our research for over a decade. Our most recent calculations concerning the lowest electronic transition of the Be atom [6] demonstrated that the experimental accuracy can be matched with theoretical calculations. However, this only happens when not only the nonrelativistic wave functions and the energies are calculated with very high precision, but also relativistic and QED corrections are included up to the order of α^4 .

In the present calculations we use an approach that does not assume the Born-Oppenheimer (BO) approximation regarding the separability of the electronic and nuclear motion. The non-BO wave functions of the ground and excited states of the studied system are expanded in terms of correlated Gaussian functions that depend explicitly on the distances between the particles (nuclei and electrons) forming the system. The work on implementation of these functions in atomic and molecular calculations has been carried out in our group for a number of years [7–12]. An important part of this development has been the use of the analytical gradient of the variational energy functional with respect to the exponential parameters of the Gaussians in the optimization of those parameters.

In this work we report the development and implementation of the algorithm for calculating the complete relativistic correction of the order of α^2 (where $\alpha=1/c$) determined as the expectation value of the sum of the electronic and nuclear mass-velocity, Darwin, spin-spin, and orbit-orbit operators. The expectation value is calculated using the non-BO wave function expanded in term of correlated Gaussians multiplied by powers of the internuclear distance (we call them “diatomic Gaussians”). Such multipliers are not necessary in non-BO calculations of atomic systems and were not used in our calculations concerning the Be atom [6], but they are indispensable in diatomic calculations because they are capable of describing the internuclear correlation effects. There have been very accurate calculations of relativistic effects in molecular systems with two and more electrons reported before (see, for example, Refs. [13–16]),

but they have only concerned the electronic corrections and have been done within the BO approximation. This work and our previous work [17] show the complete α^2 molecular relativistic correction calculated in the all-particle approach using the non-BO framework.

The algorithm developed in this work is applied to calculate all bound states of the HeH^+ ion with the zero total angular momentum (the so-called “pure vibrational states” or “S states”). We studied the hydrohelium cation, HeH^+ , before. In our most recent work [17] we used an approach employing explicitly correlated Gaussians with complex exponential parameters to determine the orbit-orbit relativistic corrections for the lowest three pure vibrational states and with those corrections added to our previous results [18] we obtained a better agreement between the experimental and theoretical transition frequencies in comparison with the calculations performed without the orbit-orbit corrections [18]. However, the nonrelativistic energies of the three states obtained with the complex Gaussians were rather poor. Encouraged by that study and now equipped with the procedure for calculating the orbit-orbit correction with Gaussians multiplied by powers of the internuclear distance (diatomic Gaussians) developed in this work we have recalculated all 11 pure vibrational states of HeH^+ at a much higher level of precision. The present calculations are performed on a two-electron heteronuclear system.

There have been several experimental high-resolution spectroscopy works on HeH^+ . The first laboratory observation of this system dates back to 1925 [19]. The interest in HeH^+ is mainly due to its relevant studies of interstellar space [20] where hydrogen and helium are the two most abundant elements. Since HeH^+ has a relatively large permanent dipole moment, there have been some highly precise measurements of the vibration-rotational and pure vibrational gas-phase spectra of this system. As we described in our previous work, only the lowest two pure vibrational transitions are determined based on the experimental spectra with a very high accuracy. We are comparing our calculated transition frequencies with those transitions. This provides a very stringent test of the approach we use.

II. METHOD USED IN THE CALCULATIONS

To generate the non-BO wave functions of the pure vibrational states of HeH^+ we used the approach employed by us before in non-BO calculations for this and other systems [12,17,18]. The approach is based on the minimization of the total energy of the system expressed as the expectation value of the internal nonrelativistic Hamiltonian, \hat{H}_{nonrel} , obtained from the “laboratory frame” Hamiltonian by separation of the center-of-mass motion,

$$\hat{H}_{\text{nonrel}} = -\frac{1}{2} \left(\sum_{i=1}^3 \frac{1}{\mu_i} \nabla_{\mathbf{r}_i}^2 + \sum_{i=1}^3 \sum_{j \neq i}^3 \frac{1}{m_0} \nabla_{\mathbf{r}_i} \nabla_{\mathbf{r}_j} \right) + \sum_{i=1}^3 \frac{q_0 q_i}{r_i} + \sum_{i < j}^3 \frac{q_i q_j}{r_{ij}}. \quad (1)$$

The center of the “internal” Cartesian coordinate system used

in (1) was placed at the helium nucleus (the reference particle). In (1) $q_0=2$ is the charge of the helium nucleus, $q_1=1$ is the charge of the proton, $q_2=q_3=-1$ are the charges of electrons, \mathbf{r}_i are the position vectors of the proton and the two electrons with respect to the reference helium nucleus, r_i are their lengths, $r_{ij}=|\mathbf{r}_j-\mathbf{r}_i|$, $m_0=7294.299\,536\,3m_e$ is the mass of the helium nucleus, $m_1=1836.152\,672\,61m_e$ is the mass of the proton, $m_2=m_3=m_e=1$ are the electron masses [21], and $\mu_i=m_0m_i/(m_0+m_i)$ is the reduced mass of particle i (prime symbol denotes vector transposition). The internal Hamiltonian (1) describes three pseudoparticles with charges equal to the charges of the original particles moving in the central potential of the charge of the reference helium nucleus.

In the calculation of the mass-velocity (MV), the Darwin (D), spin-spin (SS), and orbit-orbit (OO) corrections we start with the respective Hamiltonians in the laboratory coordinate frame and we transform them to the new coordinates comprising the three coordinates of the center of mass and the nine internal coordinates, \mathbf{r}_i , $i=1,2,3$. Upon transformation of the coordinate system the Hamiltonians representing the internal MV, D, SS, and OO corrections (in the relativistic limit we do not neglect the contributions from the anomalous magnetic moments of the particles [22]) have the following form [3]:

$$\hat{H}_{\text{MV}} = -\frac{1}{8} \left[\frac{1}{m_0^3} \left(\sum_{i=1}^3 \nabla_{\mathbf{r}_i} \right)^4 + \sum_{i=1}^3 \frac{1}{m_i^3} \nabla_{\mathbf{r}_i}^4 \right], \quad (2)$$

$$\hat{H}_{\text{D}} = -\frac{\pi}{2} \left(\sum_{i=1}^3 \frac{q_0 q_i (1 + 2\kappa_i)}{m_i^2} \delta^3(\mathbf{r}_i) + \sum_{i=1}^3 \sum_{j \neq i}^3 \frac{q_i q_j (1 + 2\kappa_i)}{m_i^2} \delta^3(\mathbf{r}_{ij}) \right), \quad (3)$$

$$\hat{H}_{\text{SS}} = -\frac{8}{3} \pi \frac{q_2 q_3 (1 + \kappa_2)(1 + \kappa_3)}{m_2 m_3} \delta^3(\mathbf{r}_{23}) (\mathbf{S}_2 \cdot \mathbf{S}_3), \quad (4)$$

$$\hat{H}_{\text{OO}} = -\frac{1}{2} \sum_{i=1}^3 \sum_{j=1}^3 \frac{q_0 q_j}{m_0 m_j} \left(\frac{1}{r_j} \nabla_{\mathbf{r}_i} \cdot \nabla_{\mathbf{r}_j} + \frac{1}{r_j^3} \mathbf{r}_j \cdot (\mathbf{r}_j \cdot \nabla_{\mathbf{r}_i}) \nabla_{\mathbf{r}_j} \right) + \frac{1}{2} \sum_{i=1}^3 \sum_{j > i}^3 \frac{q_i q_j}{m_i m_j} \left(\frac{1}{r_{ij}} \nabla_{\mathbf{r}_i} \cdot \nabla_{\mathbf{r}_j} + \frac{1}{r_{ij}^3} \mathbf{r}_{ij} \cdot (\mathbf{r}_{ij} \cdot \nabla_{\mathbf{r}_i}) \nabla_{\mathbf{r}_j} \right), \quad (5)$$

where $\mathbf{r}=\{\mathbf{r}'_1, \mathbf{r}'_2, \mathbf{r}'_3\}'$, $\kappa_1=1.792\,847\,3565$ is the anomalous magnetic moment of the proton, $\kappa_2=\kappa_3=\kappa_e=0.001\,159\,652\,1811$ are the anomalous magnetic moments of the electrons [21]. Since the spin of the reference particle (the helium nucleus) is zero, there are no contributions due to this particle to D and SS operators [23]. There is also no contribution to the SS operator due to the magnetic interaction between the proton and the two electrons because they have opposite spins. However, the D interaction in this case does not vanish and it is included in \hat{H}_{D} .

TABLE I. Total nonrelativistic and relativistic energies, and relativistic mass-velocity (MV), Darwin (D), electron spin-spin (SS), and orbit-orbit (OO) corrections for pure vibrational states of HeH^+ . All values are in a.u.

v	Basis size	E_{nonrel}	$\alpha^2\langle\hat{H}_{\text{MV}}\rangle$	$\alpha^2\langle\hat{H}_{\text{D}}\rangle$	$\alpha^2\langle\hat{H}_{\text{SS}(e-e)}\rangle$	$\alpha^2\langle\hat{H}_{\text{OO}}\rangle$	$\alpha^2\langle\hat{H}_{\text{rel}}\rangle$	E_{rel}
0	7000	-2.9710784654	-7.128170×10^{-4}	5.864615×10^{-4}	3.37531×10^{-5}	-7.6159×10^{-6}	-1.002183×10^{-4}	-2.9711786837
	8000	-2.9710784659	-7.128199×10^{-4}	5.864672×10^{-4}	3.37452×10^{-5}	-7.6159×10^{-6}	-1.002234×10^{-4}	-2.9711786893
1	7000	-2.9578148923	-7.111550×10^{-4}	5.847124×10^{-4}	3.35464×10^{-5}	-7.5116×10^{-6}	-1.004078×10^{-4}	-2.9579153001
	8000	-2.9578148944	-7.111671×10^{-4}	5.847252×10^{-4}	3.35445×10^{-5}	-7.5116×10^{-6}	-1.004090×10^{-4}	-2.9579153034
2	7000	-2.9459492595	-7.100918×10^{-4}	5.834716×10^{-4}	3.34335×10^{-5}	-7.4310×10^{-6}	-1.006177×10^{-4}	-2.9460498772
	8000	-2.9459492617	-7.101125×10^{-4}	5.834945×10^{-4}	3.34322×10^{-5}	-7.4310×10^{-6}	-1.006168×10^{-4}	-2.9460498785
3	7000	-2.9354895770	-7.095934×10^{-4}	5.827085×10^{-4}	3.34303×10^{-5}	-7.3749×10^{-6}	-1.008294×10^{-4}	-2.9355904064
4	7000	-2.9264583109	-7.096362×10^{-4}	5.823979×10^{-4}	3.35380×10^{-5}	-7.3440×10^{-6}	-1.010443×10^{-4}	-2.9265593552
5	7000	-2.9188927392	-7.102980×10^{-4}	5.826097×10^{-4}	3.37346×10^{-5}	-7.3386×10^{-6}	-1.012923×10^{-4}	-2.9189940315
6	7000	-2.9128423541	-7.115620×10^{-4}	5.833279×10^{-4}	3.40436×10^{-5}	-7.3583×10^{-6}	-1.015489×10^{-4}	-2.9129439030
7	7000	-2.9083566563	-7.133646×10^{-4}	5.845118×10^{-4}	3.44520×10^{-5}	-7.4013×10^{-6}	-1.018022×10^{-4}	-2.9084584585
8	7000	-2.9054435864	-7.156062×10^{-4}	5.860649×10^{-4}	3.49361×10^{-5}	-7.4603×10^{-6}	-1.020655×10^{-4}	-2.9055456519
9	7000	-2.9039514083	-7.177551×10^{-4}	5.876366×10^{-4}	3.53328×10^{-5}	-7.5173×10^{-6}	-1.023031×10^{-4}	-2.9040537115
10	7000	-2.9034218520	-7.190573×10^{-4}	5.885932×10^{-4}	3.55838×10^{-5}	-7.5508×10^{-6}	-1.024311×10^{-4}	-2.9035242831
11	7000	-2.9033104989	-7.195187×10^{-4}	5.889384×10^{-4}	3.56624×10^{-5}	-7.5630×10^{-6}	-1.024809×10^{-4}	-2.9034129798
He +H ⁺		-2.9033045565						

The total relativistic correction was calculated for each state as the expectation value of the Hamiltonian representing all four relativistic corrections,

$$\hat{H}_{\text{rel}} = \hat{H}_{\text{MV}} + \hat{H}_{\text{D}} + \hat{H}_{\text{SS}} + \hat{H}_{\text{OO}} \quad (6)$$

with the non-BO wave function for that state.

As in the previous non-BO calculations concerning small molecular systems with only σ electrons [9–12], here we also expanded the wave functions for the pure vibrational states of HeH^+ in terms of one-center, spherically symmetric, explicitly correlated Gaussians that included pre-exponential multipliers consisting of the internuclear distance, r_1 , raised to a non-negative even power, p_k ,

$$\phi_k = r_1^{p_k} \exp[-\mathbf{r}'(A_k \otimes I_3)\mathbf{r}], \quad (7)$$

where $\mathbf{r} = \{\mathbf{r}'_1, \mathbf{r}'_2, \mathbf{r}'_3\}'$. As our previous calculations have demonstrated, these functions are very effective in describing nonadiabatic, zero angular momentum states of diatomic systems. The presence of the $r_1^{p_k}$ factor in the function (7) allows us to describe the very strong nucleus-nucleus correlation effects. In Eq. (7), the matrix A_k of the Gaussian exponential coefficients is symmetric and positive definite. That guarantees the square integrability of the Gaussian. I_3 in Eq. (7) is the 3×3 identity matrix. Before a Gaussian was used in the expansion of the wave function, it was symmetrized with respect to the permutation of the electrons.

The reader can obtain more information on the Hamiltonian transformation and the selection of the basis functions for diatomic calculations from our recent reviews [7,8]. A more detailed derivation of the matrix elements with opera-

tors \hat{H}_{MV} and \hat{H}_{D} can be found in Ref. [24] and that with \hat{H}_{OO} , which is quite involved and lengthy, will be presented in a separate work [25].

The non-BO wave function for each vibrational state of HeH^+ was obtained in a separate calculation by minimizing the Rayleigh quotient,

$$E = \min \frac{c' H(\{p_k\}, \{A_k\}) c}{c' S(\{p_k\}, \{A_k\}) c}, \quad (8)$$

with respect to the linear expansion coefficients, c_k , the Gaussian exponential parameters, $\{A_k\}$, and the pre-exponential powers, $\{p_k\}$. In the calculations we used the Cholesky-factored form of $\{A_k\}$, $A_k \equiv L_k L_k'$, to avoid restricting the elements of the A_k matrix to make it positive definite. The positive definite character of $\{A_k\}$ is automatically achieved if L_k is a lower triangular matrix with no restrictions placed on its matrix elements. In the minimization we used the analytical gradient of the energy, $E(\{c_k\}, \{p_k\}, \{L_k\})$, calculated with respect to the elements of L_k .

The calculations have been performed for 12 pure vibrational states of HeH^+ . To achieve high accuracy we used 7000 basis functions for each state (this is by 1600 more than that used in Ref. [18]). We also recalculated the three lowest states with 8000 basis functions to assure that the nonrelativistic energies for those states are converged far beyond the accuracy of the two transition frequencies known from the experiment and used here to validate our results. We believe that with that many functions the total energies for all states are converged to within the eighth-to-ninth significant figure. The range of the pre-exponential powers, $\{p_k\}$, used was 0–250, and all the powers were partially optimized for each

TABLE II. Comparison of $v' \rightarrow v$ vibrational frequencies computed with and without inclusion of the α^2 relativistic corrections (ΔE_{rel} and ΔE_{nonrel}) with experimental frequencies obtained with two different extrapolation methods [18] (ΔE_{expt}^a and ΔE_{rel}^b). All values in cm^{-1} .

$v' \rightarrow v$	Basis size	ΔE_{nonrel}	ΔE_{rel}	ΔE_{expt}^a	ΔE_{rel}^b
1 \rightarrow 0	7000	2911.0178	2910.9762	2910.9590	2910.9572(7)
	8000	2911.0174	2910.9767		
2 \rightarrow 1	7000	2604.2054	2604.1593	2604.1472	2604.1482(12)
	8000	2604.2053	2604.1597		
3 \rightarrow 2	7000	2295.6350	2295.5885	2295.5792	2295.5340(61)
4 \rightarrow 3	7000	1982.1338	1982.0866		
5 \rightarrow 4	7000	1660.4510	1660.3966		
6 \rightarrow 5	7000	1327.9060	1327.8497		
7 \rightarrow 6	7000	984.4969	984.4413		
8 \rightarrow 7	7000	639.3449	639.2871		
9 \rightarrow 8	7000	327.4952	327.4431		
10 \rightarrow 9	7000	116.2242	116.1961		
11 \rightarrow 10	7000	24.4392	24.4283		

state. At the end of the calculations, after the wave functions for all 12 states ($v=0, \dots, 11$) were generated, we calculated the expectation value of the relativistic Hamiltonian (6) for each state and added it to its nonrelativistic energy. The total energies obtained this way were used to calculate the transition frequencies.

III. RESULTS AND DISCUSSION

The total non-BO nonrelativistic energies, the relativistic corrections, and the sum of the nonrelativistic energies and the relativistic corrections calculated with 7000 basis functions for each state and with 8000 basis functions for the lowest three states are shown in Table I. The transition energies for all 12 bound vibrational states of HeH^+ with zero total angular momentum obtained in the calculations are presented in Table II. Both nonrelativistic results and results including the relativistic corrections are shown. Those corrections result in lowering the frequencies for all transitions by $0.01\text{--}0.06 \text{ cm}^{-1}$. For the two lowest transitions ($1 \rightarrow 0$ and $2 \rightarrow 1$), where the experimental frequencies are most precisely known, the calculated results are only off from the experimental values by $0.0172\text{--}0.0190 \text{ cm}^{-1}$ and $0.0111\text{--}0.0121 \text{ cm}^{-1}$, respectively. This is approximately a

50% reduction of the discrepancies we had in our previous results [18] where we did not include the OO interaction (the discrepancies were $0.0417\text{--}0.0435 \text{ cm}^{-1}$ for the $1 \rightarrow 0$ transition and $0.0204\text{--}0.0194 \text{ cm}^{-1}$ for the $2 \rightarrow 1$ transition).

IV. SUMMARY

In conclusion, the results presented in this work demonstrate that the approach based on using the high-accuracy non-BO wave function in evaluating the α^2 relativistic correction yields results that match the high-resolution experimental transition energies with the accuracy approaching 0.01 cm^{-1} . To further increase the accuracy of the calculations one needs to include the lowest-order QED corrections as well as corrections due to the finite size of the nuclei and their polarizabilities. Our future effort will go in that direction.

ACKNOWLEDGMENTS

This work has been supported in part by the National Science Foundation. The authors are grateful to the University of Arizona Center of Computing and Information Technology for using their supercomputer resources.

[1] W. E. Caswell and G. P. Lepage, *Phys. Lett.* **167B**, 437 (1986).
 [2] T. Kinoshita and M. Nio, *Phys. Rev. D* **53**, 4909 (1996).
 [3] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron* (Publishing Corporation, New York, 1977).
 [4] P. Labelle, *Phys. Rev. D* **58**, 093013 (1998).
 [5] K. Pachucki, *Phys. Rev. A* **56**, 297 (1997).
 [6] M. Stanke, D. Kędziera, S. Bubin, and L. Adamowicz, *Phys. Rev. Lett.* **99**, 043001 (2007).

[7] M. Cafiero, S. Bubin, and L. Adamowicz, *Phys. Chem. Chem. Phys.* **5**, 1491 (2003).
 [8] S. Bubin, M. Cafiero, and L. Adamowicz, *Adv. Chem. Phys.* **131**, 377 (2005).
 [9] D. B. Kinghorn and L. Adamowicz, *J. Chem. Phys.* **110**, 7166 (1999).
 [10] D. B. Kinghorn and L. Adamowicz, *Phys. Rev. Lett.* **83**, 2541 (1999).

- [11] S. Bubin and L. Adamowicz, *J. Chem. Phys.* **118**, 3079 (2003).
- [12] M. Pavanello, S. Bubin, M. Molski, and L. Adamowicz, *J. Chem. Phys.* **123**, 104306 (2005).
- [13] L. Wolniewicz, *J. Chem. Phys.* **99**, 1851 (1993).
- [14] W. Cencek, J. Rychlewski, R. Jaquet, and W. Kutzelnigg, *J. Chem. Phys.* **108**, 2831 (1998).
- [15] G. Tarczay, A. G. Császár, W. Klopper, and H. M. Quiney, *Mol. Phys.* **99**, 1769 (2001).
- [16] O. L. Polyansky, A. G. Császár, S. V. Shirin, N. F. Zobov, P. Barletta, J. Tennyson, D. W. Schwenke, and P. J. Knowles, *Science* **299**, 539 (2003).
- [17] S. Bubin, M. Stanke, D. Kędziera, and L. Adamowicz, *Phys. Rev. A* **76**, 022512 (2007).
- [18] M. Stanke, D. Kędziera, M. Molski, S. Bubin, M. Barysz, and L. Adamowicz, *Phys. Rev. Lett.* **96**, 233002 (2006).
- [19] T. R. Hogness and E. G. Lunn, *Phys. Rev.* **26**, 44 (1925).
- [20] D. Galli and F. Palla, *Astron. Astrophys.* **335**, 403 (1998).
- [21] CODATA 2002 recommended values.
- [22] H. M. Pilkuhn, *Relativistic Particle Physics* (Springer-Verlag, New York, 1979).
- [23] R. N. Lee, A. I. Milstein, and M. Schumacher, *Phys. Rev. A* **64**, 032507 (2001).
- [24] D. Kędziera, M. Stanke, S. Bubin, M. Barysz, and L. Adamowicz, *J. Chem. Phys.* **125**, 014318 (2006).
- [25] M. Stanke, D. Kędziera, S. Bubin, M. Barysz, and L. Adamowicz (unpublished).