Precision spectroscopy of the hydrogen molecular ion HD^+

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Expectations values of the Breit operators and the \(Q\) terms are calculated for HD\(^+\) with the vibrational number \(v = 0–4\) and the total angular momentum \(L = 0–4\). Relativistic and radiative corrections to some ro-vibrational transition frequencies are determined. Numerical uncertainty in \(R_\infty\alpha^3\) order correction is reduced to sub-kHz or smaller. Our work provides an independent verification of Korobov’s calculations [Phys. Rev. A \textbf{74}, 052506 (2006); \textbf{77}, 022509 (2008)].

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I. INTRODUCTION

Hydrogen molecular ions, such as H\(_2^+\) and HD\(^+\), can be used \(^1\)\(^2\) to deduce an improved value of the proton-electron mass ratio by comparing experimental and theoretical spectroscopic data. To this end, several experiments have been setup for measuring high precision ro-vibrational transition in HD\(^+\) \(^8\) and HD\(^+\) \(^\|^9\). For HD\(^+\) in particular, the \((v, L) = (4, 3) \rightarrow (0, 2)\) transition frequency has been measured at the 2 ppb level \(^8\). In order to reduce the current uncertainty of \(4 \times 10^{-10}\) \(^6\) in the proton-electron mass ratio, both experiment and theory should reach a precision of sub-kHz or better.

For light systems, nonrelativistic QED (NRQED) \(^7\)\(^8\) approach is used to expand the energy in powers of the fine structure constant \(\alpha\). Nonrelativistic energies of H\(_2^+\) and HD\(^+\) have been variationally calculated at the precision of \(10^{-15}\) \(^2\)\(^9\)\(^10\) for a wide range of vibrational states and at the precision of \(10^{-30}\) \(^11\)\(^12\)\(^13\) for some low vibrational states. Relativistic and radiative corrections of order \(R_\infty\alpha^2\), \(R_\infty\alpha^3\), \(R_\infty\alpha^4\), and \(R_\infty\alpha^5\) have been systematically calculated \(^12\)\(^13\) for H\(_2^+\) and HD\(^+\) ro-vibrational states (\(v = 0–4\), \(L = 0–4\)). The leading order \(R_\infty\alpha^2\) relativistic corrections are now available with very high precision for the H\(_2^+\) vibrational states (0, 0), (1, 0), and (0, 1) \(^17\). Recently, improved values of \(R_\infty\alpha^3\) order corrections have been achieved by an intensive calculation of the Bethe logarithm term \(^18\).

The purpose of this Brief Report is to present our independent calculations of the Breit operators and the \(Q\) terms for the HD\(^+\) ro-vibrational states (\(v = 0–4\), \(L = 0–4\)). Some important ro-vibrational transition frequencies are determined, which provides a verification of Korobov’s theoretical work. In addition, the numerical results presented here might serve as a benchmark for other theoretical methods. We use atomic units \((\hbar = e = m_e = 1)\), unless otherwise stated. The fundamental physical constants involved are taken from the 2010 CODATA recommended values \(^6\).

II. THEORY

Consider the hydrogen molecular ion HD\(^+\). After separating the center of mass coordinates for the system, the eigenvalue problem for the nonrelativistic Hamiltonian \(H_0\) becomes \(^14\)

\[
H_0 \Psi = E_0 \Psi ,
\]

\[
H_0 = \lambda_1 \nabla_{r_1}^2 + \lambda_2 \nabla_{r_2}^2 + \lambda_{12} \nabla_{r_1} \cdot \nabla_{r_2} + V ,
\]

where \(r_1\) and \(r_2\) represent respectively the position vectors of the electron and proton, relative to the deuteron situated at the origin, \(\lambda_1 = - (1 + m_d)/(2m_d)\), \(\lambda_2 = - (1/m_d + 1/m_p)/2\), \(\lambda_{12} = - 1/m_d\), \(V = - 1/r_1 + 1/r_2 - 1/r_{12}\) is the Coulomb interaction, and \(r_{12} = r_1 - r_2\). The energy eigenvalue problem for \(H_0\) is solved variationally using the basis set in Hylleraas coordinates

\[
\phi_{ijk}(r_1, r_2) = r_1^{j} r_2^{k} e^{-\alpha r_1 - \beta r_2} \gamma_{L \ell z}^{LM}(r_1, r_2) ,
\]

where \(\gamma_{L \ell z}^{LM}(r_1, r_2)\) is the vector coupled product of spherical harmonics for the electron and the proton to form a common eigenvector of \(L^2\) and \(L_z\). More details on the construction of basis set for HD\(^+\) may be found in \(^12\)\(^13\). It should be pointed out that this basis set differs from the one used by Korobov \(^12\)\(^13\). The basic type of integrals required in the calculation of matrix elements can be evaluated analytically \(^19\) using Perkins’ expansion for \(r_{12}^k\). The procedure for handling singular integrals that appear in the evaluation of Breit operators can be found in \(^20\).

The leading-order relativistic corrections due to the Breit operators are well established, which can be found in Refs. \(^21\)\(^23\). The complete spin-independent part of order \(R_\infty\alpha^2\) term is

\[
E^{(2)} = \alpha^2 \langle H_{\text{Breit}} \rangle ,
\]

where

\[
H_{\text{Breit}} = - \frac{1}{8} \nabla_{r_1}^4 - \frac{1}{8m_p^2} \nabla_{r_2}^4 - \frac{1}{8m_d} (\nabla_{r_1} + \nabla_{r_2})^4
+ \frac{\pi}{2m_p^2} [\delta(r_{12}) + \frac{\pi}{2} (\delta(r_1) + \delta(r_{12}))]
- R_{de} + R_{dp} - R_{pe} ,
\]
\[ R_{de} = \frac{-1}{2m_d} \left( \frac{\nabla r_1 \cdot (\nabla r_1 + \nabla r_2)}{r_1} + \frac{r_1 r_1 : (\nabla r_2 + \nabla r_2)\nabla r_1}{r_1^2} \right) \]
\[ R_{dp} = \frac{-1}{2m_d m_p} \left( \frac{\nabla r_2 \cdot (\nabla r_1 + \nabla r_2)}{r_2} + \frac{r_2 r_2 : (\nabla r_1 + \nabla r_2)\nabla r_2}{r_2^2} \right) \]
\[ R_{pe} = \frac{1}{2m_p} \left( \frac{\nabla r_1 \cdot \nabla r_2}{r_{12}} + \frac{r_{12} r_{12} : \nabla r_1 \nabla r_2}{r_{12}^2} \right). \]

In the above, the Darwin term $\pi/(2m^2)\delta(r_{12})$ is the nuclear spin dependent recoil correction for the spin-$\frac{1}{2}$ particle, such as proton. This term vanishes in case of spin-0 or spin-1 nucleus, such as the $^4\text{He}$ nucleus or deuterion \[24\]. It is noted that $\delta(r)$ is virtually zero due to the molecular nature of the system.

Furthermore, the spin-independent radiative correction of order $R_{\infty}\alpha^3$ may be expressed as \[25\]–\[27\]:
\[ E^{(3)} = \alpha^3 \left\{ \frac{4}{3} \left[ -\ln \alpha^2 - \beta(v, L) + \frac{19}{30} \right] (\delta(r_1) + \delta(r_{12})) + \frac{2}{3} \left[ -\ln \alpha - 4\beta(v, L) + \frac{31}{3} \right] \langle \delta(r_1) \rangle + \langle \delta(r_{12}) \rangle - \frac{14}{3} \left[ \frac{Q(r_1)}{m_d} + \frac{Q(r_{12})}{m_p} \right] \right\}, \quad (6) \]
where $\beta(v, L)$ is the Bethe logarithm, $Q(r_1)$ and $Q(r_{12})$ are the $Q$ terms introduced by Araki and Sucher \[28\],
\[ Q(r) = \lim_{\rho \to 0} \left\{ \frac{\Theta(r - \rho)}{4\pi r^3} + (\ln \rho + \gamma_E)\delta(r) \right\}, \quad (7) \]
and $\gamma_E$ is the Euler gamma constant.

For higher order corrections, such as orders $R_{\infty}^2\alpha^4$ and $R_{\infty}^3\alpha^5$, we follow the work of Ref. \[16\]. Thus, $R_{\infty}^2\alpha^4$ order non-relativistic and radiative corrections may be express as follows \[10\]:
\[ E^{(4)} = \alpha^4 \left\{ \frac{1}{\pi} \left[ -\frac{2179}{648} + \frac{3523}{864} - \frac{1}{2}\pi^2 - 2 - \frac{9}{4} \right] \langle \delta(r_1) \rangle + \langle \delta(r_{12}) \rangle + E_{\text{rel}}^{(4)} \right\}, \quad (8) \]
where $E_{\text{rel}}^{(4)}$ is the $R_{\infty}^3\alpha^4$ order relativistic correction.

Since the electron is almost bounded in the ground state of hydrogen molecular ion, its wave function can be approximately expressed as a linear combination of two hydrogen-like wave functions $\psi_e(r_e) = C[\psi_{1s}(r_1) + \psi_{1s}(r_{12})]$. Therefore, the most important $R_{\infty}^3\alpha^5$ order correction can be estimated using this approximate wave function \[10\]–\[22\]:
\[ E^{(5)} = \alpha^5 \left[ -\ln^2 \frac{1}{(\alpha)^2} + A_{61} \ln \frac{1}{(\alpha)^2} + A_{60} + \frac{B_{50}}{\pi} \right] \times \langle \delta(r_1) \rangle + \langle \delta(r_{12}) \rangle, \quad (9) \]
where the constants $A_{61}$, $A_{60}$, and $B_{50}$ are taken to be the constants of the $1s$ state of the atomic hydrogen.

| $N$ | $\delta(r_1)$ | $\delta(r_{12})$ |
|-----|---------------|---------------|
| 2789 | 0.188 729 941 487 | 0.188 382 948 5531 | $A_{61} = 5.419 \cdots \[29\]$, $A_{60} = -30.924 \cdots \[30\]$, and $B_{50} = -21.556 \cdots \[31\].

In addition to the relativistic and radiative corrections, one also needs to consider the contribution from the finite nuclear charge distribution. The leading-order correction is
\[ E_{\text{nuc}} = \frac{2\pi}{3} \left[ \left( \frac{R_d}{a_0} \right)^2 \langle \delta(r_1) \rangle + \left( \frac{R_p}{a_0} \right)^2 \langle \delta(r_{12}) \rangle \right], \quad (10) \]
where $R_p = 0.8775(51)$ fm and $R_d = 2.1424(21)$ fm are the root-mean-square charge radii of proton and deuteron respectively.

### III. RESULTS

With the Hylleraas-type basis set of Eq. \[43\], the wave functions along with the corresponding nonrelativistic energies are obtained by solving Eq. \[11\] variationally. Then the expectation values of the Breit operators can be evaluated. In particular, the global operator method \[32\] is applied to the evaluations of $\nabla_1^4$, $\nabla_2^4$, $\nabla_1^2 + \nabla_2^2$, $\delta(r_1)$, and $\delta(r_{12})$. As an example, Table II shows a convergence study for the expectation values of $\delta(r_1)$ and $\delta(r_{12})$. One can see that an accuracy of about 11-12 significant figures is achieved for the most difficult state of $(4, 4)$, where the nonrelativistic energy is calculated only to 16 digits. For ro-vibrational states ($v = 0–4, L = 0–4$), numerical results of the Breit operators are presented in Tables III and IV together with a comparison with Korobov’s values \[13\]. Results for the $Q$ terms are listed in Tables V and VI. All expectation values are in good agreement with Korobov’s values, although our results are more precise. The largest size of basis set used here is about 9000.

We summarize the contributions up to $R_{\infty}^3\alpha^5$ to two ro-vibrational transition frequencies in Table VI where the values of the Bethe logarithm are taken from Ref. \[18\] and the $R_{\infty}^3\alpha^4$ order relativistic correction $E_{\text{rel}}^{(4)}$ taken from Ref. \[16\]. For the $(1, 0) \rightarrow (0, 0)$ transition, the numerical uncertainty in $\Delta E_{\text{rel}}$ has been reduced from 1 kHz in Korobov’s value to the present 8 Hz, which is due entirely to the uncertainties in the fundamental constants.
The correction $\Delta E_{\alpha^2}$ to this transition has been obtained in Ref. [15] and reproduced here. The recoil correction of $R_{\alpha^2} \alpha^3 (m/M)$ and higher contributes at the level of relative $10^{-10}-10^{-11}$, which causes a theoretical uncertainty of 1 kHz in $\Delta E_{\alpha^2}$. The largest uncertainty for the transition $(1,0) \rightarrow (0,0)$ comes from the theoretical uncertainty of $\Delta E_{\alpha^2}$. The uncertainty in $\Delta E_{\alpha^2}$ is due to the uncertainties in the proton and deuteron charge radii. For the transition $(4,3) \rightarrow (0,2)$, both experimental and theoretical results are available. In our calculation for this transition, although the uncertainties in $\Delta E_{\alpha^2}$ and $\Delta E_{\alpha^3}$ have been reduced to sub kHz, the
TABLE III: Expectation values of $R_{dp}$, $R_{dc}$, and $R_{pe}$ for HD$^+$ with $v = 0 − 4$ and $L = 0 − 4$. Korobov’s results \cite{13} are listed in the second entry of each ro-vibrational state.

| $(v, L)$ | $R_{dp}$ | $R_{dc}$ | $R_{pe}$ |
|----------|----------|----------|----------|
| $(0, 0)$ | 5.35463051901711943(7) | 1.17448782932605556(3) | 1.170770145051139727(2) |
| $(1, 0)$ | 15.1448258936280077(6) | 1.1504812637673131(2) | 1.1433640050405(2) |
| $(2, 0)$ | 23.5989696623698(2) | 1.1282362008927494(6) | 1.1181235693136(2) |
| $(3, 0)$ | 30.817653006822(1) | 1.1077720643593(3) | 1.094375427689(2) |
| $(4, 0)$ | 36.88807887511(1) | 1.0883992649(8) | 1.07371830917(3) |
| $(0, 1)$ | 5.589562255342723(1) | 1.1735785001855910(1) | 1.169713799366195(4) |
| $(1, 1)$ | 15.3507527986306(1) | 1.1469258855220391(3) | 1.142380739612365(7) |
| $(2, 1)$ | 23.77772089355404(4) | 1.1274352102467439(1) | 1.11720015102388(1) |
| $(3, 1)$ | 30.97134959374(1) | 1.1069233223353(1) | 1.09407389213715(9) |
| $(4, 1)$ | 37.0183653341(6) | 1.0883423109(2) | 1.072912309499(1) |
| $(0, 2)$ | 6.05510481824934733(4) | 1.17169108405540(2) | 1.1676298214835329(3) |
| $(1, 2)$ | 15.75082763752410(4) | 1.147923888699637(7) | 1.140203152040445(2) |
| $(2, 2)$ | 24.1350123361982(4) | 1.12583357622946(1) | 1.11536727098303(3) |
| $(3, 2)$ | 31.275189712792(3) | 1.105426322514(2) | 1.092365391832(2) |
| $(4, 2)$ | 37.275607599566(2) | 1.086630566009(1) | 1.07130988849887(8) |
| $(0, 3)$ | 6.74277630617217739(6) | 1.169077912520748(2) | 1.164523841766(2) |
| $(1, 3)$ | 16.35924480624(3) | 1.145927900044(2) | 1.137506628241(4) |
| $(2, 3)$ | 24.65278167001289(9) | 1.1234560568468(8) | 1.112634817630(2) |
| $(3, 3)$ | 31.7221152212(6) | 1.103194064780(2) | 1.0898050864(1) |
| $(4, 3)$ | 37.65328339(4) | 1.0845441798(5) | 1.068929626(1) |
| $(0, 4)$ | 7.640242669140628(6) | 1.1653169532956(5) | 1.160431693454(5) |
| $(1, 4)$ | 17.1426052788899(3) | 1.142081168039(4) | 1.133671151272(3) |
| $(2, 4)$ | 25.3308170266259(7) | 1.120324362118(2) | 1.10904358742(1) |
| $(3, 4)$ | 32.3023200847(1) | 1.10025795806(8) | 1.08648221081(5) |
| $(4, 4)$ | 38.14194609(1) | 1.0817974074(2) | 1.0657990275(3) |

The total uncertainty in the transition frequency remains as large as 70 kHz, which is from the $\Delta E\alpha^*$ term.

In summary, we have presented an independent calculation of the Breit operators and the $Q$ terms for the HD$^+$ ro-vibrational states ($v = 0 − 4, L = 0 − 4$), which provides a verification of previous theoretical results.

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TABLE IV: Numerical values of $Q(r_1)$ for HD$^+$ with $v = 0 - 4$ and $L = 0 - 4$, where the second entry lists Korobov’s results [15].

| $v$ | $L = 0$ | $L = 1$ | $L = 2$ | $L = 3$ | $L = 4$ |
|-----|---------|---------|---------|---------|---------|
| $v = 0$ | $-0.1348622766681903(2)$ | $-0.132113355129(1)$ | $-0.129551987571271(1)$ | $-0.1271692904455(1)$ | $-0.12495749557739(3)$ |
| $v = 1$ | $-0.13486$ | $-0.1321$ | $-0.12955$ | $-0.12717$ | $-0.12496$ |
| $v = 2$ | $-0.13474$ | $-0.13202$ | $-0.12944$ | $-0.12707$ | $-0.12486$ |
| $v = 3$ | $-0.13450$ | $-0.13177$ | $-0.12923$ | $-0.12687$ | $-0.12467$ |
| $v = 4$ | $-0.13415$ | $-0.13144$ | $-0.12891$ | $-0.12657$ | $-0.12439$ |
| $v = 5$ | $-0.13368$ | $-0.13100$ | $-0.12850$ | $-0.12617$ | $-0.12402$ |

TABLE V: Numerical values of $Q(r_{12})$ for HD$^+$ with $v = 0 - 4$ and $L = 0 - 4$, where the second entry lists Korobov’s results [15].

| $v$ | $L = 0$ | $L = 1$ | $L = 2$ | $L = 3$ | $L = 4$ |
|-----|---------|---------|---------|---------|---------|
| $v = 0$ | $-0.13459119556585105(1)$ | $-0.13183897779797(3)$ | $-0.12927929986259(7)$ | $-0.1268839283180(2)$ | $-0.12466388687278(6)$ |
| $v = 1$ | $-0.13459$ | $-0.13184$ | $-0.12927$ | $-0.12688$ | $-0.12466$ |
| $v = 2$ | $-0.13447$ | $-0.13172$ | $-0.12916$ | $-0.12678$ | $-0.12450$ |
| $v = 3$ | $-0.13423$ | $-0.13150$ | $-0.12895$ | $-0.12658$ | $-0.12438$ |
| $v = 4$ | $-0.13388$ | $-0.13116$ | $-0.12863$ | $-0.12628$ | $-0.12410$ |
| $v = 5$ | $-0.13344$ | $-0.13072$ | $-0.12822$ | $-0.12589$ | $-0.12373$ |

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[1] L. Hilico, N. Billy, B. Grémaud, and D. Delande, Eur. Phys. J. D 12, 449 (2000).
[2] S. Schiller and V.I. Korobov, Phys. Rev. A 71, 032505 (2005).
[3] J.C.J. Koelmeij, B. Roth, A. Wicht, I. Ernsting, and S. Schiller, Phys. Rev. Lett. 98, 173002 (2007); U. Bressel, A. Borodin, J. Shen, M. Hansen, I. Ernsting, and S. Schiller, Phys. Rev. Lett. 108, 183003 (2012).
[4] J.C.J. Koelmeij, Phys. Chem. Chem. Phys. 13, 18844 (2011); J.C.J. Koelmeij, D.W.E. Noom, D. de Jong, M.A. Haddad and W. Ubachs, Appl. Phys. B 107, 1075(2012).
[5] J.-Ph. Karr, F. Bielsa, A. Douillet, J. Pedregosa Gutierrez, V.I. Korobov, and L. Hilico, Phys. Rev. A 77, 063410 (2008); J.-Ph. Karr, A. Douillet, L. Hilico, Appl. Phys. B, 107, 1043(2011).
[6] http://physics.nist.gov/cuu/Constants/index.html
[7] W.E. Caswell and J.P. Lepage, Phys. Lett. B 167, 437 (1986).
[8] M. Nio and T. Kinoshita, Phys. Rev. D 55, 7267 (1997).
[9] J.-Ph. Karr, S. Klic, and L. Hilico, J. Phys. B 38, 853 (2005).
[10] V.I. Korobov, Phys. Rev. A 61, 064503 (2000).
[11] D.H. Bailey and A.M. Frolov, J. Phys. B 35, 4287 (2002).
[12] Z.-C. Yan, J.-Y. Zhang, and Y. Li, Phys. Rev. A 67, 062504 (2003).
[13] M.M. Cassar and G.W.F. Drake, J. Phys. B 37, 2485 (2004).
[14] H. Li, J. Wu, B.-L. Zhou, J.-M. Zhu, and Z.-C. Yan, Phys. Rev. A 75, 012504 (2007).
[15] V.I. Korobov, Phys. Rev. A 74, 052506 (2006).
[16] V.I. Korobov, Phys. Rev. A 77, 022509 (2008).
[17] Z.-X. Zhong, Z.-C. Yan and T.-Y. Shi, Phys. Rev. A 79, 064502 (2009).
[18] V.I. Korobov and Z.-X. Zhong, Phys. Rev. A 86, 044501 (2012).
[19] Z.-C. Yan and G.W.F. Drake, Chem. Phys. Lett. 259, 96 (1996).
[20] Z.-C. Yan and G.W.F. Drake, Can. J. Phys. 72, 822 (1994).
[21] H.A. Bethe and E.E. Salpeter, Quantum Mechanics of One- and Two-Electron Atoms (Plenum, New York, 1977).
[22] V.B. Berestetsky, E.M. Lifshitz, and L.P. Pitaevsky, Relativistic Quantum Theory (Pergamon, Oxford, 1982).
[23] M.I. Eides, H. Grotch, and V.A. Shelyuto, Phys. Rep. 342, 63 (2001).
[24] K. Pachucki and S. Karshenboim, J. Phys. B 28, L221 (1995).
[25] V.I. Korobov, Phys. Rev. A 70, 012505 (2004).
[26] K. Pachucki, J. Phys. B 31, 3547 (1998).
[27] A. Yelkhovsky, Phys. Rev. A 64, 062104 (2001).
[28] H. Araki, Prog. Theor. Phys. 17, 619 (1957); J. Sacher, Phys. Rev. 109, 1010 (1958).
TABLE VI: Summery of contributions to the HD$^+$ transition frequencies (in MHz).

| Author | Present | (4, 3) → (0, 2) | Present | (1, 0) → (0, 0) | Korobov [16] |
|--------|---------|----------------|---------|----------------|--------------|
| $\Delta E_{\text{tot}}$ | 214 976 047.328 2(6) | 57 349 439.973 34(14) | 57 349 439.9717 |
| $\Delta E_{\text{nr}}$ | 3 411.702 93(4) | 958.276 694(8) | 958.277(01)$^a$ |
| $\Delta E_{\alpha,3}$ | -891.610 9(1) | -242.126 26(4) | -242.125(02) |
| $\Delta E_{\alpha,4}$ | -6.457(1) | -1.748(1) | -1.748 |
| $\Delta E_{\alpha,5}$ | 0.388(74) | 0.105(20) | 0.105(19) |
| $\Delta E_{\text{nuc}}$ | -0.462(6) | -0.125 2(17) | -0.125(2)$^a$ |

$^a$Obtained using the data of Table V in Ref. [12].

[29] A. J. Layzer, Phys. Rev. Lett. 4, 580 (1960).
[30] K. Pachucki, Ann. Phys. (N.Y.) 226, 1 (1993).
[31] K. Pachucki, Phys. Rev. Lett. 72, 3154 (1994); M.I. Eides and V.A. Shelyuto, Phys. Rev. A 52, 954 (1995).
[32] R.J. Drachman, J. Phys. B 14, 2733 (1981).