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Ground-state energy of H-: a critical test of triple basis sets

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We report an improved variational upper bound for the ground state energy of H⁻ using Hylleraas-like wave functions in the form of a triple basis set having three distinct distance scales. The extended precision DQFUN of Bailey, allowing for 70 decimal digit arithmetic, is implemented to retain sufficient precision. Our result exceeds the previous record [A. M. Frolov, Euro. J. Phys. D **69**, 132 (2015)], indicating that the Hylleraas triple basis set exhibits comparable convergence to the widely used pseudorandom all-exponential basis sets, but the numerical stability against roundoff error is much better. It is argued that the three distance scales have a clear physical interpretation. The new variational bound is –0.527 751 016 544 377 196 590 814 469 a.u.

I. INTRODUCTION

High-precision calculations of properties of two-electron atoms and ions, requiring a treatment of electron correlation, have long served as a benchmark for the various methods of constructing wave functions, beginning with the pioneering work of Hylleraas [1]. The key property of interest is the nonrelativistic ground state energy of helium or heliumlike ions, such as H⁻, a quantity calculated previously in Refs. [2–8] that will be the subject of this paper. Variational calculations provide an upper bound to the exact ground-state energy, and by the Hylleraas-Undheim-McDonald (HUM) theorem [9], also for the excited states.

These undertakings are critically important since the variational procedure that leads to the best basis functions for the energies can then be used in the calculation of the suite of matrix elements needed for the perturbations prescribed by the NRQED program [10, 11], leading to meaningful comparisons with experiments. This is particularly important in the high-precision calculations that are used in searches for new physics, such as the calculation and measurement of the tuneout frequency of helium [12] and King plots to search for an electron-neutron interaction [13].

The difference in these variational calculations lies in the choice of basis states. A conventional Hylleraas function has the form (for S-states)

$$\varphi_{ijk}(\alpha, \beta) = r_1^i \, r_2^j \, r_{12}^k \, e^{-\alpha r_1 - \beta r_2} \pm \text{exchange}, \quad (1)$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the two electrons relative to the nucleus, $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$, and α and β are nonlinear parameters that set the distance scale. This sometimes written equivalently in terms of perimetric coordinates $s = r_1 + r_2$, $t = r_1 - r_2$ and $u = r_{12}$. In a standard Hylleraas calculation, as used in the early work by Pekeris and others [14], one starts with a variational trial function of the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2)_{\text{tr}} = \sum_{i,j,k=0}^{i+j+k\leq\Omega} a_{ijk}\varphi_{ijk}(\alpha, \beta) \quad (2)$$

where the a_{ijk} are linear variational parameters, as determined by matrix diagonalization. Ω defines a Pekeris shell of terms that typically controls the size of the basis set. If all terms are included, then the number of terms in the variational basis set is

$$N = \frac{(\Omega + 1)(\Omega + 2)(\Omega + 3)}{6} \quad (3)$$

and so grows as Ω^3. The quantity

$$E_{\text{tr}} = \frac{\langle\Psi_{\text{tr}}|H|\Psi_{\text{tr}}\rangle}{\langle\Psi_{\text{tr}}\Psi_{\text{tr}}\rangle} \quad (4)$$

is then an upper bound to the true ground-state energy for a system with Hamiltonian H. By the HUM theorem [9], the higher matrix eigenvalues are also upper bounds to the true excited states, provided only that the correct number of matrix eigenvalues lies lower. No further orthogonalization is required.

There are two main problems with this approach. First, although the Hylleraas basis set is provably complete [15], and so is guaranteed to converge to the correct answer as Ω is increased, a point of diminishing returns is reached. In addition, the matrix eigenvalue problem becomes ill-conditioned leading to a severe loss of significant figures. Second, the accuracy rapidly deteriorates with increasing principal quantum number n for the higher-lying excited states.

There have been three main approaches to circumvent these problems. The first is to include other functional forms, such as negative powers of s [16], half-integral powers [17] and logarithmic terms of the form $\ln R$ where $R = (r_1^2 + r_2^2)^{1/2}$ [3, 18, 19], as suggested by the Fock expansion [20]. This approach was carried to its ultimate conclusion by Schwartz [21], who obtained the ground state energy of helium to 38 decimal digits with the use of 104-digit arithmetic. This still stands as the record for the most accurate calculation for a three-body system, but it did not solve the problem of a loss of numerical stability, or loss of accuracy with increasing n. Also, integrals over the logarithmic terms are more difficult in the calculation of relativistic and QED corrections.

The second approach involves introducing a completely different kind of Hylleraas function, as first proposed by Frolov and coworkers [22], and further developed by Korobov [23, 24] of the form

$$\varphi_{\text{exp}}(\alpha, \beta, \gamma) = e^{-\alpha r_1 - \beta r_2 - \gamma r_{12}} \quad (5)$$

This form has a γr_{12} term in the exponent, and no powers of the radial coordinates at all. The trial function then has the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2)_{\mathrm{tr}} = \sum_{i=0}^{N} a_i \varphi_{\exp}(\alpha_i, \beta_i, \gamma_i) \qquad (6)$$

with the $3N$ nonlinear parameters $\alpha_i, \beta_i, \gamma_i$ chosen in a quasi-random manner, including complex values. The advantages of this approach is the simplicity of the basis set and the ease with which integrals over the basis set can be calculated. The disadvantage is that extended precision arithmetic is required to maintain numerical stability, and the accuracy declines with increasing n for excited states. Nevertheless, very high accuracy has been obtained with this method up to $n = 6$ [25].

The third approach involves doubling the basis set, as first proposed by Drake [26–28], so that the trial wave function becomes

$$\Psi(\mathbf{r}_1, \mathbf{r}_2)_{\mathrm{tr}} = \sum_{i,j,k=0}^{i+j+k\leq\Omega} \left[c_{ijk}^{(\mathrm{A})} \varphi_{ijk}(\alpha_\mathrm{A}, \beta_\mathrm{A}) \right. $$
$$\left. + c_{ijk}^{(\mathrm{B})} \varphi_{ijk}(\alpha_\mathrm{B}, \beta_\mathrm{B}) \right] \qquad (7)$$

In this form, each combination of powers i, j, k occurs twice with independent linear variational parameters $c_{ijk}^{(\mathrm{A})}$ and $c_{ijk}^{(\mathrm{B})}$, and four nonlinear parameters α_A, β_A and α_B, β_B. Their optimization produces a natural separation of the basis set into an asymptotic A sector with approximately (screened) hydrogenic values for α_A, β_A, and a short-range B sector with much larger values of α_B, β_B that increase systematically with Ω. In general, there is also a screened hydrogenic term $c_0 \Psi_0$, but this is omitted for $Z = 1$.

The original motivation for doubling the basis set was to improve the accuracy for the higher-lying Rydberg states of helium where there are indeed two distinct distance scales at play, and high precision results have been obtained for all states of helium up to $n = 10$ and $L = 7$ [29]. An additional bonus is that doubling the basis set also improves the accuracy for the ground state by more than an order of magnitude for basis sets of the same size [30], and with improved numerical stability. (The 1992/94 results were obtained with the 18-digit Definicon processor that was available at the time.)

If doubling the basis set helps, then it is natural to ask what happens if the basis set is tripled or quadrupled. By extension of Eq. (7), the trial wave function with a triple basis set reads

$$\Psi(\mathbf{r}_1, \mathbf{r}_2)_{\mathrm{tr}} = \sum_{ijk}^{i+j+k\leq\Omega_\mathrm{A}} \underbrace{c_{ijk}^{(\mathrm{A})} \varphi_{ijk}(\alpha_\mathrm{A}, \beta_\mathrm{A})}_{\text{A-sector}}$$
$$+ \sum_{ijk}^{i+j+k\leq\Omega_\mathrm{B}} \underbrace{c_{ijk}^{(\mathrm{B})} \varphi_{ijk}(\alpha_\mathrm{B}, \beta_\mathrm{B})}_{\text{B-sector}} \qquad (8)$$
$$+ \sum_{ijk}^{i+j+k\leq\Omega_\mathrm{C}} \underbrace{c_{ijk}^{(\mathrm{C})} \varphi_{ijk}(\alpha_\mathrm{C}, \beta_\mathrm{C})}_{\text{C-sector}}$$

The parameters Ω_X ($X = \mathrm{A, B, C}$) separately control the number of terms in each sector. Earlier calculations with a triple basis set for the ground states of He, $\mathrm{H^-}$ and $\mathrm{Ps^-}$ [5] showed that eigenvalues accurate to 21 figures could be obtained with standard quadruple precision (32 decimal digit) arithmetic. At the time, these were the most accurate values in the literature, but they have since been surpassed in accuracy by all-exponential calculations of the Korobov type with larger basis sets [6–8, 24, 25]. Although the original 21-figure accuracy is sufficient for current atomic physics applications (including the calculation of relativistic and QED corrections), it is still interesting to test the ultimate accuracy of the triple-basis-set method in comparison with the all-exponential method. The present work therefore extends the previous calculations for $\mathrm{H^-}$ [5] to much larger basis sets ($\sim$10 000 terms). At this level, it is necessary to use extended precision arithmetic. We have therefore implemented the multiprecision FORTRAN90 package of Bailey [31] with double-quadruple (dq) precision, afforded by the DQ-FUN package [32]. The resulting 70-digit arithmetic is much more than what is actually needed.

II. CALCULATIONS

The main computational step is to construct approximate variational solutions to the Schrödinger equation with a triple basis set. In centre-of-mass coordinates, the Hamiltonian is

$$H = \frac{1}{2\mu} \sum_{i=1}^{N} \mathbf{p}_i^2 + \frac{1}{M} \sum_{i=1}^{N} \sum_{j>i}^{N} \mathbf{p}_i \cdot \mathbf{p}_j$$
$$- \sum_{i=1}^{N} \left(\frac{Ze^2/4\pi\epsilon_0}{|\mathbf{r}_i|} + \sum_{j>i}^{N} \frac{e^2/4\pi\epsilon_0}{|\mathbf{r}_j - \mathbf{r}_i|} \right). \qquad (9)$$

with nuclear charge $Z = 1$ for $\mathrm{H^-}$. We present results for both the finite- and infinite-mass cases, corresponding to either including or excluding the $\mathbf{p}_i \cdot \mathbf{p}_j$ mass polarization term in Eq. (9). The variational solution is obtained by solving the generalized eigenvalue problem

$$\mathbf{H} - E\mathbf{O} = 0,$$

where $\mathbf{H}$ and $\mathbf{O}$ are the Hamiltonian and overlap matrices in the basis given by Eq. (8). The nonlinear parameters are then optimized on a six-dimensional energy surface by calculating analytically the derivatives $\partial E / \partial \alpha_x$ and $\partial E / \partial \beta_x$ [28]. The second derivatives are then estimated by differencing, and the zeros of the first derivatives located by Newton's method. Since the derivatives become exceedingly small near the minimum, the optimization is carried out on a finite grid of points to avoid excessive numerical cancellation in estimating the second derivatives by differencing.

The optimization procedure produces a natural partition of the three sectors in Eq. 8 into different distance scales with a clear physical meaning. The A sector with the smallest nonlinear parameters represents the asymptotic region $r \to \infty$; the B sector with intermediate nonlinear parameters optimizes the intermediate region; and the C sector, with the largest value for the nonlinear parameters, optimizes the short-range behaviour of the wave function. Fig. 1 shows how these nonlinear parameters vary with Ω conrolling the size of the basis set. In the asymptotic A sector, α_A, β_A remain nearly constant as Ω increases. In contrast, α_B, β_B, and especially α_C, β_C increase nearly linearly with Ω. As a consequence, the characteristic function $r^\Omega e^{-\alpha r}$ peaks at approximately the same constant distance $r_{\text{peak}} = \Omega / \alpha$ from the nucleus in the B and C regions. Thus the wave function spreads inwards with increasing Ω to represent complex inner correlation effects, and perhaps also simulate logarithmic terms.

III. RESULTS

This section describes the results of a sequence of calculations for the ground-state energy of H^-, and their convergence with increasing basis set size, as controlled by Ω_X. The nominal size of each sector is as given by Eq. (3). However, Since the triple basis set is over-complete in that each combination of powers is included three times, we have found that it is possible to introduce a few truncations that improve the efficiency and numerical stability without significantly affecting the accuracy of the final results. The truncations are as follows:

- Since the two electrons are equivalent, terms with $i > j$ are omitted. This reduces the basis set size by nearly a factor of 2.

- In sector A (the long-range sector), the highest powers j and k of r_2 and r_{12} respectively are limited to $\Omega_A - 4$.

- In sectors C, the value of Ω_C is reduced to $\Omega_C = \Omega_A - 8$, while $\Omega_B = \Omega_A$.

- In sectors $X = B$ and C, the terms are restricted to those with $i + j + k - |i - j| < \Omega_X$ for $k > 6$.
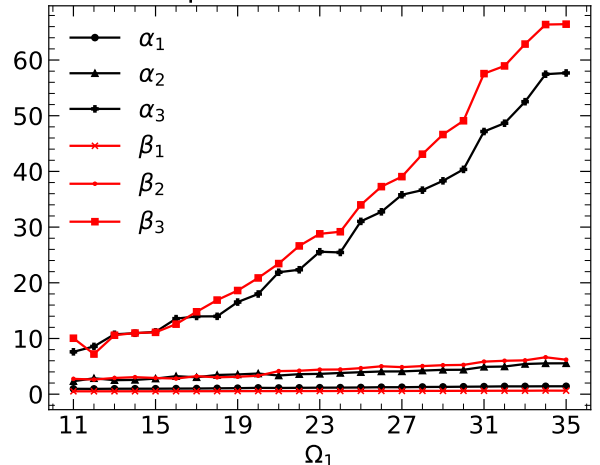

FIG. 1: Variation of the nonlinear parameters $\alpha_X, \beta_X, X = 1, 2, 3$ with basis set size (corresponds to $X = $ A, B, C in the text), determined by $\Omega_1 = \Omega_A$.

The last truncation is a modified version of one originally suggested by Kono and Hattori [36]. It suppresses terms in the short-range B and C sectors where the powers of r_1 and r_2 are very different. The second truncation on the maximum powers of r_2 and r_{12} in sector A was not used in our previous Ref. [5], making the present basis sets slightly smaller. For example, the present size is 2263 terms at $\Omega_A = 21$, instead of the previous 2276 terms. These truncations only affect the order in which the basis functions are added, and so they do not affect the completeness of the basis set or the ultimate convergence of the results.

As a test of the truncations, Fig. 3 displays the fractional energy difference between successive calculations of different basis set sizes as a function of the number of terms. The advantage of using the described truncations, particularly for larger basis sets where the energy obtained using truncated basis sets is consistently lower. The fractional difference being smaller demonstrates that convergence is being achieved faster in the case of the truncated basis sets.

The significant advantage gained by using a triple basis over a double basis set is displayed in Fig. 3. The triple basis sets give upper bounds that are several orders of magnitude more accurate for a given number of terms. Since Ω becomes large more quickly for the double basis sets with the same number of terms as a triple basis set, a point of diminishing returns is reached sooner. We therefore did not attempt to perform large ($N > 5500$) calculations for the double basis set case.

Tables IV and IV show the convergence pattern for the ground state energy of the infinite- and finite-mass cases respectively, obtained by progressively increasing Ω_A with the aforementioned truncations. Also displayed in these convergence tables is the difference in energy,
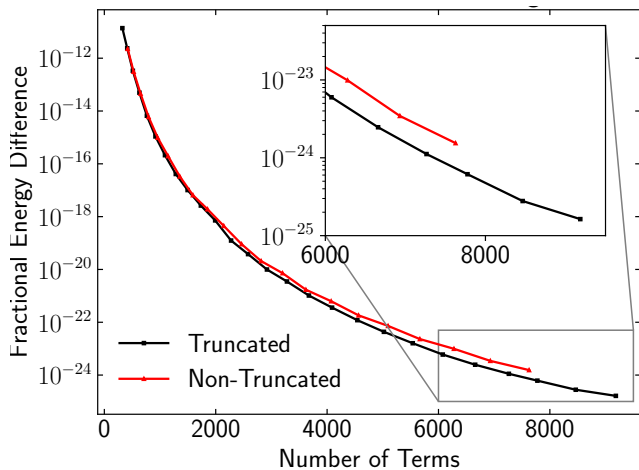
FIG. 2: The fractional energy difference, as a function of basis set size, compared for truncated and untruncated basis sets.
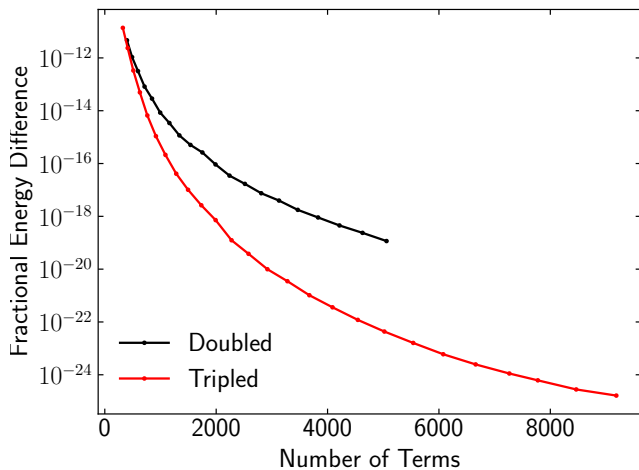

FIG. 3: Comparison of the fractional energy difference, as a function of basis set size, for doubled and tripled basis sets.

denoted Δ, between successive Ω_A values, and also their ratio defined by

$$R(\Omega) = \frac{E(\Omega - 1) - E(\Omega - 2)}{E(\Omega) - E(\Omega - 1)} \qquad (10)$$

The R values provide a direct measure of the smoothness of convergence. If R were a constant, then the series would converge as a geometric series of constant ratios. Since R is not constant, a least-squares fitting procedure was used to obtain an extrapolated energy and its uncertainty corresponding to $\Omega = \infty$) [5].

Table I compares the current result for the ground-state energy of $^\infty H^-$ with previous calculations. This result improves upon the 2015 result of Frolov [8] by setting a better (i.e. lower) upper bound for this energy. Numerical comparison of the corresponding finite-mass

TABLE I: Comparison of different calculations of the non-relativistic energy of $^\infty H^-$ (infinite nuclear mass) in atomic units. The third and fourth rows from the bottom compare the previous best upper bound from previous work [8] with the present work, while the bottom rows compare these two calculations for a similar number of terms.

Reference	$E(^\infty H^-)$
Ref. [2]	$-0.527\ 751\ 016\ 544\ 240$
Ref. [3]	$-0.527\ 751\ 016\ 544\ 240$
Ref. [4]	$-0.527\ 751\ 016\ 544\ 253$
Ref. [6]	$-0.527\ 751\ 016\ 544\ 377\ 196\ 503$
Ref. [5]	$-0.527\ 751\ 016\ 544\ 377\ 196\ 586\ 5$
Ref. [7]	$-0.527\ 751\ 016\ 544\ 377\ 196\ 589\ 733$
Ref. [8] [a]	$-0.527\ 751\ 016\ 544\ 377\ 196\ 590\ 75(10)$
This work [a]	$-0.527\ 751\ 016\ 544\ 377\ 196\ 590\ 814\ 520\ (18)$
Ref. [8] [b]	$-0.527\ 751\ 016\ 544\ 377\ 196\ 590\ 446$
This work [b]	$-0.527\ 751\ 016\ 544\ 377\ 196\ 590\ 814\ 469$
$N = 4000$ [8]	$-0.527\ 751\ 016\ 544\ 377\ 196\ 590\ 446$
$N = 4089$	$-0.527\ 751\ 016\ 544\ 377\ 196\ 590\ 625 \ldots$

[a]These extrapolated values correspond an infinitely large basis set.
[b]These numbers represent the lowest upper bound achieved in the two respective calculations.

ground state energy is not possible due to the different values of μ/M used in the two calculations; we used the currently accepted $\mu/M = 0.000544320575$, while Ref. [8] used $\mu/M = 0.000544320557$.

We further note that the convergence pattern observed in the infinite-mass case, where the triple basis set method performs equally well as the all-exponential method for the same number of terms, is also true in the finite-mass case.

The bottom two rows of Table I compare our present calculated energies with the best previous calculation [8] for a similar number of terms in the basis set. The comparison around $N = 4000$ corresponds to the maximum number of terms used in Ref. [8]. Contrary to previous claims [21, 33], these results demonstrate that the rate of convergence for the triple Hylleraas basis set is about the same as that of the all-exponential method used in Ref. [8].

The code used to generate the wavefunctions for infinite and finite mass cases, each with doubled and tripled basis sets, can be found on our GitHub page at github.com/DrakeResearcher/PublicPrograms and will be published in a forthcoming paper.

IV. DISCUSSION

The main focus of this paper is to explore the properties of triple basis sets as a method for the high-precision solution of the quantum mechanical three-body problem. The ground state of H^- serves as a test case where cor-

relation effects are of dominant importance. The results greatly extend our previous calculations for H^- [5] from 2276 terms ($\Omega = 21$) to 9500 terms ($\Omega = 35$). As shown in Table I the present result sets a new best upper bound for the nonrelativistic ground state energy of $^\infty H^-$. The new upper bound is -0.527 733 137 114 642 857 599 601 567 a.u.

The improved results required implementing extended precision arithmetic to maintain sufficient accuracy for basis sets beyond about 3000 terms, or 20 figure accuracy. However, remembering that quantities other than the energy are only accurate to about half as many figures, the old 20 figure accuracy was perfectly adequate for most atomic physics applications, including the calculation of relativistic and QED corrections.

Nevertheless, it is still of interest to explore the comparison with the quasirandom all-exponential method to test both the ultimate accuracy and numerical stability of the two methods. The comparison shows that the rate of convergence with basis set size is about the same as for the newer Frolov calculations [8], but the numerical stability of the triple basis set method is much better. Since quadruple precision (32-digit) arithmetic yields 20 figure accuracy for the energy, only about 12 figures are lost due to round-off error. In contrast, extended precision arithmetic is required for the all-exponential method even for relatively small basis sets. Although integrals are simpler for the all-exponential method because there are no powers of the radial coordinates, the corresponding integrals, including the more singular ones, are well known for the triple basis set, and analytic formulas are tabulated in ref. [37]. In addition, there are simple angular/radial recursion relations that can be used if there is no γr_{12} term in the exponent [38].

There are also differences in aesthetics and physical interpretation. As stated by Schwartz [?] "What struck me as surprising in Korobovs work was the fact that it seemed to ignore that earlier 'wisdom' about analytic properties of wave- functions." While the individual Korobov functions of the form $e^{-\alpha r_1 - \beta r_2 - \gamma r_{12}}$ are conceptually very simple, the randomized values for α, β and γ are lacking in physical meaning. On the other hand, the optimization procedure for the triple basis set is deterministic and produces a natural physical separation of the distance scales into asymptotic, intermediate and short-range distances.

In future work, we will use the triple basis sets to update all the states covered in the 1992 tabulation [29] for helium, including the relativistic and quantum electrodynamic corrections to the energies needed to make high precision comparisons with experiment. The individual optimization of distance scales will be especially valuable in extending the calculations to higher-lying Rydberg states beyond the $n = 10$ limit in Ref. [29]. It may also prove useful in other ongoing work concerning the beta decay of ^6He to form $^6Li^+$ [39] and the charge-state distributions of the decay products in the energy range of overlapping continua for $^6Li^+$ [40].

Acknowledgements

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TABLE II: Convergence table for the nonrelativistic energy of H$^-$ (infinite nuclear mass) in atomic units ($2hcR_\infty$).

Ω	N	E(Ω)	Δ	Ratio
10	324	−0.527 751 016 537 120 298 159 943 450		
11	411	−0.527 751 016 543 123 319 736 872 489	−0.000 000 000 006 003 021 576 929 039	
12	512	−0.527 751 016 544 201 052 501 972 807	−0.000 000 000 001 077 732 765 100 318	5.57
13	630	−0.527 751 016 544 351 071 898 546 381	−0.000 000 000 000 150 019 396 573 574	7.18
14	764	−0.527 751 016 544 373 706 103 115 774	−0.000 000 000 000 022 634 204 569 393	6.63
15	918	−0.527 751 016 544 376 621 448 030 789	−0.000 000 000 000 002 915 344 915 015	7.76
16	1089	−0.527 751 016 544 377 084 475 330 067	−0.000 000 000 000 000 463 027 299 278	6.30
17	1283	−0.527 751 016 544 377 174 876 272 135	−0.000 000 000 000 000 090 400 942 068	5.12
18	1495	−0.527 751 016 544 377 191 236 695 444	−0.000 000 000 000 000 016 360 423 309	5.53
19	1733	−0.527 751 016 544 377 195 203 424 642	−0.000 000 000 000 000 003 966 729 198	4.12
20	1990	−0.527 751 016 544 377 196 210 485 389	−0.000 000 000 000 000 001 007 060 747	3.94
21	2276	−0.527 751 016 544 377 196 525 161 746	−0.000 000 000 000 000 000 314 676 357	3.20
22	2581	−0.527 751 016 544 377 196 570 711 213	−0.000 000 000 000 000 000 045 549 467	6.91
23	2920	−0.527 751 016 544 377 196 585 564 730	−0.000 000 000 000 000 000 014 853 517	3.07
24	3279	−0.527 751 016 544 377 196 588 969 541	−0.000 000 000 000 000 000 003 404 811	4.36
25	3673	−0.527 751 016 544 377 196 590 271 075	−0.000 000 000 000 000 000 001 301 534	2.62
26	4089	−0.527 751 016 544 377 196 590 625 191	−0.000 000 000 000 000 000 000 354 116	3.68
27	4543	−0.527 751 016 544 377 196 590 751 247	−0.000 000 000 000 000 000 000 126 056	2.81
28	5020	−0.527 751 016 544 377 196 590 791 652	−0.000 000 000 000 000 000 000 040 405	3.12
29	5538	−0.527 751 016 544 377 196 590 806 083	−0.000 000 000 000 000 000 000 014 431	2.80
30	6077	−0.527 751 016 544 377 196 590 811 396	−0.000 000 000 000 000 000 000 005 313	2.72
31	6659	−0.527 751 016 544 377 196 590 813 254	−0.000 000 000 000 000 000 000 001 858	2.86
32	7264	−0.527 751 016 544 377 196 590 813 966	−0.000 000 000 000 000 000 000 000 712	2.61
33	7776	−0.527 751 016 544 377 196 590 814 231	−0.000 000 000 000 000 000 000 000 265	2.69
34	8465	−0.527 751 016 544 377 196 590 814 409	−0.000 000 000 000 000 000 000 000 178	1.49
35	9185	−0.527 751 016 544 377 196 590 814 469	−0.000 000 000 000 000 000 000 000 060	2.92
Extrap.		−0.527 751 016 544 377 196 590 814 520 (18)		

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TABLE III: Convergence table for the nonrelativistic energy of H$^-$ (finite nuclear mass) in atomic units ($2hcR_\infty$)), including a comparison to the best calculation to date of Ref. [8].

Ω	N	E(Ω)	Δ	Ratio
10	324	$-0.527\ 445\ 881\ 107\ 054\ 461\ 708\ 510\ 555$		
11	411	$-0.527\ 445\ 881\ 113\ 073\ 533\ 808\ 430\ 855$	$-0.000\ 000\ 000\ 006\ 022\ 350\ 188\ 988\ 639$	
12	512	$-0.527\ 445\ 881\ 114\ 153\ 096\ 903\ 218\ 911$	$-0.000\ 000\ 000\ 001\ 080\ 151\ 043\ 216\ 129$	5.58
13	630	$-0.527\ 445\ 881\ 114\ 303\ 909\ 467\ 466\ 628$	$-0.000\ 000\ 000\ 000\ 150\ 894\ 699\ 335\ 987$	7.16
14	764	$-0.527\ 445\ 881\ 114\ 325\ 984\ 737\ 285\ 183$	$-0.000\ 000\ 000\ 000\ 022\ 087\ 292\ 386\ 065$	6.83
15	918	$-0.527\ 445\ 881\ 114\ 328\ 849\ 072\ 602\ 215$	$-0.000\ 000\ 000\ 000\ 002\ 865\ 895\ 282\ 776$	7.71
16	1089	$-0.527\ 445\ 881\ 114\ 329\ 361\ 029\ 246\ 274$	$-0.000\ 000\ 000\ 000\ 000\ 512\ 235\ 464\ 358$	5.59
17	1283	$-0.527\ 445\ 881\ 114\ 329\ 451\ 399\ 166\ 410$	$-0.000\ 000\ 000\ 000\ 000\ 090\ 419\ 137\ 132$	5.67
18	1495	$-0.527\ 445\ 881\ 114\ 329\ 467\ 733\ 368\ 369$	$-0.000\ 000\ 000\ 000\ 000\ 016\ 343\ 097\ 843$	5.53
19	1733	$-0.527\ 445\ 881\ 114\ 329\ 471\ 708\ 726\ 440$	$-0.000\ 000\ 000\ 000\ 000\ 003\ 977\ 523\ 119$	4.11
20	1990	$-0.527\ 445\ 881\ 114\ 329\ 472\ 743\ 919\ 483$	$-0.000\ 000\ 000\ 000\ 000\ 001\ 035\ 756\ 826$	3.84
21	2276	$-0.527\ 445\ 881\ 114\ 329\ 473\ 017\ 208\ 250$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 273\ 437\ 605$	3.79
22	2581	$-0.527\ 445\ 881\ 114\ 329\ 473\ 062\ 778\ 989$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 045\ 595\ 558$	6.00
23	2920	$-0.527\ 445\ 881\ 114\ 329\ 473\ 077\ 430\ 676$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 014\ 659\ 666$	3.11
24	3279	$-0.527\ 445\ 881\ 114\ 329\ 473\ 080\ 997\ 928$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 003\ 569\ 195$	4.11
25	3673	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 241\ 669$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 001\ 244\ 419$	2.87
26	4089	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 585\ 099$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 000\ 343\ 616$	3.62
27	4543	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 710\ 589$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 000\ 125\ 559$	2.74
28	5020	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 750\ 677$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 000\ 040\ 110$	3.13
29	5538	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 765\ 023$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 000\ 014\ 354$	2.79
30	6077	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 770\ 315$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 000\ 005\ 295$	2.71
31	6659	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 772\ 168$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 000\ 001\ 853$	2.86
32	7264	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 772\ 917$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 000\ 000\ 750$	2.47
33	7776	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 772\ 988$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 000\ 000\ 071$	10.58
34	8465	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 773\ 319$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 000\ 000\ 332$	1.10
35	9185	$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 773\ 381$	$-0.000\ 000\ 000\ 000\ 000\ 000\ 000\ 000\ 061$	5.41
Extrap. [a]		$-0.527\ 445\ 881\ 114\ 329\ 473\ 082\ 773\ 433(30)$		
Ref. [8] [b]		$-0.527\ 445\ 881\ 119\ 767\ 477\ 071\ 665(10)$		

[a] Calculated using $\mu/M = 0.0005443205668$
[b] Calculated using $\mu/M = 0.000544320557$