The higher-order $C_n$ dispersion coefficients for hydrogen.

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The complete set of 2nd, 3rd and 4th order van der Waals coefficients, $C_n$ up to $n = 32$ for the H(1s)-H(1s) dimer are computed using pseudo-states to evaluate the appropriate sum rules. A study of the convergence pattern for $n \leq 16$ indicates that all the $C_{n\leq 16}$ coefficients are accurate to 13 significant digits. The relative size of the 4th-order $C_n^{(4)}$ to the 2nd-order $C_n^{(2)}$ coefficients is seen to increase as $n$ increases and at $n = 32$ the 4th-order term is actually larger.

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I. INTRODUCTION

The long-range interaction between two spherically symmetric atoms can be written in the general form

\[ V(R \to \infty) = -V_0(R) - V_6(R) - V_{10}(R) - V_{11}(R) - \ldots, \]

(1)

where the dispersion potential, $V_n(R)$ of order $n$ is written

\[ V_n(R) = \frac{C_n}{R^n}. \]

(2)

The $C_n$ parameters are the van der Waals dispersion coefficients. The even ($n = 6, 8, \ldots$) dispersion coefficients are calculated using sum rules derived from 2nd-order perturbation theory and provide an attractive interaction. The odd ($n = 11, 13, \ldots$) terms come from 3rd-order perturbation theory, and are repulsive. Contributions from 4th-order perturbation theory start at $n = 12$. The dispersion interaction for the simplest system, namely the hydrogen dimer, is only known precisely to $n = 11$. The latest calculations by Yan and Dalgarno (YD) 2 reported almost exact values for the 2nd-order even dispersion parameters up to $n = 16$. They also gave almost exact results for the 3rd-order coefficients, up to $n = 15$. However, it is known that contributions from 4th-order perturbation theory start at $n = 12$ so the dispersion potential computed from the YD $C_n$ is incomplete for $n > 11$.

In this article, the complete set of dispersion parameters, from $C_6$ to $C_{16}$ are computed by using a large pseudo-state expansion to evaluate the appropriate sum rules. The contributions from 4th-order perturbation theory to $C_{12}$, $C_{14}$ and $C_{16}$ are explicitly included.

II. CALCULATION OF THE DISPERSION PARAMETERS

All the dispersion coefficients computed in this paper were computed by first diagonalizing the semi-empirical Hamiltonian in a large basis of Laguerre type orbitals (LTOs) defined by

\[ \chi_\alpha(r) = N_\alpha r^{\ell+1} \exp(-\lambda_\alpha r)L_{n_\alpha-\ell-1}^{(2\ell+2)}(2\lambda_\alpha r), \]

(3)

where the normalization constant is

\[ N_\alpha = \sqrt{\frac{(2\lambda_\alpha)^{2\ell+3}(n_\alpha - \ell - 1)!}{(\ell + n_\alpha + 1)!}}. \]

(4)

The function $L_{n_\alpha-\ell-1}^{(2\ell+2)}(2\lambda_\alpha r)$ is an associated Laguerre polynomial that can be defined in terms of a confluent hypergeometric function \( _1F_1 \) as

\[ L_{n_\alpha-\ell-1}^{(2\ell+2)}(2\lambda_\alpha r) = \frac{(n_\alpha + \ell + 1)!}{(n_\alpha - \ell - 1)!(2\ell + 2)!} \times M(-n_\alpha - \ell - 1, 2\ell + 2, 2\lambda_\alpha r) \]

(5)

All the matrix elements can be written in simple compact forms provided a common $\lambda_\alpha$ is adopted throughout the calculation. However, in the present work, the radial wave functions were placed on a numerical grid and all matrix elements computed by gaussian quadratures. This was done for reasons of convenience as the diagonalisation could be done with an existing program used in previous calculations of the dispersion parameters and the structures of positronic atoms. This program can achieve close to machine precision in almost all radial matrix computations.

Since the Hamiltonian diagonalisation is complete, sum rules involving radial matrix elements were used to determine the dispersion parameters. The specific sum-rules used are those derived by Ovsiannikov, Gulyarovski and Lopatko (OGL). Their expressions are a bit simpler than those developed by other authors. There were some omissions in their published equations, and a more thorough description of the sum-rules is presented here.
The dispersion coefficients for the H-H dimer. All the results in the "Best Previous" column come from [2] except that for $C_{12}^{(4)}$ which is taken from [3]. All values are in atomic units.

| Coefficient | 10 LTOs       | 15 LTOs       | 20 LTOs       | Best previous |
|------------|--------------|--------------|--------------|--------------|
| $C_6$      | 6.499 026 705 3305 | 6.499 026 705 4057 | 6.499 026 705 4059 | 6.499 026 705 4058 |
| $C_8$      | 124.399 083 58236 | 124.399 083 58362 | 124.399 083 58362 | 124.399 083 58362 |
| $C_{10}$   | 3285.828 414 9425 | 3285.828 414 9674 | 3285.828 414 9674 | 3285.828 414 9674 |
| $C_{12}^{(2)}$ | 1.214 860 208 9691$10^5$ | 1.214 860 208 9696$10^5$ | 1.214 860 208 9686$10^5$ | 1.214 860 208 9668$10^5$ |
| $C_{14}^{(2)}$ | 6.060 772 689 1917$10^6$ | 6.060 772 689 1917$10^6$ | 6.060 772 689 1917$10^6$ | 6.060 772 689 1917$10^6$ |
| $C_{16}^{(2)}$ | 3.937 506 393 9985$10^8$ | 3.937 506 393 9985$10^8$ | 3.937 506 393 9992$10^8$ | 3.937 506 393 9992$10^8$ |
| $C_{11}$   | -3474.898 037 8919 | -3474.898 037 8822 | -3474.898 037 8822 | -3474.898 037 8822 |
| $C_{13}$   | -3.269 869 240 4549$10^5$ | -3.269 869 2440 0407$10^5$ | -3.269 869 2440 0407$10^5$ | -3.269 869 2440 0407$10^5$ |
| $C_{15}$   | -2.839 558 063 3179$10^7$ | -2.839 558 063 2997$10^7$ | -2.839 558 063 2997$10^7$ | -2.839 558 063 2998$10^7$ |
| $C_{12}^{(4)}$ | 1241.587 803 8317 | 1241.587 803 8462 | 1241.587 803 8462 | 1241.587 803 8462 |
| $C_{14}^{(4)}$ | 3.009 633 558 9570$10^5$ | 3.009 633 559 0035$10^5$ | 3.006 633 559 0035$10^5$ | 3.006 633 559 0035$10^5$ |
| $C_{16}^{(4)}$ | 4.745 455 287 4168$10^7$ | 4.745 455 287 4083$10^7$ | 4.745 455 287 4079$10^7$ | 4.745 455 287 4079$10^7$ |
| $C_{12}$   | 1.227 276 087 0002$10^5$ | 1.227 276 087 0071$10^5$ | 1.227 276 087 0071$10^5$ | 1.227 276 087 0071$10^5$ |
| $C_{14}$   | 6.361 736 045 0628$10^6$ | 6.361 736 045 0920$10^6$ | 6.361 736 045 0921$10^6$ | 6.361 736 045 0921$10^6$ |
| $C_{16}$   | 4.412 051 922 7282$10^8$ | 4.412 051 922 7393$10^8$ | 4.412 051 922 7393$10^8$ | 4.412 051 922 7393$10^8$ |

This entry adds to BM $C_{12}^{(4)}$ to the YD $C_{12}^{(4)}$.

A.  The 2nd-order terms

The 2nd-order dispersion coefficients for the H-H system have been determined to high accuracy in [2, 3, 10] even for high $n$. The working expression adopted for computation is,

$$C_{2\lambda+6}^{(2)} = \sum_{\ell_1=1}^{\lambda+1} \frac{(2\ell+4)!}{(2\ell_1+1)!(2\ell'_1+1)!} \times \frac{(0,0)\langle \ell_1, \ell_1 \rangle^2 (0,0)\langle \ell'_1, \ell'_1 \rangle^2}{(E_{\ell_1} + E_{\ell'_1} - 2E_0)}$$

where $\ell'_1 = \lambda + 2 - \ell_1$. The state vector $|\ell_1, \ell_1\rangle^2$ represents the radial part of the state $i_1$ with orbital angular momentum $\ell_1$ and energy $E_{\ell_1}$. The ground state energy is $E_0$. The sum rule

$$T^{(\ell)} = \sum_i (0,0)\langle \ell_1, \ell \rangle^2 = \frac{2(\ell + 2)!}{2(2\ell +1)!}$$

is a useful diagnostic check of the accuracy of the underlying discretization of the H-spectrum.

B.  The 3rd-order terms; $C_{11}$ and $C_{13}$

The dispersion coefficients, $C_{11}$ and $C_{13}$, arise from 3rd-order perturbation theory [1, 2, 3, 4, 11]. Close to exact dispersion parameters for the H-H system have been published [2].

The general expression for the 3rd-order $C_{2\lambda+11}$ is [1]

$$C_{2\lambda+11} = - \sum_{\ell_1 k_1 \ell_2} \sum_{\ell'_1 k'_1 \ell'_2} \sum_{\ell_1' k_1' \ell_1' k_1' \ell_2} \frac{G(\lambda, \ell_1, \ell'_1, \ell_2, \ell'_2, k_1, k'_1)}{(E_{\ell_1'} - 2E_0)(E_{\ell_2'} - 2E_0)} \times \frac{\langle 0,0|\rho^{\ell_1}|i_1, \ell_1\rangle\langle i_1, \ell_1|\rho^{k_1}|i_2, \ell_2\rangle}{\langle i_2, \ell_2|\rho^{\ell_2}|0,0\rangle\langle 0,0|\rho^{\ell'_1}|i'_1, \ell'_1\rangle} \times \langle i'_1, \ell'_1|\rho^{k'_1}|i'_2, \ell'_2\rangle\langle i'_2, \ell'_2|\rho^{\ell'_2}|0,0\rangle \langle 0,0|\rho^{\ell_2}|0,0\rangle$$

with the notation $E_{i'} = E_{i_1} + E_{i_2}$ being used in the energy denominator. The parameter $\lambda$ is defined

$$2\lambda + 8 = \lambda_1 + k_1 + \ell_2 + \ell'_1 + k'_1 + \ell'_2$$

and all of the angular momentum indices are greater than zero. Defining $J = (\ell_1 + k_1 + \ell_2)/2$ and $J' = (\ell'_1 + k'_1 + \ell'_2)/2$, the coefficient $G$ is defined as

$$G(\lambda, \ell_1, \ell'_1, \ell_2, \ell'_2, k_1, k'_1) = (\lambda + 4)!A(J, \ell_1, k_1, \ell_2) \times A(J', \ell'_1, k'_1, \ell'_2) B(\lambda, \ell_1, k_1)B(\lambda, k_1, k'_1)B(\lambda, \ell_2, \ell'_2)$$

where

$$B(\lambda, \ell_1, \ell_2) = \frac{[2(\lambda + 4 - \ell_1 - \ell_2)]!}{(\lambda + 4 - \ell_1 - \ell_2)!} \quad ,$$

and

$$A(J, \ell_1, k_1, \ell_2) = \frac{J!}{(2J + 1)!(J - \ell_1)!(J - k_1)!(J - \ell_2)!} \quad .$$


C. The 4th-order contributions to \( C_{12} \) and \( C_{14} \)

As far as we know, there have only been two explicit calculations of the 4th-order contribution to \( C_{12} \). Bukta and Meath \(^3\) gave estimates of \( C^{(2)} \) and \( C^{(4)} \) for the hydrogen dimer. Ovsianikov et al. \(^1\) developed a general and compact expression for the evaluation of \( C^{(4)} \), and in addition they reported values of \( C^{(4)} \) for all possible combinations of hydrogen and the alkali atoms. Rectifying some omissions in their published equations \(^8\), one writes

\[
C^{(4)}_{2\lambda+12} = b_{2\lambda+12} - \sum_{\lambda_1=0}^{\lambda} C^{(2)}_{2\lambda_1+6} a_{2\lambda_2+6} ,
\]

where

\[
\lambda = \lambda_1 + \lambda_2 .
\]

The factor \( a_{2\lambda_2+6} \) is

\[
a_{2\lambda_2+6} = \sum_{\ell_1=1}^{\lambda_2+1} \frac{(2\lambda_2 + 4)!}{(2\ell_1 + 1)!(2\ell_1' + 1)!} \times \sum_{i_1,i_1'} (0,0) |\ell_1,1\rangle |1,1\rangle^2 (0,0) |\ell_1',1\rangle |1,1\rangle^2 (E_{i_1} + E_{i_1'} - 2E_0)^2
\]

where

\[
\ell_1 + \ell_1' = \lambda + 2 .
\]

The expression for \( a_{2\lambda_2+6} \) is practically the same as eq. \(^{15}\) for \( C^{(2)}_{2\lambda_2+6} \); the only difference being an extra factor in the energy denominator (compare with eq. (10) of \(^1\)).

The factor \( b_{2\lambda+12} \) is more complicated and defined as

\[
b_{2\lambda+12} = \sum_{\ell_1,\ell_2, k_1, k_2, k_1', k_2'} \sum_{i_1,i_2,i_1',i_2'} \sum_{K} \left| L_1 K_1 K_2 L_3 \right| \left| 2\ell_1 2\ell_1' 2k_1 2k_1' 2k_2 2k_2' 2\ell_3' 2\ell_3 \right| \times \langle L_1 0 K_1 0 K_0 \rangle \langle K_2 0 L_3 0 K_0 \rangle \times \sum_{k_1,k_1',k_2,k_2'} \sum_{\ell_1,\ell_1'} \begin{pmatrix} k_2 & k_2' & K_2 \\ k_1 & k_1' & K_1 \\ \ell_2 & \ell_2' & K \end{pmatrix} \times \begin{pmatrix} L_1 \\ K_1 \\ 1 \end{pmatrix} \left| L_1 K_1 K_2 L_3 \right| \left| 2\ell_1 2\ell_1' 2k_1 2k_1' 2k_2 2k_2' 2\ell_3' 2\ell_3 \right| \\
\times \langle 0,0 |\ell_1,\ell_1'|i_1,1\rangle \langle i_1,1|\ell_2,k_2|2,2\rangle \times \langle i_2,2|k_2|k_3,3\rangle \langle k_3,3|\ell_3,k_3'|0,0\rangle \times \langle 0,0 |\ell_1,\ell_1'|i_1',1\rangle \langle i_1',1|\ell_2,k_2'|2,2\rangle \times \langle i_2,2|k_2'|k_3,3\rangle \langle k_3,3|\ell_3,k_3'|0,0\rangle
\]

where \( L_1 = \ell_1 + \ell_1' \), \( L_3 = \ell_3 + \ell_3' \), \( K_1 = k_1 + k_1' \) and \( K_2 = k_2 + k_2' \). We use \( \tilde{L} = (2L + 1) \). The sums are constrained by the condition

\[
L_1 + K_1 + K_2 + L_3 = 2\lambda + 8 .
\]

While \( \ell_1, \ell_1', \ell_3, \ell_3' \) must be greater than 0, it is possible for \( \ell_2 \) and \( \ell_2' \) to be equal to 0. None of \( k_1, k_1', k_2 \) or \( k_2' \) can be zero. Since \( \ell_2 \) and \( \ell_2' \) can both be equal to zero, the possibility of \( i_2 \), \( i_2' \) both occupying the ground state must be explicitly excluded from the summation.

III. RESULTS OF THE CALCULATION

The results of the calculations for the complete set of dispersion coefficients up to \( C_{16} \) are given in Table \(^{11}\). The parameters are given for basis sets with 10, 15 and 20 basis functions per angular momentum respectively. The exponent in the LTO was chosen to be \( \lambda = 1.0 \) for all angular momenta. This choice resulted in much faster convergence of the dispersion parameters than that observed by Yan and Dalgarano in their calculations of the 3rd-order dispersion coefficients. Table \(^{11}\) also gives results reported by YD and a single calculation of \( C^{(4)}_{12} \) by Bukta and Meath (BM) \(^3\).

A. The 2nd-order terms

The calculations of \( C^{(2)} \) do not give new information and Yan and Dalgarano \(^2\) have given values which are converged to better than 15 significant figures. The present calculations with the \( N = 20 \) basis are identical to 13 significant figures. The small differences in the last digit for some of coefficients arise from minor inaccuracies with the radial matrix elements. Hence we conclude that the present calculations are numerically reliable and that the pseudo-state representation of the H-spectrum is close to converged.

Besides the dispersion coefficients, the sum-rule, eq. \(^{17}\) was evaluated and seen to be correct to 12 significant digits for all polarities relevant to the evaluation of \( C_5 \) to \( C^{(2)}_8 \).

B. The 3rd-order terms

Since the 3rd-order terms, \( C^{(3)}_n \) have already been given by YD, these calculations merely serve as a test of our numerical procedures. Once again, calculations with the 20 LTO basis agree with the YD results to 14 significant figures. It is worth noting the present results required fewer terms than YD to achieve convergence. YD made the choice \( \lambda_0 = 1/(\ell + 1) \) in eq. \(^{4}\) and did not achieve convergence to the 14th digit place until the dimension of the LTO expansion was 50. The present basis with \( \lambda_0 = 1.0 \) achieves the same level of convergence with 20 LTOs.
TABLE II: The $n \geq 16$ dispersion coefficients for the H-H dimer. All values are in atomic units.

| $n$ | $C_n^{(2)}$ | $C_n^{(4)}$ | $C_n^{(2)} + C_n^{(4)}$ | $C_n^{(3)}$ |
|-----|-------------|-------------|-------------------------|-------------|
| 17  | 3.234 218 716×10¹⁰ | 7.009 061 179×10⁹ | 3.935 124 834×10¹⁰ | 2.726 099 889×10⁹ |
| 18  | 3.278 573 440×10¹² | 1.083 922 188×10¹² | 4.362 495 628×10¹² | 3.020 900 833×10¹³ |
| 19  | 4.021 082 848×10¹⁴ | 1.832 218 347×10¹⁴ | 5.853 301 195×10¹⁴ | 3.900 227 980×10¹³ |
| 20  | 5.868 996 335×10¹⁶ | 3.444 924 821×10¹⁶ | 9.313 921 156×10¹⁶ | 5.856 636 712×10¹⁵ |
| 21  | 7.249 373 286×10¹⁸ | 1.730 296 722×10¹⁹ | 2.028 440 001×10¹⁸ | 1.017 059 252×10¹⁸ |
| 22  | 1.005 294 993×10¹⁹ | 1.709 243 726×10²¹ | 3.706 188 667×10²¹ | 4.613 037 362×10²² |
| 23  | 1.996 944 941×10²¹ | 4.507 006 859×10²³ | 9.060 295 725×10²³ | 1.188 007 684×10²⁵ |
| 24  | 4.533 288 866×10²³ | 1.325 398 446×10²⁶ | 2.506 505 534×10²⁶ | 1.898 007 684×10²⁵ |

C. The 4th-order terms

The only previous explicit calculation of a 4th-order term was that made by Bukta and Meath (BM) [3], and the only parameter given was $C_n^{(4)}$. The OGL [1] estimate of $C_n^{(4)}$, 1.220×10⁵ au was made using an approximation to the Greens function and so perfect agreement is not expected. However, the present calculation agrees with BM calculation of $C_n^{(4)}$ to all digits quoted, namely seven.

The number of terms in the sum, eq. (17) increases rapidly as $n$ increases. There are 4 terms for $C_n^{(4)}$, 12 there are 64 terms for $C_n^{(4)}$, and finally there are 460 terms for $C_n^{(6)}$.

The dominant contribution to $C_n^{(4)}$ comes from $b_{2\lambda+12}$ with 96% of $C_n^{(4)}$ coming from $b_{12}$. The tendency for $b_{2\lambda+12}$ to be the dominant term in $C_n^{(4)}$ becomes more accentuated as $n$ increases and the $b_{16}$ term gives an estimate to $C_n^{(4)}$ that is correct to 0.1%.

One feature of the Table II concerns the relative size of $C_n^{(4)}$ to $C_n^{(2)}$. For $n = 12$, the $C_n^{(4)} : C_n^{(2)}$ ratio is 1.02%. However, as $n$ gets larger, the ratio also gets larger. For $n = 14$ the ratio is 4.97%, while for $n = 16$ the ratio is 12.1%.

D. The dispersion coefficients for $n \geq 17$

Higher order contributions than 4th-order begin at $n = 17$. There is a 5th-order contribution to $C_{17}$ and a 6th-order contribution to $C_{18}$ [1]. Estimates of $C_n^{(2)}$ for $n \geq 17$ have been made by a variety of authors [10, 12, 13, 14]. However, the only estimate of the 3rd and 4th-order terms with $n \geq 17$ are those of OGL [1]. By explicit calculation they obtained $C_{17}^{(3)} = -2.739 \times 10^9$ au which agrees with the present more extensive calculation to within 1%. Making an approximation to the greens function they estimated $C_{18}^{(3)} = 3.3 \times 10^9$ au, which is about half the size of the present value.

The dispersion parameters up to $C_{32}$ from the present calculation are tabulated in Table III. The reason for taking the calculations so far rests in the relative size of the $C_n^{(4)}$ and $C_n^{(2)}$ terms. It was noticed that the $C_n^{(4)} : C_n^{(2)}$ ratio got larger as $n$ increased. So the calculations were extended to $C_{32}$ in order to demonstrate explicitly that the $C_n^{(4)} : C_n^{(2)}$ ratio can actually become larger than 1.0.

The precision of the entries in Table III is not as high as those in Table II. The calculations of $C_n^{(3)}$ did become more time consuming as $n$ increased. There were 922,064 different $(\ell_1, \ell_2, \ell_3, \ldots)$ combinations by the time $n = 32$ was reached. Also the number of radial integrals in eq. (17) increases as $N^4$ where $N$ is the numbers of LTOs for any given $\ell$. So the $N = 20$ calculation is 64 times more intensive than the $N = 10$ calculation.

The $C_n^{(2)}$ and $C_n^{(3)}$ entries in Table III were taken from the calculation with 15 LTOs. The $C_n^{(4)}$ entries were taken from a $N = 15$ calculation up to $n = 20$, thereafter the $N = 10$ basis was used. The values of $C_n^{(2)}$ agree with those of Thakkar [11] for all ten digits given in Table II. Comparisons between $N = 10$ and $N = 15$ calculations for $C_n^{(3)}$ suggest that the convergence is slower as $n$ increases and that $C_n^{(3)}$ is reliable to about 6 digits. A similar level of accuracy can be expected for $C_n^{(4)}$ and a comparison between the $N = 10$ and $N = 15$ values for $C_{20}^{(4)}$ gives agreement for the first 9 digits.
IV. CONCLUSIONS

The higher \( n \) dispersion parameters from \( C_{11} \), through to \( C_{16} \) have been computed to an accuracy of 13 significant figures for the H-H dimer. Since the 4th-order contributions were included for \( C_{12}, C_{14} \) and \( C_{16} \) the adiabatic dispersion interaction can now be regarded as complete up to terms of order \( R^{-16} \).

The time taken to evaluate the dispersion coefficients was not excessive. For example, a calculation using 20 LTOs took about 17 minutes to determine all terms up \( C_{16} \) on a 850 MHz CPU. Hence the pseudo-state method adopted here, and in other similar works (e.g. \([2, 3]\)), could be used to make explicit calculations of the 5th-order correction to \( C_{17} \) and even the 6th-order correction to \( C_{18} \). Therefore, it is certainly possible with existing technology to determine the complete dispersion interaction for the H-H interaction for all terms up to and including \( C_{22} \).

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