

excitation cross section of H_2 by slow electron impact. An analysis of swarm experiments by Engelhardt and Phelps,¹⁴ using the Born approximation values for the rotational excitation cross section, yielded a synthesized vibrational excitation cross section for H_2 which was a factor of 2 larger than Schulz's for electron energies >3 eV. Our present results, while still containing major uncertainties, indicate that one must question both the magnitude and shape of the rotational excitation cross sections based upon the Born approximation, which have been used in the swarm experiment analysis. It is

hoped that calculations with a more realistic interaction potential can be done in the future.

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Perturbation-Theory Expansions Through 21st Order of the Nonrelativistic Energies of the Two-Electron Systems $(2p)^2\ ^3P$ and $(1s)^2\ ^1S^*$

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The Hylleraas-Scherr-Knight variational perturbation method has been applied to the two-electron systems $(2p)^2\ ^3P$ and $(1s)^2\ ^1S$, carrying the calculations through to tenth-order perturbation wave functions. Various forms of expansions for the trial wave functions have been considered, e.g., the Hylleraas form and the Schwartz form, and numerical results are given in naturally spaced groups up to and including 252-term expansions. Estimates of the correct perturbation-energy coefficients through 21st order are tabulated, and the resulting nonrelativistic energies for $Z=2, 3, \dots, 10$, are given with ten significant figures. To complete the tables the energies of the two states for H^- have also been calculated variationally, using the same expansions of trial wave functions as in the perturbation treatment, and for the $(2p)^2\ ^3P$ state an extrapolated energy value of -0.2507097 measured in units of $Z^2R\hbar$ has been obtained.

1. INTRODUCTION

THE $(2p)^2\ ^3P$ state of the negative hydrogen ion has already been found to be stable.¹ Using a 22-term trial wave function, Wold obtained an energy value of -0.250427 , measured in units of $Z^2R\hbar$.

In a preliminary investigation for bound states of the negative hydrogen ion² an improved 22-parameter wave function has been set up yielding an energy of

-0.250618 for H^- . In the same paper the Hylleraas-Scherr-Knight (HSK) variational perturbation method was also applied for the first time to that state, furnishing a second-order and a third-order energy coefficient of -0.078788 and 0.003631 , respectively.

The HSK variational perturbation method appears to be very well suited for atomic calculations provided that an electronic computer is available. The results are

TABLE I. Contributions to the perturbation energy coefficients $(\lambda_2-\lambda_5)$ for the state $(2p)^2\ ^3P$.

Order	Contributions to λ_2	Contributions to λ_3	Contributions to λ_4	Contributions to λ_5
3	-0.0744773381	0.0013129555	0.0257976480	-0.0010557398
7	-0.0040427166	0.0009572751	-0.0239069249	0.0015435888
13	-0.0002268368	0.0012021496	-0.0021170919	-0.0016508836
22	-0.0000340131	0.0001651968	-0.0003597004	0.0003557950
34	-0.0000063734	0.0000319708	-0.0000726308	0.0000963727
50	-0.0000014801	0.0000074218	-0.0000171772	0.0000235745
70	-0.0000004035	0.0000020003	-0.0000046640	0.0000065446
95	-0.0000001253	0.0000006093	-0.0000014133	0.0000020143
125	-0.0000000433	0.0000002059	-0.0000004710	0.0000006734
161	-0.0000000164	0.0000000761	-0.0000001707	0.0000002425
203	-0.0000000067	0.0000000303	-0.0000000667	0.0000000934
252	-0.0000000029	0.0000000129	-0.0000000278	0.0000000384

* Supported by Aeronautical Research Laboratory, OAR, and Fridtjof Nansen's Fund for Advancement of Science.

¹ E. Wold, Phys. Math. Univ. Oslo., No. 13, 1962.

² J. Midtdal, Phys. Math. Univ. Oslo., No. 21, 1964.

TABLE II. Contributions to the perturbation energy coefficients ($\lambda_2-\lambda_5$) for the state $(1s)^2\ ^1S$.

Order	Contributions to λ_2	Contributions to λ_3	Contributions to λ_4	Contributions to λ_5
3	-0.2922676282	0.0069919564	0.0604400311	-0.0034562059
7	-0.0209368521	0.0031267441	-0.0546518754	0.0053301998
13	-0.0016754968	0.0059009075	-0.0056451735	-0.0051912415
22	-0.0003312179	0.0010027080	-0.0014124818	0.0008401128
34	-0.0000822682	0.0002549806	-0.0003439043	0.0002758621
50	-0.0000247257	0.0000764071	-0.0001040998	0.0000815122
70	-0.0000085745	0.0000262370	-0.0000357128	0.0000280739
95	-0.0000033291	0.0000100439	-0.0000135743	0.0000106911
125	-0.0000014165	0.0000042058	-0.0000056174	0.0000044104
161	-0.0000006501	0.0000018988	-0.0000024995	0.0000019466
203	-0.0000003180	0.0000009138	-0.0000011840	0.0000009114
252	-0.0000001640	0.0000004643	-0.0000005919	0.0000004494

produced much faster than by using the orthodox variational treatment, owing to the fact that, in reality, no variational process is necessarily needed. Moreover, the computation furnishes the energies of the whole isoelectronic sequence of the state under consideration. In addition, the wave function obtained for excited states will automatically be orthogonal to all the lower lying discrete states of the same symmetry type. This last statement has been formulated as the general orthogonality theorem of that method.³

The approximate perturbation wave functions furnished by the variational equations of the Hylleraas-Scherr-Knight procedure, will automatically, to any order, satisfy the same orthogonality conditions as the exact perturbation wave functions.

In this paper we present a tenth-order perturbation wave function both for the $(2p)^2\ ^3P$ state and the $(1s)^2\ ^1S$ state of a two-electron system. Estimates of the correct perturbation energy coefficients through 21st order have been evaluated, giving the total nonrelativistic energies to ten significant figures.

The calculations involved in this investigation have all been performed on a UNIVAC 1107, located at the Norwegian Computing Center, using double-length floating-point arithmetic throughout in the treatment of real numbers. This implies a fraction part (mantissa) of 54 bits.

2. THE HSK METHOD AND CONVERGENCE PROPERTIES

We shall here only point out two important convergence properties concerning the perturbation energy

coefficients furnished by the Hylleraas-Scherr-Knight variational perturbation method. For a general development of the theory we like to refer to the papers of Hylleraas⁴ and Scherr and Knight.⁵

Using $Z^{-1}a_0$ as the unit of length and $Z^3R\hbar$ as the unit of energy, the correct wave function and the energy of the system may be expanded as power series in Z^{-1} :

$$\Psi = \sum_{n=0} Z^{-n}\psi_n, \tag{1}$$

$$E' = \sum_{n=0} Z^{-n}\epsilon_n, \tag{2}$$

where ϵ_n will be referred to as the exact n th-order perturbation energy coefficient.

Introducing the same notation as Scherr and Knight⁵ we write

$$G_0 = H_0 - \epsilon_0, \tag{3}$$

$$G_1 = H' - \epsilon_1, \tag{4}$$

and the general perturbation equation then reads

$$G_0\psi_n + G_1\psi_{n-1} - \sum_{k=2}^n \epsilon_k\psi_{n-k} = 0 \quad (n \geq 0), \tag{5}$$

where terms with negative indices are to be ignored.

For the trial wave function Φ we assume the expansion

$$\Phi = \sum_{n=0} Z^{-n}\varphi_n, \tag{6}$$

the first term of which is known exactly, $\varphi_0 = \psi_0$. Generally, the n th-order wave function φ_n will be

TABLE III. $(2p)^2\ ^3P$. The perturbation energy coefficients ($\lambda_2-\lambda_5$) obtained by using 70 terms of the function sets A, B, C , and D .

System	A	B	C	D
λ_2	-0.0787891616	-0.0787892684	-0.0787888273	-0.0787885857
λ_3	0.0036789699	0.0036794237	0.0036771019	0.0036748797
λ_4	-0.0006805412	-0.0006816742	-0.0006757580	-0.0006707077
λ_5	-0.0006874788	-0.0006786133	-0.0006868611	-0.0006809169

³ J. Midtdal, Phys. Math. Univ. Oslo., No. 25, 1964.

⁴ E. A. Hylleraas, Z. Physik **65**, 209 (1930).

⁵ W. Scherr and R. E. Knight, Rev. Mod. Phys. **35**, 436 (1963).

TABLE IV. $(1s)^2\ ^1S$. The perturbation energy coefficients ($\lambda_{\alpha}-\lambda_{\beta}$) obtained by using 70 terms of the function sets A , B , C , and D .

System	A	B	C	D
λ_2	-0.3153267650	-0.3153314850	-0.3153199067	-0.3153216644
λ_3	0.0173799405	0.0173938726	0.0173573876	0.0173579619
λ_4	-0.0017532166	-0.0017727239	-0.0017230515	-0.0017379791
λ_5	-0.0020916865	-0.0020749745	-0.0021083529	-0.0020435480
E_2'	-1.4518618814	-1.4518621332	-1.4518616240	-1.4518616031
E_{10}'	-1.8781360852	-1.8781361203	-1.8781360367	-1.8781360543

TABLE V. $(2p)^2\ ^3P$. Perturbation energy coefficients in rydbergs.

Order	95	125	161	203	Extrapolated
λ_0	-0.5	-0.5	-0.5	-0.5	-0.5
λ_1	0.328125	0.328125	0.328125	0.328125	0.328125
λ_2	-0.078789286860	-0.078789330175	-0.078789346552	-0.078789353231	-0.0787893588
λ_3	0.003679579117	0.003679785031	0.003679861097	0.003679891432	0.0036799159
λ_4	-0.000681954483	-0.000682425513	-0.000682596257	-0.000682662913	-0.0006827145
λ_5	-0.000678733541	-0.000678060180	-0.000677817688	-0.000677724244	-0.0006776540
λ_6	-0.000461624682	-0.000462273882	-0.000462510422	-0.000462601734	-0.0004626686
λ_7	-0.000330333269	-0.000329904267	-0.000329743148	-0.000329679673	-0.0003296346
λ_8	-0.000245740847	-0.000245939073	-0.000246014856	-0.000246045734	-0.0002460681
λ_9	-0.000189510063	-0.000189424083	-0.000189398225	-0.000189387979	-0.0001893807
λ_{10}	-0.000149319221	-0.000149254234	-0.000149266242	-0.000149268987	-0.0001492694
λ_{11}	-0.000120102790	-0.000120063454	-0.000120083288	-0.000120081483	-0.0001200814
λ_{12}	-0.000098310455	-0.000098288232	-0.000098305389	-0.000098299550	-0.000098300
λ_{13}	-0.000081690676	-0.000081673627	-0.000081685667	-0.000081679701	-0.000081682
λ_{14}	-0.000068737310	-0.000068743356	-0.000068751987	-0.000068746200	-0.000068747
λ_{15}	-0.000058523335	-0.000058507694	-0.000058514375	-0.000058510409	-0.000058512
λ_{16}	-0.000050342879	-0.000050279841	-0.000050288979	-0.000050283771	-0.000050286
λ_{17}	-0.000043432914	-0.000043585559	-0.000043592610	-0.000043589705	-0.000043592
λ_{18}	-0.000037126600	-0.000038079767	-0.000038076355	-0.000038071340	-0.000038072
λ_{19}	-0.000031119756	-0.000033464197	-0.000033485465	-0.000033485480	-0.000033485
λ_{20}	-0.000025451251	-0.000029468756	-0.000029630324	-0.000029623126	-0.000029623
λ_{21}	-0.000020279539	-0.000025887407	-0.000026360660	-0.000026365510	-0.000026365
R	-0.00009288	-0.000020086	-0.000034945	-0.000034940	-0.00003494

TABLE VI. $(1s)^2\ ^1S$. Perturbation energy coefficients in rydbergs.

Order	95	125	161	203	Extrapolated
λ_0	-2.0	-2.0	-2.0	-2.0	-2.0
λ_1	1.25	1.25	1.25	1.25	1.25
λ_2	-0.315330092511	-0.315331509050	-0.315332159193	-0.315332477164	-0.315332856
λ_3	0.017389984475	0.017394190231	0.017396088991	0.017397002781	0.017398058
λ_4	-0.001766790854	-0.001772408264	-0.001774907761	-0.001776091725	-0.001777409
λ_5	-0.002080995355	-0.002076584996	-0.002074638378	-0.002073726948	-0.002072747
λ_6	-0.001221785193	-0.001223982114	-0.001224952290	-0.001225404814	-0.001225864
λ_7	-0.000745676528	-0.000744963038	-0.000744649864	-0.000744503652	-0.000744368
λ_8	-0.000485445999	-0.000485626060	-0.000485694669	-0.000485725045	-0.000485747
λ_9	-0.000331431015	-0.000331350901	-0.000331332208	-0.000331326411	-0.000331324
λ_{10}	-0.000232550314	-0.000232341777	-0.000232354627	-0.000232357326	-0.000232358
λ_{11}	-0.000166747368	-0.000166552290	-0.000166605562	-0.000166603362	-0.000166603
λ_{12}	-0.000121836878	-0.000121709724	-0.000121773645	-0.000121760118	-0.000121761
λ_{13}	-0.000090516192	-0.000090423800	-0.000090478110	-0.000090458127	-0.000090464
λ_{14}	-0.000068195225	-0.000068131201	-0.000068174558	-0.000068154152	-0.000068160
λ_{15}	-0.000051998576	-0.000051961412	-0.000051994943	-0.000051976554	-0.000051986
λ_{16}	-0.000040091792	-0.000040050693	-0.000040076645	-0.000040060853	-0.000040067
λ_{17}	-0.000031167922	-0.000031158331	-0.000031179327	-0.000031165999	-0.000031171
λ_{18}	-0.000024263341	-0.000024443791	-0.000024458602	-0.000024447538	-0.000024451
λ_{19}	-0.000018753709	-0.000019316188	-0.000019328625	-0.000019319740	-0.000019322
λ_{20}	-0.000014295943	-0.000015344498	-0.000015376533	-0.000015369380	-0.000015372
λ_{21}	-0.000010704954	-0.000012216521	-0.000012306032	-0.000012300509	-0.000012304
R	-0.00003822	-0.00005163	-0.00005569	-0.00005569	-0.0000557

TABLE VII. Perturbation nonrelativistic energies (E') of the state $(2p)^2\ ^3P$.

Z	95 terms	125 terms	161 terms	203 terms	Extrapolated
1	-0.25044992	-0.25057073	-0.25072006	-0.25071997	-0.250720
2	-0.3552500763	-0.3552500771	-0.3552500775	-0.3552500777	-0.35525007783
3	-0.3992551317	-0.3992551326	-0.3992551330	-0.3992551331	-0.39925513327
4	-0.4228390512	-0.4228390520	-0.4228390524	-0.4228390525	-0.422839052595
5	-0.4374984777	-0.4374984783	-0.4374984786	-0.4374984787	-0.437498478792
6	-0.4474846809	-0.4474846815	-0.4474846817	-0.4474846818	-0.447484681847
7	-0.4547225458	-0.4547225462	-0.4547225464	-0.4547225465	-0.454722546526
8	-0.4602084601	-0.4602084604	-0.4602084606	-0.4602084606	-0.460208460692
9	-0.4645094429	-0.4645094432	-0.4645094433	-0.4645094433	-0.464509443383
10	-0.4679717888	-0.4679717890	-0.4679717891	-0.4679717892	-0.467971789218

expressed as a finite sum of terms taken from some auxiliary set of well-behaved basic wave functions

$$\varphi_n = \sum_{i=1}^m c_{n,i} \psi_i. \quad (7)$$

Let us define for convenience

$$\langle n | \Omega | m \rangle = \int \varphi_n^* \Omega \varphi_m d\tau, \quad (8)$$

$$\Lambda_{2n} = \langle n | G_0 | n \rangle + 2 \langle n | G_1 | n-1 \rangle - \sum_{p=2}^{2n-1} \epsilon_p \sum_{i=n-p}^n \langle i | 2n-p-i \rangle, \quad (9)$$

$$\Lambda_{2n+1} = \langle n | G_1 | n \rangle - \sum_{p=2}^{2n-1} \epsilon_p \sum_{i=n-p+1}^n \langle i | 2n+1-p-i \rangle, \quad (10)$$

where, as before, terms with negative indices are to be ignored.

Insertion of Eqs. (2) and (6) into the variational theorem

$$E' \int \Phi^* \Phi d\tau \leq \int \Phi^* H \Phi d\tau \quad (11)$$

then leads to the following variational equation,

$$\langle 0 | 0 \rangle \epsilon_{2n} \leq \langle 0 | 0 \rangle \lambda_{2n} = \Lambda_{2n} \text{ (minimum)}, \quad (12)$$

provided that φ_p , ϵ_{2p} , and ϵ_{2p+1} , $p=0, 1, 2, 3, \dots, n-1$, have already been sufficiently exactly determined, and where the minimization procedure is to be performed

with respect to the n th-order perturbation wave function φ_n .

Equation (12) now furnishes an approximation to φ_n and ϵ_{2n} , which in turn may be used to calculate an approximate value of ϵ_{2n+1} :

$$\langle 0 | 0 \rangle \epsilon_{2n+1} = \Lambda_{2n+1} - 2 \epsilon_{2n} \langle 0 | 1 \rangle,$$

i.e.,

$$\langle 0 | 0 \rangle \epsilon_{2n+1} \cong \langle 0 | 0 \rangle \lambda_{2n+1} = \Lambda_{2n+1} - 2 \lambda_{2n} \langle 0 | 1 \rangle. \quad (13)$$

Hence, the approximate perturbation-energy coefficients λ_{2n} with even indices will, beyond a certain approximation, converge downwards, whereas the coefficients with odd indices converge upwards.

Tables I and II clearly demonstrate these convergence properties. There the contributions to $(\lambda_2 - \lambda_5)$ are displayed in groups in which the number of basic functions is naturally given by the specific function system itself. The functions used in this case are all of the Hylleraas type. We also note that the sets of energy coefficients of the $(2p)^2\ ^3P$ state converge more rapidly than the corresponding sets of the $(1s)^2\ ^1S$ state.

3. SETS OF WAVE FUNCTIONS USED

For the $(2p)^2\ ^3P$ state an expansion of the form

$$\varphi_p = e^{-1/2ksP} \sum_{nml} c_{nml} p^s n^m l^l \quad (14)$$

was taken, where the angular part of the spatial wave function has to be

$$P = r_1 r_2 \sin \theta \sin \theta_1 \sin \varphi = x_1 y_2 - x_2 y_1. \quad (15)$$

The exponent l must be an even positive integer to ensure correct symmetry. The following four types of

TABLE VIII. Perturbation nonrelativistic energies (E') of the state $(1s)^2\ ^1S$.

Z	95 terms	125 terms	161 terms	203 terms	Extrapolated
1	-1.05548158	-1.05549751	-1.05550204	-1.05550191	-1.0555020
2	-1.4518620463	-1.4518621169	-1.4518621505	-1.4518621673	-1.4518621880
3	-1.6177584257	-1.6177584813	-1.6177585072	-1.6177585201	-1.6177585360
4	-1.7069456988	-1.7069457397	-1.7069457588	-1.7069457682	-1.70694577969
5	-1.7624776658	-1.7624776965	-1.7624777108	-1.7624777178	-1.76247772634
6	-1.8003469868	-1.8003470105	-1.8003470214	-1.8003470268	-1.80034703338
7	-1.8278140508	-1.8278140696	-1.8278140782	-1.8278140825	-1.82781408766
8	-1.8486435678	-1.8486435829	-1.8486435900	-1.8486435934	-1.84864359755
9	-1.8649805276	-1.8649805401	-1.8649805459	-1.8649805488	-1.86498055217
10	-1.8781361097	-1.8781361202	-1.8781361250	-1.8781361274	-1.87813613028

TABLE IX. Variational nonrelativistic energies of the $(2p)^2\ ^3P$ state of H^- and He.

Order	k	H^- E'	k	He E'
34	0.28632	-0.2503505037	0.434753	-0.3552499000
50	0.26444	-0.25058405	0.434751	-0.35525002508
70	0.2592597	-0.25061397028	0.4347501	-0.35525005893
95	0.25	-0.25067224932	0.4347501	-0.35525007048
125	0.25	-0.25068255975	0.4347500	-0.35525007474
161	0.25	-0.25069724437		
203	0.25	-0.250702012		
Extrapolated		-0.2507097		-0.3552500771

expansions have been tried: (A) The exponents n and m take only positive integral values (the Hylleraas type). (B) n is integral or half-integral, m is integral (the Schwartz type). (C) n is integral, m is integral or half-integral. (D) both n and m take integral and half-integral values (introduced by H. M. Schwartz).⁶

Some results are presented in Tables III and IV. We note that the expansion B is by far the best one, both for $(2p)^2\ ^3P$ and $(1s)^2\ ^1S$, though the improvement is not so marked in the case of the $(2p)^2\ ^3P$ state.

The expansion B is just the expansion so successfully used by Schwartz⁷ in his extensive variational calculations of the nonrelativistic energies of the $(1s)^2\ ^1S$ state of He.

However, in the following variational perturbation investigations only functions of type A have been used more extensively, and for two reasons: (1) Introduction of too many half-integral exponents makes the secular equations unnecessarily ill conditioned. (2) The results are better suited for extrapolation, which is partly due to the higher degree of stability.

It may be of some interest to compare our results with those obtained by Scherr and Knight⁵ using wave functions of the Kinoshita type. In addition, they have varied the scale factor k individually for every φ_i . We have decided not to do so, partly because of the increasing computing time, partly to obtain sets of energy coefficients better suited for extrapolation. Consequently, the scale factor has been fixed at the hydrogenic value, i.e., $k=0.5$ for the $(2p)^2\ ^3P$ state and $k=1$ for the $(1s)^2\ ^1S$ state.

TABLE X. Variational nonrelativistic energies of the $(1s)^2\ ^1S$ state of H^- . $k=0.60$.

Order	E'
91	-1.0554997900
116	-1.0555017873
146	-1.0555019195
182	-1.0555019989
224	-1.0555020125
Extrapolated	-1.055502016

⁶ H. M. Schwartz, Phys. Rev. **103**, 110 (1956).⁷ C. Schwartz, Phys. Rev. **128**, 1146 (1962).

4. NUMERICAL RESULTS. THE ENERGY COEFFICIENTS

In Tables V and VI we present the numerical values of the energy coefficients (λ_0 - λ_{21}) obtained by using trial wave functions up to order 203. These tables clearly illustrate the fact that the perturbational convergence is somewhat better for the $(1s)^2\ ^1S$ state than for the $(2p)^2\ ^3P$ state, whereas the variational convergence is best for the $(2p)^2\ ^3P$ state. For both states, however, it is sufficient to evaluate the energy coefficients up to λ_{21} to obtain the energy of He with an accuracy of ten digits.

By using an extrapolation procedure we are now able to estimate a value of the sum of the remaining coefficients; let us call it the remainder, denoting it by R . The remainders given in Tables V and VI are all calculated on the basis of the coefficients (λ_{14} - λ_{21}).

The coefficients given in the 5th column are in the same way found by extrapolation from the sets of order 70, 95, 125, 161, and 203. They are believed to be correct within several units in the last decimal place given, apart from possible rounding errors due to the comparatively too short double-length numbers (approximately 16 decimal digits) for handling our equation systems of higher order than say 250 with sufficient accuracy.

The extrapolations have all been carried out by a repeated use of Aitken's δ^2 process known from numerical analysis. This method renders a relatively good estimate of the reliability of the extrapolated values of the convergence limits.

5. ENERGY VALUES

The total nonrelativistic energies computed from the sets of coefficients listed in Tables V and VI, are given in the Tables VII and VIII, respectively, for the first ten members of the isoelectronic sequences. The values presented in the last column in each table, are most likely correct within a few units in the last decimal given.

6. SOME VARIATIONALLY CALCULATED ENERGIES

A few variationally calculated energy values will be given for comparison. For the $(2p)^2\ ^3P$ state we have used the same basic set of functions as in the perturbation calculations, system A . For $(1s)^2\ ^1S$ a mixture of systems A and B was found to be most fruitful. The first 55 terms have been taken from system B , the rest from system A .

The energy obtained for the $(1s)^2\ ^1S$ state of H^- is seen to be in excellent agreement with the best value found by Pekeris⁸: $E' = -1.0555020126$ (444 terms). The scale factor k has been fixed at 0.60, which is nearly its optimum value using a 116-term wave function.

⁸ C. L. Pekeris, Phys. Rev. **126**, 1470 (1962).