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Coupled State Calculation of Proton Hydrogen Collisions in a Gaussian Basis

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Abstract. Proton hydrogen scattering has been used to investigate the usefulness of Gaussian functions as a basis set for the description of atomic collisions. An impact-parameter close-coupling calculation is carried out and cross-sections for ground-state electron capture, total electron capture and free electron production are obtained. Generally, promising agreement of the results of this work with other theoretical and experimental investigations is observed.

Introduction

Gaussian functions have been introduced in atomic and molecular physics by Boys [1]. Boys showed that Gaussian functions offer the distinct advantage over other possible basis sets for the treatment of atomic and molecular physics problems, that multicenter integrals involving arbitrary numbers of centers may be carried out analytically. For this reason they have been used in numerous atomic and molecular structure calculations. Another attractive property of Gaussian functions, which is probably less well known, makes them suitable for the treatment of heavy particle collisions involving rearrangement of electrons, as for example electron capture. Consider the wave function ϕ of a hydrogen atom moving with velocity \vec{v} in a fixed coordinate system. Let \vec{R} and \vec{r} be the position vectors of proton and electron then,

$$\phi(\vec{r}, \vec{R}) = \psi(\vec{r} - \vec{R}) \cdot \exp(i\vec{v} \cdot \vec{r}), \quad (1)$$

where $\psi(\vec{r} - \vec{R})$ is the electronic wave function in a coordinate system attached to the proton. $\phi(\vec{r}, \vec{R})$ is called a travelling orbital [2]. Assuming that $\psi(\vec{r} - \vec{R})$ may be chosen to be of the form

$$\psi(\vec{r} - \vec{R}) = N \cdot \exp(-\alpha(\vec{r} - \vec{R})^2) \quad (2)$$

ϕ may be written as

$$\phi(\vec{r}, \vec{R}) = N^* \cdot \exp \left\{ -\alpha \left[\vec{r} - \left(\vec{R} + \frac{i\vec{v}}{2\alpha} \right) \right]^2 \right\} \quad (3)$$

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which can be interpreted as the wave function of a stationary hydrogen atom at position \vec{R}^*

$$\vec{R}^* = \vec{R} + \frac{i\vec{v}}{2\alpha}. \quad (4)$$

However, the fact that \vec{R}^* is complex is irrelevant to the evaluation of multicenter integrals. This applies, in particular, to two-electron two-center integrals [3] and one-electron three-center integrals [4], which are extremely difficult to evaluate. Because of these attractive mathematical properties it seems worthwhile to investigate the merits of Gaussians as compared to exponentials from a physical point of view. Proton-hydrogen scattering was chosen as the test case because a considerable amount of theoretical and experimental work with various degrees of refinement is available for comparison with the results of the present approach. The calculations are performed in a straight line trajectory impact parameter formalism. Atomic units are used unless otherwise specified.

The Basis Set

We have chosen the variation principle to approximate the hydrogen ground state by a Gaussian expansion. Construction of Gaussian approximations of maximum overlap with the exact ground-state function was also considered and dismissed, because it is only applicable to hydrogen. Let

$$|G, s, N, \nu\rangle = \exp\{-\alpha_\nu r^2\} \quad (5)$$

be the ν th Gaussian function in an expansion containing N linearly independent but non-orthogonal (s) terms. Then,

$$\langle E \rangle = \frac{\sum_{\lambda, \nu}^N b_\nu b_\lambda^* \langle G, s, N, \lambda | \mathcal{H} | G, s, N, \nu \rangle}{\sum_{\lambda, \nu}^N b_\nu b_\lambda^* \langle G, s, N, \lambda | G, s, N, \nu \rangle} \quad (6)$$

where \mathcal{H} is the hydrogen atom Hamiltonian. The minimum energy is given by

$$\frac{\delta E}{\delta b_\nu} = 0 \quad (7)$$

$$\frac{\delta E}{\delta \alpha_\nu} = 0. \quad (8)$$

(7) and (8) constitute a non-linear eigenvalue problem which may be solved for N eigenvalues E_λ with corresponding eigenvectors b_λ and N exponential parameters α_ν by iterative techniques. Numerical values of E_λ and α_ν are collected in Table I. The lowest eigenvalue for each N , of course, refers to the ground state. The higher eigenvalues all turn out to be positive. The corresponding eigenfunctions are pseudostates and do not have a direct physical significance. Using the methods described in a preceding paper [5] we have expanded the ground-state approximation and the pseudo-

Table I
Exponential parameters, α_v , eigen-energies E_λ , and overlap integrals with exact hydrogen wave functions for Gaussian expansions involving 1 to 4 terms

N	1	2	3				4			
α_v	0.28294	0.20153	1.3325	0.151376	0.681289	4.50036	0.121945	0.444513	1.96214	13.0100
λ	1	1	2	1	2	3	1	2	3	4
E_λ	-0.4244	-0.4858	0.8917	-0.4970	0.3076	5.929	-0.49928	0.1132	2.592	21.15
n	1	0.95684	0.99331	0.00012	0.99875	—	0.99974	—	—	—
2	0.00848	0.00287	0.07053	0.00059	0.17281	0.00787	0.00011	0.28952	0.01721	0.00176
3	0.00127	0.00028	0.02324	0.00002	0.05132	0.00197	—	0.07679	0.00309	0.00033
4	0.00041	0.00007	0.01006	—	0.02142	0.00077	—	0.03082	0.00104	0.00011
5	0.00018	0.00003	0.00520	—	0.0109	0.00038	—	0.01539	0.00047	0.00005
$\sum_{n=0}^{\infty} U_{n\lambda}^2$	0.96750	0.99661	0.11993	0.99937	0.27861	0.01172	0.99985	0.44323	0.02266	0.00235

states in hydrogen eigenfunctions. Table I gives numerical values of

$$|u_{n\lambda}|^2 = |\langle G, o, N, \lambda | H(ns) \rangle|^2 \quad (9)$$

for $N = 1-4$ and $n = 1-5$. $|G, o, N, \lambda\rangle$ is the orthonormal solution of (7, 8) corresponding to eigenvalue E_λ and $|H(ns)\rangle$ is the exact hydrogen state with principal quantum number n and angular momentum $l = 0$. The last two lines of Table I give the total contribution of all discrete states to $|G, o, N, \lambda\rangle$ and the integrated continuum contribution. An example of the spectral distribution of

$$|\langle G, o, N, \lambda | H(ks) \rangle|^2 = |u_{k\lambda}|^2, \quad (10)$$

where $H(ks)$ is a continuous hydrogen state with electron wave number k , is given for $N = 4$ in Figure 1. The amount of overlap of the pseudostates with the hydrogen continuum is consistent with their positive energy eigenvalues.

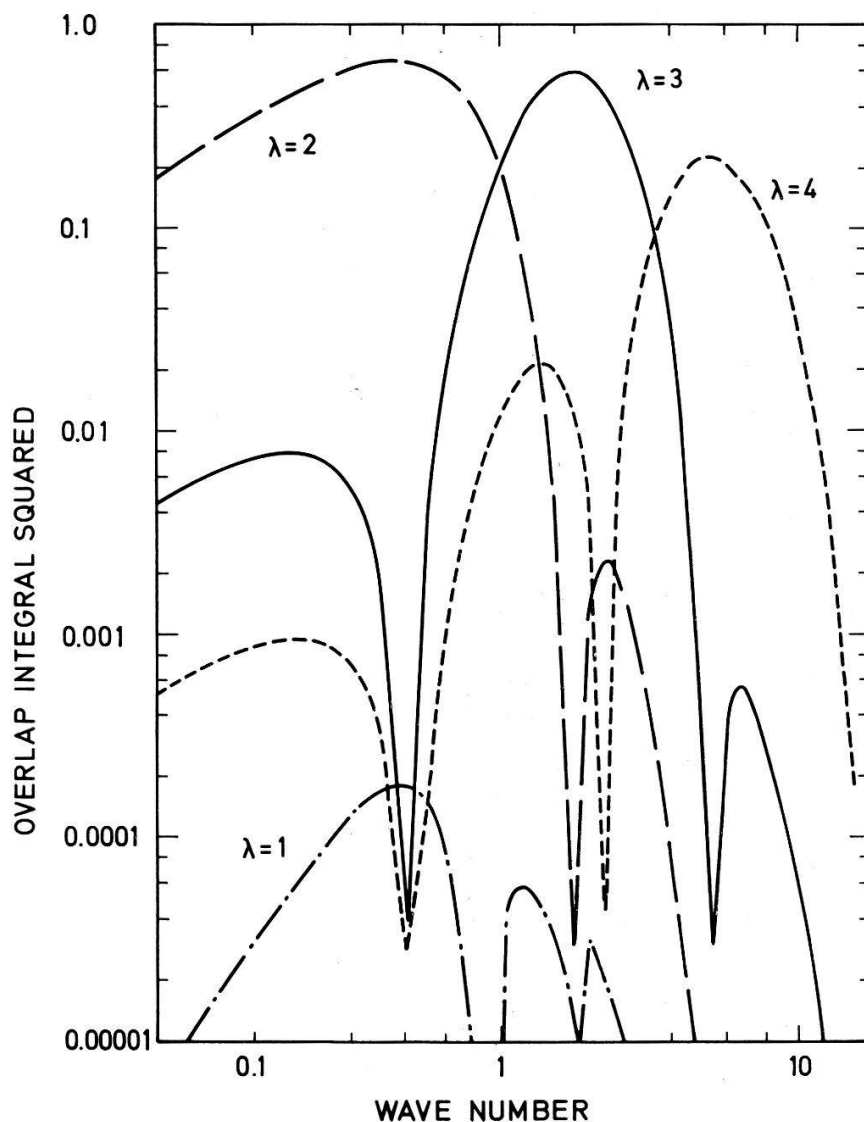


Figure 1

This figure is a log-log plot of the overlap of the orthonormal states of a four-term Gaussian expansion with the hydrogen continuum. Indices $\lambda = 1, 2, 3, 4$ correspond to eigenenergies of $-0.49, 0.11, 2.59$, and 21.15 , respectively. While the ground state representation $\lambda = 1$ hardly contains any hydrogen continuum, the pseudostates with $\lambda \geq 2$ exhibit a considerable overlap.

It is instructive to use the set of functions $|G, s, N, \nu\rangle$ with values α_ν as determined above, to calculate the electronic eigenenergies of the $1s\sigma$ and $2p\sigma$ states of the hydrogen molecular ion in an LCAO approximation. The results are given in Figure 2 together with the exact solution from the work of Bates and Reid [6]. Since the H_2^+ molecule is

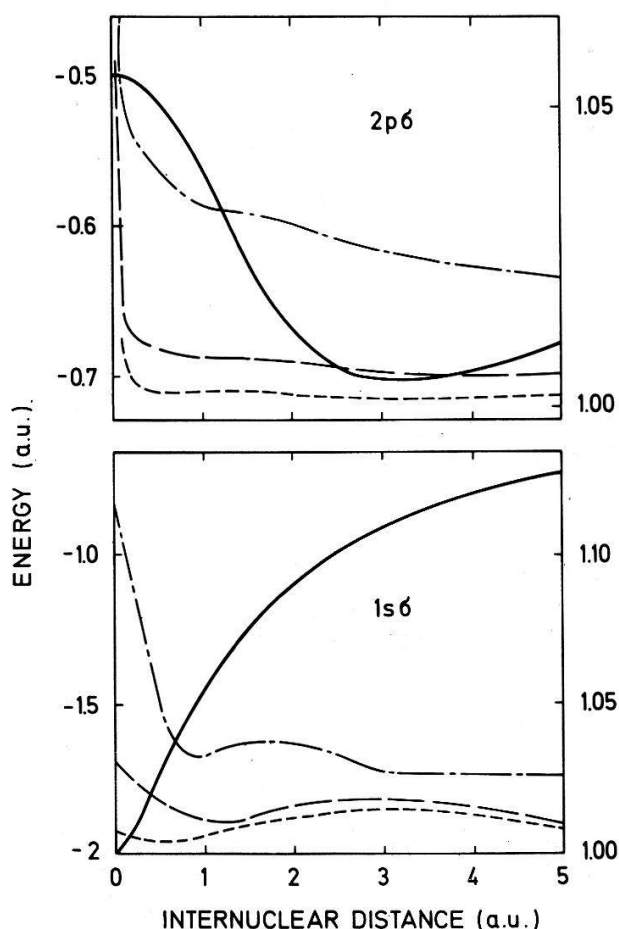


Figure 2

The solid lines in this figure are the exact potential energy curves of the H_2^+ molecular ion in the $1s\sigma$ (lower part) and the $2p\sigma$ (upper part) states as given by Bates and Reid [6]. The broken curves, whose ordinate scale is given on the right, give the factor by which results obtained with a Gaussian LCAO variation calculation for the respective states exceed the exact results. --- four-state calculation, —·—·— three-state calculation and, ····· two-state calculation.

the limiting case of H^+-H scattering as the velocity of relative motion goes to zero, a satisfactory description of low energy H^+-H collisions is expected for $N \geq 2$ from an inspection of Figure 2.

The Coupled Equations

Consider a coordinate system with its origin midway between the two protons and its Z -axis in the direction of the proton relative velocity (Fig. 3). The relative-position vector of any two points may conveniently be written as $\vec{r}_{\mu\mu'}$, where μ and μ' define the two ends of \vec{r} and take on the values 2 for the electron, 1 for the target proton, (-1) for the projectile proton, and 0 for the origin of coordinates. Using this convention, the electronic Hamiltonian is

$$\mathcal{H}_{el} = -\frac{1}{2}\Delta_{r_{02}} - \sum_{\mu=-1,1} \frac{1}{r_{\mu 2}}, \quad (11)$$

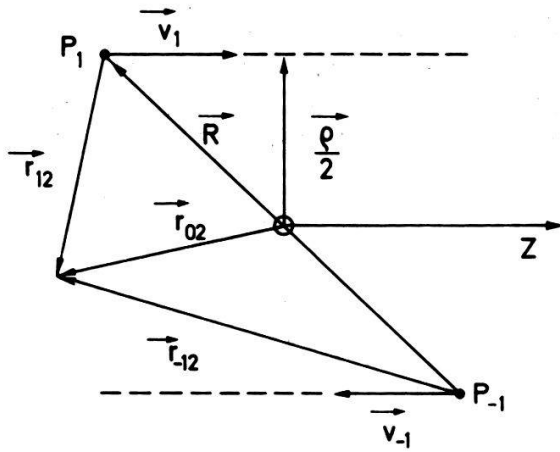


Figure 3

Coordinates chosen to describe the collision.

and the proton velocities with respect to the origin are given by

$$\vec{v}_\mu = \frac{\mu}{2} \cdot \vec{v}. \quad (12)$$

In the impact parameter approximation we let the distance from proton (1) to proton (-1) be given by

$$\vec{r}_{-11} = \vec{R} = \vec{\rho} + \vec{v} \cdot t. \quad (13)$$

We expand the electronic wave function in terms of travelling Gaussian orbitals about each proton. These basis states are given by

$$|G, S, N, \nu, \vec{r}_{0\mu}, \vec{v}_\mu\rangle = \exp \left\{ -\alpha_\nu r_{\mu 2}^2 + i \vec{v}_\mu \vec{r}_{02} - i \frac{v^2}{8} t \right\}, \quad (14)$$

with $\mu = -1, 1$ and $\nu = 1, \dots, N$. Taking

$$|a(t)\rangle = \sum_\mu \sum_\nu b_{\mu\nu}(t) |G, s, N, \nu, \vec{r}_{0\mu}, \vec{v}_\mu\rangle, \quad (15)$$

we require that the functional

$$\int_{-\infty}^{\infty} \left\langle a(t) \left| \mathcal{H}_{e1} - i \frac{\delta}{\delta t} \right| a(t) \right\rangle dt \quad (16)$$

be stationary. This leads to the coupled equations for the expansion coefficients

$$i \sum_{\mu' \nu'} S_{\mu\nu\mu'\nu'} \dot{b}_{\mu'\nu'} = \sum_{\mu' \nu'} H_{\mu\nu\mu'\nu'} b_{\mu'\nu'}, \quad \begin{array}{l} \mu = -1, 1 \\ \nu = 1, \dots, N. \end{array} \quad (17)$$

$S_{\mu\nu\mu'\nu'}$ and $H_{\mu\nu\mu'\nu'}$ are defined by

$$S_{\mu\nu\mu'\nu'} = \langle G, s, N, \nu, \vec{r}_{0\mu}, \vec{v}_\mu | G, s, N, \nu', \vec{r}_{0\mu'}, \vec{v}_{\mu'} \rangle, \quad (18)$$

$$H_{\mu\nu\mu'\nu'} = \left\langle G, s, N, \nu, \vec{r}_{0\mu}, \vec{v}_\mu \left| \mathcal{H}_{e1} - i \frac{\delta}{\delta t} \right| G, s, N, \nu', \vec{r}_{0\mu'}, \vec{v}_{\mu'} \right\rangle, \quad (19)$$

and satisfy the matrix relation

$$i\dot{S} = H^+ - H, \quad (20)$$

which may conveniently be used to check numerical calculations. While the representation (15) is convenient for the computation of matrices H and S , the numerical integration of (17) is greatly facilitated and numerically more stable if we expand $|a(t)\rangle$ as

$$|a(t)\rangle = \sum_{\mu=-1,1} \sum_{\lambda=1}^N a_{\mu\lambda}(t) |G, o, N, \lambda, \vec{r}_{0\mu}, \vec{v}_\mu\rangle \cdot \exp(-iE_\lambda t). \quad (21)$$

The states $|G, o, N, \lambda, \vec{r}_{0\mu}, \vec{v}_\mu\rangle$ are given in terms of $|G, s, N, \lambda, \vec{r}_{0\mu}, \vec{v}_\mu\rangle$ by a linear time-independent transformation,

$$|G, o, N, \lambda\rangle = \sum_{\nu=1}^N D_{\lambda\nu} |G, s, N, \nu\rangle, \quad (22)$$

with $D_{\lambda\nu}$ as determined from the solution of the eigenvalue problem (7, 8). The coupled equations for the new expansion coefficients $a_{\mu\lambda}$ are then,

$$\begin{aligned} i \sum_{\mu'\nu'} S_{\mu\nu\mu'\nu'} \left\{ \sum_{\lambda=1}^N D_{\nu'\lambda} [-iE_\lambda a_{\mu'\lambda}(t) + \dot{a}_{\mu'\lambda}(t)] \exp(-iE_\lambda t) \right\} \\ = \sum_{\mu'\nu'} H_{\mu\nu\mu'\nu'} \sum_{\lambda=1}^N D_{\nu'\lambda} \exp(-iE_\lambda t) a_{\mu'\lambda}(t). \end{aligned} \quad (23)$$

(23) is integrated from $t = -20/v$ to $t = 20/v$ subjected to the initial condition, that the electron be in the ground state around the target proton (1) before the collision

$$a_{\mu\lambda} \left(-\frac{20}{v} \right) = \delta_{\mu 1} \delta_{\lambda 1}. \quad (24)$$

Results for Ground State Capture

The total cross-section for ground-state capture in the impact parameter approximation is given by

$$\sigma_{\text{tot}} = 2\pi \int_0^\infty |a_{-11}(t \rightarrow \infty)|^2 \rho d\rho. \quad (25)$$

Numerical values are collected in Table II. Results for Gaussian functions are given in columns d–g for one- to four-term expansions, respectively. A non-systematic variation of cross-sections at different energies is observed going from column d to g. While at 1 keV the four-term results are highest, at 5 keV they are lowest. It is, however, remarkable, that there is essentially no difference between the three- and four-term expansion results, indicating a satisfactory convergence of the Gaussian expansion. Among the various calculations available in the literature [7, 8, 9, 10, 11] we have chosen the $1s-2s-2p$ hydrogen wave function calculation of Cheshire, Gallaher, and Taylor (a), the $1s-2s-2p$ hydrogenic $\overline{3s-3p}$ pseudostate calculation of the same authors (b), and the $1s-2s-2p$ Sturmian calculation of Wilets and Gallaher (c). The 5 keV and 50 keV numbers in (a, b) have been obtained by quadratic interpolation, while the Wilets and Gallaher results have been read from a drawing.

Table II
Total cross-section for ground-state capture in units of 10^{-16} cm^2

Energy (keV)	Cross-sections						
	a	b	c	d	e	f	g
1	16.6	19.12	17.4	14.3	15.17	15.91	16.04
5	10.0	10.31	10.1	9.92	9.99	9.88	9.76
15	5.79	5.82	5.7	6.12	5.50	5.07	5.24
25	2.98	2.93	3.1	2.83	2.59	2.73	2.82
50	0.68	0.67	—	0.58	0.70	0.72	0.67
100	0.092	0.088	—	0.071	0.11	0.088	0.088

Key to references

- a) Cheshire, Gallaher, and Taylor $1s-2s-2p$ close coupling.
- b) Cheshire, Gallaher, and Taylor $1s-2s-2p-\overline{3s-3p}$ pseudostate close coupling.
- c) Gallaher and Wilets, $1s-2s-2p$ Sturmian close coupling.
- d, e, f, g) This work with $N = \text{one-, two-, three-, or four-term Gaussian expansions.}$

The pseudostate calculation of Cheshire et al. is certainly the most elaborate with respect to the computational effort and uses the largest basis set. The three- and four-term Gaussian results agree satisfactorily with Cheshire's data at the three higher-energies. At the lowest energy of 1 keV the Gaussian calculation agrees with the four-state hydrogenic results (a), with the early one-state calculation of McCarroll [8], and with the molecular eigenfunction expansion of Ferguson [7], which are not given in the table. However, the Sturmian results and even more pronounced Cheshire's pseudostate results (b) are definitely higher. Assuming capture into excited states to be negligible as compared to ground-state capture at an energy as low as 1 keV (Fig. 6) we may include experimental data in the discussion. Total cross-sections for electron capture by protons in atomic hydrogen have been measured by Fite et al. [12], McClure [13], and Bayfield [14]. Only Fite's measurement extends to 1 keV where he obtains a cross-section of $20 \times 10^{-16} \text{ cm}^2$. However, at energies higher than 3 keV Fite's data are consistently higher, by a factor of 1.18, than the more recent results of McClure and Bayfield which agree perfectly with each other. If we scale Fite's results by this factor we obtain $17 \times 10^{-16} \text{ cm}^2$ at 1 keV which seems to rule out Cheshire's value. On the other hand, the Gaussian results are definitely too low, which might be attributed to the fact that a Gaussian basis will never yield asymptotically correct H_2^+ potential energy curves.

Excited States, Total Capture, and Ionization

While the calculation of ground-state capture is straightforward and does not present any difficulty, capture into the excited pseudostates does not have a simple physical meaning. If the equations for the Gaussian expansion coefficients have been integrated for $-t_e \leq t \leq t_e$, where t_e is well in the asymptotic region, then,

$$a_{\mu\lambda}(t) = a_{\mu\lambda}(t_e) \cdot \exp\{-iE_\lambda(t - t_e)\}, \quad t \geq t_e \quad (26)$$

E_λ is the energy eigenvalue of the orthonormal pseudostate $|G, o, N, \lambda\rangle$. The probability $P_{n\mu}$ of finding the electron in the n th excited state around proton μ at time t is then,

$$P_{n\mu}(t) = \left| \sum_{\lambda=2}^N a_{\mu\lambda}(t_e) u_{n\lambda} \exp\{-iE_\lambda(t - t_e)\} \right|^2, \quad t \geq t_e \quad (27)$$

with $u_{n\lambda}$ as defined earlier. The time dependence of $P_{n\mu}$ arises because $|G, o, N, \lambda\rangle$ is not an eigenstate of hydrogen. Following Gallaher and Wilets [10] we take the average over time,

$$\bar{P}_{n\mu} = \lim_{T \rightarrow \infty} \int_{t_e}^T \frac{P_{n\mu}(t)}{T - t_e} dt \quad (28)$$

which yields

$$\bar{P}_{n\mu} = \sum_{\lambda=2}^N |a_{\mu\lambda}(t_e) u_{n\lambda}|^2. \quad (29)$$

The term $\lambda = 1$, corresponding to the Gaussian approximation of the hydrogen ground state, is excluded from the summation. Including this term would give contributions to the excited states arising from the imperfect representation of the ground state independent of collision conditions. This consideration, however, becomes progressively irrelevant as N increases from 1 to 4.

Figure 4 shows cross-sections for capture into the 2s-state of hydrogen calculated with three- and four-term expansions, together with the experimental data of Bayfield [14]. Since the 2s-state is not explicitly included in the basis one would hardly expect more than an order of magnitude estimate of the 2s capture cross-section. The Gaussian expansion does definitely better than that.

The probability for capture into all discrete S-states is given by

$$P_{\text{tot } 1} = \sum_{\lambda=1}^N |a_{1\lambda}(t_e)|^2 \sum_{n=1}^{\infty} |u_{n\lambda}|^2. \quad (30)$$

Figure 5 shows this probability for an impact parameter corresponding to three degrees scattering as a function of energy together with other experimental and theoretical results. Capture probabilities obtained with the three-term expansion are essentially identical with those obtained with the four-term expansion. The present results differ only insignificantly from Cheshire's pseudostate calculation and the Sturmian results of Gallaher and Wilets and reproduce the experimental data satisfactorily in contrast to the four-term hydrogenic calculations of Wilets and Gallaher [9].

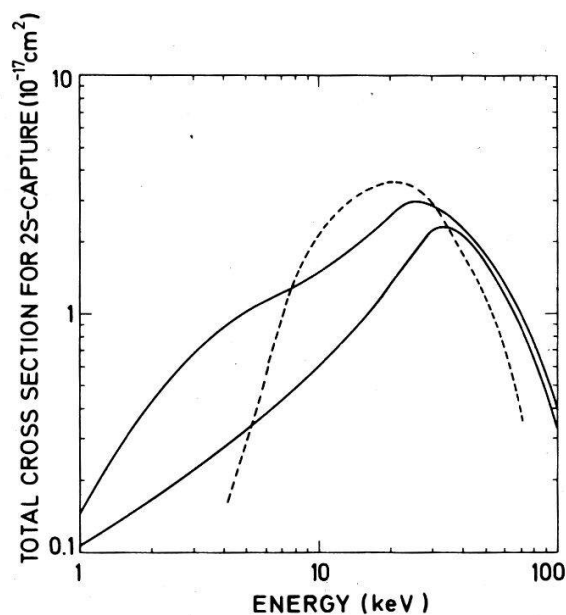


Figure 4

Cross-section for capture into the 2s-state of hydrogen. The broken curve is the experimental result of Bayfield. The upper solid curve was obtained with a four-term Gaussian expansion and the lower with a three-term expansion.

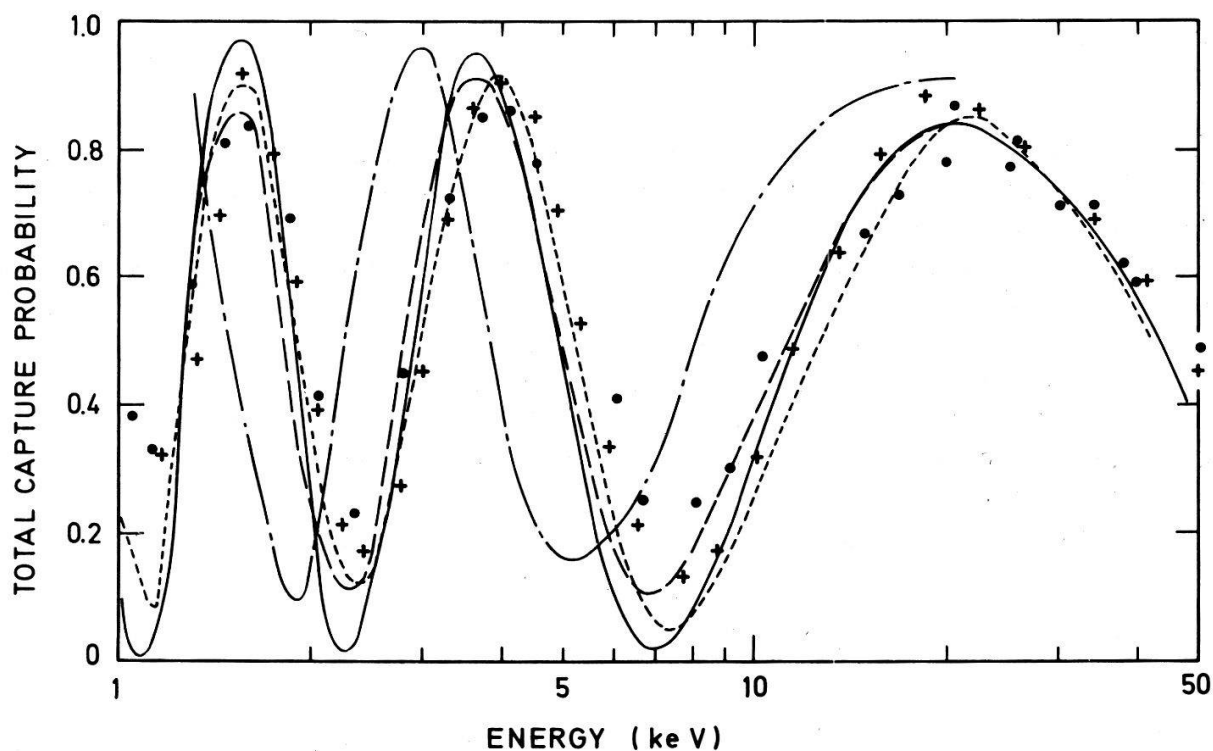


Figure 5

Total capture probability for a scattering angle of 3 degrees. — present results using three- or four-term Gaussian expansions; --- Gallaher and Wilets, four-state Sturmian [10]; —·—·— Wilets and Gallaher, four-state hydrogenic [9]; Cheshire et al., seven-state 1s-2s-2p hydrogenic $3s\ 3p$ pseudostates [11]; +++ experiment Lockwood and Everhart 1962 [15]; ••• experiment Helbig and Everhart 1965 [16].

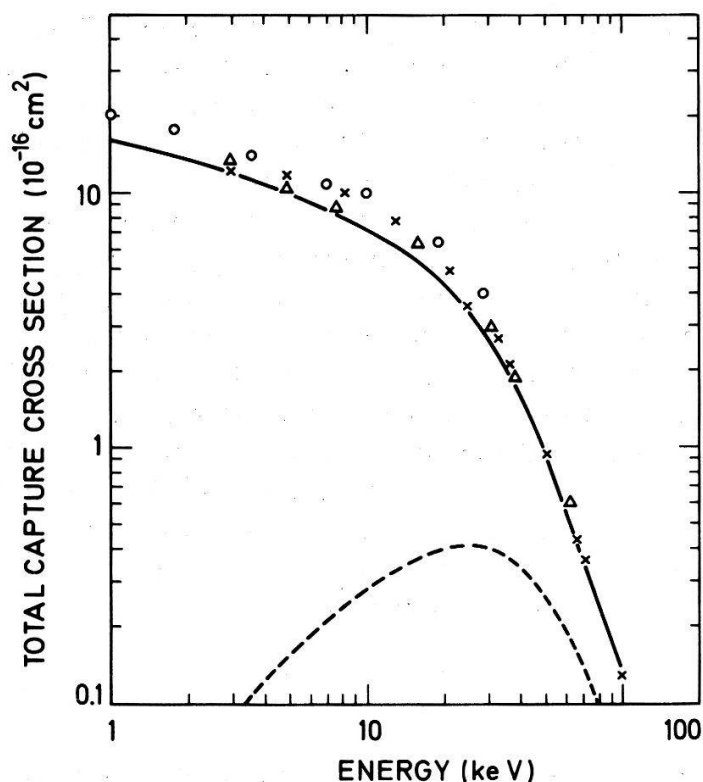


Figure 6
Total cross-section for electron capture by protons from hydrogen. — present results four-state Gaussian; --- contribution of capture into excited states from present calculation. $\circ \circ \circ$ experiment Fite et al. 1958 [12]; $\times \times \times$ experiment Bayfield 1969 [14]; $\triangle \triangle \triangle$ experiment McClure 1966.

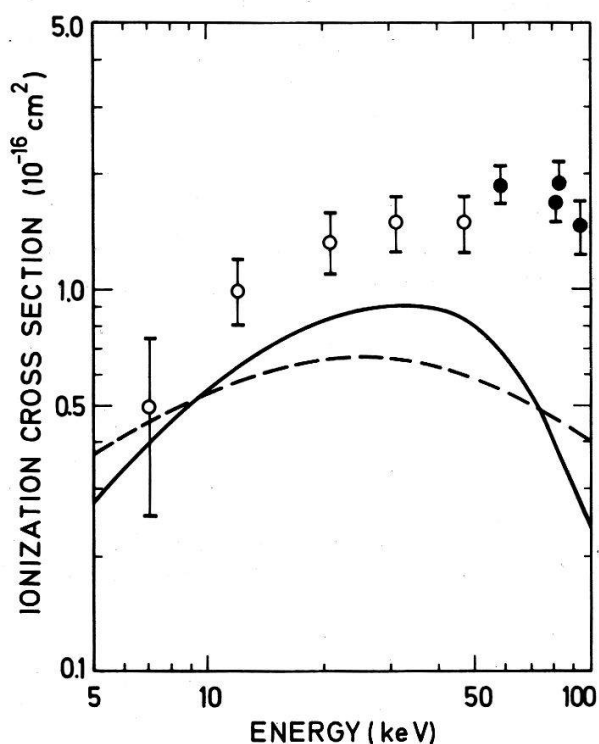


Figure 7
Total cross-section for free electron production in proton-hydrogen collisions. — present results, three-term Gaussian expansion; --- present results four-term Gaussian expansion; $\circ \circ \circ$ experiment Fite et al. 1960 [17]; $\bullet \bullet \bullet$ experiment Gilbody and Ireland 1964 [18].

Total cross-sections for capture into discrete states are shown in Figure 6 together with experimental data. Again three- and four-term Gaussian results are practically identical. Theory and experiment are in excellent agreement at higher energies. Below about 30 keV, however, the Gaussian results are too small by roughly 10%. The lower broken curve shows the contribution of capture into excited states.

Due to the large overlap of the Gaussian pseudostates with the hydrogen continuum an estimate of the cross-section for free electron production may be obtained from the present calculations. Free electrons are produced by either excitation of the target continuum or by capture into continuous states of the projectile. The latter process is quite important and contributes between 50% at 1 keV and 82% at 100 keV to the total cross-section. The total cross-section for free electron production is displayed in Figure 7 together with experimental results. Only s-wave contributions to both processes can be obtained from the present calculation and the higher energy behaviour of our data, as compared to experiment, suggests that considerably improved ionization cross-sections could be obtained if higher angular momenta were included in the expansion of the electronic wave function.

Conclusions

The present work has been carried out to investigate the suitability of Gaussian functions for the calculation of atomic collision cross-sections. The results for electron capture show that Gaussian expansions meet with considerable success. The most prominent property of the Gaussian expansions in addition to computational convenience is their large overlap with the hydrogen continuum. This can be employed to give estimates for ionization cross-sections, and, in view of the general success of the present calculation, supports Gallaher and Wilets' suggestion that continuum contributions may be of considerable importance in close coupling calculations.

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