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Coupled-State Calculations of Proton-Helium Scattering*

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Using the impact-parameter method, calculations have been done on the excitation of helium by protons in the kinetic-energy region of 10–10 000 keV. The total wave function of the system is expanded in a set of helium eigenstates including the $n=1$, $n=2$, and $n=3$ (except for 3^1S) states. The resulting linear differential equations (up to 18) have been solved numerically and compared with existing calculations and experiment. It is shown that for higher impact energies the many-state cross sections tend to the Born cross sections, but that for non-allowed transitions discrepancies exist up to very high energy. For allowed transitions, the agreement between theory and experiment is reasonable. Sublevel cross sections are shown to be very sensitive to the number of states retained in the expansion; only at the highest energies for which calculations have been done are they in agreement with Born sublevel cross sections. This fact is also shown by a comparison of calculated and measured polarization fractions of the emitted light induced by the excitations.

I. INTRODUCTION

Up till now the excitation of helium by protons in the keV energy region has been calculated in the Born and distortion approximations. Born results and a review of other work have been presented by the author in a previous paper,[1] henceforth referred to as I. The aim of this paper is to expand the total wave function of the system in an increasing number of target eigenstates and investigate whether the resulting cross sections show any convergence and at which energy, and how the theory agrees with experimental results.

For reasons of mathematical simplicity no projectile eigenstates were included, although it is felt that this severely limits the usefulness of the method. The states which have been included are 1^1S, 2^1S, 2^1P, 3^1P, and 3^1D including the magnetic substates. The collision plane was chosen to be the XZ plane, and the real representation of the substates was used, so that this set yielded a maximum of nine states. The combinations for which expansions have been made include the following: $1S$-$2S$-$2P$ [4 state], $1S$-$2P$ [3 state], $1S$-$3P$ [3 state], $1S$-$3D$ [4 state], $1S$-$2P$-$3D$ [6 state ($2P$)], $1S$-$3P$-$3D$ [6 state ($3P$)], $1S$-$2P$-$3P$-$3D$ [8 state], and $1S$-$2S$-$2P$-$3P$-$3D$ [9 state].

II. THEORY

We shall only give a short description of the theory; a more complete treatment has been given by Bates.[2] Atomic units will be used throughout, unless otherwise mentioned.

We assume that the proton is moving along a rectilinear path with collision parameter ρ and constant velocity $\vec{v}$. The trajectory is parallel to the Z axis of a fixed coordinate system with origin located at the helium nucleus. The internuclear distance is denoted by $\vec{R}$. Defining the electronic wave function of the system as $X(\vec{r},t)$, where $\vec{r}$ stands for the electron coordinates and t denotes the time, we may expand X in helium eigenstates $\Psi(\vec{r})$ with eigenenergy E_n,

$$X_p(\vec{r},t)=\sum_n a_{pn}(t)\Psi_n(\vec{r})\exp[-iE_n t]\ . \qquad (1)$$

The expansion coefficients a_n depend parametrically on ρ and $\vec{v}$. Inserting (1) in the Schrödinger equation for X,

$$(H-i\,\partial/\partial t)X=0\ , \qquad (2)$$

yields after some manipulation an infinite set of linear first-order differential equations for the coefficients $a_{pn}(t)$. These will henceforth be called transition amplitudes, a name which will become clear below:

$$i\,\frac{\partial a_{pq}}{\partial t}=\sum_n a_{pn}(t)V_{qn}(\vec{R})\exp[-i(E_n-E_q)t]\ , \qquad (3)$$

where

$$V_{qn}(\vec{R})=\int\Psi_q(\vec{r}_1,\vec{r}_2)V(\vec{R},\vec{r}_1,\vec{r}_2)\times\Psi_n(\vec{r}_1,\vec{r}_2)d\vec{r}_1 d\vec{r}_2\ , \qquad (4)$$

in which $V(\vec{R},\vec{r}_1,\vec{r}_2)=-\dfrac{1}{|\vec{R}-\vec{r}_1|}-\dfrac{1}{|\vec{R}-\vec{r}_2|}$,

and $\vec{r}$ in $\Psi(\vec{r})$ has been replaced by the two electron vectors $\vec{r}_1$ and $\vec{r}_2$ with respect to the origin.

If we define $t=0$ at the distance of closest approach, and let the projectile move in time from $t=-\infty$ to $t=+\infty$, we find for the probability that a transition from the original state p to state q has taken place,

$$P_{pq}=|a_{pq}(+\infty)|^2\ . \qquad (6)$$

Because of the cylindrical symmetry of the system, the cross section for excitation of q from p can be written as

$$Q(p-q)=2\pi\int_0^\infty|a_{pq}(+\infty)|^2\rho d\rho\ . \qquad (7)$$

III. APPROXIMATIONS AND PROCEDURE

In order to simplify the mathematics, approximate analytic functions have been used for the helium eigenstates. Generally they were of the following type:

$$\Psi_n(\vec{r}_1,\vec{r}_2)=(2+2\Delta^2)^{-1/2}[\phi_{1s}(2,r_1)\psi_n(\vec{r}_2)+\phi_{1s}(2,r_2)\psi_n(\vec{r}_1)]\ . \qquad (8)$$

Except for $n=2^1S$, Δ is equal to 0. The ground state was taken as

$$\Psi_{1s}(\vec{r}_1,\vec{r}_2)=\psi_{1s}(r_1)\psi_{1s}(r_2)\ . \qquad (9)$$

The set of $\psi_n(\vec{r})$ employed is [$\phi_{nlm}(Z,\vec{r})$ stands for a hydrogenic eigenstate nlm with nuclear charge Z]

1^1S: $\psi_{1s}(r)=N/(4\pi)^{1/2}[e^{-\alpha r}+\eta e^{-\beta r}]$,

$N=2.605\,05$,

$\alpha=1.41$,

$\beta=2.61$,

$\eta=0.799$;[3]

2^1S: $\psi_{2s}(r)=N/(4\pi)^{1/2}[e^{-\alpha r}+\eta e^{-\beta r}]$,

$N=0.645\,12$,

$\alpha=1.136$,

$\beta=0.464$,

$\eta=-0.280\,624$.

This is a slightly modified version of Marriott and Seaton's 2^1S state.[4] η is chosen such that this state is orthogonal to the ground state.

2^1P: $\psi_{2p}(\vec{r})=\phi_{2p}(Z,\vec{r})$, $Z=0.97$;[5]

3^1P: $\psi_{3p}(\vec{r})=(2N/\sqrt{3})(c-r)re^{-\mu r}Y_{1m}(\theta,\phi)$,

$\mu=0.325$, $c=5A/\mu$, $A=(1+2/2\mu)^{-1}$,

$N_{3p}{}^2=\mu^7/(25A^2-25A+15/2)$,

where c is chosen such[6] that this state is orthogonal to 2^1P;

3^1D: $\psi_{3d}(\vec{r})=\phi_{3d}(1,\vec{r})$.[6]

The particular choice of this set of states has been discussed in I. Generally we might say that this set provides energies and generalized oscillator strengths which compare very favorably with those obtained through the use of many-term Hylleraas eigenstates.

In expansion (1) from 3 up to 9 states have been retained. The resulting 3–9 complex differential equations have been solved numerically without making any further approximations.

IV. NUMERICAL PROCEDURE

The system of linear differential equations for the transition amplitudes has been numerically solved on a CDC 6400 Computer using a FORTRAN version of a Runge-Kutta procedure with self-selecting step size.[7] Sufficient convergence was obtained by replacing the infinite upper and lower

limit of time-integration by $(-100/v, +100/v)$.

A typical computing time for a transition amplitude for one particular value of ρ and v was 1 sec. Computing time increased sharply at lower energies (<20 keV). Cross sections were calculated using Simpson integration. The results are believed to be correct within error limits of 5%. Polarization fractions were calculated using the relations given by Percival and Seaton.[8]

Numerical and graphical results are presented in Tables I–VII and Figs. 1–7 together with earlier results[9,10] and some experiments.[11–14] A discussion of the experimental results is given elsewhere.[11] The Born results were taken from I except for the 2^1S cross sections, which have been calculated using a modified version of our main program.

TABLE I. Cross sections in πa_0^2 for excitation of 2^1S from the ground state as a function of proton kinetic energy E. The Born data are taken from Ref. 1.

E (keV)	Born	4 state ($2P$)	9 state
10	9.48×10^{-2}		
15	9.63×10^{-2}	5.85×10^{-3}	7.22×10^{-3}
20	9.07×10^{-2}	1.68×10^{-2}	1.97×10^{-2}
25	8.38×10^{-2}	2.92×10^{-2}	3.34×10^{-2}
30	7.70×10^{-2}	4.00×10^{-2}	4.47×10^{-2}
50	5.67×10^{-2}	5.87×10^{-2}	6.18×10^{-2}
70	4.43×10^{-2}	5.72×10^{-2}	5.82×10^{-2}
100	3.33×10^{-2}	4.79×10^{-2}	4.72×10^{-2}
150	2.34×10^{-2}	3.46×10^{-2}	3.34×10^{-2}
250	1.47×10^{-2}	2.08×10^{-2}	1.99×10^{-2}
500	7.60×10^{-3}	9.73×10^{-3}	9.33×10^{-3}
750	5.12×10^{-3}	6.19×10^{-3}	5.98×10^{-3}
1000	3.87×10^{-3}	4.51×10^{-3}	4.38×10^{-3}
2000	1.95×10^{-3}	2.13×10^{-3}	2.09×10^{-3}
5000	7.84×10^{-4}	8.16×10^{-4}	8.09×10^{-4}
10 000	3.93×10^{-4}	4.07×10^{-4}	3.99×10^{-4}

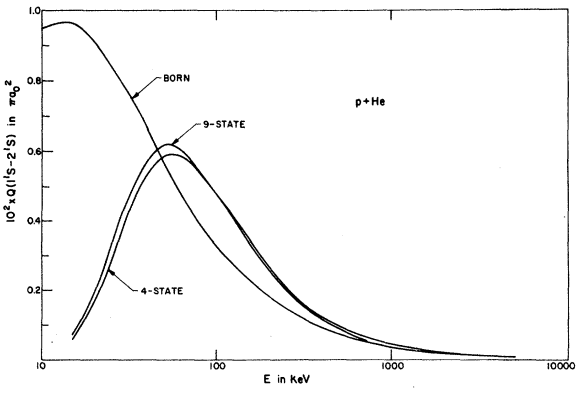

FIG. 1. Cross sections Q for excitation of 2^1S as a function of proton kinetic energy E.

V. DISCUSSION

A. Cross Sections

2^1S: Inclusion of distortion and coupling with the 2^1P state gave cross sections markedly different from the Born cross sections (see Fig. 1 and Table I). Inclusion of the 3^1P and 3^1D states did not produce significant changes, indicating that back coupling from the $n=3$ states is not very important. It is interesting to note that for the 9-state expansion QE, the cross section multiplied by the projectile energy, is decreasing with increasing energy at high energies; this is contrary to the behavior shown by the Born approximation (see I). Within the error limits, agreement between Born and many-state expansions is reached at about 2000 keV.

2^1P: Bell[9] has already shown that distortion effects significantly reduce the cross section below 100 keV. The many-state expansions confirm this (see Fig. 2 and Table II), and there also seems to be a tendency toward lower cross sections as more states are included. The shift of the curves for the many-state calculations indicates that coupling to the 2^1S state is very important. Inclusion of 3^1P and 3^1D states shows that back coupling from these states also plays an important role. Agreement with Born is found between 250 and 500 keV.

3^1P: Figure 3 and Table III show that, as was the case for 2^1P excitation, the many-state calculations give markedly reduced cross sections below about 400 keV. Comparison with Bell's[9] calculations show, as for 2^1P, that the single most important reason for this is distortion. The omission of the 3^1S state probably causes the 2^1P and 3^1P curves to be not completely comparable. Agreement with Born is again found between 250 and 500 keV. In this case, we also compared our results with two sets of experimental results.[11,12] It is seen that the agreement of distortion calculations and 3-, 8-, and 9-state calculations with experiment is very acceptable above 35 keV. At lower energies, structure exists of which no indication can be found in our calculations. Thomas's[12] experiments show best agreement with the 8- and 9-state expansions.

3^1D: The usual pattern of reduced cross sections at lower energies is again shown (see Fig. 4 and Table IV) when including distortion[10] and rotational coupling effects in the 4-state approximation. But from here on a wild pattern of cross-section curves results. Replacement in the 6-state approximation of 3^1P by 2^1P leads to a thirtyfold increase in the cross section at the maximum. Inclusion of both 2^1P and 3^1P (8 state) and also 2^1S (9 state) leads to cross sections a factor of 3 lower than the 6-state ($2P$) results, but still gives cross sections 4 times as high as

TABLE II. Cross sections for excitation of 2^1P.

E (keV)	Born	3 state	4 state	6 state	8 state	9 state
10	1.07×10^{-1}	3.65×10^{-3}		3.14×10^{-3}		
15	1.57×10^{-1}	2.06×10^{-2}	3.68×10^{-3}	1.69×10^{-2}	6.65×10^{-3}	3.91×10^{-3}
20	1.89×10^{-1}	4.62×10^{-2}	8.75×10^{-3}	3.88×10^{-2}	1.91×10^{-2}	9.32×10^{-3}
25	2.08×10^{-1}	7.40×10^{-2}	1.69×10^{-2}	6.30×10^{-2}	3.61×10^{-2}	1.77×10^{-2}
30	2.20×10^{-1}	1.00×10^{-1}	2.73×10^{-2}	8.52×10^{-2}	5.42×10^{-2}	2.80×10^{-2}
50	2.29×10^{-1}	1.62×10^{-1}	7.33×10^{-2}	1.44×10^{-1}	1.12×10^{-1}	7.35×10^{-2}
70	2.19×10^{-1}	1.83×10^{-1}	1.05×10^{-1}	1.67×10^{-1}	1.42×10^{-1}	1.05×10^{-1}
100	2.00×10^{-1}	1.86×10^{-1}	1.27×10^{-1}	1.74×10^{-1}	1.57×10^{-1}	1.27×10^{-1}
150	1.71×10^{-1}	1.72×10^{-1}	1.34×10^{-1}	1.64×10^{-1}	1.54×10^{-1}	1.34×10^{-1}
250	1.34×10^{-1}	1.40×10^{-1}	1.21×10^{-1}	1.35×10^{-1}	1.31×10^{-1}	1.21×10^{-1}
500	8.93×10^{-2}	9.30×10^{-2}	8.76×10^{-2}	9.25×10^{-2}	9.13×10^{-2}	8.75×10^{-2}
750	6.85×10^{-2}	7.23×10^{-2}	6.67×10^{-2}	7.01×10^{-2}	6.94×10^{-2}	6.75×10^{-2}
1000	5.62×10^{-2}	5.83×10^{-2}	5.65×10^{-2}	5.81×10^{-2}	5.76×10^{-2}	5.64×10^{-2}
2000	3.40×10^{-2}		3.39×10^{-2}	3.46×10^{-2}	3.42×10^{-2}	3.39×10^{-2}
5000	1.67×10^{-2}		1.66×10^{-2}	1.64×10^{-2}	1.66×10^{-2}	1.65×10^{-2}
10 000	9.55×10^{-3}		9.41×10^{-3}	9.43×10^{-3}	9.42×10^{-3}	9.40×10^{-3}

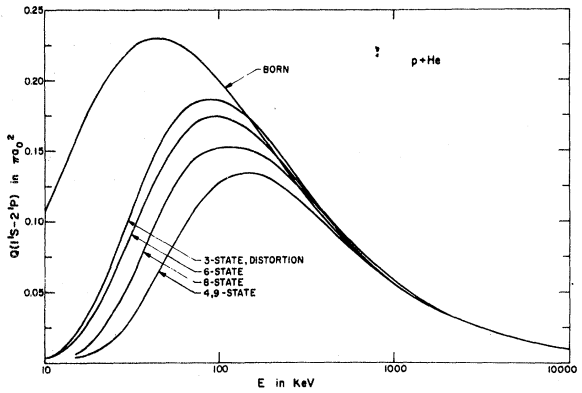

FIG. 2. Cross sections for excitation of 2^1P. The distortion curve is from Bell (Ref. 9).

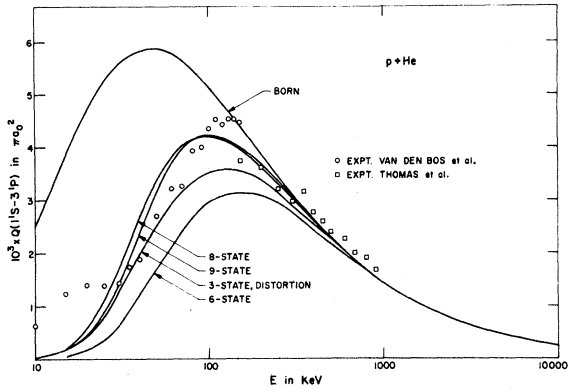

FIG. 3. Cross sections for excitation of 3^1P. The distortion curve is from Bell (Ref. 9), the experimental points are from van den Bos *et al.* (Ref. 10) and from Thomas *et al.* (Ref. 11).

TABLE III. Cross sections for excitation of 3^1P.

E (keV)	Born	3 state	6 state	8 state	9 state
10	2.52×10^{-2}	2.12×10^{-4}			
15	3.86×10^{-2}	1.64×10^{-3}	4.24×10^{-4}	2.03×10^{-3}	1.35×10^{-3}
20	4.72×10^{-2}	4.63×10^{-3}	1.64×10^{-3}	5.96×10^{-3}	4.32×10^{-3}
25	5.26×10^{-2}		3.72×10^{-3}	1.14×10^{-2}	9.00×10^{-3}
30	5.58×10^{-2}	1.26×10^{-2}	6.34×10^{-3}	1.71×10^{-2}	1.43×10^{-2}
50	5.87×10^{-2}	2.51×10^{-2}	1.70×10^{-2}	3.37×10^{-2}	3.17×10^{-2}
70	5.64×10^{-2}	3.16×10^{-2}	2.39×10^{-2}	4.02×10^{-2}	3.94×10^{-2}
100	5.15×10^{-2}	3.53×10^{-2}	2.90×10^{-2}	4.21×10^{-2}	4.22×10^{-2}
150	4.42×10^{-2}	3.54×10^{-2}	3.11×10^{-2}	3.96×10^{-2}	4.00×10^{-2}
250	3.45×10^{-2}	3.13×10^{-2}	2.90×10^{-2}	3.29×10^{-2}	3.33×10^{-2}
500	2.29×10^{-2}	2.27×10^{-2}	2.19×10^{-2}	2.28×10^{-2}	2.30×10^{-2}
750	1.76×10^{-2}	1.76×10^{-2}	1.72×10^{-2}	1.76×10^{-2}	1.77×10^{-2}
1000	1.44×10^{-2}	1.46×10^{-2}	1.43×10^{-2}	1.45×10^{-2}	1.45×10^{-2}
2000	8.71×10^{-3}	8.91×10^{-3}		8.83×10^{-3}	8.86×10^{-3}
5000	4.28×10^{-3}	4.27×10^{-3}		4.24×10^{-3}	4.24×10^{-3}
10 000	2.44×10^{-3}			2.43×10^{-3}	2.43×10^{-3}

TABLE IV. Cross sections for excitation of 3^1D.

E (keV)	Born	4 state	6 state ($2P$)	6 state ($3P$)	8 state	9 state
10	1.02×10^{-3}	3.16×10^{-5}	7.98×10^{-4}			
15	1.65×10^{-3}	2.10×10^{-4}	4.69×10^{-3}	8.71×10^{-5}	7.82×10^{-4}	6.13×10^{-4}
20	2.03×10^{-3}	5.17×10^{-4}	1.04×10^{-2}	2.18×10^{-4}	2.04×10^{-3}	1.81×10^{-3}
25	2.23×10^{-3}		1.58×10^{-2}	3.74×10^{-4}	3.58×10^{-3}	3.37×10^{-3}
30	2.31×10^{-3}	1.13×10^{-3}	2.00×10^{-2}	5.27×10^{-4}	5.04×10^{-3}	4.92×10^{-3}
50	2.21×10^{-3}	1.70×10^{-3}	2.58×10^{-2}	8.75×10^{-4}	8.42×10^{-3}	8.66×10^{-3}
70	1.94×10^{-3}	1.75×10^{-3}	2.37×10^{-2}	9.83×10^{-4}	8.75×10^{-3}	9.16×10^{-3}
100	1.60×10^{-3}	1.58×10^{-3}	1.85×10^{-2}	9.86×10^{-4}	7.46×10^{-3}	7.90×10^{-3}
150	1.21×10^{-3}	1.24×10^{-3}	1.20×10^{-2}	8.81×10^{-4}	5.15×10^{-3}	5.50×10^{-3}
250	8.07×10^{-4}	8.31×10^{-4}	5.96×10^{-3}	6.65×10^{-4}	2.67×10^{-3}	2.86×10^{-3}
500	4.37×10^{-4}	4.39×10^{-4}	1.98×10^{-3}	3.87×10^{-4}	9.57×10^{-4}	1.01×10^{-3}
750	2.99×10^{-4}	2.98×10^{-4}	1.02×10^{-3}	2.70×10^{-4}	5.27×10^{-4}	5.50×10^{-4}
1000	2.27×10^{-4}	2.25×10^{-4}	6.45×10^{-4}	2.07×10^{-4}	3.52×10^{-4}	3.65×10^{-4}
2000	1.16×10^{-4}		2.20×10^{-4}		1.43×10^{-4}	1.45×10^{-4}
5000	4.70×10^{-5}		6.24×10^{-5}		5.05×10^{-5}	5.08×10^{-5}
10 000	2.36×10^{-5}		2.71×10^{-5}		2.43×10^{-5}	2.43×10^{-5}

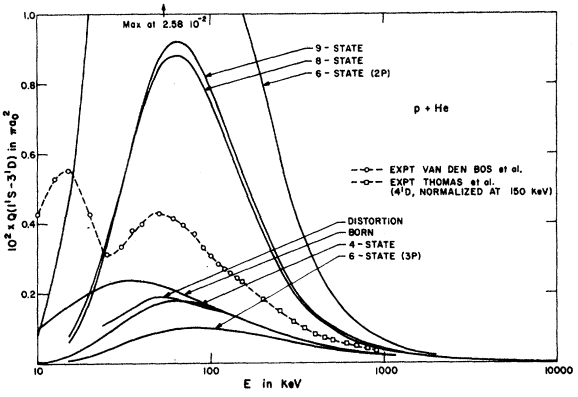

FIG. 4. Cross sections for excitation of 3^1D. For the experimental data, see Fig. 3. The distortion curve is from Davison (Rev. 15).

the Born cross sections. Agreement with experiment[11,12] is poor, also in a relative sense. Normalizing the experimental results to the Born at high energy strongly suggests $Q(\text{expt}) > Q(\text{Born})$ at lower impact energies. Again we point out the structure around 25 keV for which no indication at all is found in the calculations. Another point which has to be stressed is the bad agreement with the Born results even for very high energies. Although the 4-state results are in agreement with Born at 100 keV and the 6 state ($3P$) at 750 keV, the other many-state expansion results, especially the 6 state ($2P$), show large deviations. As was the case with the 2^1S cross sections, we mention that QE for 6 state ($2P$), 8 and 9 state is still decreasing at the highest impact energy.

A general tentative conclusion might be that for nl cross sections connected with optically allowed transitions, the Born approximation holds for energies higher than 250 keV, but that for nl cross sections connected with optically nonallowed transitions, the energy where the Born approximations start to be valid is much higher. It is also felt that the structure at around 25 keV in the ^1P and ^1D cross section curves could be due to coupling with charge-exchange processes which are known to be very important in this region of kinetic energy.

B. Polarization Fractions

In the course of the calculations cross sections for sub-levels nlm were obtained. In order to present these results in concise form, we calculated polarization fractions Π for the transitions 2^1P-1^1S, 3^1P-1^1S, and 3^1D-2^1P (see Figs. 5–7 and Tables V–VII). This kind of presentation has the added advantage that comparison can be made with experiment.

From Figs. 5 and 6 we see that the many-state calculation gave Π's which are, for energies above 200 keV, in reasonable agreement with each other but show, up to 10 000 keV, an appreciable difference with respect to the Born polarization fractions. So it seems that the validity of the Born approximation for sublevel cross sections is very questionable in the energy range investigated. Comparison with experiment[11,13] shows that even the many-state calculations give very poor results for the sublevel cross sections, assuming the experiments to be correct.

Another typical thing is that contrary to Born calculations the polarization fractions for 2^1P-1^1S and 3^1P-1^1S are not equal over the whole energy range. This is probably due to the nonsymmetrical inclusion of states with respect to 2^1P and 3^1P in the expansions.

TABLE V. Polarization fraction II as a function of proton kinetic energy E for the transition 2^1P-1^1S, in percentages. The Born data are from Ref. 1.

E (keV)	Born	3 state	4 state	6 state	8 state	9 state
10	66	87		90		
15	61	83	64	84	83	62
20	57	79	52	80	79	51
25		76	48	77	76	46
30	50	73	47	74	73	45
50	41	65	48	65	65	45
70	35	58	46	58	59	43
100	28	50	42	50	52	40
150	20	41	36	40	44	34
250	10	29	27	28	32	25
500	−3	11	13	12	15	11
750	−9	4	3	1	5	1
1000	−13	−4	−1	−3	0	−2
2000	−23		−16	−16	−16	−17
5000	−33		−28	−33	−28	−28
10 000	−40		−33	−35	−33	−34

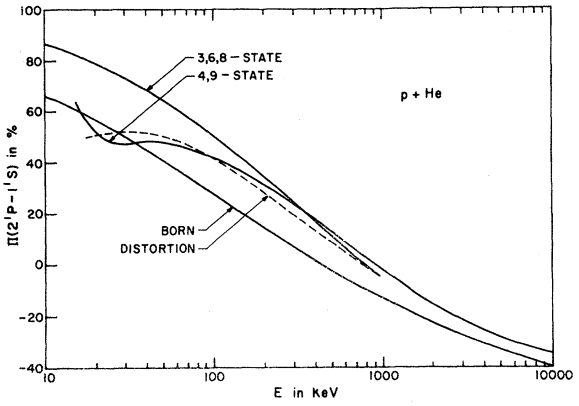

FIG. 5. Polarization fraction II as a function of proton kinetic energy E for the transition 2^1P-1^1S. The distortion curve has been caluclated from data by Bell (Ref. 9).

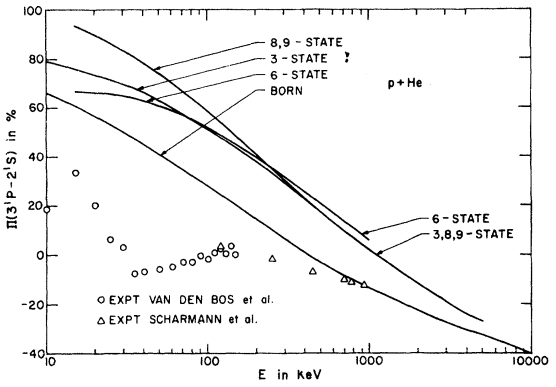

FIG. 6. Polarization fraction for the transition 3^1P-1^1S. The experimental points are from van den Bos *et al.* (Ref. 10) and from Scharmann *et al.* (Ref. 12).

TABLE VI. Polarization fraction for the transition 3^1P-1^1S.

E (keV)	Born	3 state	6 state	8 state	9 state
10	66	79			
15	61	76	67	93	92
20	57	74	66	90	88
25			66	86	86
30	50	70	65	84	83
50	41	63	61	74	74
70	35	58	57	67	67
100	28	51	52	58	59
150	20	44	45	48	49
250	10	33	35	35	36
500	−3	18	21	18	19
750	−9	8	11	8	8
1000	−13	2	6	2	2
2000	−23	−12		−12	−11
5000	−33	−27		−28	−27
10 000	−40			−32	−32

TABLE VII. Polarization fraction for the transition 3^1D-2^1P.

E (keV)	Born	4 state	6 state($2P$)	6 state($3P$)	8 state	9 state
10	40	50	57			
15	36	48	56	55	57	57
20	33	46	55	53	56	57
25			55	50	54	56
30	27	42	54	48	53	55
50	19	36	51	40	50	52
70	14	30	49	33	47	49
100	7	23	46	25	43	46
150	0	14	42	17	37	40
250	−9	2	35	7	27	31
500	−19	−14	23	−8	9	14
750	−24	−22	14	−16	−3	2
1000	−27	−26	7	−21	−11	−6
2000	−33		−10		−28	−24
5000	−38		−29		−38	−36
10 000	−40		−38		−41	−41

In Fig. 7 and Table VII we present Π for 3^1D-2^1P together with experimental results.[11,14,15] All theoretical Π's appear to be equal somewhat above 10 000 keV. Above 100 keV the agreement of 6 state ($3P$) and experiment seems reasonable. But in view of the bad agreement between the nl cross sections this conclusion is questionable.

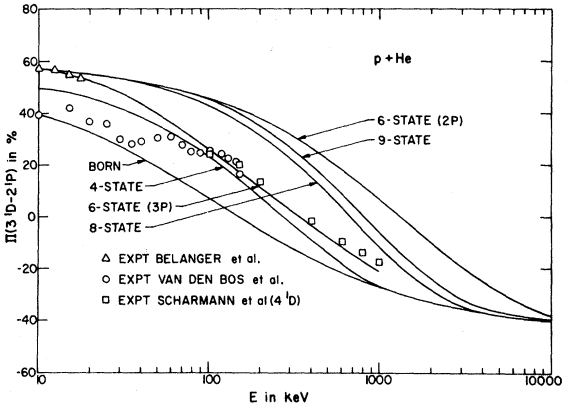

FIG. 7. Polarization fractions for the transition 3^1D-2^1P. The experimental points are from Belanger *et al.* (Ref. 13), van den Bos *et al.* (Ref. 10), and Scharmann *et al.* (Ref. 14).

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