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Sturmian treatment of excitation and ionization in high-energy proton-helium collisions

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Cross sections have been calculated for excitation of the $(2s^2)\,^1S$, $2\,^1S$, and $2\,^1P$ states and ionization of helium by MeV-energy protons. The sensitivity to couplings among these excitation and ionization channels is studied using the Sturmian-pseudostate approach applied previously by Winter [Phys. Rev. A **35**, 3799 (1987)] to one-electron systems. The inclusion of many states greatly lowers the $2s^2$ cross section and brings it closer to the recent experimental result of Giese *et al.* [Phys. Rev. A **42**, 1231 (1990)].

I. INTRODUCTION

Although more exotic projectiles and two-electron targets can now be produced in the laboratory, the colliding proton and helium atom remains of great interest theoretically and experimentally. It is a basic example of a slightly asymmetric, two-electron collision system.

The analogous one-electron system—the collision between a proton and He^+ ion—already poses difficulties at intermediate proton energies on the order of 25 keV; the strong coupling among many direct, exchange, and ionization channels necessitates a fairly large coupled-pseudostate calculation with at least $N \cong 20$ states. Such calculations have been carried out by Winter[1] with Sturmian bases, Fritsch and Lin[2] with an augmented atomic-state (AO+) basis, and others.[3] In principle, replacing He^+ by He would require $N^2 \simeq 400$ states unless the processes considered were assumed to be one-electron processes. A one-electron approach has been taken with considerable success by Jain, Lin, and Fritsch[2] to treat electron transfer to the $n=3$ levels of H at energies up to 100 keV. Winter[5] is now carrying out a large Sturmian-pseudostate calculation at energies of about 100 keV and higher using the full two-electron potential. A calculation also taking account of interatomic electron exchange, but using a smaller basis, has very recently been reported by Slim *et al.* for energies of up to 150 keV.[6]

The problem simplifies at MeV energies: there, electron transfer is very unlikely and the dominant processes are excitation and ionization. This high-energy range is thus perhaps a more suitable testing ground for treating two-electron correlation as in double excitation, without the complications introduced by one-electron transfer.

Excitation of singly excited states and ionization are generally believed to be describable at MeV energies by the high-energy limit, the first Born approximation. On the other hand, excitation of doubly excited states may, at finite (MeV) energies, still proceed through intermediate singly excited states as well as directly—a mixture of first- and second-order effects.

Fritsch and Lin[7] recently considered excitation of a number of doubly excited states, including $2s^2$, and for a variety of projectiles of increasing charge. However, they employed a limited basis in their calculations and did not study the sensitivity to basis size or coupling to ionization channels. Their calculation parallels a large recent experimental study by Giese *et al.*[8] The double-excitation processes have also been considered by McGuire and Straton.[9,10] The intent of the present paper is to consider the influence of the lower-lying singly excited states and the ionization channels on the excitation of the lowest doubly excited state, $2s^2\,^1S$, as well as on each other. Antiproton projectiles will also be considered.

The outline of the paper is as follows: In Sec. II, the Sturmian-pseudostate approach extended to two-electron systems, as well as numerical tests, will be presented. The helium-energy spectra generated by the Sturmian bases will be presented in Sec. III and cross sections will be presented in Sec. IV. Atomic units are used unless otherwise indicated.

II. METHOD AND NUMERICAL TESTS

The ^1S states of helium are represented by correlated two-electron s^2 basis functions

$$\Phi_{n_1 s n_2 s}(\mathbf{r}_1,\mathbf{r}_2)=(1/\sqrt{2})[S_{n_1 s}(r_1)S_{n_2 s}(r_2)+S_{n_2 s}(r_1)S_{n_1 s}(r_2)]\times Y_{00}(\hat{\mathbf{r}}_1)Y_{00}(\hat{\mathbf{r}}_2) \quad (1)$$

and p^2 basis functions

$$\Phi_{n_1 p n_2 p}(\mathbf{r}_1,\mathbf{r}_2)=(1/\sqrt{2})[S_{n_1 p}(r_1)S_{n_2 p}(r_2)+S_{n_2 p}(r_1)S_{n_1 p}(r_2)](1/\sqrt{3})\times[Y_{11}(\hat{\mathbf{r}}_1)Y_{1-1}(\hat{\mathbf{r}}_2)-Y_{10}(\hat{\mathbf{r}}_1)Y_{10}(\hat{\mathbf{r}}_2)+Y_{1-1}(\hat{\mathbf{r}}_1)Y_{11}(\hat{\mathbf{r}}_2)]\ , \quad (2)$$

where the $S_{nl}(r)$ are radial Sturmian functions used previously by Winter[1] in one-electron systems, following Shakeshaft[11] and earlier workers, and $Y_{lm}(\hat{\mathbf{r}})$ are spherical harmonics. Basis functions of d^2 symmetry are neglected to keep the problem to a reasonable size. These functions have only a small effect on the ^1S energies (see Sec. III) and presumably the cross section as well.

The completeness property of a Sturmian basis, as opposed to a hydrogenic basis, was emphasized and exploited many years ago by Shull and Löwdin[12] in the two-electron, atomic-structure problem, following the original work of Hylleraas.[13]

The Hamiltonian of helium is diagonalized in the s^2, p^2 basis to yield approximate ^1S energies E_k and wave functions

$$\psi_k(\mathbf{r}_1,\mathbf{r}_2)=\sum_{n_1,n_2,l} C_{kn_1ln_2l}\Phi_{n_1ln_2l}(\mathbf{r}_1,\mathbf{r}_2) \tag{3}$$

where $k=N\,^1S$, and $l=0,1$.

The ^1P states of helium are represented by the functions

$$\Phi_{1snpm}(\mathbf{r}_1,\mathbf{r}_2)=(1/\sqrt{2})[S_{1s}(r_1)S_{np}(r_2)\mathcal{Y}_{lm}(\hat{\mathbf{r}}_2) +S_{np}(r_1)\mathcal{Y}_{lm}(\hat{\mathbf{r}}_1)S_{1s}(r_2)]Y_{00}\ , \tag{4}$$

where

$$\mathcal{Y}_{lm}=\begin{cases} Y_{lm}, & m=0 \\ (1/\sqrt{2})(Y_{lm}-Y_{l-m}), & m=1 \end{cases} \tag{5}$$

and the corresponding energies E_k and wave functions

$$\psi_k(\mathbf{r}_1,\mathbf{r}_2)=\sum_n C_{k1snp}\Phi_{1snpm}(\mathbf{r}_1,\mathbf{r}_2)\ , \tag{6}$$

where $k=N\,^1P_m$. Note that the s states have here been restricted to 1s. This is an excellent approximation for singly excited states (see the energies reported in Sec. III), but a poor one for doubly excited states such as 2s2p, which have therefore not been studied here.

The one-electron Sturmian functions S_{nl} have been described previously by Winter.[1] Being simply polynomials multiplied by a fixed potential $e^{-Zr/(l+1)}$ for a given l, they form a complete set if the maximum value of n, $n_{\max}$, is sufficiently large. In practice, $n_{\max}$ must be restricted to 14 or 15 to keep the problem to a reasonable size and to avoid excessive linear dependence. The parameter Z has been taken to be the charge of the helium nucleus. This simple choice ensures good behavior with few functions for an electron near the nucleus but requires many functions when the other electron significantly screens the nucleus, as for singly excited states.

To determine transition probabilities in the semiclassical, impact-parameter method, the time-dependent electronic wave function during the collision is expanded in terms of the approximate helium wave functions $\psi_k(\mathbf{r}_1,\mathbf{r}_2)$ given by Eqs. (3) and (6). The coupled differential equations for the expansion coefficients $a_k(t)$ are

$$\frac{da_k}{dz}=\frac{-i}{v}\sum_{k'}G_{kk'}a_{k'}\ , \tag{7}$$

where the coupling matrix elements are

$$G_{kk'}(\rho,z)=\left\langle\psi_k\left|\frac{-Z_B}{r_{1B}}-\frac{Z_B}{r_{2B}}\right|\psi_{k'}\right\rangle P_{kk'}(t)\ . \tag{8}$$

Here B denotes the projectile of charge Z_B, the energy phase is $P_{kk'}=e^{i(E_k-E_{k'})t}$, z is vt, and v and ρ are the projectile's speed and impact parameter.

Since helium basis functions ψ_k are orthonormal, and since charge-exchange channels are neglected at the high energies being considered here, the coupled equations do not contain the overlap matrix or velocity-dependent coupling matrix elements which appear in coupled-state treatments of electron transfer. This is an enormous simplification. Further, the coupling matrix G defined by Eq. (8) contains only the (identical) projectile-electron interactions; the electron-electron interaction had previously been taken into account in the diagonalization of the helium Hamiltonian (to the extent that the basis is complete). The explicit form of the "direct" coupling matrix elements $G_{kk'}$ depends as follows on the symmetry of the coupled states:

$$G_{kk'}=-Z_B\sum_{n_1,n_2,n_1',n_2',l} C_{kn_1ln_2l}C_{k'n_1'ln_2'l} \times g_{n_1l0,n_2l0}O_{n_2l,n_2'l}P_{kk'} \quad (^1S\text{-}^1S\text{ coupling})\ , \tag{9a}$$

$$G_{kk'}=-Z_B\sum_{n_1,n_2}[C_{kn_1sn_2s}g_{n_1s,k'}O_{n_2s,1s} -(1/\sqrt{3})C_{kn_1pn_2p}g_{n_1pm'1s}O_{n_2pm'k'}] \times P_{kk'}\quad (^1S\text{-}^1P\text{ coupling})\ , \tag{9b}$$

$$G_{kk'}=-Z_B(g_{1s1s}\delta_{kk'}+g_{kk'})P_{kk'}\quad (^1P\text{-}^1P\text{ coupling})\ , \tag{9c}$$

where the one-electron matrix elements are

$$g_{jj'}=\left\langle\varphi_j(\mathbf{r})\left|\frac{1}{r_B}\right|\varphi_{j'}(\mathbf{r})\right\rangle\ , \tag{10a}$$

$$O_{jj'}=\langle\varphi_j(\mathbf{r})|\varphi_{j'}(\mathbf{r})\rangle\ . \tag{10b}$$

The one-center overlap matrix elements $O_{jj'}$ and two-center direct matrix elements $g_{jj'}$ can be evaluated analytically as in previous work. Some subscripts which appeared previously have been dropped: the coordinates $\mathbf{r}$ ($=\mathbf{r}_1$ or $\mathbf{r}_2$) are defined with respect to the target nucleus A, and $g_{jj'}$ was referred to previously as $g_{jj'A}$. Further, in Eq. (10) φ_j now denotes a Sturmian function if j is explicitly written as nlm in Eq. (9) and a diagonalized atomic wave function (for ^1P) if $j=k$. In Eq. (9b), the label m' ($=0$ or 1) corresponds to k'.

All matrix elements $G_{kk'}$ are proportional to the projectile nuclear charge Z_B. Cross sections are thus proportional to Z_B^2 if the processes are first order or to Z_B^4 if the processes are second order. In fact, the general dependence is a power series in Z_B, whose dominant powers are Z_B^2, Z_B^3, and Z_B^4 at higher energies; see also the discussions by Fritsch and Lin[7] and McGuire and Straton.[10] As noted by Fritsch and Lin, it is more convenient in using a coupled-state scattering program to retain all terms and thus all orders; however, the relative role of first- and second-order processes is a basic physical question which still can and should be addressed, as they have.

As done previously by Winter, the coupled Eqs. (7) are integrated numerically over z using Hamming's method with the initial condition $a_k = \delta_{1k}$ at $z = z_0$ where, in the present case, the subscript 1 denotes the $1\,^1S$ state of helium. The cross section for excitation of the kth state from the ground state is

$$Q_{1k} = 2\pi \int_0^\infty d\rho\, \rho |a_k(\rho, z_m)|^2 \; . \tag{11}$$

The range of integration over z was taken to be $(z_0, z_m) = (-30, 1000)$; however, a test run with $(z_0, z_m) = (-20, 100)$ yielded the same results to three digits. The integration over ρ in Eq. (11) was done using Simpson's rule, probably to an accuracy of at least 1%.

III. HELIUM ENERGIES

The cross section Q_{1k} depends on the quality of the helium wave function ψ_k as well as on that of other functions $\psi_{k'}$, $k' \neq k$, especially the initial state, $k'=1$. Although the corresponding energies E_k sample different regions of coordinate space than do the cross sections, these energies probably still give an indication of how good the wave functions are, and of how much correlation is included. They will therefore be reported here.

Table I shows the lowest ten ^1S energies obtained with several bases of purely $n_1 s n_2 s$ form, Eq. (1), consisting of all (symmetrized sums of) products with $n_1 \le 5$ and $n_1 \le n_2 \le n_{2\max} \le 14$. [A basis which includes all possible products for both $n_{1\max}$ and $n_{2\max} \cong 14$ would be unmanageably large for a scattering calculation which also included $(n_1 p n_2 p)\,^1S$ as well as ^1P functions. It has therefore been decided to limit n_1 while letting n_2 be larger. The effect of varying $n_{1\max}$ will be illustrated later in Table III.] It is seen in Table I that the ground-state energy is converged to within 0.0001 of the s^2 limit using only $n_{\max} = 8$. This s^2 limit, -2.8790, is an improvement not only over the one-parameter ($Z = 1.6875$) result, but also over the Hartree-Fock energy, -2.8617. The s^2 limit takes account of radial correlation, and was first obtained long ago by Shull and Löwdin[12] correct to four decimal places. It is 41% of the way from the Hartree-Fock, or uncorrelated, energy to the exact, fully correlated energy, -2.9037, obtained by Chandraseckhar *et al.*[14] (The state-of-the-art result obtained recently by Froelich and Alexander,[15] for example, has an accuracy of about 10^{-10} a.u., which far exceeds what the Sturmian basis as described here needs to do for an accurate scattering calculation.) The $2\,^1S$ energy, on the other hand, is not converged to the $n_1 s n_2 s$ limit, estimated to be -2.1443, even with $n_{\max} = 14$. However, it is only 0.002 a.u. from the

TABLE I. Lowest ten ^1S energies of helium using symmetrized bases $n_1 s n_2 s$ with $n_1 \le 5$ and $n_2 \le n_{2\max}$ (where $n_1 \le n_2$). The one-electron functions $n_1 s$ and $n_2 s$ are Sturmians with $Z=2$. The $2s^2$ energies are underlined.

$n_{2\max}$ (approx.)	$1\,^1S$	$2\,^1S$	$3\,^1S$	$4\,^1S$	$5\,^1S$	$6\,^1S$	$7\,^1S$	$8\,^1S$	$9\,^1S$	$10\,^1S$
(One-parameter)	−2.8477									
(Hartree-Fock)	−2.8617									
3	−2.8781	−1.5021	−0.147	3.622	4.847	10.110				
4	−2.8786	−1.9046	$-\underline{0.554}$	−0.159	0.874	2.295	8.938	9.719	11.604	21.206
5	−2.8789	−2.0366	−1.155	$-\underline{0.657}$	0.071	0.739	1.528	2.362	3.196	5.624
6	−2.8789	−2.0925	−1.551	$-\underline{0.701}$	−0.269	−0.159	0.246	0.910	1.647	2.886
7	−2.8789	−2.1186	−1.748	−0.946	$-\underline{0.711}$	−0.338	0.086	0.362	0.877	1.137
8	−2.8790	−2.1313	−1.860	−1.312	$\underline{-0.719}$	−0.422	−0.231	−0.016	0.143	0.705
9	−2.8790	−2.1378	−1.927	−1.529	−0.808	$-\underline{0.715}$	−0.466	−0.143	0.066	0.453
10	−2.8790	−2.1410	−1.970	−1.667	−1.141	$-\underline{0.721}$	−0.500	−0.264	−0.200	0.036
11	−2.8790	−2.1427	−1.998	−1.759	−1.358	−0.732	$-\underline{0.692}$	−0.518	−0.309	−0.012
12	−2.8790	−2.1435	−2.017	−1.824	−1.508	−1.011	$-\underline{0.720}$	−0.533	−0.364	−0.216
13	−2.8790	−2.1439	−2.030	−1.872	−1.615	−1.223	$-\underline{0.723}$	−0.625	−0.541	−0.397
14	−2.8790	−2.1440	−2.039	−1.907	−1.694	−1.376	−0.909	$-\underline{0.720}$	−0.548	−0.427
∞ (est.)	−2.8790	−2.1443	−2.06							
(exact)	−2.9037[a]	−2.1458[a]	−2.06					$-\underline{0.778}$[b]		

[a] Chandraseckhar *et al.* ($1\,^1S$) and Coolidge and James ($2\,^1S$), in Bethe and Salpeter (Ref. 14).

[b] Froelich and Alexander (Ref. 15) and references therein.

TABLE II. Lowest ten ^1S energies of helium using symmetrized bases n_1sn_2s with $n_1 \leq 5$, $n_2 \leq 14$, and $n'_1pn'_2p$ with $n'_1,n'_2 \leq n_{\max}$. The one-electron functions n_1s, n_2s, n_1p, and n_2p are Sturmians with $Z=2$

$n_{\max}$	$1\,^1S$	$2\,^1S$	$3\,^1S$	$4\,^1S$	$5\,^1S$	$6\,^1S$	$7\,^1S$	$(2s^2)8\,^1S$	$9\,^1S$	$10\,^1S$
	−2.8790	−2.1440	−2.039	−1.907	−1.694	−1.376	−0.909	−0.720	−0.548	−0.427
2	−2.8815	−2.1444	−2.040	−1.907	−1.694	−1.377	−0.913	−0.752	−0.575	−0.517
3	−2.8881	−2.1447	−2.040	−1.907	−1.694	−1.377	−0.913	−0.772	−0.587	−0.529
4	−2.8938	−2.1451	−2.040	−1.908	−1.695	−1.378	−0.914	−0.774	−0.593	−0.550
5	−2.8971	−2.1453	−2.040	−1.908	−1.696	−1.379	−0.915	−0.773	−0.596	−0.565
6	−2.8986	−2.1455	−2.040	−1.908	−1.696	−1.380	−0.917	−0.774	−0.596	−0.572
∞ (est)	−2.9002	−2.1458								
Exact	−2.9037[a]	−2.1458[a]	−2.06					−0.778[b]		

[a] Reference 14.

[b] Reference 15.

exact value, −2.1458, of Coolidge and James,[14] whereas for the ground state the corresponding difference was an order of magnitude greater; this of course reflects the lesser importance of correlation when the electrons are inequivalent. The $N\,^1S$ levels shown in Table I for $N \geq 3$ are mostly approximations to discretized, singly ionized states or doubly excited states; not until $n_{2\max}$ is increased to 12 does another energy appear below the first ionization threshold, −2.0. Without n_1pn_2p functions, the $2s^2$ doubly excited state remains 0.06 above the fully correlated value given by Froelich and Alexander.[15] Note that when an additional single-ionization energy appears near the $2s^2$ energy on enlarging the basis (as, for example, on increasing $n_{2\max}$ from 10 to 11), the effect is to repel the $2s^2$ energy away from its true value; the doubly excited states do not satisfy a variational principle. This difficulty with the stabilization method[16] will be encountered again in Sec. IV.

The effect of adding $n'_1pn'_2p$ basis functions is shown in Table II for a fixed number of n_1sn_2s basis functions. It is seen that the estimated infinite s^2,p^2 basis limit for the $1\,^1S$ state is −2.9002, which thus includes 92% of the full correlation energy. (If the $n'_1pn'_2p$ basis is terminated at $n'_1,n'_2=4$, the included correlation is reduced to 76%, but, as will be seen, there is apparently little effect of p^2 basis functions on the $2\,^1S$ cross section.) The basis limit for the $2\,^1S$ state, −2.1458, is seen to be exact to four decimal places—i.e., it includes 100% of the correlation energy. The next energy, a rather poor approximation to the $3\,^1S$ energy, is hardly affected by adding p^2 functions to the basis. The fourth through seventh ^1S levels, discretized singly ionized levels, are also insensitive. The eighth level, undoubtably the $2s^2$ doubly excited level, appears stable to 0.001 or 0.002 using $n'_1pn'_2p$ with $n'_1,n'_2 \leq 4$. The ninth and tenth levels are probably rough approximations to the $(2p^2)\,^1S$ and $(2s3s)\,^1S$ levels, but the states are not sufficiently converged to yield stable cross sections. Not surprisingly, the last three out of ten states, being doubly excited states, are much more affected by the inclusion of p^2 functions than are the first seven states.

Finally, as indicated earlier, Table III shows the sensitivity of the lowest ten ^1S energy levels to "doubly excited" n_1sn_2s basis functions. The doubly excited functions have little effect on the first seven, singly excited levels, but an essential effect on the next three levels in making them doubly excited. However, there does not appear to be much affect on $2s^2$ of increasing $n_{1\max}$ beyond 5. (A test for $n_2 \leq 10$ shows that increasing $n_{1\max}$ to 6 only reduces the $2s^2$ energy by 0.001.)

The lowest ^1P energies are shown in Table IV. The $2\,^1P$ energies agree closely with that of a simple variationally determined effective charge wave function used in a He^+-He charge-transfer calculation many years ago by Winter and Lin.[17] The $3\,^1P$ energy, on the other hand, does not appear well converged. Based on cross-section results to be presented in the next section, the roots above the first ionization threshold, although few in number, appear to be well enough distributed to represent single ionization to $l=1$, which is the dominant excitation channel at high energies.

IV. CROSS SECTIONS

Coupled-Sturmian cross sections for excitation of the $2\,^1S$, $(2s^2)\,^1S$, and $2\,^1P$ states and for ionization into ^1S and ^1P levels are given in Tables V–VII. Tables V and VI indicate the sensitivity of the ^1S cross sections at 1.5 MeV to the size of the n_1sn_2s basis and of the $n'_1pn'_2p$

TABLE III. Lowest ten ^1S energies of helium using symmetrized bases n_1sn_2s with $n_1 \leq n_{1\max}$ and $n_2 \leq 14$ (where $n_1 \leq n_2$).

$n_{1\max}$	$1\,^1S$	$2\,^1S$	$3\,^1S$	$4\,^1S$	$5\,^1S$	$6\,^1S$	$7\,^1S$	$(2s^2)8\,^1S$	$9\,^1S$	$10\,^1S$
1	−2.8725	−2.1433	−2.039	−1.906	−1.692	−1.373	−0.901	−0.193	0.913	2.762
2	−2.8784	−2.1440	−2.039	−1.906	−1.694	−1.376	−0.907	−0.212	0.072	0.579
3	−2.8788	−2.1440	−2.039	−1.907	−1.694	−1.376	−0.909	−0.619	−0.379	−0.258
4	−2.8789	−2.1440	−2.039	−1.907	−1.694	−1.376	−0.909	−0.706	−0.516	−0.390
5	−2.8790	−2.1440	−2.039	−1.907	−1.694	−1.376	−0.909	−0.720	−0.548	−0.427

TABLE IV. Lowest ${}^1P$ energies of helium using symmetrized bases $1snp$, $n \le n_{\max}$. The one-electron functions $1s$ and np are Sturmians with $Z=2$.

$n_{\max}$	$2\,{}^1P$	$3\,{}^1P$	$4\,{}^1P$	$5\,{}^1P$	$6\,{}^1P$	$7\,{}^1P$	$8\,{}^1P$
6	−2.1221	−2.018	−1.810	−1.217	1.099		
7	−2.1224	−2.037	−1.904	−1.604	−0.792	2.304	
8	−2.1224	−2.046	−1.954	−1.765	−0.363	−0.304	3.690
One-parameter[a]	−2.1224	−2.060					

[a] Winter and Lin (Ref. 17).

TABLE V. ${}^1S$ cross sections (in units of 10^{-20} cm^2) for excitation and ionization[a] of helium by 1.5-MeV protons using various symmetrized bases n_1sn_2s, $n_1 \le n_2$, where n_1s, n_2s denote one-electron Sturmians with $Z=2$.

$n_{1\max}$	$n_{2\max}$	$2\,{}^1S$	${}^1S$ ionization	$(2s^2)\,{}^1S$
4	4	87.6	134	3.6
5	5	65.9	70	0.30
5	6	50.2	(86)	0.93
5	7	40.8	96	0.12
5	8	34.9	99	0.54
5	9	31.3	(98)	0.35
5	10	29.2	109	0.40
5	11	27.9	(99)	11.
5	12	27.1	92(78)	0.30
5	13	26.8	(83)	1.4
5	14	26.6	(81)	0.20
3	10	29.2	109	0.37
4	10	29.2	109	0.49
5	10	29.2	109	0.40
6	10	29.2	109	0.38

[a] Some of the cross sections were obtained by retaining only the lowest 16 states after diagonalization of the Hamiltonian. The values for ionization obtained in this way are in parentheses. This approximation probably affects values of the excitation cross sections by at most one unit in the last digit reported here.

TABLE VI. ${}^1S$ cross sections (in units of 10^{-20} cm^2) for excitation and ionization of helium by 1.5-MeV protons using various symmetrized bases n_1sn_2s $(n_1 \le n_2)$ and $n_1'pn_2'p$.

$n_{1\max}$	$n_{2\max}$	$n'_{1\max}$	$n'_{2\max}$	$2\,{}^1S$	${}^1S$ ionization	$(2s^2)\,{}^1S$
5	12	4	4	26.7	(81)[a]	0.14
5	14	4	4	26.3	(80)[a]	0.11
5	14	none		26.6	(81)	0.20

[a] For the first basis, 28 states were retained after diagonalization of the Hamiltonian; for the other two, 16 states were retained.

TABLE VII. ${}^1S$ and ${}^1P$ cross sections (in units of 10^{-20} cm^2) for excitation and ionization of helium by proton and antiproton impact using ${}^1S$ bases $n_1sn_2s \le 5s14s$ $(n_1 \le n_2)$ and $n_1pn_2p \le 4p^2$, and ${}^1P$ bases $1snp$ with $np \le 6p$ or $7p$.

					Ionization		
np	Projectile	Energy (MeV)	$2\,{}^1S$	$2\,{}^1P$	${}^1S$	${}^1P$	$(2s^2)\,{}^1S$
$\le 6p$	Proton	1.5	27.3	392	(84)[a]	1040	0.14
$\le 7p$	Proton	1.5	27.3	385	(84)	1140	0.14
$\le 6p$	Antiproton	1.5	24.7		(76)		0.14
$\le 7p$	Antiproton	1.5		379		1130	
$\le 6p$	Proton	6.0	6.73	130	(21)	353	0.012

[a] Values were obtained by retaining only the lowest 16 ${}^1S$ states after diagonalizing the Hamiltonian.

basis, respectively. Table VII gives all excitation and ionization cross sections with larger bases including ^1P channels; this table also gives results for 1.5-MeV antiprotons and 6-MeV protons. The $2\,^1S$ and $2\,^1P$ cross sections will be considered first, followed by the ^1S and ^1P ionization cross sections. Lastly, the sensitive $(2s^2)\,^1S$ cross section will be considered.

A. 2^1S cross section

It is seen in Table V that the $2\,^1S$ cross section decreases monotonically and appears to be converging with respect to increasing the number of singly excited basis functions as $n_{2\max}$ is increased for the n_1sn_2s basis (with $n_1 \leq n_2$ and $n_{1\max}$ fixed at 5); the last noted change, on increasing $n_{\max}$ from 13 to 14, is about 0.7%. (This change, though small, is much greater than the corresponding change in the $2\,^1S$ energy, 0.005%.) On the other hand, if $n_{2\max}$ is fixed (at 10) and $n_{1\max}$ is increased from 3 to 6, the $2\,^1S$ cross section is unchanged to three digits; this is not surprising: doubly excited basis functions should have little effect on single-excitation cross sections. The effect of adding $n'_1pn'_2p$ basis functions is also slight: 1% if all functions up to $4p^2$ are included, and an estimated additional 0.3% if functions up to $5p^2$ are also included. This result with $4p^2$ functions, 26.3×10^{-20} cm^2, is identical to the first Born result of Bell, Kennedy, and Kingston[18] who also used correlated wave functions. The only effect of the large ^1S basis in the present calculation is apparently to define the initial and final states accurately and is not to provide second-order couplings among the many ^1S channels. This is confirmed directly by deleting all but the $1\,^1S$ and $2\,^1S$ states after diagonalizing the Hamiltonian: the effect is only one unit in the third digit. However, $2\,^1S$ excitation is *not* entirely first order at 1.5 MeV: including ^1P excitation and ionization channels raises the cross section by 4%. For antiproton projectiles, including ^1P channels *lowers* the cross section by 6%. At a higher energy of 6 MeV the full-basis cross section for proton impact still lies above the first Born result,[19] but now only by 1.5% rather than 4%.

B. $2\,^1P$ cross sections

Cross sections for excitation of the $2\,^1P$ state appear to be stable with respect to the addition of basis functions defining the dominant processes (^1P excitation and ionization): For 1.5-MeV protons, augmenting the ^1P basis with $1s7p_{0,1}$ functions is seen in Table VII to reduce the cross section by only 1.8%. To identify which of the many ^1P states are important, the calculation was reduced to a three-state one by deleting all states except $1\,^1S$ and $2\,^1P_{0,1}$ after diagonalizing the Hamiltonian of the helium atom. The $2\,^1P$ cross section is thereby increased 1.5%. Within this three-state approximation, the convergence was further tested by adding $1s8p_{0,1}$ functions; these functions lower the cross section by less than 0.8%. The resulting three-state value, 388×10^{-20} cm^2, is 3% above the first Born value of Bell, Kennedy and Kingston, 376×10^{-20} cm^2.

Large-basis, proton and antiproton results at 1.5 MeV are seen to differ by less than 2%. At 6 MeV, large-basis results for protons agree to three digits with the first Born value of Bell, Kennedy, and Kingston.[19]

In conclusion, second-order couplings to ^1P ionization channels affect the $2\,^1P$ cross section by less than 2% at 1.5 MeV. The percent effect of ionization channels on the $2\,^1S$ cross section was noted in Sec. IV A to be about twice as large. Finally, the first Born cross section approximates the three-state $(1^1S,2\,^1P_{0,1})$ cross section to within 3% at 1.5 MeV, whereas the two-state $(1\,^1S,2\,^1S)$ and first Born $2\,^1S$ cross sections were noted to agree to better than 1% at this energy.

C. ^1S ionization cross section

There are two purely computational difficulties in extracting ^1S ionization cross sections from the present calculation. First, as the ^1S basis is enlarged with more "singly excited" functions, bound-state roots appear which were previously of positive energy. (Recall Table I.) There is thus a sudden change of flux associated with ionization, rather pronounced when lower bound states of significant cross section are being formed. This introduces a sensitivity of perhaps 20% in the ^1S ionization cross section at 1.5 MeV. However, the differential cross section dQ/dE for direct ionization (not shown) is insensitive to these basis changes at lower energies E, so, by extrapolation to the threshold limit, $E=-2$, this problem could be circumvented. Secondly, to reduce the large amount of computing time, most of the cross sections were calculated retaining only the lowest states—typically 16 states—after diagonalizing the Hamiltonian of the helium atom. This is observed to have only little effect on the excitation cross sections of primary interest, but the arbitrary closing of higher ionization channels naturally has some effect on the ^1S ionization cross section. Referring to Table V, a test with the full and reduced n_1sn_2s basis (for $n_1 \leq 5$, $n_2 \leq 12$) shows the reduced cross section to be about 15% too low at 1.5 MeV.

Also shown in Table V are results using different numbers of "doubly excited" basis functions. These doubly excited functions, not surprisingly, have a negligible effect on the overall ^1S ionization cross section, in which the double-ionization component is small.

The addition of $p^2\,^1S$ functions negligibly affects the lower-lying positive energy states and their contribution to the ^1S ionization cross section. The effect on the overall ^1S ionization cross section shown in Table VI is also very slight.

Table VII shows that ^1P channels have a (second-order) effect of 5% on the ^1S ionization cross section at 1.5 MeV.

Overall, the ^1S ionization cross section at 1.5 MeV, about 80×10^{-20} cm^2, is probably accurate to 30%. The intent is not primarily to obtain an accurate ^1S ionization cross section, but, rather, to retain a sufficient group of ionization channels to yield reliable excitation cross sections.

D. ^1P ionization cross sections

Table VII gives the ^1P ionization cross section at a proton energy of 1.5 MeV using two large ^1S, ^1P bases with different numbers of $(1snp_{0,1})\,^1P$ functions. The addition of $1s7p_{0,1}$ functions increases the cross section by 10%, but the basis convergence has not been explored further by internal tests. The ^1P result, 1.14×10^{-17} cm^2, agrees within 1% with the value obtained from the graphical first Born results of Peach.[20] The present result for ionization at 1.5 MeV, including the ^1S contribution noted above, is 1.22×10^{-17} cm^2. Using a simple helium wave function in the first Born approximation, McGuire estimates that 82% of ionization is into s and p waves.[21] Using this to account for the neglected higher partial waves, the total ionization cross section is estimated to be 1.49×10^{-17} cm^2, which is 10% below the experimental value of Shah and Gilbody.[22]

The combined (s,p) ionization cross section for antiproton impact at 1.5 MeV lies only 1.5% below that for proton impact.

E. $(2s^2)\,^1S$ cross section

The four channels of excitation and ionization considered up to now have all involved the excitation or ionization primarily of a single electron. The $(2s^2)\,^1S$ state is the lowest doubly excited ^1S state of helium and is embedded in the single-ionization continuum. As described by Fano,[23] this degeneracy requires the inclusion of the continuum just to define the doubly excited state. The potentially complete Sturmian basis discretizes the ^1S continuum; this discretized continuum is coupled automatically to the single-configuration $2s^2$ state when the Hamiltonian of the helium atom is diagonalized. The resulting correlated $2s^2$ state was seen in Sec. III and Table II to be quite close in energy to the exact value for a sufficiently large basis including p^2 functions.

However, it was seen in Table I that, as the singly excited component of the basis is enlarged, there are some fluctuations when new positive roots appear adjacent to the $2s^2$ root. These adjacent states interact strongly with the $2s^2$ state, causing energy fluctuations of as much as 0.03 a.u., or 4%. The variation in the $2s^2$ excitation cross section at a proton energy of 1.5 MeV corresponding to the variation in the helium energy is displayed in Table V. It is seen that the fluctuations, when adjacent states appear, now become enormous: up to a factor of 30. Evidently, a 4% change in the energy is enough to drive the state into the continuum, where it acquires a large ionization component. (Whether the displaced state has a larger or smaller cross section cannot, however, be easily predicted, since it depends also on whether the roots are too dense or too sparse in the continuum.) (In the case of the much less sensitive $2\,^1S$ state, it was noted in Sec. IV A that a 0.005% change in the energy can give rise to a 0.7% change in the cross section, a 140-fold amplification of sensitivity; the above data reveal that for the $2s^2$ state, the amplification of sensitivity can be 750-fold.)

A new root adjacent to the $2s^2$ root appears for every other basis in Tables I and V (i.e., for bases with $n_{2\max}$ odd). For each of the other, "even" bases, the adjacent root moves away from the $2s^2$ root. The "even" basis cross sections in Table V *decrease smoothly* (by a factor of 20) as the basis is enlarged. The last reduction, on increasing $n_{2\max}$ from 12 to 14, is 33%, and in the presence of p^2 and ^1P functions, the change is reduced to 15%. Stability may be setting in.

The sensitivity to the s^2 *doubly* excited component is less dramatic. As $n_{1\max}$ is increased from 3 to 6 (with $n_{2\max}$ here fixed at 10), the successive changes to the cross section in Table V are +32%, −24%, and −5%. The overall effect is small and convergence seems to be setting in. A test with other bases is consistent with these observations.

The sensitivity to the p^2 doubly excited component is somewhat larger. As seen in Table VI, adding functions up to $4p^2$ to a purely s^2 basis reduces the cross section by a factor of 1.8. However, a test at one impact parameter suggests that including, also, functions up to $5p^2$ changes the $2s^2$ probability by less than 1%.

The question now arises: Does the full ^1S basis affect the $(2s^2)\,^1S$ cross section *after* the Hamiltonian of helium is diagonalized, the states thereby being accurately defined; in other words, is there second-order coupling to other ^1S states? This question is answered by tests (at the dominant impact parameter, $\rho=0.25$) in which states are deleted from a 56-state correlated ^1S basis: The removal of the bound $2\,^1S$ state is found to have a 24% effect on the $2s^2$ probability at 1.5 MeV. The removal of the next

TABLE VIII. Comparison of the present coupled-Sturmian cross sections for excitation of the $(2s^2)\,^1S$ state of helium with the coupled-state results of Fritsch and Lin (Ref. 7) and the experimental results of Giese *et al.* (Ref. 8).

Energy (MeV)	Projectile	Authors	Cross section (10^{-20} cm^2)
1.5	Proton	Fritsch and Lin	0.74
1.5	Antiproton	Fritsch and Lin	0.73
1.5	Proton	Winter	0.14
1.5	Antiproton	Winter	0.14
1.5	Electron	Giese *et al.*	0.0816
1.5	Proton	Giese *et al.*	0.0318
6.0	Proton (and antiproton)	Fritsch and Lin	0.20
6.0	Proton	Winter	0.012

four states has a combined effect of 33% on the $2s^2$ probability at 1.5 MeV, the lowest one having the largest effect (12%), and the one nearest the $2s^2$ state, the least (3%). (For the particular basis chosen, the three states $4\,^1S$ through $6\,^1S$ lie above the first ionization threshold, and the $7\,^1S$ state is the $2s^2$ state.) The two states immediately above the $2s^2$ state are probably other doubly excited states and have small contributions of 1–2% each. Higher-lying states up to $16\,^1S$ have an effect ranging from a few percent for the 56-state bias to 30% for a 70-state basis. (With a larger basis, the contributing discretized ionization states are spread over a greater range and, further, the $2s^2$ probability is smaller and more sensitive.) The composite effect of all higher-order ^1S couplings can be summarized by comparing the two-state result (9.6×10^{-22} cm^2), obtained by keeping only the initial state and the $2s^2$ state after diagonalizing the He Hamiltonian, with the estimated full 56-state result (in Table VI, first row): The difference of 40% is significant. It is clear that couplings between the $2s^2$ and ionization channels and other bound ^1S states—couplings of at least second order—cannot be neglected.

Singlet *P* channels are the dominant ionization channels at high energies. A comparison of the results in Tables VI and VII shows that ^1P states have a significant effect on the $2s^2$ cross section at 1.5 MeV, *raising* it by 20%. This effect is comparable in magnitude to, but somewhat smaller than, the effect from ^1S states.

In spite of the importance of second-order couplings noted above, proton and antiproton cross sections at 1.5 MeV are the same to three digits. (There are significant differences at "larger" impact parameters $\rho\simeq1$, but these do not contribute much to the integrated cross sections.) This observation is in agreement with that of Fritsch and Lin,[7] who, however, neglected coupling to ionization channels.

The present coupled-state results are compared in Table VIII with the recent coupled-state results of Fritsch and Lin[7] and the recent experimental results of Giese *et al.*[8] These results are also shown in Fig. 1, along with the theoretical results of McGuire and Straton.[9,10] The present result for antiprotons (and protons) at 1.5 MeV nearly touches the upper error bar of Giese *et al.* for electrons, whereas the result of Fritsch and Lin is a factor of 5 higher. The experimental result for protons is a factor of 2.5 lower than that for electrons, in contrast to both the present and Fritsch and Lin's proton-antiproton results. (However, in view of the large error bars, the experimental results for electrons and protons may not be significantly different.) The present theoretical $2s^2$ cross section decreases by more than an order of magnitude as the energy is increased from 1.5 to 6 MeV. The cross section of Fritsch and Lin does not decrease as rapidly. There is therefore an even greater discrepancy between the two sets of coupled-state results at the higher energy than at the lower one.

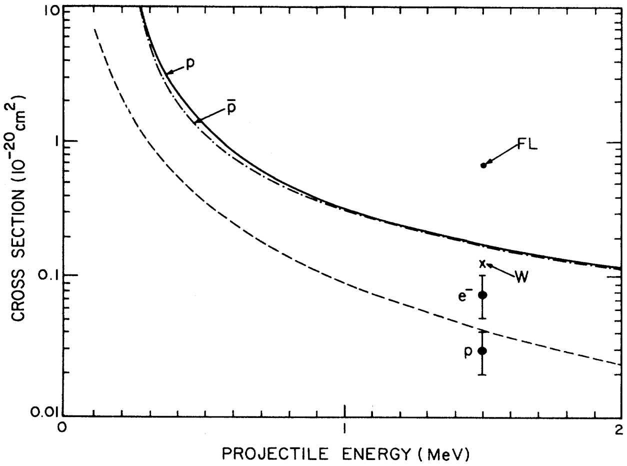

FIG. 1. Cross sections for excitation of the $(2s^2)\,^1S$ state of helium by proton or antiproton ($\bar{p}$) impact. Theoretical results: *W*, present coupled-Sturmian results for protons or antiprotons; FL, coupled-pseudostate results of Fritsch and Lin (Ref. 7) for protons or antiprotons; dotted curve, second-order result in the independent-electron approximation and solid and dash-dotted curves, second-order results with correlation of McGuire and Straton (Ref. 10). Experimental results for protons and electrons: circles with error bars, Giese *et al.* (Ref. 8).

Although McGuire and Straton made an energy-averaging approximation, their second-order cross section with correlation[10] is a significant improvement over the previous second-order result in the independent-particle approximation. These results are shown in Fig. 1. The correlated result of McGuire and Straton agrees fairly well with the experimental result and with the present Sturmian results at 1.5 MeV.

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