Coupled-Sturmian treatment of electron transfer and ionization in proton-neon collisions

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Total cross sections are reported for electron transfer and ionization from the K shell of neon atoms by proton impact at proton energies from 250 to 1500 keV using a coupled-Sturmian-pseudostate approach. This approach was recently generalized by Winter [Phys. Rev. A **47**, 264 (1993)] to quasi-one-electron systems using an analytic Hartree-Fock potential and applied to proton-carbon collisions. After a binding-energy correction is made to the single-particle energy phase, the calculated p-Ne cross sections for both ionization and electron transfer agree with the experimental values of Rødbro *et al.* [Phys. Rev. A **19**, 1936 (1979)] within the range of basis sensitivity.

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I. INTRODUCTION

Electron transfer and ionization from the K shell of carbon atoms by proton impact have recently been considered by the author [1]. For this somewhat asymmetric system, both the electron-transfer and ionization cross sections [2] are small: the peak ionization cross section is only 10^{-18} cm^2 (at a proton energy of 800 keV) and the electron transfer cross section is about an order of magnitude smaller still. Electron transfer is therefore influenced strongly by ionization channels in a coupled-state treatment of this system, and so it is important that sufficiently many such channels be included in the basis. Using a two-center coupled-Sturmian-pseudostate approach, it was found that excellent basis stability (within a few percent) can be achieved using between 35 and 54 basis functions. The results for both ionization and electron transfer agree well with the experimental results of Rødbro *et al.* [2].

The proton-carbon calculation was an extension of earlier calculations for hydrogenic-ion targets (such as C^{5+} studied by the author [3]) to quasi-one-electron targets. An analytic Hartree-Fock potential is used to represent the interaction of the active electron with the target-atom core. It was found that the basis convergence for neutral (C) targets is much faster than for ionic (C^{5+}) targets. This was attributed by Alston [4] to the weaker Coulombic behavior of the carbon potential at long range and the consequent better distribution of positive-energy roots representing ionization.

The purpose of the present paper is to test the coupled-state approach for the substantially more asymmetric proton-neon system. For this collisional system, the ionization cross section [2] is an order of magnitude smaller than for the p-C system at comparable energies and the ratio of the capture to ionization cross section is very small [2]. Thus, both processes, and particularly the influence of ionization channels on the capture process, might be expected to be difficult to treat in a coupled-state approach; for example, the unitarity of coupled-state approaches only allows one to monitor the accuracy of the dominant transition probabilities. On the other hand, the recent (nonunitary) perturbative approaches of Marxer and Briggs [5] and Alston [6] become more reliable, the more asymmetric the system. For a projectile to target nuclear-charge ratio of 1/10, as in the present case, such perturbative approaches might be expected to be quite good and provide tests of the consistency of the present theory, beyond a comparison with experimental results [2].

The outline of the paper is as follows. In Sec. II, the method will be summarized briefly; in Sec. III, numerical tests will be summarized; and, in Sec. IV, the cross sections will be presented and compared with the experimental results [2] and recent perturbative results [5,6]; this presentation will be placed in the context of the previous study for carbon targets [1]. Atomic units are used unless otherwise indicated.

II. METHOD

The coupled-Sturmian-pseudostate approach was originally carried out by Gallaher and Wilets [7] and Shakeshaft [8] for proton–hydrogen-atom collisions. Winter extended this approach to arbitrary hydrogenic-ion targets [9,3,10] and, more recently, to quasi-one-electron targets [1].

A set of Sturmian basis functions is centered on each nucleus. Each Sturmian is a polynomial multiplied by a fixed exponential $\exp[-\zeta_\alpha r_\alpha/(l_\alpha+1)]$ for a given angular momentum l_α, where r_α is the distance from nucleus α (the proton A or target nucleus B) to the electron, multiplied by a spherical harmonic. Since these polynomials form a complete set, the Sturmians do as well.

The two fixed Sturmian charges ζ_α are arbitrary. They could for simplicity be set equal to the nuclear charges Z_α. Alternatively, the target Sturmian charge ζ_B could be set equal to the effective nuclear charge $Z_B-0.3$ (according to Slater's rule) or perhaps some other value to improve basis convergence.

As for carbon targets [1], the analytic Hartree-Fock potential for the active electron has been assumed to be the potential of Green, Sellin, and Zachor (GSZ) [11]:

$$V(r_B)=\frac{-[(Z_B-1)\Omega(r_B)+1]}{r_B}\ , \tag{1a}$$

where

$$\Omega(r_B)=\frac{1}{Kd(e^{r_B/d}-1)+1}\ . \tag{1b}$$

This potential has the correct asymptotic forms $-Z_B/r_B$ as $r_B\to 0$ and $-1/r_B$ as $r_B\to\infty$. The parameters K and d have been tabulated by Szydlik and Green [12] for various neutral atoms. For neon, $K=2.71$ and $d=0.558$.

The one-electron Hamiltonian of neon, $-\frac{1}{2}\nabla^2+V(r_B)$, is diagonalized in the Sturmian basis centered on nucleus B, and the one-electron Hamiltonian of hydrogen, $-\frac{1}{2}\nabla^2-Z_A/r_A$, is diagonalized in the Sturmian basis centered on nucleus A. The eigenvectors for atom A with negative eigenvalues are approximate representations of electron-transfer states. Those with positive eigenvalues represent charge transfer to the continuum, while those for atom B with positive eigenvalues represent direct-ionization states.

The lowest neon eigenvalue obtained by the diagonalization of the one-electron Hamiltonian is $-30.754\,969$ a.u.; this is about 1.23 a.u. (4.0%) above the experimental $1s$ binding energy [13], which would be obtained from a full multielectron approach. For carbon [1], the corresponding energy and error are $-10.308\,170$ and about 0.27 a.u. (2.6%), respectively. The binding-energy correction to the cross section is very significant for carbon [1] and will be seen to be significant in Sec. IV B for neon as well.

As in the carbon paper, the two-center direct matrix elements of the GSZ potential and the two-center, charge-exchange matrix elements of both potentials have been evaluated numerically in prolate spheroidal coordinates over $\lambda=(r_A+r_B)/R$ and $\mu=(r_A-r_B)/R$ (where R is the internuclear distance).

III. NUMERICAL TESTS

The integration over λ was carried out by Gauss-Laguerre quadrature using at least 16 points for proton energies $E\le 600$ keV and, in all cases, 24 points for $E\ge 1000$ keV. Comparison with test values obtained using different numbers of points indicates that the error introduced in the ionization and electron-transfer cross section usually does not exceed 1.6% using the above-stated numbers of points except possibly for electron transfer for $E\ge 1000$ keV [14].

The integration over μ was carried out by Gauss-Legendre integration using 32 points in all cases for all proton energies. A 42-state test carried out with 40 points at the highest energy, $E=1500$ keV, indicates errors in using 32 points of 0.1% in the ionization cross section and 1.5% in the electron-transfer cross section. The errors are smaller at lower energies.

The overall limit of about 2% in the errors in integrating over λ and μ (except possibly for the error in integrating over λ at higher energies) is consistent with that reported previously for carbon [1] and purely hydrogenic [3] targets.

The coupled equations have been integrated numerically as before over the variable $z=vt$ using Hamming's method, with the absolute truncation error automatically kept between 5×10^{-6} and 5×10^{-4} in most cases. Previous work [1,9] indicates that with the use of these limits, the transition probabilities are accurate to 0.2%. Present tests for neon targets reveal errors of usually at most 0.3% [15]. To reduce the computing time to under 2000 CPU sec per impact parameter for the largest-basis (52-state) calculations, the truncation-error limits have sometimes been increased by a factor of 10 for small impact parameters; although the errors incurred in the electron-transfer probabilities at these impact parameters are up to a few percent, the error in the integrated electron-transfer cross section is probably not more than 2%.

There are two additional parameters whose values must be set before integrating the coupled equations. First, the internuclear separation beyond which charge-exchange matrix elements are neglected has been set to $25a_0$ (or, in some cases, a larger value, up to $30a_0$). Varying this cutoff over the range $25a_0$–$30a_0$ changed tested transition probabilities and cross sections by at most one unit in the third significant figure. Finally, the overall range of the z integration of the coupled equations was set to be $(-100a_0, 100a_0)$. In a single test at one impact parameter, halving this range affected the transition probabilities by at most 0.4%. These cutoffs are the same as or close to those previously used.

With the smallest (33-state) basis, the summed probability after integrating the coupled equations is usually unity to within 5×10^{-5} [16]. This is comparable to the extent of unitarity in the previous calculation for carbon targets [1]. However, in the present case of neon targets, the electron-transfer probability is at least an order of magnitude smaller than for carbon targets, on the order of 5×10^{-4} at the maximum of probability times ρ; thus, the extent of unitarity now only checks the numerical accuracy to roughly 10%. For the larger (42- and 52-state) bases, unitarity is usually valid only to within 2×10^{-4} [17]. Considering the numerical tests of parameters reported above, the numerical accuracy of the transition probabilities is probably greater than this departure from unitarity would suggest.

As in previous work, the probabilities have been integrated over impact parameters ρ using Simpson's rule. For the present case, the interval $\rho\le 1a_0$ is sufficient, due to the compactness of the p-Ne system. Since the probability times ρ versus ρ has but a single maximum, nine integration points are enough [18] for about 1% accuracy.

IV. CROSS SECTIONS

A. Sensitivity to basis

1. *Sturmian charge $\zeta_B=10$*

Shown in Table I are coupled-Sturmian cross sections for electron transfer and ionization from the K shell of neon atoms. (These cross sections, and all Sturmian cross sections presented later, contain a factor of 2 to account

for the possibility of either K-shell electron being active.) The cross sections were obtained using a Sturmian charge ζ_B equal to the nuclear charge Z_B ($=10$ for neon). To facilitate comparison, the bases used in the present study for neon and in the recent study for carbon are the same 36-, 45-, and 55-state bases used for hydrogenic targets [3], except that the filled states unavailable to the active, K-shell electron ($2s$ for C, $2s$ and $2p_{0,1}$ for Ne) have been removed from each basis after diagonalizing the GSZ Hamiltonian. The basis convergence for neutral carbon targets was previously noted to be substantially better than for C^{5+} targets. For neon targets, averaged over proton energies, the change in the cross section for electron transfer to all states on increasing the Sturmian basis from 33 to 42 states, or from 42 to 52 states, is 15%, while for ionization the change is 7%. For carbon targets, the average changes are only 13% and 4% for electron transfer and ionization, respectively, versus 18% and 7% for electron transfer and ionization from neon targets at *corresponding* scaled proton energies E/Z_B^2. Thus, the *relative* basis sensitivity (in percent) is somewhat increased on moving to the more asymmetric system, with smaller cross sections.

2. *Sturmian charges $\zeta_B = 9.7$ and 7.84*

Shown in Tables II and III are coupled-Sturmian cross sections for electron transfer and ionization from the K shell of neon atoms using the Sturmian charges $\zeta_B = 9.7$ and 7.84. Cross sections obtained using $\zeta_B = 9.7$, the value determined from Slater's rule, are reported only at 600 and 1500 keV. Averaged over these two energies, the change in the cross section for electron transfer to all states on increasing the Sturmian basis from 33 to 42 states, or from 42 to 52 states, is 14%, while for ionization the average change is 5%. These sensitivities are virtually the same as when using $\zeta_B = 10$ (13% and 6%) at the same energies. For carbon targets, the basis sensitivity using $\zeta_B = 5.7$ was previously found not to be significantly different from that using $\zeta_B = 6$. Thus, for neither target does Slater's rule give a more suitable Sturmian charge than does the choice of the nuclear charge.

The coupled-Sturmian cross sections in Table III have been obtained using the substantially smaller Sturmian charge $\zeta_B = 7.84$. (This choice was determined by setting $-\frac{1}{2}\zeta_B^2 = -30.75$ a.u., the Hartree-Fock $1s$ energy of neon. It is analogous to the previous choice, $\zeta_B = 4.54$, for carbon targets [1].) Using $\zeta_B = 7.84$, the energy-averaged change in the cross section for electron transfer to all states on increasing the Sturmian basis from 33 to 42 states, or from 42 to 52 states, is 18%, while for ionization the corresponding change is 3%. The basis sensitivities using $\zeta_B = 10$ have been noted to be 15% and 7% for electron transfer and ionization, respectively. Thus, there is less basis sensitivity with the smaller value of ζ_B only for ionization, whereas for carbon targets the smaller value of ζ_B (4.54 versus 6) yields less basis sensitivity both for ionization and electron transfer—substantially less basis sensitivity for electron transfer (5% using $\zeta_B = 4.54$ versus 13% using $\zeta_B = 6$ [1]). At corresponding scaled energies, the sensitivities with $\zeta_B = 4.54$ are only 4% and 3% for electron transfer and ionization from carbon targets versus 20% and 4% for neon targets using $\zeta_B = 7.84$. The greater basis sensitivity for neon targets using $\zeta_B = 7.84$ may in part be traced to an anomalously

TABLE I. Coupled-Sturmian cross sections (in units of 10^{-20} cm^2) using a Sturmian charge $\zeta_B = 10$ for electron transfer and ionization from the K shell of neon atoms by proton impact at a laboratory energy E.

E (keV)	Number of basis functions[a]	Electron transfer		Ionization
		$1s$	All[b]	
250	33	0.11	0.13	1.46
250	42	0.08	0.17	1.63
250	52	0.08	0.10	1.81
400	33	0.24	0.32	3.45
400	42	0.29	0.34	3.81
400	52	0.30	0.37	3.92
500	33	0.33	0.39	5.05
500	42	0.34	0.43	5.48
500	52	0.41	0.48	5.56
600	33	0.35	0.43	6.53
600	42	0.38	0.48	7.01
600	52	0.40	0.49	7.16
1000	33	0.39	0.48	9.92
1000	42	0.32	0.44	10.7_1
1000	52	0.37	0.43	11.0_4
1500	33	0.30	0.40	10.5_3
1500	42	0.28	0.35	11.3_8
1500	52	0.21	0.26	11.9_8

[a]The 36-, 45-, or 55-state basis of the proton–hydrogenic-ion paper [3], less the $2s$ and $2p_{0,1}$ states of neon after diagonalizing the GSZ neon Hamiltonian.

[b]Cross sections marked "All" are for electron transfer into all *available* bound states.

TABLE II. Coupled-Sturmian cross sections as in Table I, but using a Sturmian charge $\zeta_B = 9.7$.

E (keV)	Number of basis functions	Electron transfer 1s	Electron transfer All	Ionization
600	33	0.33	0.41	6.62
600	42	0.40	0.50	7.04
600	52	0.37	0.47	7.21
1500	33	0.27	0.36	10.5_8
1500	42	0.32	0.40	11.3_7
1500	52	0.21	0.31	12.0_4

large 52-state electron-transfer cross section at 1500 keV. The highest-lying p state has energy eigenvalue $E_{8p_B} = +29.6$ a.u. (obtained from diagonalizing the target Hamiltonian in the 52-state Sturmian basis) which is nearly equal to the Thomas energy $\frac{1}{2}v^2 = 30$ a.u. [19]. A similar situation obtains for the 42-state basis at 1000 keV [19].

The *absolute* sensitivity of cross sections to basis size is actually quite small: Averaged over energy, the range of cross sections for electron transfer to all states obtained with the three bases using $\zeta_B = 7.84$ is about 0.1×10^{-20} cm^2 while for ionization the range is about 0.6×10^{-20} cm^2. For proton-carbon collisions, the corresponding ranges, averaged over comparable scaled energies, are actually substantially larger: 0.6×10^{-20} and 3×10^{-20} cm^2 (using the analogous Sturmian charge $\zeta_B = 4.54$). Since the p-Ne ionization cross section is about an order of magnitude smaller than the p-C ionization cross section, the *percent* basis sensitivities are comparable, as previously noted. For electron transfer, on the other hand, the p-Ne cross section is about one and a half orders of magnitude below the p-C cross section, so the percent basis sensitivity is greater for neon targets, as previously noted.

For each choice of ζ_B, considering the cross sections with the three different size bases to be error bars, the graph (not shown) of cross section versus energy with $\zeta_B = 7.84$ overlaps the graph with $\zeta_B = 10$, both for electron transfer and ionization. This was previously noted to be the case for carbon targets with $\zeta_B = 4.54$ and 6, the error bars on a *logarithmic* scale being smaller for that case.

B. Binding-energy correction

The role of a binding-energy correction to the coupled-state cross sections has been discussed by the author in the context of p-C collisions [1], following earlier work by Lin and Tunnell [20] in the context of a two-state calculation. Specifically, the correction in the coupled equations is to the time-dependent energy phase between the target and projectile-centered states. All target-centered energies have been shifted by the *same* amount, the difference between the Hartree-Fock 1s energy and the many-body energy. For carbon targets, this correction of -0.27 a.u. to the Hartree-Fock 1s energy has a substantial effect on the cross sections, lowering them into agreement with the experimental results of Rødbro *et al.* [2]. For neon, the binding-energy correction to the Hartree-Fock 1s energy is -1.23 a.u. As will

TABLE III. Coupled-Sturmian cross sections as in Table I, but using a Sturmian charge $\zeta_B = 7.84$.

E (keV)	Number of basis functions	Electron transfer 1s	Electron transfer All	Ionization
250	33	0.08	0.18	1.59
250	42	0.12	0.14	1.71
250	52	0.10	0.13	1.76
400	33	0.22	0.27	3.89
400	42	0.28	0.35	3.99
400	52	0.26	0.31	4.08
500	33	0.32	0.40	5.54
500	42	0.34	0.41	5.72
500	52	0.36	0.43	5.75
600	33	0.43	0.53	7.00
600	42	0.36	0.45	7.29
600	52	0.42	0.48	7.31
1000	33	0.34	0.43	10.4_8
1000	42	0.48	0.57	10.8_5
1000	52	0.34	0.45	11.2_1
1500	33	0.19	0.23	10.9_3
1500	42	0.17	0.25	11.6_6
1500	52	0.30	0.38	12.1_2

TABLE IV. Coupled-Sturmian cross sections as in Table I, but using a Sturmian charge $\zeta_B = 7.84$ and a binding-energy correction -1.23 a.u.

E (keV)	Number of basis functions[a]	Electron transfer 1s	Electron transfer All	Ionization
250	30	0.06	0.11	1.14
250	39	0.10	0.11	1.35
250	49	0.09	0.12	1.46
400	33	0.15	0.18	3.57
400	42	0.17	0.21	4.09
400	52	0.19	0.24	4.40
500	33	0.23	0.30	4.71
500	42	0.19	0.23	4.95
500	52	0.23	0.28	5.13
600	33	0.34	0.43	5.69
600	42	0.21	0.26	5.96
600	52	0.25	0.29	5.99
1000	33	0.22	0.28	8.44
1000	42	0.38	0.50	8.40
1000	52	0.21	0.29	8.34
1500	33	0.11	0.14	9.10
1500	42	0.10	0.18	9.54
1500	52	0.24	0.32	9.18

[a]At 250 keV, the highest-lying $p_{0,1}$ states on B and the highest-lying s state on A have been removed after diagonalization; the bases are otherwise the same as for higher energies.

be seen in the comparison of cross sections in Sec. IV C, the binding-energy correction is also important for neon targets to achieve agreement with experimental results.

Binding-energy-corrected cross sections are given in Table IV for $\zeta_B = 7.84$ and, for $E \geq 600$ keV, in Table V for $\zeta_B = 10$. Particularly for electron transfer, but also for ionization, the binding-energy-corrected cross sections are, on the average, substantially lower than the corresponding uncorrected values in Tables III and I. As for carbon targets, the relative basis sensitivity is greater with the binding-energy correction than without. (For carbon targets, only $\zeta_B = 4.54$ was used in making the binding-energy correction, since this choice of ζ_B was found to lead to less sensitivity without the binding-energy correction than the choice $\zeta_B = Z_B$.) For $\zeta_B = 7.84$, the energy-averaged basis sensitivity in the electron-transfer cross section is 35% versus the previously noted sensitivity of 20% without the binding-energy correction; for carbon targets at corresponding scaled energies, the sensitivity is 9% versus 4% without the binding-energy correction. For ionization, the energy-averaged sensitivity is 5% versus 4% without the binding-energy correction; this 5% sensitivity is actually less than the corresponding sensitivity (10%) for carbon targets.

Although the *relative* basis sensitivity for electron transfer from neon targets is greater than that for carbon targets, the *absolute* basis sensitivity is actually less, as was previously noted to be true in the absence of a binding-energy correction.

Binding-energy-corrected cross sections using $\zeta_B = 10$ are given in Table V for proton energies of 600, 1000, and 1500 keV. Averaged over these energies, the basis sensitivity of cross sections for electron transfer to all states is 28%, whereas using $\zeta_B = 7.84$ it is 47% for these energies. Thus, for electron transfer from neon targets, the

TABLE V. Coupled-Sturmian cross sections as in Table I, but using a Sturmian charge $\zeta_B = 10$ and a binding-energy correction -1.23 a.u.

E (keV)	Number of basis of functions	Electron transfer 1s	Electron transfer All	Ionization
600	33	0.21	0.26	5.05
600	42	0.24	0.31	5.64
600	52	0.35	0.47	6.38
1000	33	0.26	0.32	7.56
1000	42	0.17	0.24	8.22
1000	52	0.25	0.33	8.79
1500	33	0.22	0.30	8.33
1500	42	0.19	0.25	9.04
1500	52	0.11	0.20	9.71

choice $\zeta_B = Z_B$ appears preferable to the choice $\zeta_B = 7.84$, regardless of whether the binding-energy correction is included, whereas for ionization, the choice $\zeta_B = 7.84$ is preferable.

The binding-energy correction has been noted to lead to nonunitarity of the scattering results, which is unavoidable if one describes a many-body process with a strictly one-body method. Thus, conservation of probability no longer provides a good check of numerical accuracy in integrating the coupled equations and in evaluating the charge-exchange matrix elements. Consider, for example, a calculation of the 33-state cross sections for electron transfer to all states at 600 and 1000 keV using $\zeta_B = 7.84$. Without a binding-energy correction, nonunitarity implies a *numerical* inaccuracy of no worse than 1.5%, whereas numerical inaccuracy, in principle, could be 20% with a binding-energy correction [21].

C. Comparison with experimental results

Shown in Fig. 1 are coupled-Sturmian cross sections together with the experimental cross sections of Rødbro *et al.* [2] for electron transfer and ionization from the K shell of neon by proton impact. For comparison, recent Sturmian [1] as well as experimental [2] cross sections for carbon targets are also given. Ranges of values shown indicate sensitivity to basis size as described in Sec. IV B. Values for the Sturmian charge $\zeta_B = 7.84$ are shown for neon targets, since this Sturmian charge is analogous to the Sturmian charge $\zeta_B = 4.54$ for which results are displayed for carbon targets. Although not necessarily optimal, the choice $\zeta_B = 4.54$ was shown previously [1] to give smaller sensitivity to basis size for carbon targets than other choices of ζ_B; the choice $\zeta_B = 7.84$ has been shown in Sec. IV A to give smaller sensitivity to basis size for ionization from neon targets, but not for electron transfer.

These Sturmian results include a binding-energy correction. To avoid confusion, values without a binding-energy correction are omitted. When this correction is included, the cross section for electron transfer from neon (into all states of H) agrees (or almost agrees) at all energies with the experimental values of Rødbro *et al.* within the combined experimental and large theoretical error bars. The comparison is similar to that made previously for carbon targets, except that for carbon targets the theoretical error bars were noted to be smaller, and some discrepancy was noted at 200 and 300 keV, as can be seen in Fig. 1.

For ionization from both neon and carbon targets, the Sturmian cross sections have much smaller error bars than for electron transfer. Even within these small error bars, there is generally excellent agreement with the experimental results [2].

D. Comparison with perturbative results for electron transfer

Shown in Fig. 2 are coupled-Sturmian and perturbative [5,6] results for K-K electron transfer in collisions between protons and neon atoms. The Sturmian results are as in the comparison with the experimental results in Fig. 1, but now for transfer into the ground state only, in order to be consistent with the other theoretical results. All the theoretical calculations incorporate a similar Hartree-Fock potential to represent the interaction of the active electron with the neon-atom core. All the calculations employ some form of binding-energy correction.

As has been pointed out in the recent p-C paper [1], the coupled-state calculation, at least without the binding-energy correction, is automatically normalized: Changing the normalization of the intermediate ionization channels would not affect the results. However, the perturbative results of Marxer and Briggs [5] show clearly that this is not the case with the strong-potential-Born (SPB) calculation: a renormalization is necessary on theoretical grounds alone [5], and doing so brings the SPB result closer to the experimental result (not shown). It is seen that this renormalized result is within the range

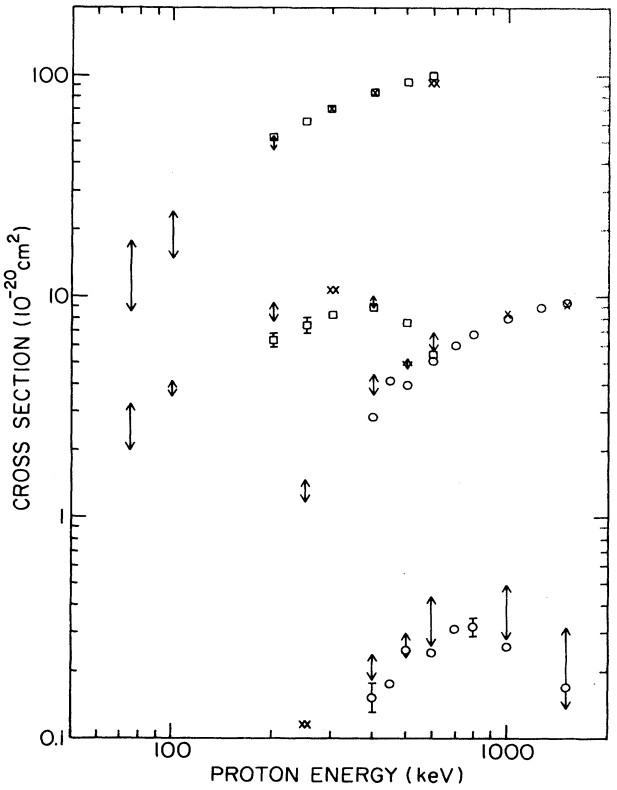

FIG. 1. Coupled-Sturmian (present results for neon targets, Ref. [1] for carbon targets) and experimental cross sections of Rødbro *et al.* [2] for electron transfer into all states and ionization from the K shell of carbon and neon atoms by proton impact. Circles and circles with error bars, the experimental results for ionization (upper set of data), and electron transfer (lower set of data) from neon targets. Squares and squares with error bars, the experimental results for ionization (upper set of data), and electron transfer (lower set of data) from carbon targets. The arrows indicate the range of Sturmian results with various bases when a binding-energy correction is included. (For clarity, the average Sturmian value for ionization is instead indicated by a cross when the range is small, and the range of values for ionization from neon at 600 keV is omitted.)

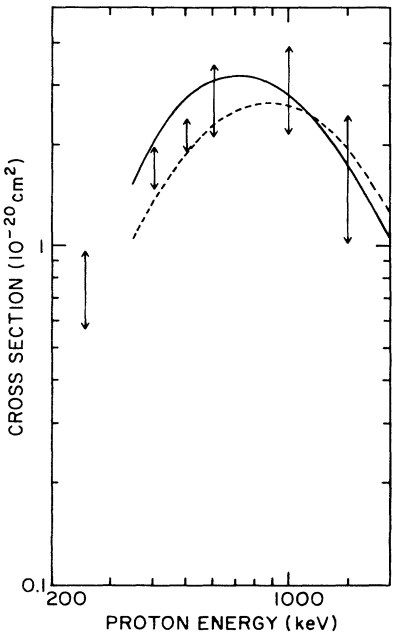

FIG. 2. Coupled-Sturmian and perturbative cross sections for K-K electron transfer in proton–neon-atom collisions. Arrow "error bars" are the range of Sturmian cross sections with a binding-energy correction. Dashed curve, renormalized SPB (Marxer and Briggs, Ref. [5]). Solid curve, distorted SPB (Alston, Ref. [6]).

of the Sturmian results for $E > 500$ keV. Previously it was noted that for carbon targets [1], the renormalized SPB results agree with the Sturmian results for $E > 300$ keV. The agreement thus actually persists to lower scaled energies E/Z_B^2 for neon targets.

Also shown in Fig. 2 are the recent distorted SPB (DSPB) results of Alston [6]. The DSPB approach avoids the need to renormalize the intermediate states by properly accounting for the Coulombic nature of the interaction. It is seen that the DSPB results are within the range of the Sturmian results for $E \gtrsim 600$ keV. [Surprisingly, for carbon, the agreement persists down to energies as low as 200 keV (not shown).] For neon, at energies $E \leq 500$ keV, the range of Sturmian results lies between the perturbative theories, almost bridging the gap between them.

V. CONCLUSION

Within a one-electron model the coupled-Sturmian approach has been extended to K-shell capture and ionization in quite asymmetric collisions, specifically between protons and neon atoms. The ionization cross section and even the very small electron-transfer cross section agree well with experimental results, within the range of basis sensitivity. The agreement with perturbative results for electron transfer is also good.

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[1] T. G. Winter, Phys. Rev. A **47**, 264 (1993).
[2] M. Rødbro, E. Horsdal Pedersen, C. L. Cocke, and J. R. MacDonald, Phys. Rev. A **19**, 1936 (1979).
[3] T. G. Winter, Phys. Rev. A **35**, 3799 (1987).
[4] S. G. Alston (private communication).
[5] H. Marxer and J. S. Briggs, J. Phys. B **25**, 3823 (1992).
[6] S. G. Alston, Phys. Rev. A (to be published).
[7] D. F. Gallaher and L. Wilets, Phys. Rev. **169**, 139 (1968).
[8] R. Shakeshaft, Phys. Rev. A **14**, 1626 (1976).
[9] T. G. Winter, Phys. Rev. A **25**, 697 (1982).
[10] Additional Sturmian papers are cited in Refs. [1,9].
[11] A. E. S. Green, D. L. Sellin, and A. S. Zachor, Phys. Rev. **184**, 1 (1969).
[12] P. P. Szydlik and A. E. S. Green, Phys. Rev. A **9**, 1885 (1974).
[13] M. O. Krause, Oak Ridge National Laboratory Report No. ORNL-OM-2943, 1970 (unpublished).
[14] A comparison was made at 1000 and 1500 keV with cross sections obtained using only 16 λ points. There were more underflows in the computations using 24 points, possibly causing greater numerical error. For electron transfer to all states, the 52-state cross sections at 1500 keV obtained with the different numbers of points differ by about 10%; 42-state cross sections, however, agree to at least 2%, as do the 52-state cross sections at 1000 keV. For electron transfer into the ground state, the 52-state (or 42-state) cross sections obtained with different numbers of points differ by 2–6% at 1000 and 1500 keV.
[15] These tests were carried out at a single impact parameter at 600 and 1000 keV using 42- or 52-state bases and for integrated cross sections using the 33-state basis. At 1500 keV for larger impact parameters with some bases, truncation-error limits an order of magnitude smaller were used due to greater sensitivity.
[16] The single exception is for small impact parameters at the highest energy, 1500 keV, using $\zeta_B = 7.84$ and a (nonunitary) binding-energy correction. The extent of this departure from unitarity is attributed to the chosen truncation-error limits (5×10^{-6}, 5×10^{-4}) which, however, still give sufficiently accurate transition probabilities at this energy for the smaller impact parameters.
[17] One of two exceptions is as noted in Ref. [16]. The other is for the 52-state calculation for smaller impact parameters at 1500 keV using $\zeta_B = 10$ and a (nonunitary) binding-energy correction. It is attributed to the use of larger truncation-error limits (10^{-5}, 10^{-3}) to reduce the computing time.
[18] Indeed, values using only seven points (i.e., fewer points in the peak region $\rho \leq 0.25$) generally agree closely: usually to within 3% for electron transfer at the lowest energy

and 1% at the highest energy, and to within 15% for ionization at the lowest energy and 3% at the highest energy.
[19] See also the discussion in T. G. Winter and S. G. Alston, Phys. Rev. A **45**, 1562 (1992) for p-He^+ collisions.
[20] C. D. Lin and L. N. Tunnell, Phys. Rev. A **22**, 76 (1980).
[21] These test calculations employ reduced truncation error limits $[10^{-6}, 10^{-4}]$ rather than the usual $[5\times10^{-6}, 5\times10^{-4}]$; although unitarity is thereby significantly improved, the cross sections are negligibly affected.