Collisional excitation and alignment of $np^5(n+1)s^2$ autoionizing states of the alkali-metal atoms

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The excitation cross sections and the alignment of the lowest autoionizing states, $np^5(n+1)s^2$, of Na, K, Rb, and Cs, induced by impact of various projectiles, have been calculated. The alignment by projectiles heavier than electrons is seen to exhibit a rich structure as a function of impact energy and it is anticipated that its overall behavior should be observable by experiment. Good agreement is found with the available data on sodium.

I. INTRODUCTION

The alkali-metal atoms have traditionally been a favorite object of study by experimentalists and theorists alike because of their relatively simple electronic structure and spectra. The study of their medium-to-high Rydberg states, obtained by excitation of the valence electron has become especially a frequent research subject with the advent of the laser and the ability to obtain substantial populations of such states; these states subsequently decay by fluorescence via optically "allowed" or "forbidden" transitions and can be monitored by photon emission spectroscopy. On the other hand, the states resulting from the excitation of an inner-shell electron decay predominantly via emission of an electron (autoionization) and thus are studied by electron spectroscopy.

Although the K, Rb, and Cs autoionizing states were observed early by Beutler and Guggenheimer,[1-3] in photoabsorption spectra, analogous studies for Na were performed more than 35 years later by photoabsorption[4] and electron-impact excitation.[5] For all four atoms these states have large excitation probabilities but very small widths (i.e., long lifetimes). In a series of experiments Nygaard[6-9] measured their contribution to the total electron-impact excitation cross section of the alkali-metal atoms, whereas Ross *et al.*,[10] Breuckmann *et al.*,[11] and DuBois *et al.*[12] performed state-selected measurements and studied the angular distribution of the autoionization electrons in Na. Pejčev and Ross[13] measured the Cs excitation cross section as a function of energy over a broad electron energy range and observed sharp maxima of the cross section near threshold. The excitation cross sections of the lowest autoionizing states $np^5(n+1)s^2$ of the alkali-metal atoms were theoretically calculated using a variety of approximations for the collision dynamics and for the atomic wave functions by Rai and co-workers,[14-17] this author,[18-20] Tiwary,[21,22] and Peterkop and Liepinsh.[23-25]

The study of autoionizing states provides information about the atomic structure and the dynamics of a state's excitation since the cross section depends strongly on the impact energy. Specifically, the different magnetic substates can be populated to a different, i.e., nonstatistical, extent, depending on the relevant partial excitation cross sections, thus resulting in a nonzero *alignment*. As is shown below, parallel measurement of the alignment, together with the excitation cross section, provide a stringent test of the validity of theoretical approximations, especially for the treatment of the collisional dynamics.

The electron-impact excitation cross sections of the lowest autoionizing states $np^5(n+1)s^2\,^2P_{3/2}$ of Na ($n=2$), K ($n=3$), Rb ($n=4$), and Cs ($n=5$) have been studied experimentally[6-13] and theoretically[14,16-25] but do not show any interesting structure, apart from sharp maxima just above threshold.[13,16] DuBois *et al.*[12] have inferred a prominent minimum in the *alignment* of the Na state at low impact energies. However, it has been speculated in the literature[26,27] that this minimum is probably due to effects of post-collision interaction (PCI)[28] on the detected electrons and might not represent structure in the alignment of the excited state. Similar minima have been observed and attributed to PCI-type effects by Heideman *et al.*[29] in the polarization of fluorescence radiation, following the electron-impact excitation of helium and lithium.

The alignment of the Na $2p^5 3s^2\,^2P_{3/2}$ state obtained by proton and/or He^+ impact was reported by Ziem *et al.*,[30] Theodosiou *et al.*,[31] and DuBois *et al.*[12] The isoelectronic state in Mg^+ was also studied by DuBois *et al.*[12] by Mg^+ on He impact. The experimental data on both atoms exhibited interesting structure and verified the overall predictions of the first Born approximation.[30-32]

To further elucidate the origin of the observed structure in the alignment and its variation (as a function of atomic number) for heavier alkali-metal atoms, the present work extends the calculations to K, Rb, and Cs and to diverse projectiles. In addition, an improved theoretical approach, the Vainshtein-Presnyakov-Sobelman (VPS) approximation,[33-35] is applied to calculate the necessary partial and total excitation cross sections.

As established by this author,[19,36] the effect of interference between the autoionizing and direct ionization transitions in the processes

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$$P + A\,[np^6(n+1)s\,^2S_{1/2}] \longrightarrow \begin{matrix} \nearrow P + A^+[np^6\,^1S_0] + e^- \\ \searrow P + A^*[np^5(n+1)s^2\,^2P_{1/2,3/2}] \end{matrix} , \tag{1}$$

where $P = e^-$, H^+, He^+, etc., and A = Na, K, Rb, and Cs is negligibly small because the direct ionization process is very weak. The autoionizing intermediate states have decay widths of only a few meV (Refs. 18, 36, and 37) and generalized Fano profile parameters $q(K)$ on the order of 100.[18,36] Some of the well-established properties of these states are summarized in Tables I–III.

In the limit of zero amplitude for the direct ionization, the alignment of the autoionizing state is equal to the anisotropy parameter in the angular distribution

$$I_{3/2}(\theta) = 2I_0[1 + \beta P_2(\cos\theta)] , \tag{2a}$$

$$I_{1/2}(\theta) = I_0 \tag{2b}$$

of the electrons emitted through autoionization. In this limit, we have[19]

$$\beta = \frac{\int_{K_{\min}}^{K_{\max}} d(Ka_0)(Ka_0)^{-3}\langle (n+1)s \mid j_1(Kr) \mid np \rangle^2 P_2(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{K}})}{\int_{K_{\min}}^{K_{\max}} d(Ka_0)(Ka_0)^{-3}\langle (n+1)s \mid j_1(Kr) \mid np \rangle^2} = [Q(np0) - Q(np1)]/[Q(np0) + 2Q(np1)] , \tag{3}$$

where $Q(npm_l)$ is the excitation cross section of an npm_l electron to a $(n+1)s0$ state, and K is the momentum transfer.

II. METHOD OF CALCULATION

The transition matrix elements and excitation cross sections have been calculated using atomic wave functions obtained within the Hartree-Slater approximation.[39] A series of calculations was actually performed to test the significance of using Hartree-Slater,[39] Hartree-Kohn-Sham,[39] and Hartree-Fock[40] single-configuration wave functions. The matrix elements were essentially the same in all cases. This was also true even when separate self-consistent calculations were performed for the ground and excited configurations, respectively, provided that the excited configuration orbitals were Schmidt orthogonalized to the orbitals of the ground configuration.

The transition probabilities where calculated in two approximations: (a) using the plane-wave first Born approximation (PWBA) form factor

$$T_{if}^B = \langle f \mid \exp(i\mathbf{K}\cdot\mathbf{r}) \mid i \rangle , \tag{4}$$

and (b) using the Vainshtein-Presnyakov-Sobelman approximation[33–35] (VPSA). The VPSA accounts to some extent for the distortion of the projectile's wave function during the collision. Its application entails the replacement of the above Born form factor by

$$T_{if}^{\mathrm{VPS}} = -T_{if}^B(4\pi Z_p/K^2)\left[\frac{K+\mu\Delta E}{\mu(K^2+\Delta E)}\right]^{-i\nu^*} N^*(\nu)\,{}_2F_1(-i\nu^*, i\nu, 1, (K^2-\mu\Delta E)^2/[(K^2+\Delta E)(K^2+\mu^2\Delta E)]) , \tag{5a}$$

$$N(\nu) = \mu^{-i\nu^*} \mid \Gamma(1-i\nu) \mid^2 , \tag{5b}$$

TABLE I. ns binding energies in eV of the alkali-metal atoms in their ground state. HS, Hartree-Slater model; HKS, Hartree-Kohn-Shamm model; HF, Hartree-Fock model.

Element	State	Theoretical HS	Theoretical HKS	Theoretical HF	Experimental[a]
Na	3s	5.137	4.855	4.956	5.139
K	4s	4.196	3.903	4.013	4.339
Rb	5s	3.950	3.645	3.752	4.176
Cs	6s	3.564	3.272	3.366	3.893

[a]Reference 38.

TABLE II. Spin-orbit splittings in eV.

Element	State	Theoretical (HF)	Experimental
Na	$2p^5 3s^2\,^2P$	0.166	0.166[a]
K	$3p^5 4s^2\,^2P$	0.249	0.260[b]
Rb	$4p^5 5s^2\,^2P$	0.810	0.845[c]
Cs	$5p^5 6s^2\,^2P$	1.431	1.217[d]

[a]Connerade *et al.*, Ref. 4.
[b]Beutler and Guggenheimer, Ref. 1.
[c]Beutler, Ref. 2.
[d]Beutler and Guggenheimer, Ref. 3.

where $\mathbf{K}=\mathbf{k}_i-\mathbf{k}_f$ is the momentum transfer, μ is the projectile's reduced mass, ΔE is the excitation energy, Z_p is the projectile's charge, ${}_2F_1$ is a hypergeometric function, and

$$\nu=-\mu Z_p/[k_f-i\,\mathrm{sgn}(Z_p)\mu\sqrt{\varepsilon_f}]\,, \tag{6}$$

ε_f being the binding energy of the active atomic electron in the final state.

The excitation cross section for a bare or structureless projectile of incident energy T_i and charge Z_p is given by

$$\sigma_{if}^{(0)}=8\pi a_0^2\frac{M}{m}\frac{R}{T_i}Z_p^2\int_{K_{\min}}^{K_{\max}}\frac{d(Ka_0)}{(Ka_0)^3}\,|\,T_{if}\,|^2\,, \tag{7}$$

where $K_{\min}=k_i-k_f$ and $K_{\max}=k_i+k_f$. When the projectile carries electrons and has nuclear charge Z, and the electrons' role is taken into account explicitly, the above expression is changed. For the sake of simplicity in the following, we discuss only projectiles carrying a *single* electron. Two distinct cases are present: (a) the projectile remains in its ground state after collision, or (b) it may be excited to any state (including continuum). For case (a) Eq. (7) applies again except that the quantity Z_p^2 is simply replaced by a momentum-transfer-dependent charge,[41] i.e.,

$$\sigma_{if}^{(1)}=8\pi a_0^2\frac{M}{m}\frac{R}{T_i}\int_{K_{\min}}^{K_{\max}}\frac{d(Ka_0)}{(Ka_0)^3}\,|\,T_{if}\,|^2 \times|\,Z-1/[1+(Ka_0/2Z)^2]^2\,|^2\,. \tag{8}$$

When the projectile state is not detected after the collision, i.e., case (b) applies, the excitation cross-section formula is increased by the addition of new terms,[41] which, using a closure relation, can be approximated[41] by

$$\Delta\sigma_{if}=8\pi a_0^2\frac{M}{m}\frac{R}{T_i}\int_{\langle K\rangle}^{K_{\max}}\frac{d(Ka_0)}{(Ka_0)^3}\,|\,T_{if}\,|^2 \times\{1-1/[1+(Ka_0/2Z)^2]^4\}\,, \tag{9}$$

where $\langle K\rangle$ is taken as equal to the value of $K_{\min}$ appropriate to the lowest excited state of the projectile (here $n=2$). Therefore, the total cross section in case (b) is given by

$$\sigma_{if}^{(2)}=\sigma_{if}^{(1)}+\Delta\sigma_{if}\,. \tag{10}$$

Even though only the alignment of the $J=\frac{3}{2}$ level from the doublet is non-negligible and was calculated, the excitation cross-section values presented in the graphs below correspond to the whole configuration $np^5(n+1)s^2\,^2P$, i.e., the sum of $\sigma(^2P_{3/2})+\sigma(^2P_{1/2})$. Another issue that the present calculations address is whether one uses theoretical or experimental values for the excitation energy. Results were obtained for both cases and they are compared with experimental observations below.

III. RESULTS AND DISCUSSION

A. Calculations

As a first step, the excitation cross section and alignment of the lowest autoionizing state of Na were calculated using a set of projectiles of varying mass and number of electrons they carry along, i.e., we considered e^-, H^+, He^{2+}, He^+, and Li^+. The screening of the He^+ and Li^+ nuclear charge due to their electrons was properly taken into account.

Figures 1 and 2 present our results versus the velocity ratio of a projectile and a $2p$ electron. We see that, as expected from the validity of the Born approximation, at medium to large velocities the results are the same for projectiles with equal velocity and charge. Because of its

TABLE III. Excitation energy in eV of the $np^5(n+1)s^2$ autoionizing states of the alkali-metal atoms.

Element	State	Theoretical HS	Theoretical HKS	Theoretical HF	Experimental $J=\frac{3}{2}$	Experimental $J=\frac{1}{2}$
Na	$2p^5 3s^2\,^2P$	38.215	31.438	30.359	30.768	30.934[a]
K	$3p^5 4s^2\,^2P$	22.738	18.672	18.937	18.713	18.973[b]
Rb	$4p^5 5s^2\,^2P$	18.674	15.430	15.865	15.308	16.153[c]
Cs	$5p^5 6s^2\,^2P$	15.381	12.747	13.288	12.303	13.519[d]

[a]Connerade *et al.*, Ref. 4.
[b]Beutler and Guggenheimer, Ref. 1.
[c]Beutler, Ref. 2.
[d]Beutler and Guggenheimer, Ref. 3.

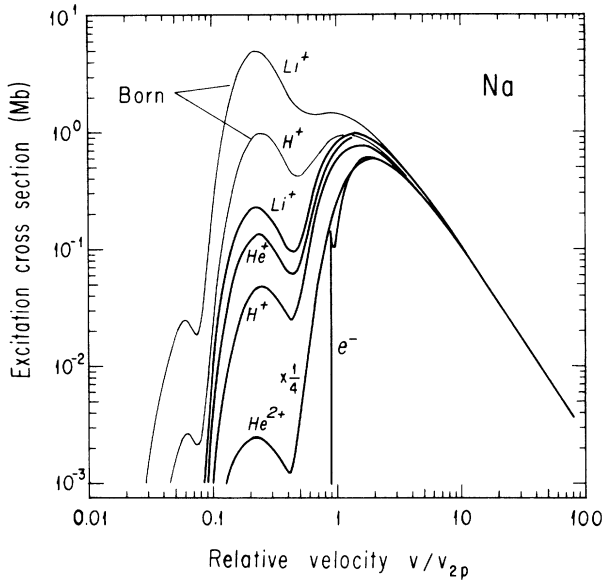

FIG. 1. Excitation cross section $\sigma(2p^6 3s \rightarrow 2p^5 3s\,^2\,^2P)$ for Na by various projectiles. Light lines, Born approximation; heavy lines, VPS approximation. Experimental excitation energies are used and electron-carrying projectiles are assumed to remain in their ground state after collision.

small mass, an electron's ability to excite the atom is limited to velocity ratios $v/v_{np} \geq 0.9$. For this reason an electron cannot probe the inner structure of the target wave functions.[31] This can be attained, however, by the heavier projectiles also considered here: As seen from Figs. 1 and 2, they yield interesting structure for both the cross section and the alignment. This structure is directly related to the nodal properties of the $2p$ and $3s$ wave functions, with zero and two nodes, respectively.[31] Each node of each wave function involved in the transition contributes a minimum to the excitation cross section and the alignment.

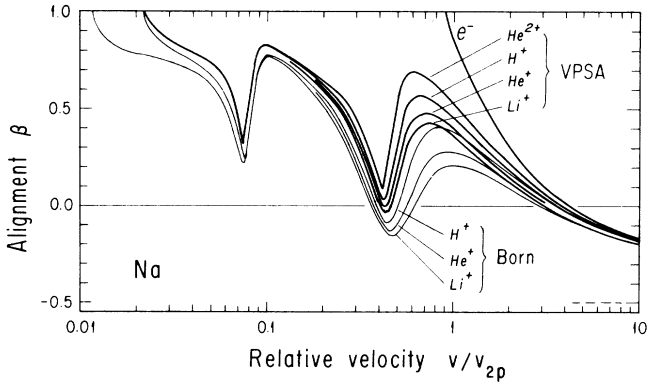

FIG. 2. Alignment of the collisionally excited $Na(2p^5 3s^2\,^2P_{3/2})$ state induced by various projectiles. Light lines, Born approximation; heavy lines, VPS approximation. Experimental excitation energies are used and electron-carrying projectiles are assumed to remain in their ground state after collision.

Figure 1 clearly indicates the effects at lower impact energies due to the different masses of the projectiles and to the number of electrons they carry: At slow collisions with electron-carrying projectiles the projectile nuclear charge is less completely shielded and the cross section is appropriately increased over the proton-impact case. The pattern is the same within either approximation used. The effect of the VPSA, i.e., some accounting for the projectile's wave-function distortion due to the collision,[33] is to reduce the cross section at low velocities by an order of magnitude or more. The sharp maximum above threshold predicted[16,21] for other alkali-metal atoms and measured[13] for Cs in the case of electron impact is clearly visible also in the case of Na.

The general behavior of the alignment of a state excited via collisions can be predicted on the basis of physical arguments:[42] At asymptotically large impact energies the alignment becomes $-\frac{1}{2}$, corresponding to the momentum transfer $\mathbf{K}$ being predominantly transverse to the direction of incidence $\mathbf{k}_i$, whereas at the excitation threshold it is $+1$, corresponding to $\mathbf{K}$ being predominantly parallel to $\mathbf{k}_i$. At threshold the projectile *must* be scattered inelastically into an s state; otherwise, the centrifugal barrier forbids the transition. Therefore, at threshold only the $Q(np0)$ partial cross section is nonzero in Eq. (3).

For electron impact the transition between the two values is smooth. For heavier projectiles, however, the alignment curve shows sharp minima (two for Na and more for heavier alkali metals). These minima appear at relative velocities $V_{\rm rel} = V_{\rm proj}/v_{np} < 1$. As seen from Fig. 2, the general shape of the alignment produced by all heavier than electron projectiles is mostly the same. As in the cross-section case, the results vary to some extent depending on the mass of the projectiles and on whether they carry electrons. The effect of distortion of the projectile wave function, treated approximately via the VPS approximation, is to basically change the overall magnitude of the Born approximation results but not their basic shape. Near $v_{\rm rel} = 0.1$ all approximations and pertinent projectiles yield similar values. DuBois *et al.*[12] were, therefore, largely justified to use the $H^+ + Na$ curve of Ref. 31 in order to explain their $Mg^+ + He$ data for the isoelectronic to Na transition. Thus they verified the existence of a peak in this general velocity range.

After the detailed analysis of Na the calculations were extended to the excitation cross section and alignment of the homologous states of K, Rb, and Cs. The overall picture obtained in Na is generally reproduced in these cases. Figures 3 and 4 show only the results obtained for proton impact in order to illustrate the similarities and point out any different features of these cases.

From Fig. 3 we notice that the excitation cross section for K, Rb, and Cs is almost an order of magnitude larger than that for Na at relative velocities above 0.2. This fact will facilitate their experimental investigation, still to be carried out. The more complicated wave-function nodal structure is evident at lower impact energies.

Figure 4 presents the alignment results for K, Rb, and Cs. One significant feature of this figure is that the

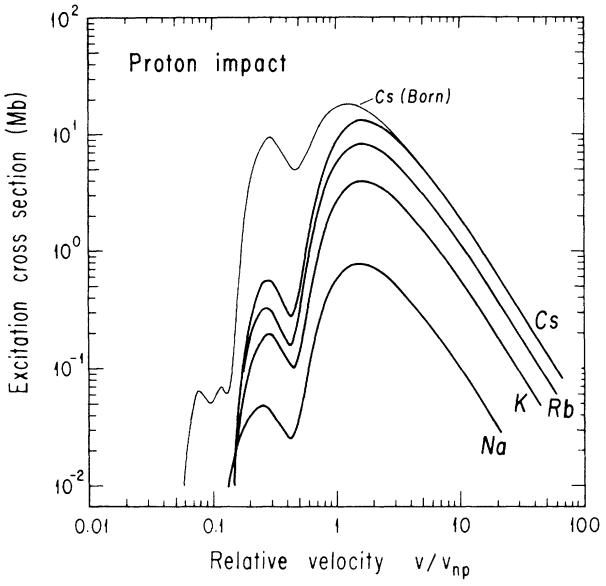

FIG. 3. Excitation cross section $\sigma[np^6(n+1)s \rightarrow np^5(n+1)s^2\,^2P]$ for Na, K, Rb, and Cs by proton impact. Light line, Born approximation; heavy lines, VPS approximation. Experimental excitation energies are used.

alignment has a lot of structure as a function of the incident energy, and this structure is basically unaffected by the approximation used. The amount of structure is really impressive and should be tantalizing for the experimentalists to investigate and verify it, at least qualitatively.

Theodosiou *et al.*[31] showed in detail the dependence of the alignment minima in Na on the properties of the $2p$ and $3s$ wave functions. Generally, the rich structure seen in Figs. 2–4 can be traced back to the nodal structure of the atomic wave functions np and $(n+1)s$ of the ground and excited states, respectively. Figure 5 shows the reduced radial wave functions $rR(r)$ of the the np and $(n+1)s$ orbitals involved in the autoionizing transitions of Na, K, Rb, and Cs studied here. One can easily map a correspondence between wave-function nodes and alignment minima, except when the node positions are at the same distance r for both the s and the p orbitals involved in the transition. Each of the extrema (lobes) of the wave functions corresponds to the location of a subshell that is occupied in the respective ion. The reason that the location of some of the inner nodes and the extrema of the s and p orbitals overlap is due to the fact that, at least for the inner electrons, the various subshells, i.e., various l, of a given shell, i.e., principal quantum number n, are, more or less, located at the same distance from the nucleus. In view of this correspondence

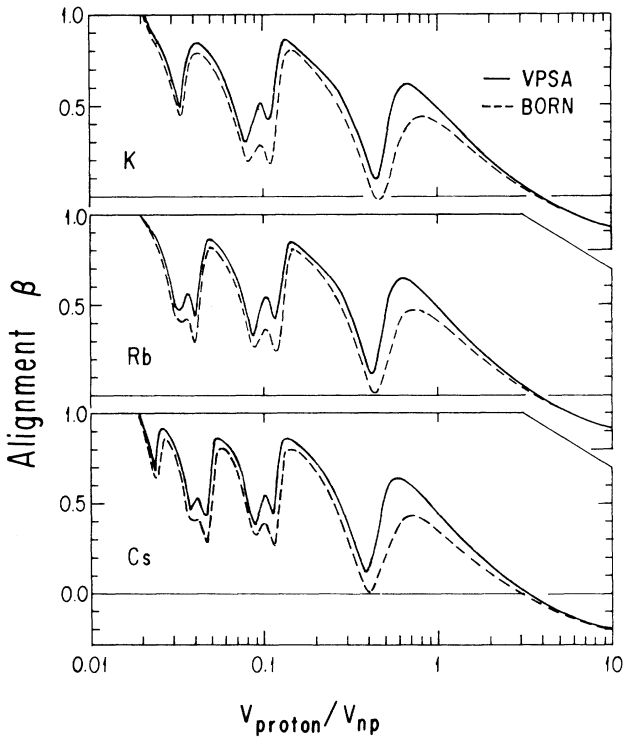

FIG. 4. Alignment of the excited $np^5(n+1)s^2\,^2P_{3/2}$ state of K, Rb, and Cs, induced by proton impact. — — —, Born approximation; ——, VPS approximation. Experimental excitation energies are used.

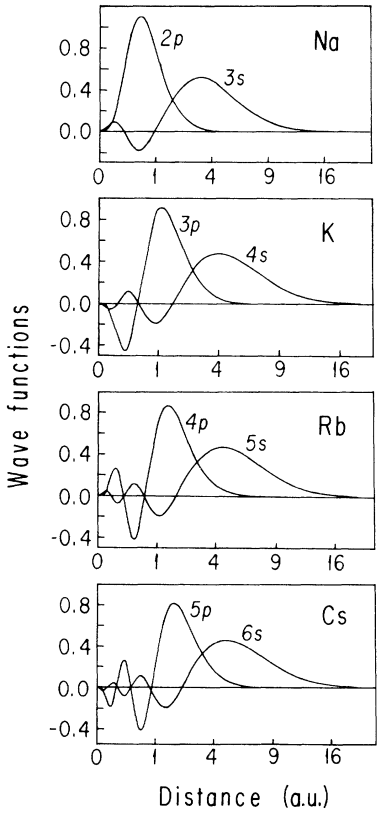

FIG. 5. Radial wave functions of the outer-shell p and s orbitals of Na, K, Rb, and Cs.

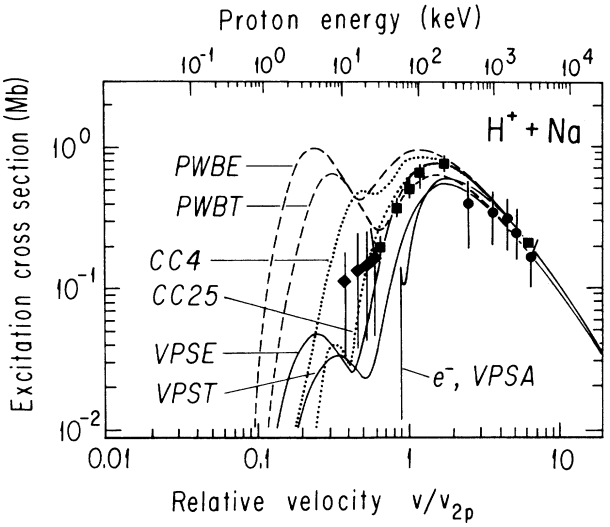

FIG. 6. Comparison between experimental and theoretical values of the excitation cross sections for proton- and electron-impact excitation of the Na $2p^5 3s^2$ term. *Experimental:* ♦, ♦, proton impact, Ref. 43; ♦, electron impact, Ref. 44. *Theoretical: CC*4 and *CC*25, 4- and 25-state close-coupling calculations, respectively, Ref. 45; *PWBE*, *PWBT*, *VPSE*, and *VPST*, present plane-wave Born and VPS approximation calculations. Labels ending in *E* denote use of experimental excitation energy values, whereas the ones ending in *T* denote results using theoretical energies.

between wave-function nodes and alignment minima, measurements of the alignment may be a unique way of explicitly observing the existence of nodes in atomic wave functions as well as a measure of their exact location.

It is true, of course, that some of this structure at low velocities will be "washed out" by the effects of temporary molecule formation by projectile and target, but it is to be seen to what extent. Experimental determination of alignment by detecting the autoionization electrons may also fail to reveal all of the features of Figs. 2

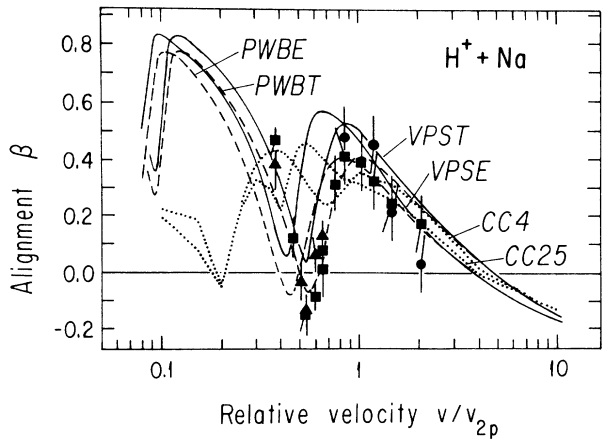

FIG. 7. Comparison between experimental and theoretical values of alignment of the Na $2p^5 3s^2\,^2P_{3/2}$ state excited by proton impact. *Experimental*: ♦, Ref. 30; ♦, Ref. 31; ♦, Ref. 43. *Theoretical*: See Fig. 6 for explanation of the curves.

and 4 due to post-collision interaction effects, i.e., when the later-emitted electrons are faster than and eventually overtake the scattered projectile, forcing it to experience two different atomic fields along its path receding from the target.

B. Comparison with experiment

Of all the alkali-metal atoms there exist experimental measurements only for Na, both for cross-section and alignment values. Figure 6 compares the present and close-coupling calculations with the available excitation cross-section measurements.[43,44] The agreement between experiment and essentially all theories is satisfactory for the case of electron impact, since the measurements are for fast electrons only. The agreement is also good for proton impact, at least down to about 30 keV, when comparison is made with the 25-state close-coupling calculation of Schöller and Briggs[45] and the present VPS approximation using experimental excitation energy values (curve *VPSE*). The two sets of measurements of Ref. 43 use different normalization techniques, the ones at higher energies have been normalized to the Born approximation value at $v_{\rm rel}=6.3$. If theoretical values are used for the excitation energy (see Table III, HS) the cross-section curves (*VPST* and *PWBT*) move to the right and have slightly decreased magnitude. If normali-

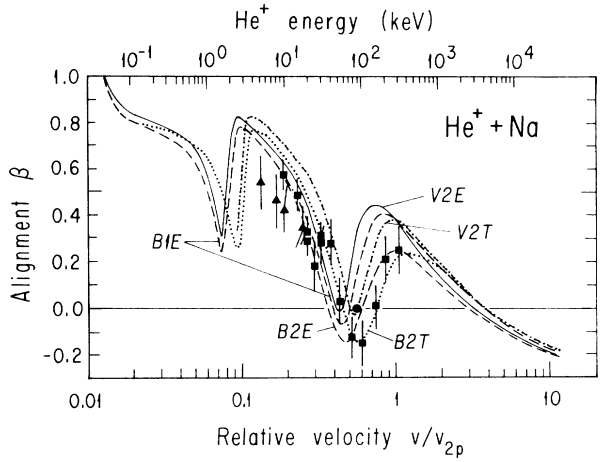

FIG. 8. Comparison between experimental and theoretical values of alignment of the Na $2p^5 3s^2\,^2P_{3/2}$ state excited by He^+ impact. *Experimental*: ●, Ref. 30; ♦, Ref. 31; ♦, Ref. 46. *Theoretical*: — — —, · · · ·, Born approximation; ——, —·—·—·, VPS approximation (see below). *B*1*E*, Born approximation assuming structureless projectile and experimental excitation energy; *B*2*E*, Born approximation assuming that the electron of the projectile is left in any state after collision and experimental excitation energy; *B*2*T*, Born approximation assuming that the electron of the projectile is left in any state after collision and theoretical excitation energy; *V*2*E*, VPS approximation assuming that the electron of the projectile is left in any state after collision and experimental excitation energy; *V*2*T*, VPS approximation assuming that the electron of the projectile is left in any state after collision and theoretical excitation energy.

zation were to be made with respect to these curves, the two experimental data sets would match very well around 20 keV energy. Agreement with the *VPST* curve would then also improve. A disagreement between experiment and the above theories should be expected below about 20 keV proton energies since the charge exchange channel becomes a significant contributor even to target excitation.[33] The above theoretical results do not include such contributions.

The obvious difference, from Fig. 2, between alignment values caused by protons and He^+ of equal impact velocity is also borne out by the experimental investigation of Hintermayer *et al.*[46] The two cases are shown separately on Figs. 7 and 8. In Fig. 7 the alignment measurements[46] for the Na excitation by proton impact are compared with the present Born and VPS approximation results as well as the close-coupling calculations of Schöller and Briggs.[45] Obviously, the Born approximation is yielding the best prediction of the measured data. It is surprising that although they predict the correct magnitude and shape of the alignment at higher impact energies, neither the 4-state nor the 25-state close-coupling calculations are able to predict the, by now, well-established minimum[30,31,46] around $v_{\rm rel}=4.5$. Since the alignment can essentially be expressed as a ratio of partial excitation cross sections [cf. Eq. (3)], the overall agreement in Fig. 7 implies that although the Born approximation overestimates the cross section at low energies, it predicts correctly the *relation* between the *partial* excitation cross sections. This appears not to be true for the VPS approximation or the close-coupling calculations[45] referred to here.

The systematic shift between the experimental curve and the Born approximation using experimental excitation energy (30.8 eV), has been the subject of considerable discussion in the past.[30–32] Theodosiou *et al.*[31] were able to reproduce the experimental curve by assuming that the $3s$ orbital wave function was radially expanded by the attraction of the incident proton and by using an energy-dependent expansion factor. Ziem and Morgenstern[32] performed semiclassical approximation calculations essentially identical in approximation level to the Born approximation. Their impact parameter analysis of the collision dynamics yielded that around $v_{\rm rel}=4.5$ the excitation of the target takes place when the proton is at about 1 a.u. in distance from the Na nucleus, i.e., well inside the $3s$ electronic cloud with average distance of about 4 a.u. Thus, one may imply that the $3s$ electron wave function should contract rather than expand. One could, however, also argue that the electron's passage through a sphere of radius 4 a.u. lasts a short time, compared to the total collision time between proton and Na. Therefore, the expansion, certain to take place at the beginning and end of the collision, is not compensated by the tendency, over a short time scale, to contract. This whole discussion dealing with time-independent fixed-in-space wave functions might be unnecessary, had we available potential curves and wave-function values of the system NaH^+ treated as a time-evolving molecule. In the absence of such information, I decided to repeat the calculation using the theoretically obtained excitation energy within the Hartree-Slater approximation, i.e., 38.2 eV (cf. Table III), since such a value would be more consistent with the wave functions used. The new results for both Born and VPS approximations are also shown in Fig. 7 as curves *PWBT* and *VPST*, respectively. The agreement of the Born prediction with experiment is impressive. Even the *VPST* curve is respectably close to experiment. A conclusion that might be drawn from this result is that the transition takes place, in the temporarily formed NaH^+ molecule, at the distance at which the potential curves corresponding to the target atom in $2p^6 3s$ and $2p^5 3s^2$ configurations, respectively, are about 38 eV apart. Again, this could be proven by a detailed molecular calculation which is presently not available to this author.

Figure 8 compares the experimental and theoretical alignment values for the case of He^+ impact excitation of Na. As discussed in Sec. II, various levels of approximation could be made in treating the contributions to the cross section and alignment from the projectile electron. The figure shows as a reference the Born curve *B1E* for a structureless projectile and experimental excitation energy. Since the experimental setup of Refs. 30, 31, and 46 did not determine the state of excitation of the projectiles after the collisions, the experimental data ought to be compared to the quantity $\sigma^{(2)}$, Eq. (10). The corresponding curves in the Born and VPS approximations are shown in Fig. 8 for both cases when experimental and theoretical energies are used. The feature of curve shifting, in going from experimental to theoretical excitation energies, which was observed in the proton-impact case is also present in the He^+ case. We see that the Born approximation results improve the agreement with experiment[30,46] when the contribution of the projectile's electron is fully accounted for. Again, the theoretical-energy Born curve yields an excellent agreement. the corresponding *VPS* curve gives also a respectable agreement.

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[1]H. Beutler and K. Guggenheimer, Z. Phys. **87**, 188 (1933).
[2]H. Beutler, Z. Phys. **91**, 131 (1934).
[3]H. Beutler and K. Guggenheimer, Z. Phys. **88**, 25 (1934).
[4]J. P. Connerade, W. R. S. Garton, and M. W. D. Mansfield, Astrophys. J. **165**, 203 (1971).
[5]H. W. Wolff, K. Radler, B. Sonntag, and R. Haensel, Z. Phys. **257**, 353 (1972).
[6]K. J. Nygaard, J. Chem. Phys. **49**, 1995 (1968).

[7]K. J. Nygaard, Phys. Lett. **51A**, 171 (1975).
[8]K. J. Nygaard and Y. B. Hahn, Phys. Rev. A **8**, 151 (1973).
[9]K. J. Nygaard and Y. B. Hahn, J. Chem. Phys. **58**, 3493 (1973).
[10]K. J. Ross, T. W. Ottley, V. Pejčev, and D. Rassi, J. Phys. B **9**, 3237 (1976).
[11]E. Breuckmann, B. Breuckmann, W. Melhorn, and W. Schmitz, J. Phys. B **10**, 3135 (1977).
[12]R. D. DuBois, L. Mortensen, and M. Rødbro, J. Phys. B **14**, 1613 (1981).
[13]V. Pejčev and K. J. Ross, J. Phys. B **10**, L291 (1977).
[14]S. N. Tiwary and D. K. Rai, J. Phys. B **8**, 1109 (1975).
[15]R. Srivastava and D. K. Rai, Phys. Lett. **57A**, 429 (1976).
[16]R. Srivastava and D. K. Rai, J. Phys. B **10**, 269 (1977).
[17]R. Srivastava, C. S. Singh, and D. K. Rai, J. Phys. B **15**, 1899 (1982).
[18]C. E. Theodosiou, Phys. Rev. A **16**, 2232 (1977).
[19]C. E. Theodosiou, J. Phys. B **10**, L353 (1977).
[20]C. E. Theodosiou, Abstracts of XII International Conference on the Physics of Electronic and Atomic Collisions, Gatlinburg 1981, edited by S. Datz, p. 769 (unpublished).
[21]S. N. Tiwary, J. Phys. B **14**, 2951 (1981).
[22]S. N. Tiwary, J. Phys. B **16**, L459 (1983).
[23]A. K. Liepinsh and R. K. Peterkop, [Opt. Spectrosc. **44**, 621 (1979)] Opt. Spektrosk. **44**, 1060 (1978).
[24]R. Peterkop and A. Liepinsh, J. Phys. B **11**, L27 (1978).
[25]R. Peterkop and A. Liepinsh, J. Phys. B **16**, L505 (1983).
[26]V. Schmidt, in *X-Ray and Atomic Inner-Shell Physics—1982,* Proceedings of the International Conference, University of Oregon, AIP Conf. Proc. No. 94, edited by B. Crasemann (AIP, New York, 1982), p. 544.
[27]R. Huster and W. Mehlhorn, Z. Phys. A **307**, 67 (1982).
[28]A. Niehaus, J. Phys. B **10**, 1845 (1977).
[29]H. G. M. Heideman, W. van de Water, and L. J. M. van Moergestel, J. Phys. B **13**, 2801 (1980).
[30]P. Ziem, R. Morgenstern, and N. Stolterfoht, Abstracts of the Proceedings of the Tenth International Conference on the Physics of Electronic and Atomic Collisions (Commissariat à l'Energie, Paris, 1977), p. 1002 (unpublished).
[31]C. E. Theodosiou, E. Breuckmann, B. Breuckmann, and W. Mehlhorn, J. Phys. B **12**, L689 (1979), and references therein; E. Breuckmann, Ph. D. thesis, University of Freiburg, Germany, 1979.
[32]P. Ziem and R. Morgenstern, J. Phys. B **13**, L299 (1980).
[33]C. E. Theodosiou, Phys. Rev. A **22**, 2556 (1980), and references therein.
[34]C. E. Theodosiou, J. Phys. B **13**, L113 (1980).
[35]C. E. Theodosiou, Phys. Lett. **83A**, 254 (1981).
[36]C. E. Theodosiou (unpublished).
[37]D. Petrini, J. Phys. B **14**, L617 (1981).
[38]C. E. Moore, *Atomic Energy Levels,* Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) Circ. No. 35 (U.S. GPO, Washington, D.C., 1971).
[39]J. P. Desclaux, Comput. Phys. Commun. **1**, 216 (1969).
[40]C. Froese-Fischer, Comput. Phys. Commun. **4**, 107 (1972).
[41]J. S. Briggs and K. Taulbjerg, *Structure and Collisions of Ions and Atoms,* Vol. 5 of *Topics in Current Physics,* edited by I. A. Sellin (Springer, Berlin, 1978), p. 105.
[42]U. Fano and J. H. Macek, Rev. Mod. Phys. **45**, 553 (1973).
[43]W. Mehlhorn, G. Kessler, T. Passarge, and W. Rave, Nucl. Instrum. Methods (to be published).
[44]G. Kessler, Diplomarbeit, University of Freiburg, Germany, 1984.
[45]O. Schöller and J. S. Briggs, in *Fundamental Processes in Atomic Collision Physics,* Vol. 134 of *NATO Advanced Study Institute, Series B: Physics,* edited by H. O. Lutz, J. S. Briggs, and H. Kleinpoppen (Plenum, New York, 1985); Abstracts of the XIV International Conference on the Physics of Electronic and Atomic Collisions, Palo Alto, 1985, edited by J. Coggiola, D. L. Huestis, and R. P. Saxon, p. 384 (unpublished).
[46]R. Hintermayer, T. Passarge, Z. Roller, R. Ruckteschler, and W. Mehlhorn, J. Phys. B **20**, 1059 (1987); R. Hintermayer, Diplomarbeit, Univeristy of Freiburg, Germany, 1983.