

nates the single-scattering cross sections of WDM and KC. The data at 90° was not compared with FM because of the non-normal incident electron beam direction, but the difference here between the experimental data and the WDM and KC calculations indicates that multiple scattering is even more of a problem, probably because the effective target thickness is greater than at 60° or 120° . Further investigations with atomic-beam targets are necessary

to determine whether the agreement with FM is fortuitous or whether multiple-scattering effects are really so important, even for so thin a low-atomic-number target. The other possibility is that the discrepancies between the experimental data and WDM and KC arise because of the breakdown of the plane-wave approximation. This possibility can only be examined after calculations based on exact wave functions become available.

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Photoionization of Sodium, Lithium, and Potassium by a Pseudopotential Method*

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A pseudopotential formalism is used to calculate the cross section for photoionization of sodium, lithium, and potassium for ejected electron energies from threshold to about 15 eV. Both the dipole length and dipole velocity matrix forms are computed. For sodium, the dipole length results are in good agreement with experiment away from the lowest threshold. The dipole velocity results for sodium, on the other hand, severely underestimate the cross section except very near threshold. For lithium, the dipole length and velocity results are less than the experimental results but agree well with other theoretical results. For potassium, the cross section exhibits the general shape of experimental curves.

I. INTRODUCTION

In principle, the cross sections for photoionization can be calculated when accurate wave functions are known for the states of the atoms and ions. In practice, assumptions have to be made in order to obtain the necessary wave functions. In a previous publication by the authors,¹ a pseudopotential formalism was used to calculate the photoionization cross section of sodium. The photoionization cross-section results, using the dipole length form of the matrix, were in very good agreement with experi-

ment. The object of this paper is to extend the work on sodium to include polarization effects and to apply the pseudopotential method to obtain photoionization cross sections of lithium and potassium.

The pseudopotential method² has been used extensively in solid-state physics and has only recently been applied to atomic collision processes.³⁻⁶ The general concept of the pseudopotential method is that a valence electron in an atom or a solid sees a weak net effective potential. Inside the core of the atom the nuclear potential acting on a valence electron is very strong and attractive. Also, in this

region the Pauli principle requires that the valence wave function be orthogonal to the orbitals of the core electrons. Thus the valence-electron wave function oscillates rapidly, corresponding to a high kinetic energy. The large negative potential energy inside the core of the atom and the large positive kinetic energy which the valence electron has there cancel to give a weak net effective potential. Thus a system of $(Z-1)$ core electrons and a valence electron can be approximated as a one-electron system with the effect of the core electrons and $(Z-1)$ protons being replaced by a weak (and usually repulsive) potential called the "pseudopotential." The pseudopotential used in this paper is not developed along the line of Philips and Kleinman² or Austin, Heine, and Sham,⁷ but along the model-potential method of Abarenkov and Heine.⁸ The only requirement on the pseudopotential is that it gives the same energy eigenstates as the real problem.

The pseudopotential formalism is especially suited to the alkali atoms. The valence electron and the closed-shell core are known to interact rather weakly, and thus the effects of the core upon the valence electron may be represented to a good approximation by some effective central potential. The alkali atoms are also well suited for comparison of theory to experiment, due to the ease with which they may be obtained as approximately monatomic vapors and to the conveniently low ionization potential.

The plan of the paper is as follows: In Sec. II the pseudopotential is used to calculate photoionization cross sections; in Sec. III the method of determining the pseudopotential is discussed; in Sec. IV our results are compared to experimental results and other theoretical work; and our conclusions are presented in Sec. V.

II. THEORY

The ionization of an atomic system by an external electromagnetic field is readily treated by perturbation theory using a semiclassical model for the interaction between bound electrons and the radiation field.⁹ In the dipole approximation, an electron ejected from the valence s state of an alkali atom will go into a continuum p state. Using a "single-channel" approximation and assuming that the differences in the core wave functions for the atom and the ion are negligible, the dipole length (L) and the dipole velocity (V) forms of the photoionization cross section are

$$\sigma^{(L,V)} = \frac{4}{3} \pi \alpha a_0^2 (I + k^2) |M^{(L,V)}|^2, \quad (1)$$

where I is the first ionization potential, k^2 is the energy of the ejected electron,

$$M^{(L)} = \int \psi_{ns}(r) r \psi_{kp}(r) dr, \quad (2)$$

and

$$M^{(V)} = \frac{2}{I + \epsilon} \int \psi_{ns}(r) \left(\frac{1}{r} \psi_{kp}(r) + \frac{d}{dr} \psi_{kp}(r) \right) dr. \quad (3)$$

In the above formulas, $\frac{4}{3} \pi \alpha a_0^2 = 8.56 \times 10^{-19} \text{ cm}^2$ and the remaining quantities are taken in the system of atomic units $\hbar = 1$, $e^2 = 1/m = 2$. The wave functions ψ_{ns} and ψ_{kp} are normalized reduced radial wave functions for the valence electron. The two alternative forms M^L and M^V are identical when the wave functions $\psi_{ns}(r)$ and $\psi_{kp}(r)$ are exact eigenstates of the same Hamiltonian.

One interesting feature about valence electrons of alkali atoms is the extent to which their observed properties parallel those to be expected from apparently crude models. One such model is the pseudopotential formalism. In introducing the pseudopotential formalism, the actual system is replaced by a one-electron system. The effect of the core electrons is represented by the pseudopotential V_p , where we choose the model form

$$V_p = Q_1 \frac{e^{-\delta_1 r}}{r^n} - \frac{\alpha_a}{(r^2 + d^2)^2} - \frac{\alpha_a}{(r^2 + d^2)^3}. \quad (4)$$

The pseudo-wave-functions satisfy the Schrödinger equation: for the bound s state

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} - V_p + \epsilon \right) \Phi_s(r) = 0 \quad (5)$$

and for the continuum p wave

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} - \frac{2}{r^2} - V_p + k^2 \right) \Phi_k(r) = 0. \quad (6)$$

The bound-state pseudo-wave-function is normalized so that

$$\int |\Phi_s(r)|^2 dr = 1. \quad (7)$$

The continuum pseudo-wave-function has the asymptotic form

$$\Phi_k(r) \sim k^{-1/2} \sin \left[kr - \frac{1}{2} \pi + (1/k) \ln(2kr) + \sigma_1 + \delta_1(k^2) \right]. \quad (8)$$

$\delta_1(k^2)$ is the non-Coulomb phase shift and $\sigma_1 = \arg \Gamma(2 + i/k)$.

The pseudo-wave-function Φ is a smoothly varying function inside the core. Since the wave function of the valence electron $\psi(r)$ must be orthogonal to the core states, $\psi(r)$ is obtained by

$$\psi(r) = \Phi(r) - \sum_c \langle \psi_c | \Phi \rangle \psi_c(r), \quad (9)$$

where ψ_c are the core-state wave functions. For the bound state, core states of the atom are used and for the continuum-state core states of the ion should be used. However, for the alkalis the differences in the core states of the atom and the singly ionized ion are negligible. Accurate core states have been calculated within the Hartree-Fock approximation by Clementi and others.¹⁰ The orthogonalized bound-state wave function ψ_{ns} is renor-

malized so that

$$\int |\psi_{ns}(r)|^2 dr = 1 \quad (10)$$

The continuum wave function ψ_{kp} is asymptotically normalized by Eq. (8). The pseudo-dipole-length cross section mentioned in this paper is

$$\sigma_p = 8.56(I + k^2) |M^{(p)}|^2 \times 10^{-19} \text{ cm}^2, \quad (11)$$

where the matrix element is calculated with the non-orthogonalized pseudo-wave-functions

$$M^{(p)} = \int \Phi_e(r) r \Phi_k(r) dr \quad (12)$$

III. EVALUATION OF PSEUDOPARAMETERS

The pseudopotential V_p is defined by Eq. (4). Values for the dipole polarizability α_d are taken from the best estimates available in the literature.¹¹ The values of the α_q and the screening constant d are chosen so that the pseudopotential reproduces, as closely as possible, the spectrum of f -state levels for the valence electron.¹² The resulting values of d are on the order of the radius of the core. The values of α_q are usually smaller than the corresponding quadrupole polarizabilities. The parameters Q_l and β_l are evaluated by requiring that the pseudo-wave-functions have the same energy spectrum as the lower l states of the valence electron of the alkali atom. Experimental energies with spin-orbit splitting subtracted off¹³ are used to evaluate Q and β .

Two methods are used to evaluate Q and β . The first method, suggested by Callaway and Laghos,⁵ requires that Q and β be chosen so that the eigenenergies of the first s and p pseudo-wave-functions agree exactly with the experimental energies of ns and np states of the valence electron of the alkali atom, where $n = 2, 3,$ and 4 for lithium, sodium, and potassium, respectively. Thus in the first method the parameters Q and β are independent of the orbital angular momentum l . Although the l -independent pseudopotentials give good results for sodium, in the general case Q and β should be functions of l . The effect of exchange can be considered as giving rise to a different potential for states of different angular momentum. The fact that this effect is small in sodium is evidenced by the success of Prokofjew¹⁴ in accounting for all the spectral levels of sodium on the basis of a single potential. For Li and K the effects of exchange can not be neglected.

Bardsley¹² has found values of Q and β for $n = 1$ (Yukawa form) for Li, Na, and K which are l dependent. He has also determined these with $n = 0$ (exponential form) for Li and Na. For a state with $l = 0$, the pseudoparameters Q_s and β_s are chosen so that the first two s -state energy levels of the pseudosystem agree exactly with the energies of the ground and first excited s state of the valence elec-

tron. Similarly, for a state with $l = 1$, Q_p and β_p are chosen so as to reproduce the correct energies for the first and second excited p states of the valence electron.

For bound states, the only requirement of the potential is that it yield correct energies over the energy range in which the potential is being used. However, for the continuum states, the requirement of the pseudopotential is that the potential yield accurate phase shifts.⁸ Bardsley's values of Q_p and β_p led to non-Coulomb p -wave phase shifts, which are shown in Table I to be in good agreement to the quantum defect values.

IV. RESULTS AND DISCUSSION

Equations (5) and (6) for the pseudo-wave-functions were solved numerically using Numerov's method. All integrals were evaluated numerically using a five-point formula. The results of our calculations are presented in Figs. 1-7, where they are compared with other calculations and experimental data (the ordinate axis in these figures is labeled in terms of the energy of the ejected electron in units of electron volts; $\epsilon = 13.6k^2$ eV). We shall discuss these separately in relation to each atom.

A. Sodium

In an earlier paper,¹ the authors have applied a pseudopotential method for sodium and obtained good agreement between the dipole length and experiment away from the lowest threshold. The pseudopotential in that work was of the form

$$V_p(r) = (Q/r)e^{-\beta r},$$

where $Q = 20.43$ and $\beta = 2.0475$. This potential exactly reproduces the experimental $3s$ and $3p$ energy levels of the valence electron but neglects polarization effects. Better agreement between theory and experiment is obtained by including polarization terms in the pseudopotential. Upon using the same

TABLE I. Calculated and quantum-defect non-Coulomb p -wave phase shifts in rads.

Element	k^2	$\delta_1(k^2)$		$\pi\mu(k^2)$
		Yukawa	Expt	Quantum defect
Na	0.0	2.684	2.685	2.687 ^a
	0.1	2.650	2.650	2.656
	0.2	2.618	2.619	2.632
Li	0.0	0.1482	0.1481	0.1488 ^b
	0.1	0.1549	0.1547	0.1568
	0.2	0.1614	0.1611	0.1652
K	0.0	2.235		2.234 ^c
	0.1	2.164		2.152
	0.2	2.100		2.070

^aReference 15.

^bCalculated from the tables in Ref. 13

^cReference 16.

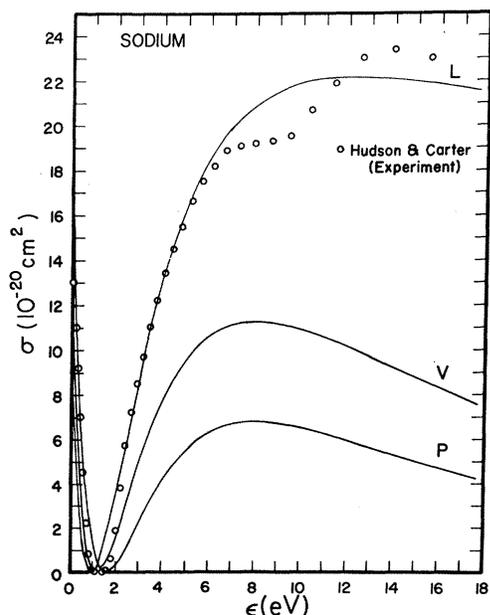


FIG. 1. Photoionization cross sections of sodium, using l -independent pseudopotential and including polarization effects. L and V indicate the length and velocity results from the full pseudopotential formalism while P is the pseudo-dipole-length cross section defined by Eq. (11). Experimental results of Hudson and Carter (Ref. 17) are given by the circles.

polarization terms as in Eq. (4) and setting $\alpha_d = 0.945a_0^3$, $\alpha_q = 1.523a_0^5$, and $d = 1.1$, the resulting potential exactly reproduces the experimental $3s$ and $3p$ energy levels of the valence electron for $Q = 16.437$ and $\beta = 1.77448$. The photoionization cross section for the pseudopotential with polarization included is compared to the experimental results of Hudson and Carter¹⁷ in Fig. 1. The l -independent pseudopotential method works for sodium but not for lithium and potassium.

A more general formalism is to make the pseudopotential parameters Q and β l dependent as indicated in Eq. (4). When this is done, Bardsley obtains the following parameters for the Yukawa form ($n=1$): $Q_s = 329.792$, $\beta_s = 3.858$ and $Q_p = 52.736$, $\beta_p = 2.403$.¹² The values of α_d , α_q , and d are the same as stated above. The resulting photoionization cross sections are compared to experiment in Fig. 2. Although the l -dependent pseudopotential cross sections do not seem to agree as well with experiment, the results are still good when compared to other theoretical results.

A slight improvement of the cross section can be obtained by changing from the Yukawa form to an exponential form ($n=0$). The corresponding pseudopotential parameters are $Q_s = 635.024$, $\beta_s = 4.534$ and $Q_p = 79.542$, $\beta_p = 2.922$. The resulting photoion-

ization cross sections are also shown in Fig. 2. The pseudopotential of the Yukawa form seems to give better results near the threshold, whereas the exponential form tends to give better results for higher photon energies. However, the difference does not seem to be significant for sodium.

The theoretical works of Seaton and Burgess and Seaton, Cooper, Boyd, Sheldon, and McGuire are compared to experiment in Fig. 3. Seaton¹⁸ computes the cross section using Hartree-Fock wave functions. Cooper¹⁹ uses a Hartree-Fock bound state and a localized form of the same Hartree-Fock potential as found in the bound-state calculations to compute the continuum orbital. The calculations of Boyd²⁰ consist of a central Hartree field approximation modified to include some correlation and polarization effects. Burgess and Seaton¹⁶ use the quantum-defect method to obtain the cross sections. Sheldon²¹ also used the quantum-defect method but adjusted the parameters to obtain agreement with the experimental cross section at threshold. McGuire²² used a central potential formalism with a model potential of the form $V(r) = 2z/r - \Delta$, $r \leq r_1$; $V(r) = 2/r$, $r \geq r_1$; $r_1 = 2(z-1)/\Delta$, where z and Δ are chosen to fit observed term values for the

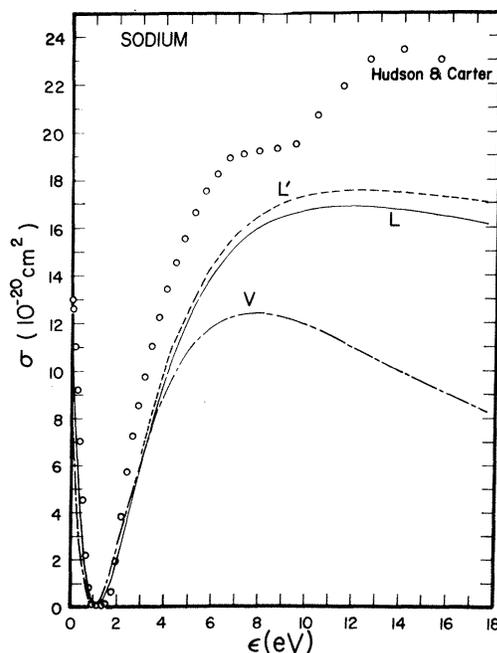


FIG. 2. Photoionization cross section of sodium using the l -dependent pseudopotential of Bardsley. L and V indicate the length and velocity forms of the matrix elements for the Yukawa form of pseudopotential. The dashed curve L' indicates the length form of the matrix element for the exponential form of the pseudopotential. Experimental results of Hudson and Carter (Ref. 17) are given by the circles.

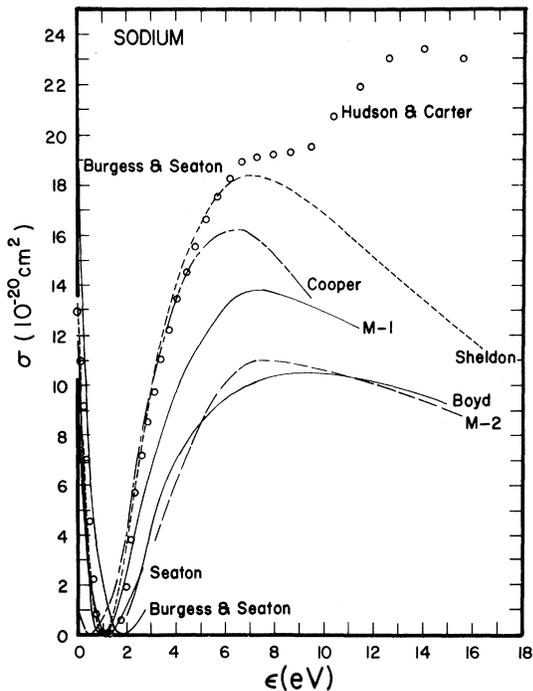


FIG. 3. Circles indicate the experimental results of Hudson and Carter (Ref. 17). The other curves are the theoretical calculations of Seaton (Ref. 18), Burgess and Seaton (Ref. 16), Cooper (Ref. 19), Boyd (Ref. 20), and Sheldon (Ref. 21). *M-1* indicates the curve for McGuire (Ref. 22) with $\Delta=18.6$ and *M-2* indicates the later results of McGuire (Ref. 23) using the Herman-Skillman potential.

various atoms. In a later calculation, McGuire²³ approximated the Herman and Skillman²⁴ potential by a series of straight lines. The parameters were then adjusted so that the model eigenvalues and those of Herman and Skillman were in reasonable agreement.

B. Lithium

The effect of replacing the core by a pseudopotential usually leads to a repulsive potential. This can be attributed to the Pauli exclusion principle, which inhibits an electron from penetrating into a region already occupied by electrons of the same symmetry. For lithium an electron in a *p* state is not excluded from the core by the Pauli principle. As a result, the *p*-state energy levels for lithium are lower than the hydrogen levels. The pseudopotential for the *p* states of lithium must thus be attractive, and thus a single pseudopotential will not generate both the *s* and *p* states.

Bardsley has also obtained the parameters for the *l*-dependent pseudopotential (4) for lithium.¹² The polarization terms in the pseudopotential are $\alpha_d = 0.1925a_0^3$, $\alpha_q = 0.112a_0^5$, and $d = 0.75$. The remaining parameters are as follows: for the Yukawa

form ($n = 1$), $Q_s = 53.524$, $\beta_s = 2.896$ and $Q_p = -3.710$, $\beta_p = 2.676$; for the exponential form ($n = 0$), $Q_s = 113.010$, $\beta_s = 3.616$ and $Q_p = -10.30$, $\beta_p = 3.569$.

The photoionization cross sections for lithium obtained for the Yukawa form and the exponential form of the pseudopotential are the same to three significant figures. Thus only one plot of cross section versus photon energy is shown, and this is given in Fig. 4 in comparison with the experimental results of Hudson and Carter.¹⁷ The results of our calculations for lithium are in good agreement with experiment near the threshold. However, away from threshold our calculations fall off faster than experiment.

Some previous theoretical results are given in Fig. 5. Stewart,²⁵ Sewell,²⁶ and Chang and McDowell²⁷ have each found the photoionization cross section using wave functions calculated within the Hartree-Fock approximation. Sewell's results are in good agreement with experiment, but disagree with the results of Stewart and of Chang and McDowell which are in agreement. Matese and LaBahn²⁸ have also done a Hartree-Fock calculation, but did not report their results which were for all purposes the same as Chang and McDowell's results. Thus it would seem that the results of Stewart given in Fig. 5 are a good indication of the photoionization cross section of lithium within the Hartree-Fock approximation. It is not known why the results of Sewell are different. Also shown in

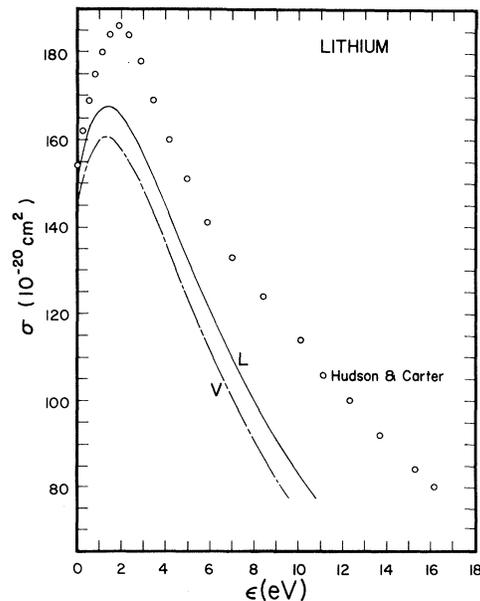


FIG. 4. Photoionization cross sections of lithium, using the Yukawa form of Bardsley's pseudopotential. *L* and *V* indicate the length and velocity forms of the matrix elements. Experimental results of Hudson and Carter (Ref. 17) are given by the circles.

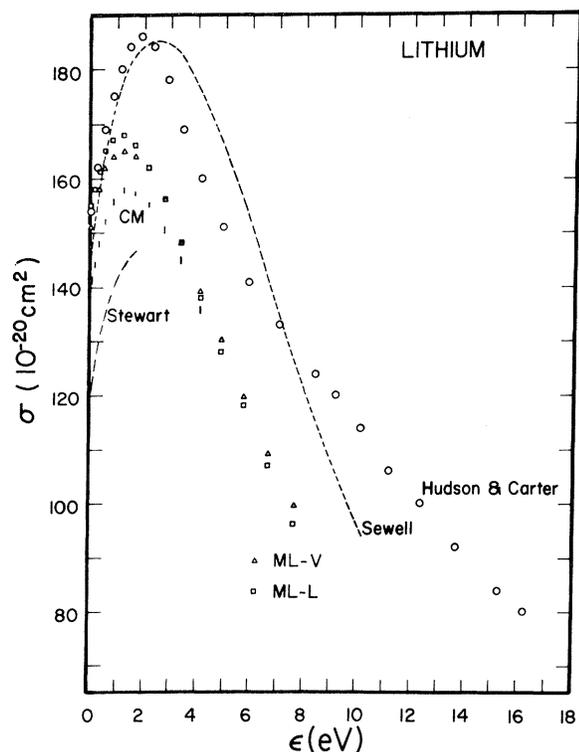


FIG. 5. Other calculations of photoionization cross section of lithium. The dashed curve is the length form of the Hartree-Fock result of Stewart (Ref. 25). The short dashes represent the length form of the Hartree-Fock result of Sewell (Ref. 26). The vertical bars marked CM indicate the extent of the length and velocity calculations of Chang and McDowell (Ref. 27), using many-body perturbation theory. ML-L and ML-V indicate the length and velocity results of Matese and LaBahn (Ref. 28), using the method of polarized orbitals. Experimental results of Hudson and Carter (Ref. 17) are given by circles.

Fig. 5 are the results Chang and McDowell²⁷ obtained by using the Brueckner-Goldstone many-body perturbation theory, and the results of Matese and LaBahn²⁸ who obtained the photoionization cross section of lithium by method of polarized orbitals.

C. Potassium

A pseudopotential which is independent of angular momentum l can be found for potassium. The parameters are $Q = 7.5656$, $\beta = 0.88715$, $\alpha_d = 5.40a_0^3$, $\alpha_q = 17.6a_0^5$, and $d = 1.5$. The dipole length form of the cross section at threshold was $2.34 \times 10^{-20} \text{ cm}^2$, but the cross section increased monotonically with energy. This is similar to the results Bates²⁹ obtained for a dipole polarizability greater than $11a_0^3$. Bates used solutions of the Hartree-Fock equations solved by Hartree and Hartree³⁰ for the bound states, and for the continuum state he neglected exchange in the Hartree-Fock equations but included

a polarization potential of the form $V(r) = -P/(r^2 + d^2)^2$. He found that the polarizability P had a great influence on the behavior of the cross section versus energy. His best agreement with experiment was obtained for $P = 10.46a_0^3$. In the present work, calculations were made using the pseudopotential method and varying the dipole polarizability between 0 and $10.46a_0^3$. But for the dipole length form, a minimum was never obtained using the l -independent pseudopotential.

In the case of the l -dependent pseudopotential, the energy dependence of the photoionization cross section closely resembles the general shape of the experimental data. The parameters obtained from Bardsley¹² for the Yukawa form ($n=1$) of the pseudopotential are $\alpha_d = 5.47a_0^3$, $\alpha_q = 12a_0^5$, $d = 1.4$, $Q_s = 1337.0724$, $\beta_s = 3.424834$, $Q_p = 115.37214$, and $\beta_p = 1.877117$. The quadrupole polarizability was chosen so as to reproduce the correct f -state energy levels of potassium. It is somewhat smaller in magnitude than the best theoretical calculations which give $\alpha_q = 16.2$. The l -dependent pseudopotential results are compared to the experimental results of Hudson and Carter³¹ in Fig. 6. Although the curve does have a minimum, the agreement between theory and experiment is not as good for potassium as it is for sodium and lithium.

Calculations were also made using different values for the polarizability. Somewhat better agreement between theory and experiment is obtained by increasing the polarizability. For $\alpha_d = 10.46a_0^3$, α_q

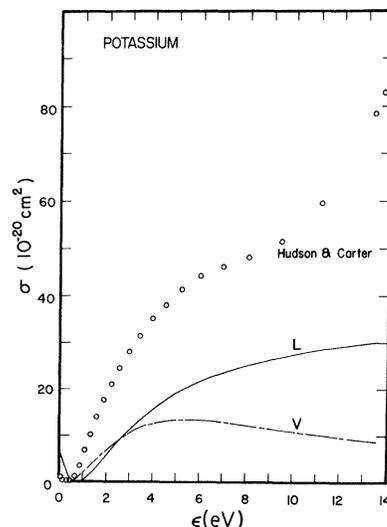


FIG. 6. Photoionization cross section of potassium, using the pseudopotential of Bardsley. L and V indicate the length and velocity forms of the matrix element. The circles indicate the experimental results of Hudson and Carter (Ref. 31) using the vapor-pressure data of Nesmeyanov.

$= 0.0$, $d = 1.4$, $n = 1$, $Q_s = 129.101$, $\beta_s = 2.11725$, $Q_p = 40.025$, and $\beta_p = 1.3924$, the adjusted dipole length curve falls about midway between the dipole length curve and the experimental points in Fig. 6. However, the position of the minimum does not seem to be extremely sensitive to changes in the polarization parameters, contrary to the results obtained by Bates.²⁹ The cross section is sensitive, though, to small changes in the energy spectrum used to compute the pseudopotential (cf. the best-fit curve L' in Fig. 7).

Other theoretical results for potassium are illustrated in Fig. 7. The results of Sheldon²¹ and McGuire²² are obtained by adjusting parameters to give a best fit to experimental results. Also included in Fig. 7 is a best-fit curve obtained using the pseudopotential method. The best-fit curve was obtained by varying the parameters Q_p and β_p and using Bardsley's values for the remaining parameters. For a fixed Q_p , β_p is chosen so that the energy of the first p state of the pseudosystem equals the $4p$ energy level of potassium. For each set of values Q_p and β_p , the cross section is calculated and compared to experimental results at threshold. For $Q_p = 30$ and $\beta_p = 1.37117$, the calculated results is approximately equal to the experimental results of $1.2 \times 10^{-20} \text{ cm}^2$. For this Q_p and β_p , the energy of the second p state of the pseudosystem is -0.0942076 Ry , compared to -0.0938238 Ry , the energy¹³ of the $5p$ level of potassium. For energies

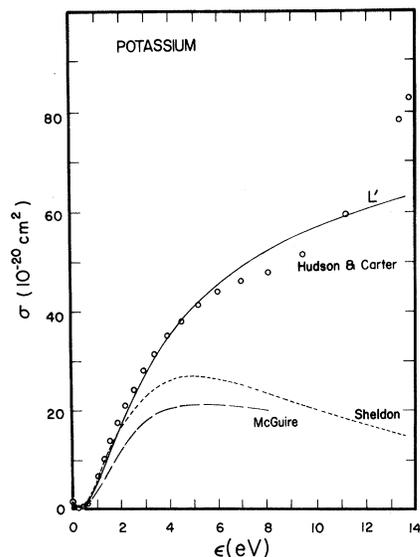


FIG. 7. Photoionization cross section of potassium. The short-dash curve indicates the adjusted quantum-defect results of Sheldon (Ref. 21). The dash curve indicates the results of McGuire (Ref. 22) for $\Delta = 6.20$. L' is a best-fit curve obtained in this paper by adjusting the pseudopotential parameters. The experimental results of Hudson and Carter (Ref. 31) are given by the circles.

above 2 eV, the cross section obtained by adjusting the pseudopotential are in much better agreement with experiment than previous theoretical calculations.

Calculations for the photoionization of potassium are complicated by many factors. The minimum in the cross section occurs very near threshold. The spin-orbit effect for potassium is much larger than for sodium. Also the $(3p)^5(4s)^2$ transitions in potassium are very important in the absorption spectrum and probably affects the photoionization cross section for the energy range discussed in this paper. Thus it is not too surprising that the results for potassium do not seem to be as good as the results of sodium and lithium.

V. CONCLUSION

The photoionization cross sections for the alkalis are very sensitive to the wave functions because of the high degree of cancellation which occurs in the matrix elements, Eqs. (5) and (6). This sensitivity seems to be greatest in potassium.¹⁶ Previous theoretical calculations are in good agreement with experiment near threshold, but for energies above a few electron volts the calculated cross sections decrease with increasing energy much faster than the experimental results would indicate. The present pseudopotential calculations also fall off faster than experiment for higher energies, but much less so than previous theoretical works. Thus it is found that pseudopotentials, evaluated from experimentally determined energy spectra, yield qualitatively good approximations for the photoionization cross section.

A comparison of the pseudopotential method and the quantum-defect method¹⁶ shows many similarities. In both methods, model parameters are chosen to fit selected experimental information and the results used to predict additional phenomena. The quantum-defect method has the advantages of being more analytical with essentially all the analytical analysis already done by Seaton and co-workers. The pseudopotential method entails specific calculations for each system being studied. However, the pseudopotential method might be expected to give better results than the quantum-defect method, since the quantum-defect method is equivalent to setting the pseudopotential equal to zero and truncating the wave functions at some finite radius to avoid the singularity at the origin.

In regard to predicting photoionization cross sections, a relatively crude model pseudopotential yields superior results over the quantum-defect method for at least simple hydrogenlike systems such as the alkali metals.

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High-Energy Atomic Charge Transfers*

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The usual conclusions concerning the energy dependence of high-energy atomic charge transfer are shown to depend critically upon the short-range singularity of the Coulomb potential. The problem is reexamined for the case of smooth potentials. All the previous conclusions concerning the high-energy dependence of the various approximations are changed.

The problem of the high-energy dependence of the charge-exchange cross section is a subtle mathematical problem which has received a good deal of attention.¹ Briefly, the current situation is this: The first Born approximation for the charge-exchange cross section of a proton plus an atom behaves as E^{-6} at sufficiently high energy with the precise coefficient in doubt.¹ For the *very special case* of distinguishable protons on hydrogen, there is a backward peak which yields a cross section

proportional to E^{-3} with an extremely small coefficient.² A further complication of the situation arises from the inclusion of second-order processes through the second Born approximation or the impulse approximation.³ These contribute a term to the cross section proportional to $E^{-11/2}$. Again the coefficient depends upon the theoretical approach. Thus, the second-order terms dominate the leading first-order terms, (E^{-6}). This has been taken as evidence to substantiate the doubt which has been