The Photoionization of Lithium, Sodium, and Potassium and the Photodetachment of the Negative Hydrogen Ion.

Richard Lee Smith
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## Part I: PHOTOIONIZATION OF LITHIUM, SODIUM, POTASSIUM

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ABSTRACT

The dissertation is a two part work. Part I is a separable entity from Part II. In Part I 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 compare favorably with other theoretical results. For potassium the cross section exhibits the general shape of experimental curves.

In Part II the variational method proposed by F.E. Harris and extended by R.K. Nesbet is employed to obtain wave functions for the singlet p-wave continuum functions of the negative hydrogen ion, using a 1s-2s-2p close coupling approach. The bound-free absorption coefficient is calculated using length, velocity, and acceleration forms of the dipole matrix element. The results of these calculations are presented. Particular attention is given to the energy region near 0.751 ryd where the $^1P$ shape resonance exists. Comparison of the results from the length, velocity and acceleration operator methods indicate that the wave functions obtained by this variational method are sufficiently accurate for calculating the photodetachment of $H^-$. 

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PART I - PHOTOIONIZATION OF LITHIUM, SODIUM, POTASSIUM
SECTION I-1

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 author,\textsuperscript{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 experiment. The object of this work 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 method\textsuperscript{2} has been used extensively in solid state physics and has only recently been applied to atomic collision processes.\textsuperscript{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 Kleinman\(^2\) 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 Part I is as follows: Section I-2 presents the pseudopotential method as applied to calculate photoionization cross sections; in Section I-3 the method of determining the pseudopotential is discussed; in Section I-4 the results are compared to experimental results and other theoretical work; the conclusions are presented in Section I-5.
SECTION I-2

THEORY

The ionization of an atomic system by an external electromagnetic field is readily treated by perturbation theory using a semi-classical 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

\[
\sigma^{(L,V)} = \frac{\hbar}{3} \pi a_o^2 \left(I + k^2\right) |M^{(L,V)}|^2
\]

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

\[
M^{(L)} = \int \psi_{ns}(r) r \psi_{kp}(r) dr
\]

and

\[
M^{(V)} = \frac{2}{I + k^2} \int \psi_{ns}(r) \left[ \frac{1}{r} \psi_{kp}(r) + \frac{d}{dr} \psi_{kp}(r) \right] dr.
\]

In the above formulas \(\frac{\hbar}{3} \pi a_o^2 = 8.56 \times 10^{-19} \text{cm}^2\) and the remaining quantities are taken in the system of atomic units \(\hbar = 1\), \(e^2 = \frac{1}{m} = 2\).
The wave functions \( \psi_{ns} \) and \( \psi_{kp} \) are normalized reduced radial wave functions for the valence electron. The two alternative forms, \( M^L \) and \( N^V \), 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

\[
V_p = Q \frac{e^\frac{-\beta}{r}}{r^n} - \frac{\alpha_d}{(r^2+d^2)^2} - \frac{\alpha_q}{(r^2+d^2)^3}
\]

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

\[
\left[ \frac{d^2}{dr^2} + \frac{2}{r} - V_p + \epsilon \right] \phi_s(r) = 0
\]

and for the continuum p-wave

\[
\left[ \frac{d^2}{dr^2} + \frac{2}{r} - \frac{2}{r^2} - V_p + k^2 \right] \phi_k(r) = 0.
\]

The bound state pseudo wave function is normalized so that

\[
\int |\phi_s(r)|^2 dr = 1
\]
The continuum pseudo wave function has the asymptotic form
\[ \psi_k(r) \sim k^{-\frac{1}{2}} \sin [k r - \frac{\pi}{2} + \frac{1}{2} \ln(2kr) + \sigma_1 + \delta_1(k^2)]. \tag{I.8} \]

\( \delta_1(k^2) \) is the non-coulomb phase shift and \( \sigma_1 = \arg \Gamma(2 + \frac{i}{k}). \)

The pseudo wave function \( \psi \) is a smoothly varying function inside the core. The actual wave function of the valence electron must be orthogonal to the core states. \( \Psi(r) \) is the pseudo wave function properly orthogonalized to the core state wave functions \( \psi_c \),

\[ \Psi(r) = \psi(r) - \sum_c \langle \psi_c | \psi \rangle \psi_c(r). \tag{I.9} \]

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 \( \Psi_{ns} \) is re-normalized so that

\[ \int |\Psi_{ns}(r)|^2 \, dr = 1. \tag{I.10} \]

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

\[ \sigma_p = 8.56 \, (1 + k^2) |M(p)|^2 \times 10^{-19} \, \text{cm}^2. \tag{I.11} \]
where the matrix element is calculated with the non-orthogonalized pseudo wave functions,

\[ M(p) = \int \hat{\phi}_e(r) r \hat{\phi}_k(r) dr \]
EVALUATION OF PSEUDO PARAMETERS

The pseudopotential $V_p$ is defined by Eq. (1.4). Values for the dipole polarizability, $\alpha_q$ are taken from the best estimates available in the literature.\textsuperscript{11} The values of the $\alpha_q$ 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.\textsuperscript{12} The $f$-levels are used to determine $\alpha_q, d$ because for a large $\ell$ value the centrifugal term will dominate over the first term in Eq. (1.4) and one can set $Q_\ell = 0$. The resulting values of $d$ are on the order of the radius of the core. The values of $\alpha_q$ are usually smaller than the corresponding quadrupole polarizabilities. The parameters $Q_\ell$ and $\beta_\ell$ are evaluated by requiring that the pseudo wave functions have the same energy spectrum as the lower $\ell$ states of the valence electron of the alkali atom. Experimental energies with spin-orbit splitting subtracted off\textsuperscript{13} are used to evaluate $Q$ and $\beta$.

Two methods are used to evaluate $Q$ and $\beta$. The first method, suggested by Callaway and Laghos\textsuperscript{5}, requires that $Q$ and $\beta$ be chosen so that the eigen-energies of the first $s$- and $p$-pseudo wave functions agree exactly with the experimental energies of the $ns$- 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 $\beta$ are independent of the orbital angular momentum $\ell$. Although the $\ell$-independent pseudopotentials give good results for sodium, in the general case $Q$ and $\beta$ should be functions of $\ell$. 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 Prokof'jew 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.

Bardsley has found values of $Q$ and $\beta$ for $n = 1$ (Yukawa form) for Li, Na, and K which are $\ell$-dependent. He has also determined these with $n = 0$ (exponential form) for Li and Na. For a state with $\ell = 0$, the pseudo parameters $Q_s$ and $\beta_s$ are chosen so that the first two $s$-state energy levels of the pseudo system agree exactly with the energies of the ground and first excited $s$-state of the valence electron. Similarly for a state with $\ell = 1$, $Q_p$ and $\beta_p$ 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 pseudo-potential is that the potential yield accurate phase shifts. Bardsley's values of $Q_p$ and $\beta_p$ led to non-coulomb $p$-wave phase shifts which are shown in Table I to be in good agreement to the quantum defect values.
SECTION I-4

RESULTS AND DISCUSSION

Equations (I.5) and (I.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 the calculations are presented in Figures 1 through 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; $\epsilon(eV) = 13.6 k^2$).

A - SODIUM

In an earlier paper the author has 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

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

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 polarization terms as in Eq. (I.4)
and setting $\alpha_d = 0.945 a^3_0$, $\alpha_q = 1.523 a^5_0$ 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 Carter$^{17}$ in Figure 1. $L$ and $V$ indicate the dipole length and velocity results from the full pseudopotential formalism while $P$ is the pseudo-dipole length cross section defined by Eq. (1.11).

A more general formalism is to make the pseudopotential parameters $Q$ and $\beta$ $\ell$-dependent as indicated in Eq. (1.4). When this is done, Bardsley obtains the following parameters for the Yukawa form ($n=1$); $Q_s = 329.792$, $\beta_s = 3.858$ and $Q_p = 52.736$, $\beta_p = 2.403$. The values of $\alpha_d$, $\alpha_q$, and $d$ are the same as stated above. The resulting photoionization cross sections are compared to experiment in Figure 2. Although the $\ell$-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 dipole length photoionization cross sections, labeled $L'$, are shown in Figure 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, Burgess and Seaton, Cooper, Boyd, Sheldon, and McGuire are compared to experiment in Figure 3. Seaton\textsuperscript{18} computes the cross section using Hartree-Fock wave functions. Cooper\textsuperscript{19} 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 Boyd\textsuperscript{20} consist of a central Hartree field approximation modified to include some correlation and polarization effects. Burgess and Seaton\textsuperscript{16} use the quantum defect method to obtain the cross sections. Sheldon\textsuperscript{21} also used the quantum defect method but adjusted the parameters to obtain agreement with the experimental cross section at threshold. McGuire\textsuperscript{22} uses a central potential formalism with a model potential of the form $V(r) = 2z/r - \Delta$, $r < r_1$; $V(r) = 2/r$, $r > r_1$; $r_1 = 2(z-1)/\Delta$, where $z$ and $\Delta$ are chosen to fit observed term values for the various atoms. In a later calculation, McGuire\textsuperscript{23} approximated the Herman and Skillman\textsuperscript{24} 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 so a single pseudopotential will not generate both the s-states and p-states.

Bardsley has also obtained the parameter for the l-dependent pseudopotential (I.4) for lithium. The polarization terms in the pseudopotential are, \( \alpha_d = 0.1925 \ a_0^3 \), \( \alpha_p = 0.112 \ a_0^5 \), and \( \alpha = 0.75 \). The remaining parameters are as follows: for the Yukawa form (n=1), \( \alpha_s = 53.524 \), \( \beta_s = 2.896 \) and \( \alpha_p = -3.710 \), \( \beta_p = 2.676 \); for the exponential form (n=0) \( \alpha_s = 113.010 \), \( \beta_s = 3.616 \) and \( \alpha_p = -10.30 \), \( \beta_p = 3.569 \).

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. The results of the calculations for lithium are in good agreement with experiment near the threshold. However, away from threshold the calculations fall off faster than experiment.

Some previous theoretical results are given in Figure 5. Stewart, Sewell, and Chang and McDowell have each found the photoionization cross section using wave functions calculated within
the Hartree-Fock approximation. Sewell's results are in good agree-
ment with experiment, but disagree with the results of Stewart and
of Chang and McDowell which are in agreement. Matese and LaBahn\textsuperscript{28}
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
Figure 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 Figure 5
are the results Chang and McDowell\textsuperscript{27} obtained by using the Brueckner-
Goldstone many-body perturbation theory, and the results of Matese
and LaBahn\textsuperscript{28} 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: \( Q = 7.5656, \)
\( \beta = .88715, \alpha_d = 5.40 a_o^3, \alpha_q = 17.6 a_o^5, \) and \( d = 1.5. \) The dipole
length form of the cross section at threshold was \( 2.34 \times 10^{-20} \) cm\(^2\),
but the cross section increased monotonically with energy. This is
similar to the results Bates\textsuperscript{29} obtained for a dipole polarizability
greater than \( 11 a_o^3. \) Bates used solutions of the Hartree-Fock
equations solved by Hartree and Hartree\textsuperscript{30} 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
\[ V(r) = - \frac{P}{(r^2 + d^2)^2} \]. 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 \( P = 10.46 \, a_o^3 \).

In the present work calculations were made using the pseudopotential method and varying the dipole polarization between zero and \( 10.46 \, a_o^3 \). But for the dipole length form a minimum was never obtained using the \( \lambda \)-independent pseudopotential.

In the case of the \( \lambda \)-dependent pseudopotential, the energy dependence of the photoionization cross section closely resembles the general shape of the experimental data. The parameters obtained from Bardsley\(^1\)\(^2\) for the Yukawa form (\( n=1 \)) of the pseudopotential are: 

\[ \alpha_d = 5.47 \, a_o^3, \quad \alpha_q = 12, \quad a_o^5, \quad d = 1.4, \quad Q_s = 1337.0724, \quad \beta_s = 3.424834, \quad Q_p = 115.37214 \] and \( \beta_p = 1.87717 \). 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 \( \lambda \)-dependent pseudopotential results are compared to the experimental results of Hudson and Carter\(^3\)\(^1\) in Figure 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 \( \alpha_d = 10.46 \, a_o^3 \), \( \alpha_q = 0.0 \), \( d = 1.4 \), \( n = 1 \), \( Q_s = 129.101 \), \( \beta_s = 2.11725 \), \( Q_p = 40.025 \), and \( \beta_p = 1.3924 \), the adjusted dipole length curve falls about midway between the dipole length curve and the experimental points in Figure 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. 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 Figure 7).

Other theoretical results for potassium are illustrated in Figure 7. The results of Sheldon and McGuire are obtained by adjusting parameters to give a best fit to experimental results. Also included in Figure 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 pseudo system 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 β_p = 1.37117, the calculated result is approximately equal to the experimental result of 1.2 x 10^{-20} cm^2. For this Q_p and β_p, the energy of the second p-state of the pseudo system is -0.0942076 ry, compared to -0.0938238 ry the energy of the 5p level of potassium. For energies 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 effects 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.
SECTION I-5

CONCLUSION

The photoionization cross sections for the alkalis are very sensitive to the wave functions due to the high degree of cancellation which occurs in the matrix elements, Eq. (I.5 - I.6). This sensitivity seems to be greatest in potassium. 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 sections.

A comparison of the pseudopotential method and the quantum defect method 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 coworkers. 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 pseudo-potential 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 hydrogen-like systems such as the alkali metals.
Table I. Calculated non-coulomb and quantum defect p-wave phase shifts in radians

<table>
<thead>
<tr>
<th>Element</th>
<th>$K^2$</th>
<th>$\delta_1(k^2)$ Yukawa</th>
<th>Exp.</th>
<th>$\pi\mu(k^2)$ Quantum Defect</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na</td>
<td>0.0</td>
<td>2.684</td>
<td>2.685</td>
<td>2.687$^a$</td>
</tr>
<tr>
<td></td>
<td>0.1</td>
<td>2.650</td>
<td>2.650</td>
<td>2.656</td>
</tr>
<tr>
<td></td>
<td>0.2</td>
<td>2.618</td>
<td>2.619</td>
<td>2.632</td>
</tr>
<tr>
<td>Li</td>
<td>0.0</td>
<td>0.1482</td>
<td>0.1481</td>
<td>0.1488$^b$</td>
</tr>
<tr>
<td></td>
<td>0.1</td>
<td>0.1549</td>
<td>0.1547</td>
<td>0.1568</td>
</tr>
<tr>
<td></td>
<td>0.2</td>
<td>0.1614</td>
<td>0.1611</td>
<td>0.1652</td>
</tr>
<tr>
<td>K</td>
<td>0.0</td>
<td>2.235</td>
<td></td>
<td>2.234$^c$</td>
</tr>
<tr>
<td></td>
<td>0.1</td>
<td>2.164</td>
<td></td>
<td>2.152</td>
</tr>
<tr>
<td></td>
<td>0.2</td>
<td>2.100</td>
<td></td>
<td>2.070</td>
</tr>
</tbody>
</table>

$^a$Reference 15

$^b$Calculated from the tables in Ref. 13

$^c$Reference 16
Figure 1  Photoionization cross sections of sodium, using $\lambda$-independent pseudopotential and including polarization effects. $L$ and $V$ indicate the length and velocity results from the full pseudopotential formalism while $P$ is the pseudodipole length cross section defined by Eq. (I.11). Experimental results of Hudson and Carter (Ref. 17) are given by the circles.
Figure 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.
Figure 3 The 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.
Figure 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.
Figure 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.
Figure 6 Photoionization cross section of potassium, using the pseudo-potential 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.
Figure 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.
PART II - PHOTODETACHMENT OF NEGATIVE HYDROGEN ION
SECTION II-1

INTRODUCTION

The negative hydrogen ion, \( H^- \) is the principle source of opacity in the solar atmosphere. This astrophysical importance of negative ions was first noted by Wildt\(^{32}\) in 1939. Wildt pointed out that in an atmosphere containing both metal and hydrogen atoms the ionization of the metal atoms can supply the electrons necessary for the formation of negative hydrogen ions.

The electron affinity of hydrogen is due to incomplete screening of the nucleus and to the polarization of the hydrogenic core. Although a neutral atom exerts an attractive force on an electron, there are a limited number of stationary states for attached electrons. This is due to the short range of the effective attractive field in which the electron moves. Also the Pauli Principle limits the number of available states. For the negative hydrogen ion there is only the one bound state; excited bound states do not exist. Thus the atomic absorption coefficient is identical to the cross-section for the photodetachment of an electron.

In 1940, using the photodetachment results of Massey and Bates,\(^{33}\) Stromglen\(^{34}\) was able to produce a theory of the solar atmosphere with no principal discrepancies. However Wildt's\(^{35}\) investigation on the theoretical relation between the color-temperature and the effective-temperature of stars did have discrepancies. The maximum of the
photodetachment curve needed to be moved from 4000Å toward larger wavelengths.

By 1959 the photodetachment curve was known precise enough for astronomical purposes. The maximum of the photodetachment curve was approximately $4.5 \times 10^{-17} \text{ cm}^2$ and located near 8200Å. The improvement in the photodetachment results was mainly due to Chandrasekhar and his co-workers. Chandrasekhar was the first to point out the need for more variational parameters in the expansion of the bound state wave function of $\text{H}^-$. He also noted that the dipole velocity photodetachment results are more stable to different bound states than the length results and thus are probably more accurate. The main motivation of the work after 1960 was not necessarily to obtain more accurate photodetachment results, but rather to show the capabilities of other theories in predicting accurate photodetachment results. This is one reason that the present work was undertaken.

Nesbet has formulated a procedure that is readily applied to atomic scattering problems. Seiler, Oberoi, and Callaway have applied this method to the slow collisions of electrons and positrons with atomic hydrogen. They calculated the appropriate phase shifts and cross sections. Using the Nesbet procedure or algebraic close coupling method one can also determine the wave function of the scattered electron in an analytic form. If an accurate wave function is known many other properties of the scattered electron can be easily obtained. Thus it is of interest to investigate the
accuracy of a wave function generated by the algebraic close coupling method. Using the knowledge that the photodetachment results are equal in the length, velocity, and acceleration dipole approximation for exact wave functions, one can use photodetachment calculations for H\textsuperscript{-} to determine the accuracy of the wave functions generated by the algebraic close coupling method.

Once the wave functions were found to be accurate, the work was extended into the energy region where inelastic processes are possible and a multichannel formalism is needed. Just above the n=2 level there exists a \textsuperscript{1}P resonance. Its contribution to the photoabsorption cross section is investigated.

The plan of Part II is as follows: in Section II-2 the analysis for determining the wave functions is given; in Section II-3 the method of determining photodetachment cross-sections is discussed; in Section II-4 the photodetachment results in the non-resonance region are discussed; in Section II-5 the photodetachment results for the \textsuperscript{1}P resonance are discussed and the conclusions are presented.
SECTION II-2

WAVE FUNCTIONS

A - Bound State

In this section, the wave functions which are needed for calculating the photodetachment cross section of H\(^-\) are discussed. The procedure for calculating the bound state wave function of H\(^-\) is discussed in part A and in part B the Nesbet method for obtaining the scattered wave function is described.

Three different bound states are used in this work. The author obtained two bound states, one which includes the three hydrogen channels 1s, 2s, and 2p and one which includes four channels 1s, 2s, 2p, and 2p. The 2p is the pseudo state of Burke, Gallaher, and Geltman\(^{39}\) which was chosen to reproduce the full polarizability of the ground state of H.

\[
R_{2p} = -0.966 \ r(1 + \frac{1}{2}r)e^{-r} + 0.340 \ r e^{-r/2}
\]  

A six channel bound state obtained by Matese and Oberoi\(^{40}\) which consists of three hydrogen states 1s, 2s, and 2p and three pseudo states 3s, 3p, and 3d was also used. The pseudo-states were chosen to be of the form
\[ R_{3s} = N_s (1 + \alpha_s r) e^{-\eta_s r} + \lambda_{ls} R_{ls} + \lambda_{2s} R_{2s} \]

\[ R_{3p} = N_p (1 + \alpha_p r) e^{-\eta_p r} + \lambda_{2p} R_{2p} \]

\[ R_{3d} = N_d (1 + \alpha_d r) e^{-\eta_d r} \]

where the \( \lambda_n \) and \( N_n \) are such that the six basis functions are mutually orthonormal. The pseudo-state parameters were obtained, by using conventional variational techniques to minimize the energy of \( H^\prime \).

The two-electron Hamiltonian is given by

\[ H(1,2) = -\frac{1}{r_1} - \frac{1}{r_2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_{12}}. \]

Atomic units are to be used consistently throughout this work; the energy being measured in Rydbergs and \( \hbar = 1, m = \frac{1}{2}, \) and \( e^2 = 2. \)

The trial wave function is of the form

\[ \Psi^{\Gamma'}(1,2) = [1 + P_{12}] R_\Gamma(1) F_\Gamma(2) Y^M_{\ell_1 \ell_2} (\Omega_{12}). \]

Here \( \Gamma' \) and \( \Gamma \) are channel indices and designate sets of quantum numbers

\[ \Gamma = (n_\Gamma, \ell_\Gamma, s_\Gamma, \ell, L, S, M_L, M_S, \pi) \]
where:

1. \( n_r \) is the principal quantum number of the atomic state;
2. \( \ell_r, s_r \), specify the orbital angular momentum and spin of the atomic state;
3. \( \ell \) is the orbital angular momentum of the scattered particle;
4. \( L, S, M_L, M_S, \pi \) specify the total orbital and spin angular momentum of the two particle system, their components on the axis of quantization, and the total parity respectively. These quantities are conserved in the collision.

\( P_{12} \) is the space exchange operator. The function \( Y \) couples the angular momentum of the electron and the atom

\[
\frac{\mathcal{M}_L}{\mathcal{L}_r^\ell} \phi_{12}(\Omega_1, \Omega_2) = \sum_m C(\ell, \ell_r; m; M_L, m_L) Y_{\ell_m r}(\Omega_1) Y_{m r}(\Omega_2). \tag{II.6}
\]

The single particle wave function \( F_r(r) \) is expanded in the form

\[
F_r(r) = \sum_n c_n f_n(r). \tag{II.7}
\]

where the \( f_n \) are normalized Slater orbitals

\[
f_n = c_n r^{\ell} e^{-r^2} \tag{II.8}
\]

The index \( n \) designates the number of basis function (Slater orbitals) considered. The coefficients \( c_n \) are chosen so as to span the range \( 0 < r < 100a_0 \).
The Ritz variational method is used to solve the eigenvalue problem

\[ H \mathbf{b} = E \mathbf{S} \mathbf{b}. \]

Here \( H \) is the Hamiltonian matrix and \( S \) is the overlap matrix. \( \mathbf{b} \) is a vector of the elements \( b_{\Gamma n} \). The smallest eigenvalue of the matrix equation is the energy of \( H^- \) and the corresponding eigenvector is the bound state wave function. A local minimum for the energy of \( H^- \) is obtained by treating the smallest eigenvalue as a non-linear function of the pseudo-state parameters \( a^\_, \eta^\_. \). Using ten basis functions for each of the coupled channels Matese and Oberoi obtained \(-1.0537\) Ryd.\textsuperscript{41} for the energy of \( H^- \). The exact value is \(-1.0555\) Ryd.\textsuperscript{42}
B - Continuum State

The variation method proposed by Nesbet is used to calculate singlet continuum p-wave electron hydrogen wave functions. The trial wave function is taken to be of the form

$$\Psi'(1,2) = \sum_{\Gamma}^{N} \Psi'(1,2)$$

where $\Psi'(1,2)$ is the component of the total wave function in the $\Gamma$th channel. This function may be expressed as

$$\Psi'(1,2) = \chi'_{\Gamma}(1,2) + \alpha'_{0\Gamma} A_{0\Gamma}(1,2) + \alpha'_{1\Gamma} A_{1\Gamma}(1,2)$$

where $\chi'_{\Gamma}$ is a normalizable function and $A_{0\Gamma}$ and $A_{1\Gamma}$ are functions having a specified asymptotic form.

The function $\chi'_{\Gamma}(1,2)$ may be expressed as

$$\chi'_{\Gamma}(1,2) = \sum_{b=1}^{N} \Phi_{b}(1,2) C_{b}^{\Gamma'}$$

where $b$ is the basis index and

$$\Phi_{b} = (\frac{1+\sqrt{2}}{\sqrt{2}}) R_{\Gamma}(1) \eta_{b}^{\Gamma}(2) \lambda_{\Gamma L L}(\Omega_{1}, \Omega_{2}).$$

The normalizable basis functions $\eta_{b}(r) = \frac{[(2\xi_{b})^{2\xi+3}]^{1/2} r^{L} e^{-\xi_{b} r}}{\Gamma(2L+3)}$.

And above the threshold for the excitation of the n=2 states, two additional basis functions are included of the form
\[(1-e^{-\beta r})^{\ell+2} \sin(k_1 r)/r^2\]
\[(1-e^{-\beta r})^{\ell+2} \cos(k_1 r)/r^2\].

The function \(R_\Gamma\) is the hydrogenic radial function. In this work three states are included the ls, 2s, and 2p states of hydrogen. The operator \(P_12\) is the two particle exchange operator.

The asymptotic functions may be expressed as

\[A_i\Gamma = \frac{1+P_{12}}{\sqrt{2}} R_\Gamma(r_1) S_i(G, r_2) Y_{L_i, \ell_i, \ell_i} (\Omega_1, \Omega_2) \quad i = 0,1\].

The functions \(S_0\) and \(S_1\) are proportional to \(r^{-1}\sin(k_1 r - \ell\pi/2)\), respectively, at large distance. The specific forms used were

\[S_0(G, r) = k_\Gamma (1-e^{-\beta r})^{2\ell+1} j_{\ell}(k_1 r)\]

and

\[S_1(G, r) = k_\Gamma (1-e^{-\beta r})^{2\ell+1} N_{\ell}(k_1 r)\]

in which \(j_{\ell}\) and \(N_{\ell}\) are spherical Bessel and Neumann functions. The quantity \(\beta\) is an arbitrary parameter. The factor \((1-e^{-\beta r})^{2\ell+1}\) is introduced so that the function \(S_1\) will behave as \(r^{\ell}\) close to the origin. For \(S_0\) the factor \((1-e^{-\beta r})^{2\ell+1}\) is included solely for convenience in calculating the necessary integrals.
The wave function as it stands has three unknowns, $\alpha_{o\Gamma'}^\Gamma$, $\alpha_{1\Gamma'}^\Gamma$, and $C_b^{\Gamma'\Gamma'}$. However the $C_b^{\Gamma'\Gamma'}$ can be expressed in terms of $\alpha_{o\Gamma'}^\Gamma$ and $\alpha_{1\Gamma'}^\Gamma$. And either $\alpha_{o\Gamma'}^\Gamma$ or $\alpha_{1\Gamma'}^\Gamma$ can be defined to be a delta function $\delta_{\Gamma'\Gamma'}$, leaving only one unknown. In the Kohn Variational Method $\alpha_{o\Gamma'}^\Gamma = \delta_{\Gamma'\Gamma'}$, and in the Inverse Kohn Variational Method $\alpha_{1\Gamma'}^\Gamma = \delta_{\Gamma'\Gamma'}$.

The trial wave function $\Psi^{\Gamma'}$ must satisfy the Schrödinger equation in the subspace of Hilbert space spanned by the basis functions $\eta_b^{\Gamma}$. This condition is used to determine the short range coefficients $C_b^{\Gamma'\Gamma'}$ in terms of the asymptotic coefficients $\alpha_{1\Gamma'}^\Gamma$. The initial channel index $\Gamma'$ will be suppressed in the remainder of this discussion.

The demand that the trial wave function $\Psi$ satisfy the Schrödinger equation in the subspace spanned by the short range functions $\eta_b^{\Gamma}$ leads to the system of linear equations.

$$\sum_{\Gamma} \langle \varphi^{\gamma}(1,2) | H - E | \chi_{\Gamma}(1,2) + \alpha_{o\Gamma} A_{o\Gamma}(1,2) + \alpha_{1\Gamma} A_{1\Gamma}(1,2) \rangle = 0, \quad \text{II.18}$$

for a channel index $\gamma = 1, \ldots, N$ and basis index $a = 1, \ldots, n_{\gamma}$.

An equivalent expression for Eq. II.18 is

$$\sum_{s} \sum_{b} M_{s}^{pq} c_{b}^{s} = -\sum_{q} (\alpha_{oq} a_{s}^{q} + \alpha_{1q} a_{c}^{q}), \quad \text{II.19}$$
where
\[
M_{pq}^{ab} = (\phi_a^{P}|H-E|\phi_b^q),
\]
\[
M_{pq}^{as} = (\phi_a^{P}|H-E|A_{oq}),
\]
\[
M_{pq}^{ac} = (\phi_a^{P}|H-E|A_{1q}).
\]

In the remaining discussion p, q, and s are channel indices. And a and b are basis indices. The problem can be simplified by noting that the coefficients $c^s_b$ can be expressed as linear combination of $\alpha'$s,
\[
c^s_b = \sum_q (\alpha_{oq} c^{sq}_{bo} + \alpha_{1q} c^{sq}_{bl})
\]
where for $p = 1, \ldots, N$ and $a = 1, \ldots, n_p$
\[
\sum_s \sum_b \langle \phi_a^{a}|H-E|\phi_b^s \rangle c^s_{bo} = -\langle \phi_a^{a}|H-E|A_{oq} \rangle
\]
\[
\sum_s \sum_b \langle \phi_a^{a}|H-E|\phi_b^s \rangle c^s_{bl} = -\langle \phi_a^{a}|H-E|A_{1q} \rangle.
\]

These $2N$ inhomogeneous linear equations of Eq. (II.22) may be solved by two methods. One method is an eigenvalue problem and the other method consists of matrix inversion.
In the eigenvalue method one first obtains the homogeneous solution. The homogeneous equation may be expressed as

\[ \sum_s \sum_b (H^{s}_{ab} - \mathcal{E}_a^{s}_{ab})c^s_{b\alpha} = 0. \]

Eq. (II.23) is an eigenvalue problem of dimension \( \Sigma n_p \).

The eigenfunctions,

\[ \gamma_\alpha(1,2) = \sum_s \gamma^s_\alpha(1,2) = \sum_s \sum_b \gamma^s_b(1,2) c^s_{b\alpha} \]

span the same subspace of Hilbert space as the basis functions \( \eta^\Gamma_b \).

Thus, Eq. II.22 may also be expressed as,

\[ \sum_s \sum_b \langle \psi^p | H - \mathcal{E} | \psi^s_b \rangle c^s_{b\alpha} = -\langle \psi^p | H - \mathcal{E} | A_{0q} \rangle \]

\[ \sum_s \sum_b \langle \psi^p | H - \mathcal{E} | \psi^s_b \rangle c^s_{b\Gamma} = -\langle \psi^p | H - \mathcal{E} | A_{1q} \rangle. \]

It is convenient to introduce the functions \( \xi^s_{1q} \),

\[ \xi^s_{1q} = \sum_b \gamma^s_b(1,2) c^s_{b\Gamma} \quad i=0,1, \]

and to express them in terms of the eigenfunctions \( \gamma_\alpha \). This leads to the expression

\[ \sum_s \langle \psi^p | H - \mathcal{E} | \gamma^s \rangle c^s_{\alpha'1} = -\langle \psi^p | H - \mathcal{E} | A_{1q} \rangle \]
for \( i = 0,1 \) where

\[
\hat{\phi}_i^s = \sum_{\alpha'} \psi_{\alpha'}^s (1,2) K_{\alpha',1}^q.
\]

Since the eigenfunctions \( \psi_{\alpha} \) are taken to be orthonormal

\[
K_{\alpha d}^q = (E - E_{\alpha})^{-1} \sum_{\alpha'} \langle \psi_{\alpha} | H - E | A_{1q} \rangle
\]

and

\[
\hat{\phi}_i^s = \sum_{\alpha} \psi_{\alpha} (E - E_{\alpha})^{-1} M_{\alpha d}^q \quad i = 0,1.
\]

The function \( \chi_s^v \) may be expressed as

\[
\chi_s^v(1,2) = \sum_{\alpha} [\alpha_{i q}^v \hat{\phi}_i^s (1,2) + \alpha_{i q}^v \hat{\phi}_i^s (1,2)].
\]

Thus the short range coefficients \( C_{dq}^v \) are expressed in terms of the asymptotic coefficients \( \alpha_{i q}^v \), and the eigenfunctions \( \psi_{\alpha} \) and eigenenergies \( E_{\alpha} \) by Eq. II.30 and Eq. II.31.

Eq. II.21 can also easily be solved by using matrix inversion in Eq. II.22. Here

\[
C_{b0}^{sq} = - \sum_{\alpha} (M^{-1})_{ba} M_{\alpha d}^q
\]

\[
C_{b1}^{sq} = - \sum_{\alpha} (M^{-1})_{ba} M_{\alpha c}^q
\]
ASYMPOTIC COEFFICIENTS - $\alpha_{i_1 q}$

The asymptotic coefficients are determined variationally. The variational functional is taken to be

$$I_{\sigma u} = \langle \Psi^\sigma | H - E | \Psi^\nu \rangle$$

$$= \sum_F \sum_S \langle \Psi^\sigma_F(1,2) | H - E | \Psi^\nu_S(1,2) \rangle.$$

The trial function was expressed as

$$\Psi^\nu(1,2) = \sum_S \Psi^\nu_S(1,2)$$

$$\Psi^\nu_S(1,2) = \chi^\nu_S(1,2) + \alpha^\nu_{os} \alpha_{0s}^{os}(1,2) + \alpha^\nu_{1s} \alpha_{ls}^{1s}(1,2).$$

For the variational calculation it is convenient to express the trial function $\Psi^\nu$ with component in channel $s$ as

$$\Psi^\nu_S(1,2) = \sum_{i_1 q} \sum_{i_1 q} \alpha^\nu_{i_1 q} \Psi^s_{i_1 q}(1,2)$$

where the functions $\Psi^s_{i_1 q}$ are defined by

$$\Psi^s_{i_1 q}(1,2) = \phi^s_{i_1 q}(1,2) + \delta \alpha_{i_1 q}^{s}(1,2).$$
Then the variational functional can be expressed as

\[ I_{\sigma^\nu} = \sum_{ij} \sum_{pq} \alpha_i^\sigma \beta_j^\nu M_{ij}^{pq} \alpha_j^\nu \]  

or

\[ I_{\sigma^\nu} = \sum_{ip} \sum_{pq} \alpha_i^\sigma \beta_j^\nu I_{ip}^{pq} \]  

where

\[ I_{ip}^{pq} = \sum_{jq} M_{ij}^{pq} \alpha_j^\nu, \quad i,j = 0,1; \quad p,q = 1,\ldots,N. \]

The matrix elements \( M_{ij}^{pq} \) are defined by

\[ M_{oo}^{pq} = \sum_{rs} \sum_{st} \left( \psi_r^x | H_{rs} - E \delta_{rs} | \psi_s^o \right) \]

\[ = \sum_{s} \left( S_p \left| H_{ps} - E \delta_{ps} | \psi_s^s \right. \right) \]

\[ M_{ol}^{pq} = \sum_{rs} \sum_{st} \left( \psi_r^x | H_{rs} - E \delta_{rs} | \psi_s^l \right) \]

\[ = \sum_{s} \left( S_p \left| H_{ps} - E \delta_{ps} | \psi_s^s \right. \right) \]

\[ M_{lo}^{pq} = \sum_{rs} \sum_{st} \left( \psi_r^x | H_{rs} - E \delta_{rs} | \psi_s^o \right) \]

\[ = \sum_{s} \left( S_p \left| H_{ps} - E \delta_{ps} | \psi_s^o \right. \right) \]

\[ M_{ll}^{pq} = \sum_{rs} \sum_{st} \left( \psi_r^x | H_{rs} - E \delta_{rs} | \psi_s^l \right) \]

\[ = \sum_{s} \left( S_p \left| H_{ps} - E \delta_{ps} | \psi_s^l \right. \right) . \]
The matrix elements $M_{pq}^{ij}$ can be determined by either of two methods.

If the eigenvalue problem has been solved then

$$M_{oo}^{pq} = M_{ss}^{pq} + \sum_{a} M_{sa}^{pq} (E - E_{a})^{-1} M_{as}^{os},$$

$$M_{ol}^{pq} = M_{sc}^{pq} + \sum_{a} M_{ca}^{pq} (E - E_{a})^{-1} M_{ac}^{os},$$

$$M_{lo}^{pq} = M_{cs}^{pq} + \sum_{a} M_{ac}^{pq} (E - E_{a})^{-1} M_{ca}^{os},$$

$$M_{ll}^{pq} = M_{cc}^{pq} + \sum_{a} M_{ca}^{pq} (E - E_{a})^{-1} M_{ac}^{os}. \tag{II.41}$$

And if the eigenvalue problem has not been solved, the $M_{ij}^{pq}$ are easily determined using the following equations,

$$M_{oo}^{pq} = M_{ss}^{pq} - \sum_{rs} \sum_{ab} M_{sa}^{pr} (M^{-1})^{rs}_{ab} M^{sq}_{bs},$$

$$M_{ol}^{pq} = M_{sc}^{pq} - \sum_{rs} \sum_{ab} M_{ca}^{pr} (M^{-1})^{rs}_{ab} M^{pq}_{bc}, \tag{II.42}$$

$$M_{lo}^{pq} = M_{cs}^{pq} - \sum_{rs} \sum_{ab} M_{ca}^{pr} (M^{-1})^{rs}_{ab} M^{sq}_{bs},$$

$$M_{ll}^{pq} = M_{cc}^{pq} - \sum_{rs} \sum_{ab} M_{ca}^{pr} (M^{-1})^{rs}_{ab} M^{sq}_{bc}.$$

Using the identity

$$M_{ij}^{pq} = M_{ji}^{qp} + k_{p} \delta_{pq} (\delta_{io} \delta_{jl} - \delta_{il} \delta_{jo}) \tag{II.43}$$
where
\[ k_p^2 = E_p - E \]

the variational functional may be expressed alternatively as
\[ I_{\sigma\nu} = \sum_{j} (I_{j\sigma}^{q} \alpha_{j}^{\nu} + k_{q}(\delta_{jl} \alpha_{oq}^{\sigma} - \delta_{jo} \alpha_{lq}^{\sigma} \alpha_{j}^{\nu})) \]

If the coefficients \( \alpha^{\sigma} \) and \( \alpha^{\nu} \) are independent, from Eq. II.38
\[ \frac{\delta I_{\sigma\nu}}{\delta \alpha_{ip}^{\sigma}} = I_{ip}^{\nu} \]
and from Eq. II.45
\[ \frac{\delta I_{\sigma\nu}}{\delta \alpha_{j}^{\nu}} = I_{j}^{q} + k_{q}(\delta_{jl} \alpha_{oq}^{\sigma} - \delta_{jo} \alpha_{lq}^{\sigma}). \]

Thus the first order variation of \( I_{\sigma\nu} \) is given in general by
\[ \delta I_{\sigma\nu} = \sum_{i} \sum_{p} \delta \alpha_{ip}^{\sigma} \frac{I_{ip}^{\nu}}{I_{ip}} + \sum_{i} \sum_{j} I_{j}^{q} \delta \alpha_{j}^{\nu} \]
\[ + \sum_{q} \frac{k_{q}(\alpha_{oq}^{\sigma} \delta \alpha_{lq}^{\nu} - \alpha_{oq}^{\sigma} \delta \alpha_{lq}^{\nu})}{I_{ip} I_{ip}^{\nu}}. \]

Using the Kohn Variational Method the \( R \) matrix is defined as
\[ R_{pq} = \left( \frac{k_{q}}{k_{p}} \right) \frac{1}{2} \gamma_{pq} \]

where
\[ \gamma_{pq} = \alpha_{pq}, \]

\[ \gamma_{pq} = \alpha_{lq}^{p}, \]
and

\[ \alpha_{pq} = \delta_{qp} \quad q = 1, \ldots, N \]  

where \( p \) is the initial channel index.

For the above definition of the \( R \) matrix, the first variation of the variational functional simplifies considerably. All coefficients \( \alpha \) are real and the variations of \( \alpha_{pq} \) vanish. Eq. II.48 reduces to

\[ \delta I_{\sigma \nu} = \sum_p I_{p \nu}^p \delta \gamma_{p \sigma} + \sum_q I_{q \sigma}^q \delta \gamma_{q \nu} + k_\sigma \delta \gamma_{\nu \sigma} \]  

The integrals \( I_{p \nu}^p \) that occur in Eq. II.52 can all simultaneously be reduced to zero by an appropriate choice of coefficients \( \gamma_{q \nu} \).

Using Eqs. II.43, II.50, II.51

\[ I_{p \nu}^p = M_{p \nu}^p + \sum_q M_{pq} \gamma_{q \nu} \]  

\[ 0 = M_{p \nu}^p + \sum_q M_{pq} \gamma_{q \nu}^{(o)} \]  

Thus the coefficients \( \gamma_{q \nu}^{(o)} \) satisfy the set of linear equations

\[ \sum_q M_{pq} \gamma_{q \nu}^{(o)} = -M_{p \nu}^p \]  

If \( I_{p \nu}^p = 0 \) for all \( p, q \) then Eq. II.52 becomes

\[ \delta (I_{\sigma \nu} - k_\sigma \gamma_{\nu \sigma}) = 0. \]
This gives approximately stationary values of the coefficients

\[ \gamma_{\nu q} = \gamma_{\nu q}^{(o)} - \left( \frac{1}{k_q} \right) I_{\nu q}^{\nu}(\gamma_{\nu q}^{(o)}) \]  \hspace{1cm} \text{(II.57)}

\[ \gamma_{\nu q} = \gamma_{\nu q}^{(o)} - \left( \frac{1}{k_q} \right) (M_{oo}^{\nu q} + \sum_p M_{ol}^{qp} \gamma_{\nu q}^{(o)}). \]  \hspace{1cm} \text{(II.58)}

This completes the calculation of \( \alpha_{1q}^{\nu} = \gamma_{\nu q} \). However there are difficulties with spurious singularities for the Kohn method if \( |M_{11}^{pq}(E)| \) should have isolated zeroes. These can be avoided by computing elements of the \( R^{-1} \) matrix for these isolated energy regions.

A method, similar to that used for the \( R \) matrix, can be used for computing elements of \( R^{-1} \) matrix. This method is called the Inverse Kohn by Nesbet. In the single-channel problem it reduces to second Hulthen method. A brief equation outline of the method follows.

\[ R^{-1} = \left( \frac{k_q}{k_p} \right)^{\frac{1}{2}} \beta_{pq} \]

\[ \beta_{\sigma q} = \alpha^{\sigma}_{oq} \]  \hspace{1cm} \text{(II.59)}

\[ \alpha^{\sigma}_{1q} = \delta_{q\sigma} \]

\[ \delta_{I_{\sigma \nu}} = \sum_p I_{o\nu}^{p} \delta_{\sigma p} + \sum_q I_{o\sigma}^{q} \delta_{\nu q} - k_\sigma \delta_{\nu \sigma} \]

\[ \sum_q M_{oo}^{pq} \beta_{\nu q}^{(o)} = -M_{ol}^{\nu} \]
\[ \delta(I_{O^V} + 1 \, k \beta_{O^V}) = 0 \]

\[ \beta_{V^q} = \beta_{V^q}^{(o)} + (1/k)I_{V^V}^{(o)} \beta_{V^q}^{(o)} \]

\[ \beta_{V^q} = \beta_{V^q}^{(o)} + (1/k)(M_{11}^q + \sum_p^q M_{1p}^q \beta_{V^p}^{(o)}) \]

Spurious singularities also occur in the Inverse Kohn Method, if \( |M_{oo}^{pq}(E)| \) has isolated zeroes. However a point of singularity in the Kohn method is almost never a singularity in the Inverse Kohn method and vice versa. Thus the spurious singularities can be avoided. Nesbet suggests using the Kohn formula when the ratio of determinants

\[ \frac{|M_{oo}^{pq}|}{|M_{11}^{pq}|} \]

is less than unity, and using the Inverse Kohn formula when this ratio is greater than unity. This type of spurious singularity did not create any difficulties in the present work.
SECTION II-3

MULTICHANNEL PHOTODETACHMENT

Having determined the needed wave functions in the previous section, in this section we will describe how these wave functions can be used to determine the photodetachment cross section. Because inelastic processes are to be allowed, a multichannel formalism is needed.

Henry and Lipsky\(^43\) have described a theory for multichannel photoionization which includes coupling between final-state channels. They applied the formalism to the photoionization of neon. Matese and Oberoi also used this formalism in computing the photodetachment of H\(^-\) below the n=2 threshold. The description which follows is that found in the paper by Matese and Oberoi.\(^40\)

The total cross section, with contributions from all open channels is given by

\[
\sigma(j) = \sum_{\Gamma} \sigma_{\Gamma}(j) \tag{II.61}
\]

where

\[
\sigma_{\Gamma}(j) = \frac{8\pi}{3} a_0^2 \left( \frac{\hbar v}{2 \text{Ryd}} \right)^{3-2j} \sum_{\Gamma',\Gamma''} M_{\Gamma,j}^{(j)} A_{\Gamma',\Gamma''}^{\Gamma} M_{\Gamma''}^{(j)}
\]

and

\[
A_{\Gamma',\Gamma''}^{\Gamma} = (1-iR)_{\Gamma',\Gamma''}^{-1} (1+iR)_{\Gamma''}^{-1}.
\]
Here $j = 1, 2, 3$ indicates the length, velocity or acceleration dipole approximation. $\Gamma$, $\Gamma'$ and $\Gamma''$ indicate open final state channels. $R$ is the reactance matrix and is determined by Eq. (II.49).

$$M^{(j)}_{\Gamma \Gamma} = N \sum_{\gamma_f \gamma_{1}} \sum_{\sigma = \pm 1}$$

$$\begin{align*}
\delta_{l_{2f}, l_{1f}, l_{if}, \ell + \sigma} \left[ \langle u_{\gamma_f} \mid 0^{(j)} \rangle \mid v_{\gamma_{1}} \rangle \langle \Gamma_{\gamma_f} \Gamma_{\gamma_{1}} \Gamma_{\gamma_{1}} \rangle 
+ \langle u_{\gamma_f} \mid 0^{(j)} \rangle \langle \Gamma_{\gamma_f} \Gamma_{\gamma_{1}} \Gamma_{\gamma_{1}} \rangle 
\right] \\
+ \delta_{l_{1f}, l_{2f}, l_{if}, \ell + \sigma} \left[ \langle \Gamma_{\gamma_f} \mid 0^{(j)} \rangle \langle u_{\gamma_f} \mid v_{\gamma_{1}} \rangle 
\right] \\
+ \langle \Gamma_{\gamma_f} \mid 0^{(j)} \rangle \langle u_{\gamma_f} \mid v_{\gamma_{1}} \rangle 
\end{align*}$$

$\Gamma$ is a channel index. $u$ is either a $1s$, $2s$, $2p$ reduced hydrogenic state or a reduced pseudo state wave function. Using the notation of Section II-2, the reduced final state single particle wave function $F_{\Gamma}$ is

$$F_{\Gamma}^{\Gamma'} = r \kappa \frac{1}{2} \left[ \sum_{l} \sum_{q} \gamma_{l}^{a} q^{b} \gamma_{l}^{a} q^{b} + \alpha_{\Gamma}^{\Gamma'} (1 - e^{-\beta r})^{2l+1} j_{l}(K_{r}x) 
+ \alpha_{\Gamma}^{\Gamma'} (1 - e^{-\beta r})^{2l+1} N_{l}(K_{r}x) \right]$$

$$II.63$$
N is the bound state normalization, \( l=l_{11}=l_{21} \), and the dipole operator \( O_{\ell \sigma}^{(j)} \) is given by

\[
O_{\ell \sigma}^{(j)} = -\sigma \left[ \frac{\ell+\frac{1}{2}(1+\sigma)}{2\ell+1} \right]^2 \begin{cases} 
0 & j=1 \\
\frac{\partial}{\partial r} - \sigma [\ell+\frac{1}{2}(1+\sigma)]/r & j=2 \\
\frac{1}{r^2} & j=3
\end{cases}

\]

For energies below the n=2 threshold, only the 1s channel is open. In this case Eq. (II.61) becomes

\[
\sigma(j) = \frac{8\pi}{3} \alpha a_o^2 \left( \frac{\hbar \nu}{\text{Ryd}} \right)^{3-2j} M_{\Gamma_1}^{(j)}(d) \cos^2 \delta \tag{II.65}
\]

where \( \delta \) is the \( ^1P \) phase shift and \( \Gamma_1 \) is the 1s channel.
PHOTODETACHMENT RESULTS AND CONCLUSIONS BELOW THE INELASTIC THRESHOLD

In this section the photodetachment cross section is calculated using Eq. (II.65) and the wave functions described in Section II-2. The photon energies considered in this section ($\lambda > 1131$) are not large enough to produce an inelastic collision, thus only a single channel formalism is needed. The purpose of this section is to demonstrate that the wave functions obtained using the algebraic close coupling method are sufficiently accurate to compute the photodetachment cross section of $H^-$. First the photodetachment cross section is computed for the same continuum wave function and three different bound states. The continuum state is a three state expansion composed of the $1s$, $2s$, $2p$ hydrogen states. The three bound states are those described earlier. In Figure 8 the dipole velocity photodetachment results are shown. Curve 1 in Figure 8 represents the results using the six channel bound state of Matese and Oberoi. In Figure 9 this same curve is shown to be in good agreement to a similar calculation by Doughty and Fraser. Doughty and Fraser computed the photodetachment cross section of $H^-$ using the seventy parameter Schwartz bound state. They used a three state close coupling calculation for the continuum state. Note in Figure 8 that the four state expansion which includes the $2p$ pseudo state yields results which are
significantly better than the results obtained using the three state expansion. The photodetachment results in the dipole length approximation are shown in Figure 10.

In Figure 11 the six state expansion of Matese and Oberoi is used to compute both the bound and the continuum state. Also shown in Figure 11 are the results of Doughty, Frasier, and McEachran. They used the Schwartz bound state of H⁻. They calculated the continuum state using the close coupling method with the first six hydrogenic states included in the expansion of the wave function.

Figures 8-11 illustrate the already known facts that the dipole velocity approximation yields the best photodetachment cross sections, and that the photodetachment results are not as sensitive to the continuum state as they are the bound state. Figures 8-11 should also establish that accurate wave functions can be obtained by using the algebraic close coupling method. However there is one difficulty that arises in using the algebraic close coupling method. If the total energy of the system is very close to one of the eigenvalues of Eq. (II.23) then the wave functions exhibit spurious resonance structure, spurious in the sense that this eigenstate doesn't exist in the real or actual physical problem and thus the resonance structure also doesn't exist in the real problem. Therefore the energy region of the non-physical eigenvalues should be avoided. If an energy region containing a non-physical eigenvalue needs to be investigated, the eigenvalue spectrum is easily shifted by changing the exponential coefficients of the basis set. A description of this difficulty in
regard to the photodetachment of H\(^-\) is given in the paper by Mate\(\text{se}^{40}\) and Oberoi.
SECTION II-5

1P RESONANCE

In the electron hydrogen problem there exists a 1P resonance just above the n=2 threshold. Because the n=2 channels are open, the problem of determining the singlet p-wave function is more difficult in this energy region. The source of the difficulty is the coupling of the degenerate 2s and 2p states of atomic hydrogen, which gives rise to a long-range off-diagonal dipole potential.\(^4\)\(^6\)

E. R. Smith, R. S. Oberoi, and R.J.W. Henry have investigated this problem by considering a two channel model problem which contained an off-diagonal dipole potential. They found that in the model problem, for degenerate energies, the asymptotic solution of the wave function could not be accurately approximated using spherical Bessel and Neumann functions. They suggested two means of correcting for this. One method was to include energy-dependent sinusoidal terms in the basis set. Two such additional terms were added in the present work (Eq. II.14). The addition of the energy-dependent sinusoidal terms means that the eigenvalue equation (Eq. II.23) must be solved for every energy, whereas before it needed to be solved only once. Since the alternate method of matrix inversion is much quicker, one would naturally want to solve the problem using that procedure. However, one would like to know the eigenvalue spectrum, as mentioned in the last section. Knowing the eigenvalue spectrum is even more
important in the inelastic work, because the energy-dependent sinusoidal terms seem to cause a clustering of eigenvalues about the energy being considered.

The problem of non-physical eigenenergies does not seem to arise in calculating the $L=1$ cross sections of the $1s-2s$ and $1s-2p$ transitions. These cross sections are given in Figure 12 along with the results of Taylor and Burke.\textsuperscript{47} Taylor and Burke used the close-coupling method for two expansions, one including three states and the other three states plus twenty correlation terms. Although the maximums in the cross section occurred at the same energies, the values of the maximums are slightly less in the present work. This might be caused by not including enough sinusoidal terms in the basis expansion.\textsuperscript{48} The agreement between the present work and that of Taylor and Burke seems to indicate that the present work has been extended above $n=2$ threshold correctly. Thus the wave functions are used to compute the contribution of the $^1P$ resonance to the photodetachment cross section.

The photodetachment cross section for the $^1P$ resonance was determined using the bound state of Matese and Oberoi. The final state was obtained using the algebraic close coupling method with three states ($1s-2s-2p$) included in the expansion. Sixteen basis functions were used in the expansion of the single particle function $F_q^V$ fourteen Slater type and two harmonic. The photodetachment cross section was computed using three different sets of sixteen basis functions. Figure 13 represents a best fit curve for the three sets of photodetachment data. The data points in the energy region
(0.75-0.76 Ryd.) do not fit a smooth curve. However the same smooth curve gives a good best fit curve to all three sets of data. The author feels that the given curve is accurate to within 10%. Also included in Figure 13 are the velocity results obtained by Macek using the bound state 20-parameter Hylleraas-type wave function for H⁻ of Hart and Herzberg and a 1s-2s-2p close coupling final state. The difficulty in obtaining a smooth curve is attributed to two reasons. One is the difficulty with an eigenvalue being too close to the total energy E. The other source of difficulty is the cut off parameter β. A good cut off parameter for channel one is $\beta = k_1$ or approximately $= 0.8 a_o^{-1}$. Whereas a good cut off parameter for channel four is $\beta = k_2$ or $0.05 a_o^{-1}$. The same cut off parameter was used for all channels. Beta was chosen to be the average of $k_1$ and $k_2$ or $\beta$ equal approximately $0.45-0.50 a_o^{-1}$. This $\beta$ is as small as possible if one is to obtain reasonable results for the 1s channel. However it is much too large, to accurately cut off the spherical Neumann function $\gamma_2$ in channel four. This is illustrated in Table II, which shows the contribution to the photodetachment cross section of a collision where the hydrogenic electron is left in the excited 2p state of hydrogen and the other electron is scattered with angular momentum $l=2$.

In summary, accurate wave functions can be obtained using the Algebraic Close Coupling Method. However the appearance of spurious singularities as noted by Matese and Oberoi in their paper seems to be even a larger source of difficulty for energies above the $n=2$. 
threshold. Also a single cut-off parameter for all open channels should not be used for energies very near the threshold.

Work is presently underway to make these two changes in the program: to make the cut off parameter equal to the wave vector of the channel and to include two additional harmonic terms in the basis set. When this is completed the work will be extended to six channels.
TABLE II

PHOTODETACHMENT CROSS SECTIONS: FINAL STATE CHANNEL FOUR
\(^{12}n_4=2, \lambda =1, \ell=2\)

<table>
<thead>
<tr>
<th>(k^2) (Ryd.)</th>
<th>(\text{LENGTH } \sigma \times 10^{-17} \text{cm}^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(\text{BASIS} A)</td>
</tr>
<tr>
<td>0.751</td>
<td>0.05</td>
</tr>
<tr>
<td>0.752</td>
<td>0.79</td>
</tr>
<tr>
<td>0.753</td>
<td>0.34</td>
</tr>
<tr>
<td>0.754</td>
<td>0.65</td>
</tr>
<tr>
<td>0.755</td>
<td>0.60</td>
</tr>
<tr>
<td>0.756</td>
<td>0.77</td>
</tr>
<tr>
<td>0.757</td>
<td>0.39</td>
</tr>
<tr>
<td>0.758</td>
<td>0.37</td>
</tr>
<tr>
<td>0.759</td>
<td>0.33</td>
</tr>
</tbody>
</table>

Basis A: \(\xi_b = [0.005, 0.015, 0.03, 0.075, 0.1, 0.3, 0.6, 0.8, 1.1, 1.3, 1.6, 2.0, 3.0, 5.0]\)

Basis B: \(\xi_b = [0.005, 0.01, 0.04, 0.07, 0.2, 0.4, 0.6, 0.8, 1.2, 1.4, 1.8, 2.5, 3.5, 4.5]\)

Basis C: \(\xi_b = [0.005, 0.015, 0.03, 0.075, 0.1, 0.3, 0.45, 0.6, 0.8, 1.3, 1.6, 2.0, 3.0, 5.0]\)
Figure 8 Photodetachment cross sections in the dipole velocity approximation for H⁻ using an algebraic close coupling three state continuum wave function and three different bound states.
Figure 9 Photodetachment cross sections of $H^-$ in the dipole velocity approximation. The dashed curve is the result using a four channel bound state. The solid curve is the result using the six channel bound state. The circles are the result of Doughty and Fraser using the Schwartz bound state.
Figure 10 Photodetachment cross sections of H⁻ in the dipole length approximation. The dashed curve is the result using a four channel bound state. The solid curve is the result using the six channel bound state. The circles are the results of Doughty and Fraser using the Schwartz bound state.
Figure 11 Six channel photodetachment cross sections of H⁻ in the dipole length and velocity approximation. The solid curves labeled L and V are the length and velocity results using a six channel bound state and a six channel continuum state. The dashed curves labeled L and V are the length and velocity results of Doughty, Fraser, and McEachran. They used a close coupling continuum wave function with six hydrogen states included, and they used the Schwartz bound state.
Figure 12 Partial P Cross Sections of the 1s-2s and 1s-2p Transition above the n=2 Threshold: the dots are this work and the dashed and solid curves are the results of Taylor and Burke.
Figure 13 The photodetachment cross section of H^- in the energy region of the 1P resonance. The solid curve is the best fit curve of this work. The dashed curve is the result of Macek. Macek used a three state close coupling continuum state and the twenty parameter bound state wave function of Hart and Herzberg.
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VITA

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