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## Phase-Shift Calculation for Low-Energy Electron-Rb Scattering

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Total elastic and total spin-exchange cross sections have been calculated numerically for low-energy electrons incident on rubidium atoms. The effects of electron exchange and of target distortion are treated through the use of the adiabatic exchange approximation and the method of polarized orbitals.

## I. INTRODUCTION

Several authors have, in recent years, computed elastic scattering cross sections for electron-alkali atom collisions at low energies. Of these, the calculations by Garrett<sup>1</sup> for sodium and lithium appear to be the most successful. His calculated cross sections are in excellent agreement with the experimental data of Brode<sup>2</sup> and with that of Perel, *et al.*<sup>3</sup> in the energy range 0.25–16.0 eV. In addition, optical-pumping experiments<sup>4,5</sup> yield a spin-exchange cross section

for electron-sodium collisions at thermal energies in good agreement with Garrett's results.

The optical-pumping data is useful because it gives information about the phase shifts at extremely low energies. At the lowest energies, the theoretical phase shifts are particularly sensitive to the approximations made in the calculation.

Recently, it has become feasible to carry out spin-exchange optical-pumping experiments over a wide range of thermal energies.<sup>6</sup> It appears reasonable that the energy dependence of alkali

atom-electron spin-exchange cross sections will be measured over a temperature range 300–800°K. Rubidium is a very convenient element to optically pump, and the same kind of cross section data is available for rubidium as is available for sodium. For this reason, it appeared useful to repeat Garrett's phase shift calculation for the case of electron-rubidium collisions. The follow-

ing is a report of this effort. First, the theoretical basis of the calculation will be briefly reviewed. Next, the specific application to rubidium will be discussed, and departures from Garrett's procedure explained. Finally, the results of the calculation will be presented and compared with existing experimental data.<sup>2,7</sup>

## II. METHOD OF CALCULATION

A detailed description of the theoretical basis for the calculation discussed in this report is contained in Ref. 1. The effect of the distortion of the target atom by the electric field of the incident electron is taken into account through the use of a polarization potential in the scattering equation. The polarization potential is calculated by the method of polarized orbitals.<sup>8,9</sup> The distortion due to the incident electron is assumed to occur adiabatically and is treated by an application of first-order perturbation theory to the Hartree-Fock electron orbitals of the unperturbed atom. Under the influence of the perturbation, the electron orbitals depend upon the coordinates of the incoming electron.

The present calculation involves a further simplifying approximation in that the unperturbed wave functions are calculated by means of the Slater approximation. In this approximation, exchange integrals in the Hartree-Fock equations are replaced by an average exchange potential.

The radial equations (in atomic units), which must be solved for the perturbation of the atomic orbitals due to the incident electron, are

$$\left( \frac{d^2}{dr_1^2} - \frac{l'(l'+1)}{r_1^2} - V(r_1) + A_s(r_1) + \epsilon_1^0 \right) U_{nl \rightarrow l'}(r_1, r_f) = \frac{2r_1}{r_f^2} P_{nl}(r_1), \quad r_f > r_1, \quad (1a)$$

and

$$\left( \frac{d^2}{dr_1^2} - \frac{l'(l'+1)}{r_1^2} - V(r_1) + A_s(r_1) + \epsilon_1^0 \right) U_{nl \rightarrow l'}(r_1, r_f) = \frac{2r_f}{r_1^2} P_{nl}(r_1), \quad r_1 > r_f, \quad (1b)$$

$$\text{with } V(r_1) = -2Z/r_1 + \sum_j \int |\phi_j(\vec{r}_2)|^2 (2/r_{12}) d\vec{r}_2, \quad (2)$$

$$\text{and } A_s(r_1)g(r_1) = 6[(3/8\pi) \sum_j \phi_j^*(\vec{r}_1) \phi_j(\vec{r}_1)]^{1/3} g(r_1). \quad (3)$$

The  $\phi_j$  are the unperturbed Hartree-Fock-Slater (HFS) wave functions,  $A_s$  is the Slater exchange potential, the  $P_{nl}$  are the radial HFS functions and the  $U_{nl \rightarrow l'}$  are the radial perturbations of the orbitals. The coordinate of the incident electron is  $r_f$ ;  $l' = l \pm 1$  for  $l > 0$  and  $l' = 1$  for  $l = 0$ . In obtaining these equations only the dipole part of the perturbing interaction was used.

The polarization potential  $V_p$  which must be calculated is

$$V_p(r_f) = \sum_{nl} V_{nl \rightarrow l'}(r_f), \quad (4)$$

where

$$V_{nl \rightarrow l'}(r_f) = K_{nl \rightarrow l'} [(2/r_f^2) \int_0^{r_f} P_{nl}(r_1) r_1 U_{nl \rightarrow l'}(r_1, r_f) dr_1 + 2r_f \int_{r_f}^{\infty} P_{nl}(r_1) U_{nl \rightarrow l'}(r_1, r_f) r_1^{-2} dr_1]. \quad (5)$$

The constants  $K_{nl \rightarrow l'}$  are numbers which depend upon  $l'$  and on the number of electrons in an  $nl$  shell. The polarization potential should approach  $-\alpha/r_f^4$  as  $r_f \rightarrow \infty$ , where  $\alpha$  is the dipole polarizability of rubidium.

The scattering equation is written as a two-electron equation for the incident electron and the valence electron in the field of the perturbed core. The adiabatic exchange approximation is used to express the wave function  $\psi(\vec{r}_1, \vec{r}_2)$  for the two electrons as

$$\psi(\vec{r}_1, \vec{r}_2) = \psi'(\vec{r}_1, \vec{r}_2)F(\vec{r}_2) \pm \psi_0(\vec{r}_2)F(\vec{r}_1), \quad (6)$$

where  $\psi_0$  is the ground-state wave function of the valence electron,  $F$  is the free electron wave function, and  $\psi'$  is the ground-state wave function which is perturbed adiabatically in the collision. The plus and

minus signs refer to the singlet and triplet states, respectively, of the two electrons. Applying first-order perturbation theory and expanding  $F$  in partial waves, one obtains the radial equations for each partial wave  $f_l$ .

$$\frac{d^2}{dr^2} f_l + \left( k_0^2 - V_0 + A_s - V_p - \frac{l(l+1)}{r^2} \right) f_l = \pm U_0 \left[ (E_0 - k_0^2) \delta_{l0} \int_0^\infty f_0 U_0 dr \right. \\ \left. + [2/(2l+1)] (r^l \int_0^\infty f_l U_0 r^{-(l+1)} dr + r^{-(l+1)} \int_0^r f_l U_0 r^l dr - r^l \int_0^r f_l U_0 r^{-(l+1)} dr) \right], \quad (7)$$

$$\text{where } V_0(r_2) = V(r_2) + \langle \psi_0 | 2/r_{12} | \psi_0 \rangle, \quad (8)$$

which is the screened Hartree-Fock potential. The kinetic energy of the free electron is  $k_0^2 = E - E_0$ , where  $E_0$  is the ground-state energy of the bound electron.  $U_0$  is the radial part of the normalized ground-state wave function for the bound electron.

### III. APPLICATION TO RUBIDIUM

Equations (1) and (7) must be solved by numerical methods. The calculations were performed on a CDC 3600. The calculation of the HFS wave functions is, of course, the starting point. These were obtained from a program written by Herman and Skillman.<sup>10</sup> In their discussion, Herman and Skillman note that the use of the Slater approximation leads to a potential which goes to zero at large  $r$  rather than to  $-2/r$ , the potential of a singly ionized atom. They attempt to partially correct this deficiency by replacing  $V(r) - A_s(r)$  by  $-2/r$  for  $r > r_0$  where  $r_0$  is the value of  $r$  for which

$$V(r_0) - A_s(r_0) = -2/r_0.$$

This modification of the HFS potential was used throughout this calculation because it should pull the valence wave function in closer to the origin. The approximate wave functions which are typically generated for the larger alkali atoms have the defect that the valence wave function does not fall off fast enough with increasing values of  $r$ . This results in an undesirably large value for the polarizability of the atom and, hence an incorrect polarization potential.

The Herman and Skillman program furnished  $P_{nl}(r)$ ,  $V(r)$ ,  $A_s(r)$  and  $\epsilon_1^0$ . The  $P_{nl}(r)$  were calculated on a 512 point mesh. This same mesh was used to obtain the solutions to Eq. 1. The method of solving Eq. (1) is completely analogous to the technique used by Sternheimer<sup>11</sup> in his calculation of atomic dipole polarizabilities. The boundary conditions are that  $U_{nl} \rightarrow l' \rightarrow 0$  as  $r \rightarrow 0$  and that  $U_{nl} \rightarrow l'$  be exponentially decreasing at  $\infty$ . Starting with a series expansion at the origin and an exponential at large  $r$ , the two solutions of Eq. (1) were integrated by the Numerov<sup>12</sup> process and matched at a convenient radius to five significant figures. The  $U_{nl} \rightarrow l'$  were calculated for values of  $r_f$  at every fourth point on the mesh in order to obtain  $V_p(r_f)$ . The contribution to  $V_p$

from every electron orbital was included.

The polarization potential calculated on the basis of the HFS wave functions obtained from the Herman and Skillman program was unsatisfactory. The dipole polarizability of rubidium<sup>13,14</sup> is experimentally  $264 \pm 27$  in atomic units. Thus, one expects  $V_p$  to approach  $-264/r^4$  at large  $r$ . The calculated  $V_p$ , however, approached  $-405/r^4$  at large  $r$ . This was too large a discrepancy to continue with because of the extreme sensitivity of the scattering cross section to the form of the polarization potential.

The principal contribution to  $V_p$  at large  $r$  is from the perturbation of the valence orbital. Therefore, an attempt was made to improve the unperturbed valence wave function. The magnitude of the valence eigenenergy  $\epsilon_1^0$  generated by the self-consistent HFS procedure is slightly smaller than the experimental value. A first-order correction to the valence wave function was made by simply replacing the HFS value for  $\epsilon_1^0$  in the Schrödinger equation for the valence orbital by the experimental value. The valence wave function was then recalculated. With this new wave function, together with the other electron orbitals (unmodified) from the Herman and Skillman program,  $V_p$  was calculated again. This time  $V_p \rightarrow -325/r^4$  at large  $r$ , which was a considerable improvement. A plot of the recalculated  $V_p$  is shown in Fig. 1.

It should be pointed out that Garrett's<sup>1</sup> calculation for sodium was in far better shape at this stage. His HFS wave functions were adequate to give complete agreement between the experimental value of the dipole polarizability and his calculated value. Although the recalculation here of the valence orbital improved the situation, the calculated polarizability is still  $\sim 25\%$  too large. In addition, since the valence contribution to  $V_p$  obtained from the HFS wave functions was so much in error, the core contribution to  $V_p$ , which dominates at small  $r$ , is automatically suspect.

In the solution of Eq. (7), it was decided to use the improved polarization potential along with the

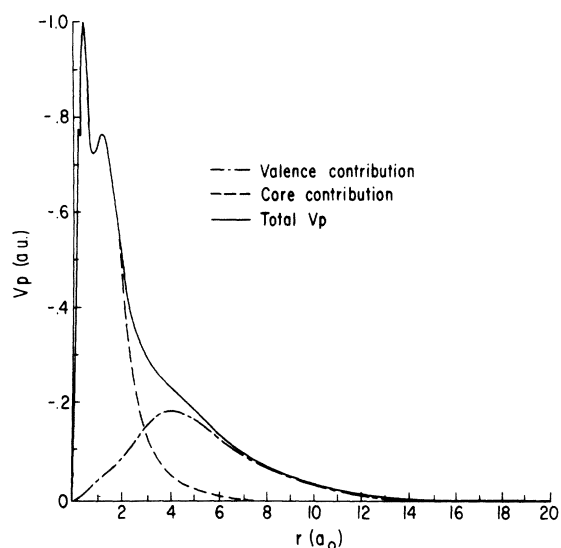


FIG. 1 Contributions to the polarization potential from the core electrons and from the valence electron together with their sum  $V_p$ .

recalculated valence wave function and the experimental value for the valence ground-state energy.

Equation (7) was solved by a successive iteration procedure and the phase shifts  $\delta_l^+$  and  $\delta_l^-$  were obtained from the solutions. The solutions  $f_l$  were started at the origin by a series expansion and with the right-hand side of Eq. (7) set equal to zero. They were integrated by the Numerov method out to a value of  $r$  for which

$$(V_0 + V_p)/k^2 < 10^{-4}$$

for each value of  $k^2$ . The solutions to the homogeneous equation were substituted into the integrals on the right-hand side to obtain the first iteration. This process was continued until the integrals on the right-hand side were self-consistent to within 0.01%. The  $f_l$  were compared with the appropriate spherical Bessel functions at the largest values of  $r$  to obtain the phase shifts. The multiple of  $\pi$  to be added to the phase shift was taken to be the difference between the number of nodes appearing in the  $f_l$  and the number of nodes in the corresponding Bessel functions. The values for  $\delta_l^+$  and  $\delta_l^-$  are listed on Tables I, II, and III.

TABLE I. Singlet phase shifts.

$E$ (Ry)	$\delta_0^+ - 5\pi$	$\delta_1^+ - 3\pi$	$\delta_2^+ - 2\pi$	$\delta_3^+$	$\delta_4^+$	$\delta_5^+$	$\delta_6^+$	$\delta_7^+$	$\delta_8^+$
0.00025	-0.035	0.001	-0.002	-0.001	0.000				
0.00050	-0.044	0.014	-0.004	-0.001	0.001				
0.00075	-0.055	0.036	-0.005	-0.002	-0.001	-0.001			
0.0010	-0.070	0.063	-0.006	-0.003	-0.001	-0.001			
0.0015	-0.105	0.128	-0.005	-0.004	-0.002	-0.001			
0.0020	-0.143	0.203	-0.002	-0.005	-0.003	-0.001			
0.0025	-0.182	0.281	0.002	-0.005	-0.003	-0.002			
0.0030	-0.220	0.361	0.008	-0.005	-0.004	-0.002	-0.001		
0.0040	-0.291	0.517	0.022	-0.004	-0.005	-0.003	-0.002		
0.0050	-0.355	0.664	0.037	-0.001	-0.005	-0.004	-0.002		
0.0060	-0.412	0.796	0.051	0.004	-0.005	-0.004	-0.003		
0.0075	-0.487	0.963	0.069	0.012	-0.003	-0.004	-0.003		
0.010	-0.595	1.160	0.095	0.026	0.003	-0.004	-0.004		
0.020	-0.913	1.422	0.193	0.063	0.026	0.010	0.001	-0.003	
0.030	-1.126	1.470	0.280	0.102	0.041	0.020	0.011	0.004	-0.001
0.050	-1.412	1.474	0.414	0.179	0.074	0.038	0.020	0.012	0.008
0.065	-1.558	1.466	0.483	0.238	0.099	0.050	0.029	0.017	0.010
0.075	-1.636	1.457	0.517	0.277	0.115	0.059	0.033	0.021	0.013
0.085	-1.703	1.448	0.543	0.315	0.131	0.067	0.039	0.024	0.016
0.100	-1.788	1.433	0.571	0.370	0.156	0.080	0.046	0.029	0.019
0.125	-1.902	1.404	0.597	0.455	0.197	0.102	0.059	0.037	0.025
0.150	-1.994	1.373	0.607	0.531	0.237	0.123	0.071	0.045	0.030
0.250	-2.273	1.229	0.577	0.745	0.380	0.206	0.122	0.077	0.052
0.500	-2.761	0.891	0.408	0.980	0.595	0.373	0.237	0.155	0.106
0.750	-3.113	0.629	0.251	1.130	0.688	0.475	0.325	0.224	0.157
1.000	-3.391	0.418	0.122	1.303	0.736	0.533	0.387	0.278	0.201

TABLE II. Triplet phase shifts.

$E$ (Ry)	$\delta_0^- - 5\pi$	$\delta_1^- - 4\pi$	$\delta_2^- - 2\pi$	$\delta_3^-$	$\delta_4^-$	$\delta_5^-$	$\delta_6^-$	$\delta_7^-$	$\delta_8^-$
0.00025	0.590	-0.004	-0.002	-0.001	0.000				
0.00050	0.671	-0.000	-0.004	-0.002	0.001				
0.00075	0.689	0.008	-0.005	-0.002	-0.001	-0.001			
0.0010	0.685	0.018	-0.006	-0.003	-0.001	-0.001			
0.0015	0.656	0.042	-0.005	-0.004	-0.002	-0.001			
0.0020	0.619	0.064	-0.002	-0.005	-0.003	-0.001			
0.0025	0.581	0.084	0.003	-0.006	-0.003	-0.002			
0.0030	0.546	0.100	0.009	-0.005	-0.004	-0.002	-0.001		
0.0040	0.483	0.123	0.023	-0.004	-0.005	-0.003	-0.002		
0.0050	0.428	0.134	0.039	-0.001	-0.005	-0.004	-0.002		
0.0060	0.379	0.139	0.054	0.004	-0.005	-0.004	-0.003		
0.0075	0.312	0.139	0.074	0.012	-0.003	-0.004	-0.003		
0.010	0.212	0.128	0.104	0.026	0.003	-0.004	-0.004		
0.020	-0.087	0.028	0.227	0.063	0.026	0.010	0.001	-0.003	
0.030	-0.298	-0.096	0.348	0.104	0.041	0.020	0.011	0.004	-0.001
0.050	-0.603	-0.321	0.558	0.189	0.074	0.038	0.020	0.012	0.008
0.065	-0.777	-0.464	0.674	0.259	0.099	0.050	0.029	0.017	0.010
0.075	-0.876	-0.550	0.732	0.309	0.116	0.059	0.033	0.021	0.013
0.085	-0.965	-0.629	0.776	0.359	0.133	0.067	0.039	0.024	0.016
0.100	-1.085	-0.736	0.825	0.435	0.160	0.080	0.046	0.029	0.019
0.125	-1.256	-0.893	0.868	0.560	0.205	0.102	0.059	0.037	0.025
0.150	-1.401	-1.026	0.883	0.674	0.250	0.124	0.072	0.045	0.030
0.250	-1.839	-1.425	0.828	0.977	0.422	0.213	0.123	0.078	0.052
0.500	-2.513	-2.004	0.580	1.198	0.686	0.404	0.246	0.158	0.107
0.750	-2.947	-2.358	0.376	1.296	0.783	0.520	0.344	0.231	0.159
1.000	-3.270	-2.615	0.218	1.425	0.822	0.582	0.412	0.290	0.206

TABLE III. Phase shifts for higher  $l$  values where  $\delta_l^+ = \delta_l^-$ .

$E$ (Ry)	$\delta_9$	$\delta_{10}$	$\delta_{11}$	$\delta_{12}$	$\delta_{13}$	$\delta_{14}$	$\delta_{15}$	$\delta_{16}$	$\delta_{17}$
0.050	0.004								
0.065	0.007	0.005							
0.075	0.008	0.006							
0.085	0.010	0.006							
0.10	0.013	0.009							
0.125	0.017	0.012	0.009						
0.150	0.021	0.015	0.011						
0.250	0.037	0.026	0.020						
0.500	0.075	0.055	0.042	0.032					
0.750	0.113	0.083	0.063	0.049	0.039	0.031	0.025	0.020	
1.000	0.148	0.111	0.084	0.066	0.052	0.042	0.034	0.028	0.023

#### IV. TOTAL ELASTIC AND SPIN-EXCHANGE CROSS SECTIONS

The total elastic cross section  $\sigma$  in units of  $\pi a_0^2$  is

$$\sigma = \frac{1}{k^2} \sum_{l=0}^{\infty} (2l+1)(\sin^2 \delta_l^+ + 3 \sin^2 \delta_l^-). \quad (9)$$

The elastic scattering cross section obtained

from the phase shifts in Tables I, II, and III is plotted as a function of energy in Fig. 2. The cross section for rubidium-electron collisions as measured by Brode<sup>2</sup> is shown for comparison in the same figure. The qualitative behavior of the experimental cross section is in reasonable agreement with the calculation, but the magnitude of the calculated cross section is too small roughly by a factor of two.

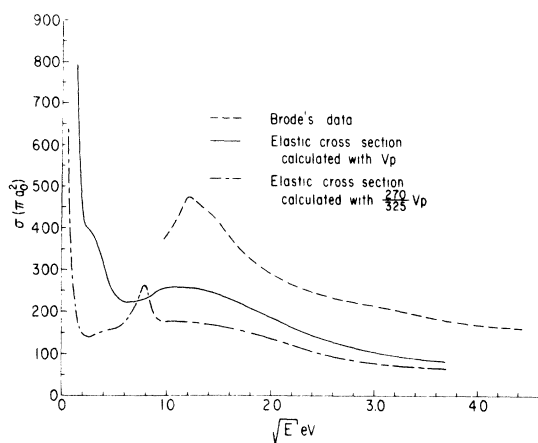


FIG. 2 Total elastic scattering cross section computed from the phase shifts in Tables I, II, and III compared with Brode's experimental results and with the total cross section computed from the modified polarization potential  $(270/325) V_p$ .

Primarily to test the sensitivity of the calculated cross section to the form of the polarization potential, the polarization potential  $V_p$  was normalized by the factor  $(270/325)$  and the cross section recalculated. This, of course, brings the asymptotic behavior of the polarization potential into line with experiment by brute force. This approach was tried in the calculation of Crown and Russek<sup>15</sup> for cesium-electron scattering. The cross section resulting from this modified  $V_p$  is also plotted in Fig. 2. This normalization of  $V_p$  pulls the cross section further away from agreement with experiment and introduces a narrow resonance due to  $p$ -wave scattering. A  $p$ -wave resonance (much larger) was also produced in the Crown and Russek calculation when they normalized their polarization potential in the same way. There is no experimental verification or disproof of the existence of this resonance.

A comparison of the Crown and Russek calculated cross section for cesium-electron scattering with Brode's data and a similar comparison for Garrett's sodium calculation are given in Figs. 3 and 4, respectively. The results of the present calculation for rubidium with the unmodified  $V_p$  are in much poorer agreement with experiment than was the case for sodium, but more satisfactory than the calculation for cesium. The cross sections for rubidium and cesium are monotonically increasing at the lowest energies, while the sodium cross section has turned around and is decreasing.

The only experimental check for the phase shifts at very low energy is the spin-flip cross section obtained from optical-pumping experiments. In

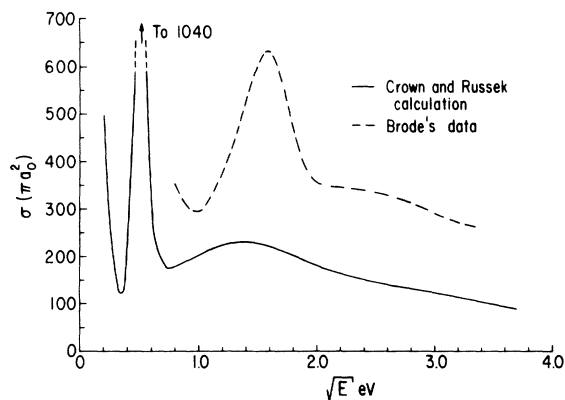


FIG. 3 Total elastic scattering cross section for cesium calculated by Crown and Russek compared with Brode's experimental data for cesium.

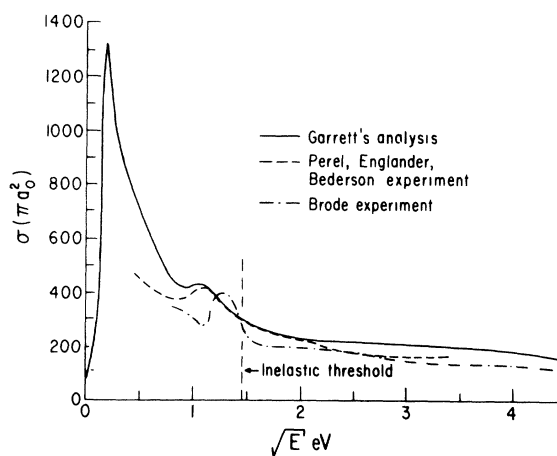


FIG. 4 Total elastic scattering cross section for sodium as calculated by Garrett compared with the experimental results of Brode and of Perel *et al.*

these experiments, the conditions can be adjusted so that the linewidth of the electron spin resonance is a function of the electron-alkali atom spin-flip cross section  $\sigma_{sf}$ . The linewidth is calculated by averaging the expression  $VN\sigma_{sf}$  over a Boltzmann distribution characterized by the temperature of the electrons. The velocity of the electrons is  $V$ ,  $N$  is the volume-density of the rubidium atoms and  $\sigma_{sf}$  is given by

$$\sigma_{sf} = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\delta_l^- - \delta_l^+). \quad (10)$$

Here the cross section is in units of  $\text{cm}^2$  and  $\hbar k = mV$  is the momentum of the electrons. The experimental linewidth for rubidium-electron collisions at 293°K is  $1500 \pm 200$  Hz. The calculated linewidth using the phase shifts in Table I is 700

Hz and the calculated linewidth using the modified  $V_p$  is 350 Hz. Again, the *ad hoc* normalization of  $V_p$  makes things worse.

Thus, the calculated spin-exchange cross section for rubidium averaged over the energy spread of the optical pumping experiment is about a factor of two too small. Garrett's phase shifts for sodium yielded an averaged spin-exchange cross section in good agreement with experiment.<sup>5</sup>

#### V. CONCLUSION

Though HFS wave functions are apparently quite adequate for scattering calculations involving the lighter alkalis, they proved less adequate for rubidium. The quantitative agreement between this calculation and experiment is poor compared to Garrett's calculation for sodium, but a good deal better than for cesium. This probably simply reflects the relative size and complexity of the target atoms. Recently, it has been reported<sup>16</sup> that Brode's numbers for the  $K - e$  collision cross section are too large by a factor of 2. If it turns out that his results for Rb are in

error in the same way, the agreement between the present calculation and experiment at the upper end of the energy range may be better than it now appears. There would still be poor agreement with the optical-pumping experiment at thermal energies. The results for rubidium are sufficiently reasonable, however, to encourage one not to abandon the method of polarized orbitals and the adiabatic approach to the scattering equation without first trying again with more accurate wave functions. The *ad hoc* normalization of the polarization potential to yield the correct dipole polarizability at large  $r$  did not appear to be useful in this calculation.

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