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Electron—hydrogenlike-ion scattering

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The *s*-, *p*-, and *d*-wave phase shifts have been calculated for elastic scattering of electrons by hydrogenlike ions He^+, Li^{2+}, Be^{3+}, and B^{4+} with the use the polarized-orbital method of Callaway *et al.* The present method takes account of exchange polarization explicitly following Sloan. Our *s*-wave triplet phase shifts are in very good agreement with those of the variational method. In the case of e^--He^+ scattering, our singlet *s*-wave phase shifts differ by about 7.5% whereas for e^--B^{4+} scattering, agreement is very good.

INTRODUCTION

The scattering of electrons by positive hydrogenlike ions has been investigated theoretically. There are some theoretical attempts that warrant mentioning. The polarized-orbital method of Temkin, Lamkin, and Sloan[1,2] has been employed by Sloan[2] to investigate e^--He^+ scattering at low incident energies. Burke *et al.*[3] have applied a three-state (1*s*-2*s*-2*p*) close-coupling method to investigate the same problem. The results are not very satisfactory. Burke and Taylor[4] have used a three-state close-coupling method with 16 correlation terms in the expansion of total wave function. This problem was first treated variationally by Bransden and Dalgarno[5] who have used the three-parameter trial wave function. Shimamura[6] has used the Harris variational method[7] to investigate the electron-hydrogenlike ion scattering problem using 50-term Schwartz-type trial functions. These variational phase shifts are in close agreement with those of Burke and Taylor.

The difficulties and limitations of close-coupling and variational methods are well known. The method of polarized orbitals has been found to be suitable in studying electron-atom scattering. Here we have used the polarized-orbital method of Callaway *et al.*[8] This method is variationally consistent.[9] The formalism of Callaway *et al.*[8] gives rise to a correction term to adiabatic polarization potential which is repulsive in nature. The effect of the exchange polarization that is attractive in nature has been neglected by them in the calculation of phase shifts. In our study we have included the effect of exchange polarization explicitly following Temkin, Lamkin, and Sloan. Here we have taken He^+, Li^{2+}, Be^{3+}, and B^{4+} as our targets and have given the elastic *s*-, *p*-, and *d*-wave phase shifts.

THEORY

Total wave function for electron-hydrogenlike ions in the framework of polarized-orbital methods can be written as

$$\Phi(\vec{r}_1,\vec{r}_2)=(1+P_{12})\chi(\vec{r}_1,\vec{r}_2)F(\vec{r}_1) , \qquad (1)$$

with

$$\chi(\vec{r}_1,\vec{r}_2)=\Phi_0(\vec{r}_2)+\Phi_d(\vec{r}_1,\vec{r}_2) .$$

Projecting onto $\Phi_0(\vec{r}_2)+\Phi_d(\vec{r}_1,\vec{r}_2)$, one can obtain the following integro-differential equation (Banerjee *et al.*[10]):

TABLE I. Elastic *s*-wave phase shifts.

	e^--He$^+$				e^--Be^{3+}		
Energy (eV)	Present Singlet	Present Triplet	Variational Triplet	Energy (eV)	Present Singlet	Present Triplet	Variational Triplet
0.774	0.4019	0.9311	0.9241	2.489	0.1487	0.4024	0.4004
2.164	0.3922	0.9193	0.9121	8.042	0.1485	0.3983	0.3959
5.098	0.3745	0.8953	0.8896	16.459	0.1484	0.3923	0.3911
7.662	0.3616	0.8752	0.8683	28.256	0.1485	0.3843	0.3834
11.092	0.3475	0.8498	0.8461	33.625	0.1486	0.3808	0.3775
20.457	0.3225	0.7884	0.7858	50.834	0.1492	0.3701	0.3667
29.139	0.3107	0.7422	0.7393	66.785	0.1499	0.3609	0.3609
32.060	0.3082	0.7270	0.7181	97.300	0.1515	0.3451	0.3459
38.040	0.3049	0.7005	0.8315	106.580	0.1520	0.3406	0.3372
				143.040	0.1538	0.3247	0.3299

	e^--Li^{2+}				e^--B^{4+}		
Energy (eV)	Present Singlet	Present Triplet	Variational Triplet	Energy (eV)	Present Singlet	Present Triplet	Variational Triplet
1.295	0.2132	0.5621	0.5590	8.829	0.1151	0.3117	0.3109
6.799	0.2103	0.5514	0.5462	21.396	0.1156	0.3074	0.3063
14.735	0.2072	0.5368	0.5325	31.436	0.1160	0.3040	0.3009
21.456	0.2054	0.5250	0.5251	39.206	0.1163	0.3015	0.3009
45.760	0.2026	0.4880	0.4833	48.353	0.1167	0.2986	0.2955
63.990	0.2027	0.4644	0.4595	62.768	0.1173	0.2942	0.2957
83.530	0.2039	0.4427	0.5547	74.435	0.1178	0.2098	0.2873
				111.440	0.1194	0.2806	0.2773
				159.820	0.1213	0.2688	0.2658
				216.470	0.1233	0.2567	0.2563

$$[\nabla^2_{r_1}+K_i^2-V_c(\vec{r}_1)-V_p(\vec{r}_1)-V_d(\vec{r}_1)]F(\vec{r}_1)=\int d\vec{r}_2\chi^*(\vec{r}_2,\vec{r}_1)(H-E)\chi(\vec{r}_1,\vec{r}_2)F(\vec{r}_2)\ . \tag{2}$$

subject to the normalization condition

$$\int |\chi(\vec{r}_1,\vec{r}_2)|^2 d\vec{r}_2=1 \tag{3}$$

for all values of incident electron coordinate $\vec{r}_1$. Here V_c and V_p are the static and adiabatic polarization potentials, respectively. The first-order correction term to adiabatic polarization potential V_p is given by the V_d.

Equation (2) with normalization constraints [Eq. (3)] is variationally consistent. The solution of Eq. (2) is not an easy task. It is not true that the solution of Eq. (2) necessarily predicts reliable results, for the choice of our trial function may not be sufficiently good. Oberoi and Callaway[11] have solved Eq. (2) for the calculation of binding energy of H$^-$. Their result is very unpromising. It is well known that Temkin-Lamkin-Sloan potential contains excess attraction. It has been seen from the work of Daskhan *et al.*[12] that the inclusion of V_d in the framework of Temkin-Lamkin-Sloan formalism makes the effective potential slightly less attractive than the exact one. Their *s*-wave phase shifts are always less than the exact variational results. Keeping this in mind we have solved the following equations as used by Daskhan *et al.*[12]:

$$[\nabla^2_{r_1}+K_i^2-V_c(\vec{r}_1)-V_p(\vec{r}_1)-V_d(\vec{r}_1)]F(\vec{r}_1)=\int d\vec{r}_2\Phi_0^*(\vec{r}_2)(H-E)\chi(\vec{r}_1,\vec{r}_2)F(\vec{r}_2)\ . \tag{4}$$

We have solved this integro-differential equation making the partial-wave analysis as given by Daskhan *et al.*[12] We have taken the expressions for V_p and V_d from the work of Callaway *et al.*[8]

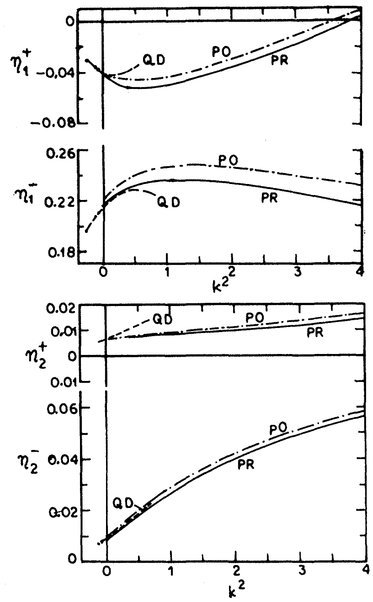

FIG. 1. *p*- and *d*-waves phase shifts (in radians) for e^--He$^+$ scattering; present results PR, Sloan PO, and quantum-defect theory QD.

RESULTS AND DISCUSSIONS

We have solved the integro-differential equations using the method as employed by Tamkin and Lamkin[2] and Sloan.[3] We have reproduced the phase shifts of Sloan as a check of our program by using suitable step size. For the case of e^--He$^+$ scattering the required step size is 0.05 a.u.. But it has been found for e^--B^{4+} scattering that step size of 0.01 to 0.005 are required to have a stable phase shift. Moreover, one has to integrate for all energies up to $r = 10$ to obtain converged phase shifts.

Shimamura[6] has used a different set of energies to calculate singlet and triplet phase shifts. We have selected the energies that were taken by him for triplet case. Table I gives our *s*-wave phase shifts along with triplet phase shifts of Shimamura for comparison. Our triplet phase shifts are in very good agreement with corresponding variational results. Singlet phase shifts are more sensitive to the choice of effective potential. Our present singlet results differ by about 7.5% from these of

TABLE II. Present *p*-wave elastic phase shifts.

Energy (eV)	e^--He$^+$ Singlet	Triplet	Energy (eV)	e^-Be^{3+} Singlet	Triplet
0.774	−0.0393	0.2141	2.489	−0.0387	0.1298
2.164	−0.0417	0.2188	8.042	−0.0376	0.1293
5.098	−0.0451	0.2260	16.459	−0.0357	0.1283
7.662	−0.0465	0.2301	28.256	−0.0330	0.1268
11.092	−0.0469	0.2333	33.625	−0.0317	0.1262
20.457	−0.0421	0.2341	50.834	−0.0274	0.1238
32.060	−0.0408	0.2280	66.785	−0.0230	0.1216
38.040	−0.0342	0.2240	97.300	−0.0161	0.1174
			106.580	−0.0140	0.1162
			143.040	−0.0059	0.1114
Energy (eV)	e^--Li^{2+} Singlet	Triplet	Energy (eV)	e^--B^{4+} Singlet	Triplet
1.295	−0.0504	0.1683	8.829	−0.0184	0.0985
6.799	−0.0495	0.1684	21.396	−0.0159	0.0972
14.735	−0.0473	0.1679	31.436	−0.0138	0.0962
21.456	−0.0451	0.1670	39.206	−0.0123	0.0954
40.347	−0.0352	0.1621	48.353	−0.0104	0.0944
45.760	−0.0354	0.1618	62.768	−0.0074	0.0929
63.990	−0.0271	0.1572	74.435	−0.0051	0.0917
83.530	−0.0188	0.1523	111.440	+0.0024	0.0880
			159.820	+0.0116	0.0831
			216.470	+0.0218	0.0778

TABLE III. Present *d*-wave elastic phase shifts.

Energy (eV)	e^--He$^+$ Singlet	Triplet	Energy (eV)	e^--Be^{3+} Singlet	Triplet
0.774	0.0059	0.0104	2.489	0.00081	0.0086
2.164	0.0064	0.0125	8.042	0.00066	0.0095
5.098	0.0070	0.0167	16.459	0.00045	0.0109
7.662	0.0074	0.0201	28.256	0.00021	0.0128
11.092	0.0077	0.0242	33.625	0.00012	0.0135
20.457	0.0086	0.0341	50.834	−0.00007	0.0158
29.139	0.0095	0.0414	66.785	−0.00014	0.0177
32.060	0.0099	0.0435	97.300	−0.00002	0.0208
38.040	0.0108	0.0473	106.580	−0.00008	0.0216
			143.040	0.00062	0.0244

Energy (eV)	e^--Li^{2+} Singlet	Triplet	Energy (eV)	e^--B^{4+} Singlet	Triplet
1.295	0.0026	0.0098	8.829	−0.00016	0.00785
6.799	0.0025	0.0121	21.396	−0.00037	0.00891
14.735	0.0023	0.0152	31.436	−0.00051	0.00978
21.456	0.0021	0.0176	39.206	−0.00061	0.01032
40.347	0.0021	0.0248	48.353	−0.00070	0.01099
45.760	0.0025	0.0249	62.768	−0.00083	0.01199
63.990	0.0024	0.0289	74.435	−0.00089	0.01276
83.530	0.0032	0.0325	111.440	−0.00098	0.01494
			159.820	−0.00085	0.01728
			216.470	−0.00042	0.01946

Shimamura for the case of e^--He$^+$ scattering, our values being lower. Similar discrepancy has also been noticed by Daskhan *et al.* for e^--H scattering. This discrepancy decreases with the increase of charge of the ion. For the case of e^--B^{4+}, our results are in excellent agreement with those of Shimamura. With the increase of ionic charge, Z, polarizability decreases. This may be probable reason for better agreement of *s*-wave phase shifts with the increase of Z.

Our *p*- and *d*-wave phase shifts for e^--He$^+$ scattering are shown in Fig. 1. The corresponding results of Sloan and those of quantum defect are also given for comparison. From our experience for e^--H scattering (Ref. 12) we conclude that the present results are expected to be more reliable than those of Sloan. Purely adiabatic hypothesis fails with the increase of incident energies. Sloan has considered only the adiabatic dipole polarization potential in the direct channel. Therefore it is expected that their results at intermediate energies are less reliable.

We have tabulated our *p*- and *d*-waves phase shifts for four ionic targets (Tables II and III). As no other results are available in the literature, we are not able to compare our results.

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[1] A. Temkin and J. C. Lamkin, Phys. Rev. 121, 788 (1961).

[2] I. H. Sloan, Proc. R Soc. London, Ser. A 281, 151 (1969).

[3] P. G. Burke, D. D. Mevicar, and K. Smith, Proc. Phys. Soc. London 84, 749 (1964).

[4] P. G. Burke and A. J. Taylor, Proc. Phys. Soc. London 88, 549 (1966).

[5] B. H. Bransden and A. Dalgarno, Proc. Phys. Soc. London, Sec. A 66, 268 (1953).

[6] I. Shimamura, J. Phys. Soc. Jpn. 31, 217 (1971).
[7] F. E. Harris, Phys. Rev. Lett. 19, 173 (1967).
[8] J. Callaway, R. W. LaBahn, T. R. Pu, and W. M. Duxler, Phys. Rev. 168, 12 (1968).
[9] J. Callaway, Comput. Phys. Commun. 6, 265 (1974).
[10] G. Banerji, P. Mandal, and A. S. Ghosh, Phys. Lett. 83A, 62 (1981).
[11] R. S. Oberoi and J. Callaway, Phys. Rev. A 1, 45 (1970).
[12] M. Daskhan, P. Khan, A. S. Ghosh, and Carlos Falcon, Phys. Rev. A 23, 728 (1981).