Coherence, alignment, and spin asymmetry in electron-hydrogen inelastic scattering

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The coherence and alignment in electron excitation of hydrogen (1s-2p) is studied for electron energies of 35 and 54.4 eV using a two-potential approach. We also study the spin asymmetry in the scattering of spin-polarized electrons with spin-polarized hydrogen atoms and compare our results with other available calculations.

Atoms which have been collisionally excited usually possess an anisotropy in the population of the excited states. The anisotropy has been related to the observables of the subsequent decay *viz* the photon angular distribution and polarization. The investigation of the three components of the polarization of radiation (P_1, P_2, and P_3) emitted normal to the scattering plane can be used to determine the coherence of the excitation of an atomic state. Normally the condition for the coherent excitation of states (without significant hyperfine structure) is given by $|P| = (P_1^2+P_2^2+P_3^2)^{1/2} = 1$. The measurements of P_1 and P_2 also yield information about the alignment (γ) of the charge cloud with respect to the incident beam direction.

In recent years considerable advances have been made in the development of polarized electron sources as well as polarized atomic targets. This has initiated experiments on polarized-electron–polarized-target scattering, to probe the spin-dependent features of the scattering. The study of spin asymmetry in the scattering of spin-polarized electrons with spin-polarized atoms provides useful information about the exchange contribution to the scattering. In this paper we report results for coherence parameter (P), the alignment angle (γ), and spin asymmetry (A) in electron-hydrogen inelastic (1s-2p) scattering. We follow a two-potential approach.

Dividing the total interaction potential $V = U + W$, the T matrix for electron-hydrogen inelastic scattering in the two-potential approach, is given by[1,2]

$$T = \langle \phi_f^-(\mathbf{r}_1,\mathbf{r}_2) \,|\, W \,|\, \psi_i^+(r_1,r_2)\rangle , \tag{1}$$

where ψ and ϕ satisfy

$$H\psi = E\psi \text{ and } (H_0+U)\phi = E\phi . \tag{2}$$

H_0 is the unperturbed Hamiltonian and E is the total energy. $\mathbf{r}_1$ and $\mathbf{r}_2$ are the atomic and incident electron coordinates respectively. Including exchange, and retaining the first term in the expansion of ψ_i^+ with respect to H_2 $(=H_0+U)$, Eq. (1) can be rewritten as

$$T_\pm = -2\pi(f \pm g) , \tag{3}$$

with

$$f = -(2\pi)^{-1}\langle X_f^-(\mathbf{r}_2)v_f(\mathbf{r}_1) \,|\, W \,|\, X_i^+(\mathbf{r}_2)v_i(\mathbf{r}_1)\rangle , \tag{4}$$

and

$$g = -(2\pi)^{-1}\langle X_f^-(\mathbf{r}_2)v_f(\mathbf{r}_1) \,|\, W \,|\, X_i^+(\mathbf{r}_1)v_i(\mathbf{r}_2)\rangle . \tag{5}$$

$v_{i,f}$ $(\mathbf{r}_1)$ is the atomic wave function and $X_{i,f}^\pm$ $(\mathbf{r}_2)$ are the distorted waves of the scattered electron and $\phi_{i,f}^\pm$ $(\mathbf{r}_1,\mathbf{r}_2) = X_{i,f}^\pm(\mathbf{r}_2)v_{i,f}(\mathbf{r}_1)$.

The local approximation to the exchange amplitude is obtained as[2]

$$g = -\left\langle X_f^-(\mathbf{r}_2)v_f(r_2) \left| \left[\frac{1}{K_i^2} + \frac{1}{K_f^2} \right] \right| X_i^+(\mathbf{r}_2)v_i(\mathbf{r}_2)\right\rangle ,$$

with

$$K_j^2 = k_j^2 - 2[V_s^j + V_p^j(r_2)]$$

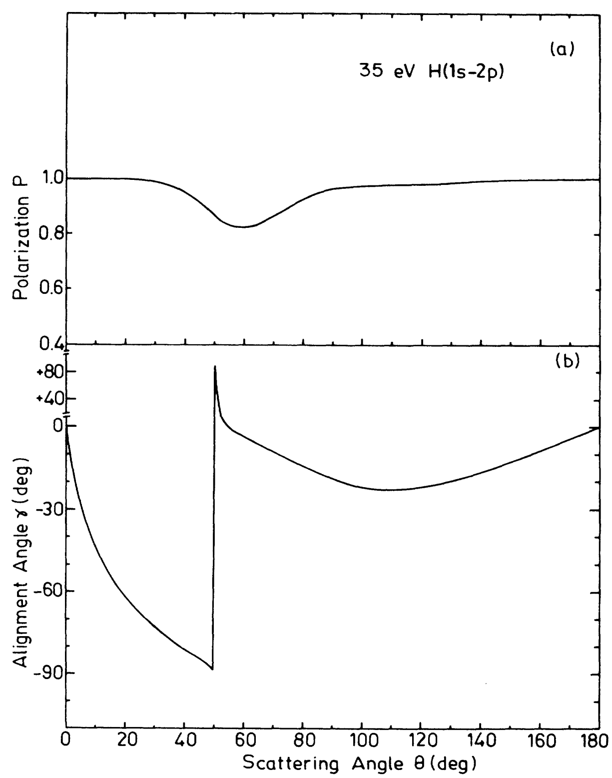

FIG. 1. (a) Polarization and (b) alignment at 35 eV electron energy. ——, present results.

and

$$V_s^j = \langle v_j(\mathbf{r}_1) \,|\, V \,|\, v_j(\mathbf{r}_1) \rangle \ .$$

$\mathbf{k}_j$ is the momentum of the scattered electron. V_s^j and V_p^j are the static and polarization potentials in the channel j. For U we take $U^i = V_s^i + V_p^i$ and $U^f = V_s^f$.

The polarization potential is of the form[2]

$$V_p^j = \frac{-\alpha_j}{2r^4}\{1-\exp[-(r/r_{0j})^6]\} \ .$$

r_{0j} is the cutoff parameter. The nonadiabatic polarization potential is obtained[2] from the above through the prescription of Onda and Truhlar.[3]

The differential cross section σ is given by

$$\sigma = \frac{k_f}{k_i}\left(\tfrac{1}{4}\,|f+g|^2 + \tfrac{3}{4}\,|f-g|^2\right) \ .$$

The polarization components P_1, P_2, and P_3 can be expressed in terms of the angular correlation parameters[4,5] λ, A_{1+}^c, O_{1-}^c as

$$P_1 = 2\lambda - 1 \ ,$$

$$P_2 = -2A_{1+}^c \ ,$$

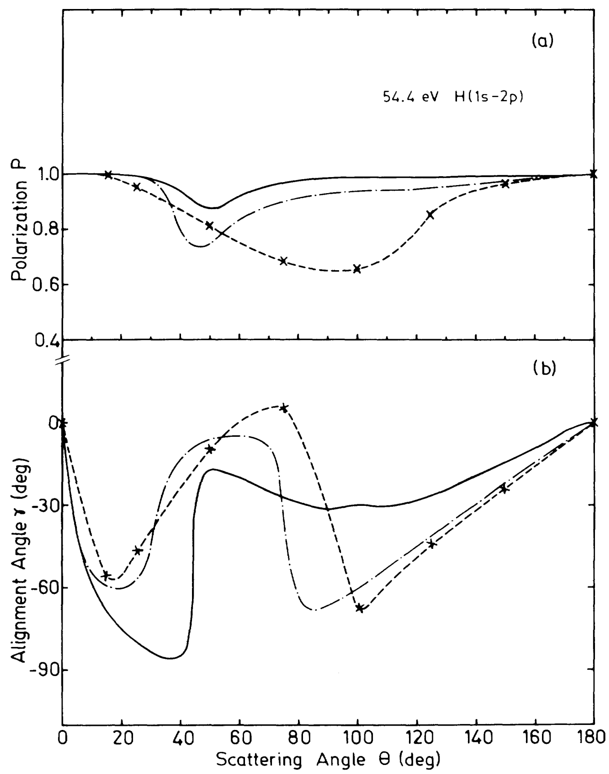

FIG. 2. (a) Polarization and (b) alignment at 54.4 eV electron energy. ——, present results; –✕–✕–, UEBS results (Ref. 8); and —·—·—·, SODW calculations (Ref. 7).

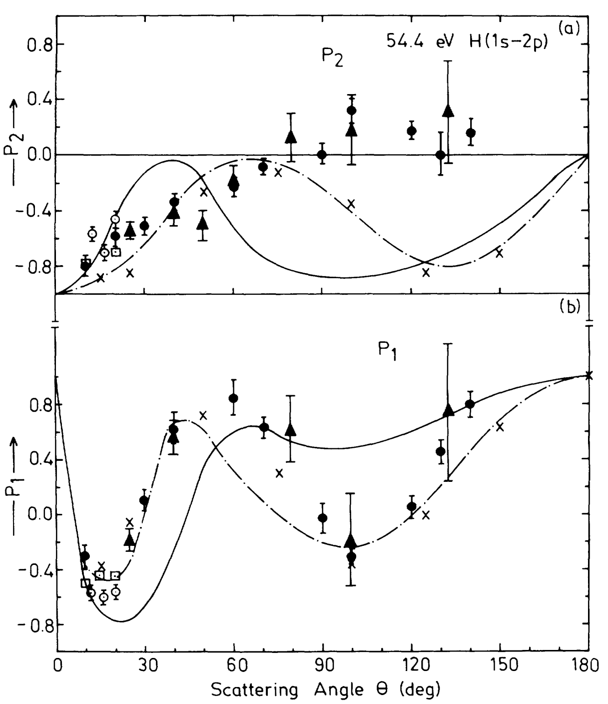

FIG. 3. Polarization components (a) P_2 and (b) P_1 at 54.4 eV electron energy. ——, present results; —·—·—·, SODW calculation (Ref. 7); ×, UEBS calculation (Ref. 8); ⊡, Hood *et al.* (Ref. 12); ●, Williams (Ref. 10); ○, Slevin *et al.* (Ref. 9); and ▲, Weigold *et al.* (Ref. 11).

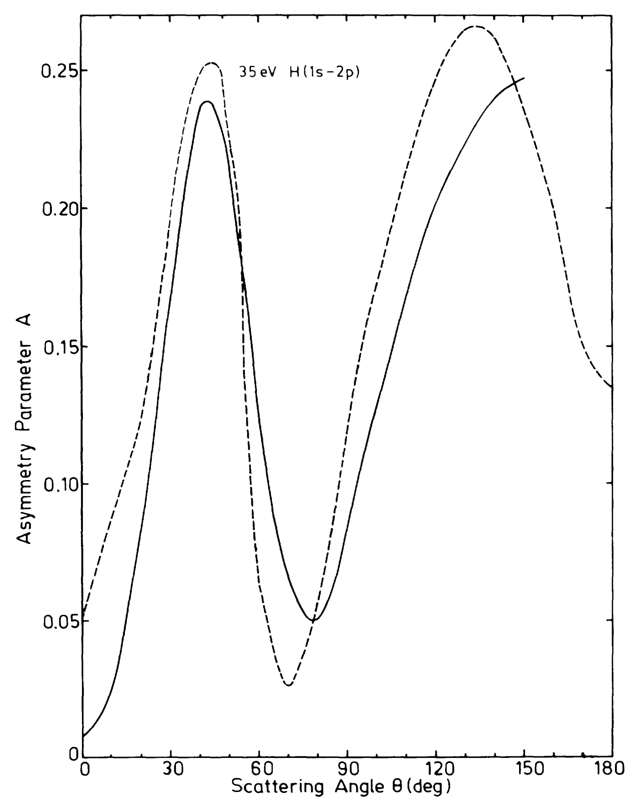

FIG. 4. Spin asymmetry A at 35 eV electron energy. ——, present results; — — —, 10CCLE results of McDowell *et al.* (Ref. 13).

and

$$P_3 = -2O^c_{1-} \ (= -\langle L_y \rangle) .$$

The total polarization P is

$$P = (P_1^2 + P_2^2 + P_3^2)^{1/2} .$$

The alignment angle γ is then given by

$$\gamma = \tfrac{1}{2}\arg(P_1 + iP_2) .$$

The parameters λ, A^c_{1+}, and O^c_{1-} are related to the scattering amplitudes (Saxena and Mathur[5]).

In the situation when both the projectile and the target are spin polarized, the differential cross section for spin antiparallel and spin parallel scattering can be expressed as[6]

$$\sigma(\uparrow\downarrow) = |f|^2 + |g|^2$$

and

$$\sigma(\uparrow\uparrow) = |f - g|^2 .$$

TABLE I. Coherence and alignment parameters at incident electron energy of 35 and 54.4 eV.

Scattering angle (deg)	P_1	P_2	P_3	γ
		$E_i = 35$ eV		
0	1.0	0.0	0.0	0.0
5	0.618	−0.784	−0.059	−25.9
10	0.049	−0.987	−0.151	−43.6
15	−0.314	−0.907	−0.278	−54.6
20	−0.511	−0.754	−0.412	−62.1
25	−0.606	−0.583	−0.537	−68.1
30	−0.620	−0.410	−0.656	−73.2
40	−0.426	−0.144	−0.836	−80.7
50	−0.050	0.005	−0.866	87.4
60	0.388	−0.052	−0.727	−3.8
80	0.790	−0.427	−0.238	−14.2
100	0.691	−0.679	−0.043	−22.2
120	0.697	−0.694	−0.038	−22.5
140	0.820	−0.561	−0.044	−17.2
160	0.946	−0.320	−0.036	−9.3
180	1.0	0.0	0.0	0.0
		$E_i = 54.4$ eV		
0	1.0	0.0	0.0	0.0
5	0.194	−0.980	−0.048	−39.4
10	−0.443	−0.883	−0.157	−58.3
15	−0.682	−0.663	−0.308	−57.9
20	−0.766	−0.466	−0.442	−74.4
25	−0.770	−0.283	−0.565	−79.9
30	−0.671	−0.135	−0.711	−84.3
40	−0.275	−0.052	−0.898	−84.6
50	0.325	−0.221	−0.792	−17.1
60	0.591	−0.499	−0.504	−20.1
80	0.558	−0.807	0.032	−27.7
100	0.506	−0.838	0.150	−29.4
120	0.626	−0.760	0.141	−25.3
140	0.799	−0.589	0.098	−18.2
160	0.938	−0.343	0.035	−10.0
180	1.000	0.0	0.0	0.0

The spin asymmetry A between spin parallel and spin antiparallel scattering is

$$A = [\sigma(\uparrow\downarrow) - \sigma(\uparrow\uparrow)]/[\sigma(\uparrow\downarrow) + \sigma(\uparrow\uparrow)] .$$

For the $1s$-$2p$ excitation, A can be explicitly written as

$$A_{1s\text{-}2p} = \sum_{m=-1}^{1} [\sigma_{2pm}(S=0) - \sigma_{2pm}(S=1)]/\sigma_{2p} ,$$

where S denotes the total spin and σ_{2p} the total differential cross section.

Results. Figure 1(a) gives the variation of the polarization P with respect to the scattering angle. It is observed that for scattering angles between 0° and 35° and beyond 100° the polarization remains close to unity, thereby showing complete coherence of the excitation process. Around 60° the lowest value of polarization ($P = 0.82$) is obtained. Figure 1(b) gives the variation of the alignment angle γ of the charge cloud with scattering angle. A rapid decrease in alignment is noticed at low scattering angles. A minima in the alignment angle ($\gamma = -85°$) is obtained at an electron scattering angle of about 45° followed by sudden jump between 49° and 50° scattering angles. γ attains a value close to zero around 55° scattering angle, beyond which it shows a gradual variation. The sudden jump in the alignment angle is related to the maximum transfer of angular momentum ($\langle L_y \rangle$).

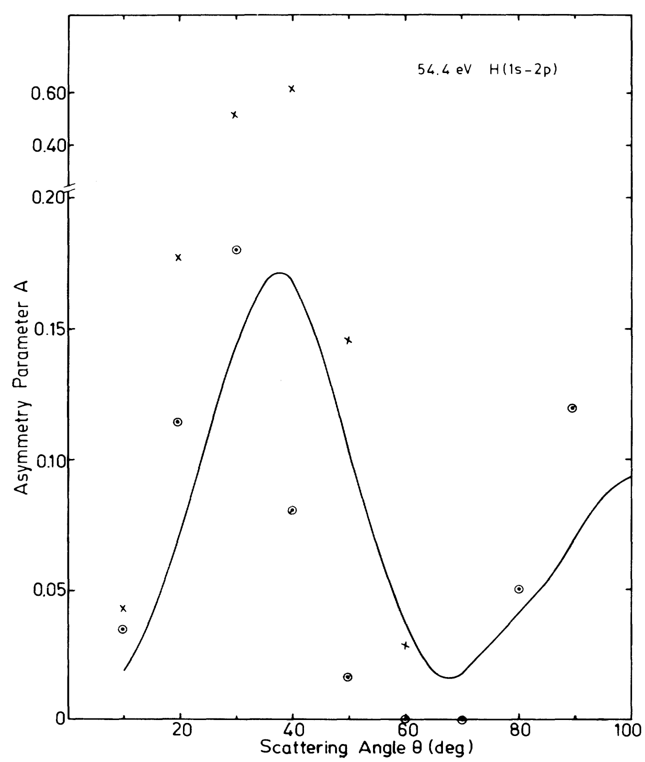

FIG. 5. Spin asymmetry A at 54.4 eV electron energy. ——, present results; ×, CCSOP results of McDowell *et al.* (Ref. 13); and ⊙, pseudostate approximation calculation of Wyngaarden and Walters (Ref. 14).

Figures 2(a) and 2(b) show the variations of our results of polarization P and the alignment angle γ with respect to the scattering angle at 54.4-eV energy. Comparison with the second-order distorted wave (SODW) calculation of Madison *et al.*[7] and the unitarized eikonal Born series (UEBS) results[8] is also shown. The present results for P show a behavior similar to the SODW calculation. The dip in the SODW calculation, however, is more pronounced and shifted towards lower angles in comparison to the present calculation. Further, it is noted that our results of P show a good agreement with the UEBS results for scattering angles up to 50°, and also beyond 150°. However, at intermediate scattering angles the UEBS results tend to be significantly lower than our results. For the alignment angle, we find that there is a qualitative agreement between our results and those based on the SODW and UEBS methods. The future experimental results would provide a test for theory.

Figures 3(a) and 3(b) show the present results of the polarization components P_2 and P_1, along with the SODW (Ref. 7) and UEBS (Ref. 8) calculations and the experimental values, derived from the λ and R measurements of Slevin *et al.*,[9] Williams,[10] Weigold *et al.*,[11] and Hood *et al.*[12] It is observed that for P_2 none of the theoretical calculations agree with the data in the large scattering angle region beyond 70°. For low scattering angles the present calculations are in reasonable agreement with the data, whereas in the angular region between 30° and 70° the SODW and the UEBS calculations are in better agreement with the data. For P_1 [Fig. 3(b)], the SODW and UEBS calculations provide a better agreement with the data compared to the present calculation.

In Table I we give the numerical values of the coherence and alignment parameters (P_1, P_2, P_3, and γ) at 35 and 54.4 eV incident electron energies.

Figure 4 shows the present results for the spin asymmetry parameter A at 35 eV energy. The calculations of McDowell *et al.*,[13] based on the ten-state close-coupling method with local exchange (10CCLE) are also shown for comparison. From the figure we note that there is a reasonably good agreement between our calculation and that of McDowell *et al.* The peaks and minima in the two calculations are fairly close and their locations are also within a 10° scattering angle.

Figure 5 shows our results of spin asymmetry A at 54.4 eV energy. The comparison with the close-coupling second-order potential (CCSOP) calculation of McDowell *et al.*[13] and the pseudostate approximation calculation of Wyngaarden and Walters[14] is shown. It is observed that below 50° a peak is obtained in all the three calculations at nearly the same location. The peak height in our calculation (0.17) is closer to that of Wyngaarden and Walters (0.18). The CCSOP calculation predicts a very high value of peak height (≈ 0.6). The measurements of the asymmetry parameter, now in progress in various laboratories, will provide a direction for further improvement in the available theories.

In conclusion, we expect that the two-potential approach would be a reasonable procedure for the study of these finer aspects (coherence, alignment, and spin asymmetry) in electron atom collisional excitations.

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