Alignment and orientation parameters in positron-sodium resonant scattering

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The two-potential approach is used to study the differential and integrated cross sections, the alignment and orientation parameters $(\lambda,\chi,\langle L_y\rangle,\gamma)$, and the coherence of excitation in the resonant scattering of positrons with sodium atoms at three intermediate energies 12.1, 22.1, and 30 eV. These parameters are compared with the corresponding parameters in electron-sodium resonant scattering. Such a comparison between electron and positron scattering leads to useful information about the role of different interaction potentials in the scattering process.

I. INTRODUCTION

The study of alignment and orientation in atomic collision provides a deep insight into the understanding of the dynamics of the collision process. An extensive study of alignment and orientation parameters for electron-impact excitation of atoms has been performed during the last two decades. A comprehensive review of the same has been given recently by Andersen *et al.*[1] Most of the theoretical and experimental work on positron impact excitation of atoms is limited to the study of differential and total cross sections.[2] Fargher and Roberts[3] have studied angular correlation parameters in positron hydrogen scattering and Willis *et al.*[4] and Madison and Winters[5] for positron helium scattering. Saxena and Mathur[6] have studied the angular correlation parameters for e^+-Li resonant scattering. Recently Pangantiwar and Srivastava[7] have studied λ and χ parameters in electron-positron scattering from a rubidium atom. To our knowledge no theoretical or experimental work is available for alignment and orientation studies on positron-sodium ($3s$-$3p$) scattering. Such studies are, however, important. In this paper we report a theoretical study of positron-sodium atom scattering using a two-potential approach at three intermediate energies, 12.1, 22.1, and 30 eV, and give a relative comparison between positron and electron orientation and alignment parameters. The effect of positronium formation which is important near the excitation threshold would be negligible in the energy region studied here.

II. THEORY

We consider the sodium atom as a one-electron system and incorporate the effect of core electrons in the form of a core potential. The total Hamiltonian for the projectile positron plus sodium atom system is written as

$$H=H_0+V\ , \tag{1}$$

where the unperturbed Hamiltonian is

$$H_0=-\tfrac{1}{2}(\nabla_1^2+\nabla_2^2)-\frac{1}{r_1}+V_c(r_1) \tag{2}$$

and the total interaction potential is

$$V=-\frac{1}{r_{12}}+\frac{1}{r_2}+V_c(r_2)\ , \tag{3}$$

where $V_c(r_2)$ is the core potential and $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the atomic electron and incident positron, respectively. Dividing the total interaction potential V as

$$V=U_i+W_i\ ,\quad \text{initial channel} \tag{4}$$

$$V=U_f+W_f,\quad \text{final channel} \tag{5}$$

the T matrix in the two-potential approach is given by

$$T=\langle\phi_f|U_i|\chi_i^+\rangle+\langle\chi_f^-|W_f|\psi_i^+\rangle\ , \tag{6}$$

where the functions ϕ, χ, and ψ satisfy the Schrödinger equations

$$\begin{aligned} &H_0\phi=E\phi\ ,\\ &(H_0+U_i)\chi_i^+=E\chi_i^+\ ,\\ &(H_0+U_f)\chi_f^-=E\chi_f^-\ ,\\ &H\psi=E\psi\ , \end{aligned} \tag{7}$$

respectively. If the potential U is chosen to depend on the incident positron coordinate only, then the first term of Eq. (6) vanishes for inelastic scattering. In the distorted-wave approximation, to the first order we replace ψ_i^+ by χ_i^+ and obtain

$$T=\int[\chi_f^-(\mathbf{r}_1,\mathbf{r}_2)]^*W_f\chi_i^+(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1d\mathbf{r}_2\ . \tag{8}$$

The function χ can be expanded as

$$\chi_i^+(\mathbf{r}_1,\mathbf{r}_2)=F_i^+(\mathbf{r}_2)v_i(\mathbf{r}_1)$$

and

$$\chi_f^-(\mathbf{r}_1\mathbf{r}_2)=F_f^-(\mathbf{r}_2)v_f(\mathbf{r}_1)\ , \tag{9}$$

where F_i^+ and F_f^- are the scattered positron wave functions in the initial and final channels, respectively, and v_i and v_f are electron wave functions in the initial and final states.

The distorting potentials U_i and U_f used in Eq. (7) are chosen similar to our earlier work[8] on electron-lithium

scattering as

$$U_i(r_2)=V_s^i(r_2)+V_p^i(r_2)+V_c(r_2)\ , \tag{10}$$

where

$$V_s^i(r_2)=\left\langle v_i(\mathbf{r}_1)\left|-\frac{1}{r_{12}}+\frac{1}{r_2}\right|v_i(\mathbf{r}_1)\right\rangle$$

is the static potential in the initial channel. For the polarization potential $V_p^i(r_2)$ we use a nonadiabatic potential which is energy dependent.[9,10] It is given by

$$V_p^i(r_2)=V_p^a(r_2)/(1+6K_i^2/\omega_i^2 r_2^2)\ , \tag{11}$$

where $V_p^a(r_2)$ is the adiabatic polarization potential, which is chosen to be of the following form:

$$V_p^a(r_2)=-\frac{\alpha_i}{2r_2^4}\{1-\exp[-(r_2/r_0)^6]\}\ . \tag{12}$$

α_i is the dipole polarizability of the sodium atom, ω_i is the average excitation energy, and r_0 is the cutoff parameter. r_0 is determined from the following relations:

$$\begin{aligned} r_0&=\tfrac{3}{8}K_i/\omega_i\ ,\\ \omega_i&=\frac{2}{\alpha_i}\langle v_i(\mathbf{r}_1)|Z^2|v_i(\mathbf{r}_1)\rangle\ . \end{aligned} \tag{13}$$

Z is the dipole operator.

For the final channel we take

$$U_f=V_s^f(r_2)+V_c(r_2) \tag{14}$$

where

$$V_s^f(r_2)=\left\langle v_f(\mathbf{r}_1)\left|-\frac{1}{r_{12}}+\frac{1}{r_2}\right|v_f(\mathbf{r}_1)\right\rangle\ .$$

The valence-electron wave functions $v_i(\mathbf{r}_1)$ and $v_f(\mathbf{r}_1)$ and the core potential $V_c(r_2)$ are taken from Danielle.[11]

The differential cross section for a collision in which the sodium atom is excited from the initial state i to the final state f is given by

$$\sigma=\sigma_0+2\sigma_1\ , \tag{15}$$

with

$$\sigma_{m_f}^{i\to f}=\frac{1}{4\pi^2}\frac{k_f}{k_i}|T_{m_f}^{i\to f}|^2\ .$$

m_f denotes the magnetic quantum number of the final state. The alignment and orientation parameters are defined by Fano and Macek[12] as

$$\begin{aligned} &\lambda=\sigma_0/\sigma,\quad \chi=\arg(a_1/a_0)\ ,\\ &O_{1-}^c=-\sqrt{2}\,\mathrm{Im}\langle a_0a_1\rangle/\sigma,\quad A_{1+}^c=\sqrt{2}\,\mathrm{Re}\langle a_0a_1\rangle/\sigma\ , \end{aligned} \tag{16}$$

where a_0 and a_1 are the excitation amplitudes for the $m_f=0$ and $m_f=\pm1$ magnetic substates. σ_0 and σ_1 are the corresponding differential cross sections. $\langle\ \rangle$ denotes the spin average value.

The components P_1, P_2, and P_3 of the polarization of the radiation emitted perpendicular to the scattering plane and the alignment angle are defined as

$$\begin{aligned} P_1&=[I(0°)-I(90°)]/[I(0°)+I(90°)]\ ,\\ P_2&=[I(45°)-I(135°)]/[I(45°)+I(135°)]\ ,\\ P_3&=[I(\mathrm{RHC})-I(\mathrm{LHC})]/[I(\mathrm{RHC})+I(\mathrm{LHC})]\ ,\\ \gamma&=\tfrac{1}{2}\arg(P_1+iP_2)\ , \end{aligned} \tag{17}$$

where $I(\alpha)$ is the number of coincidence counts when the optic axis of polarizer is at $\alpha°$ to the incident-beam direction. I(RHC) and I(LHC) are the right and left polarization components, respectively. These polarization parameters are related to the parameters of Eq. (16) as[1]

$$\begin{aligned} P_1&=0.141(2\lambda-1)\ ,\\ P_2&=-0.282\,A_{1+}^c\ ,\\ P_3&=-1.116O_{1-}^c\ ,\\ \langle L_y\rangle&=-P_3\ . \end{aligned} \tag{18}$$

The depolarizing influence of the unresolved fine and hyperfine structure of the excited state of sodium is in-

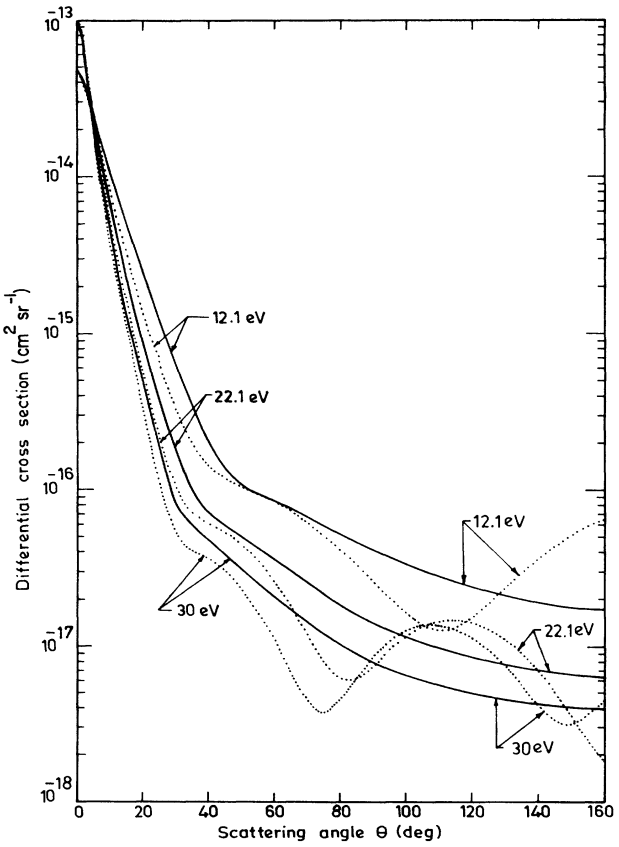

FIG. 1. Differential cross sections for positron- and electron-impact resonant excitation of sodium at 12.1, 22.1, and 30 eV. ——, positron results; · · ·, electron results.

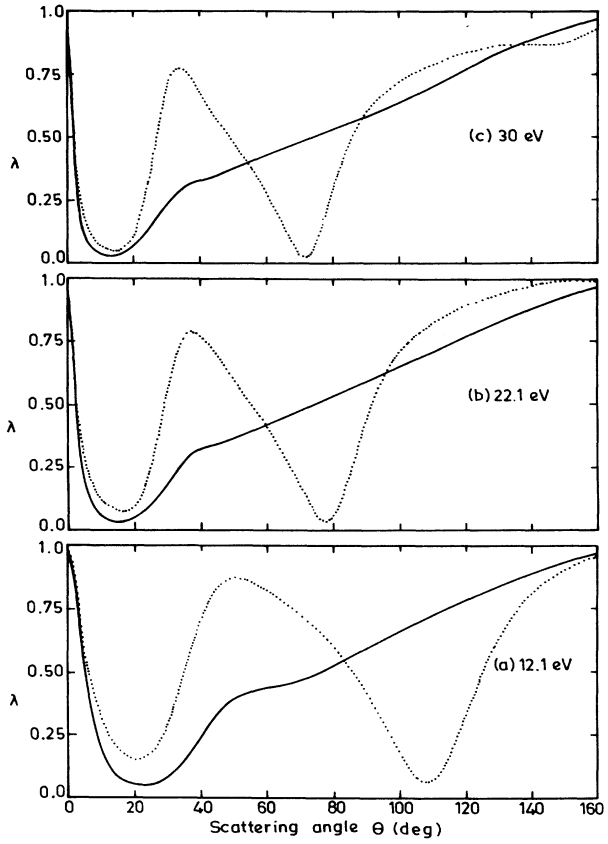

FIG. 2. λ parameter in positron- and electron-impact resonant excitation of sodium at (a) 12.1 eV, (b) 22.1 eV, and (c) 30 eV energy. Caption is the same as in Fig. 1.

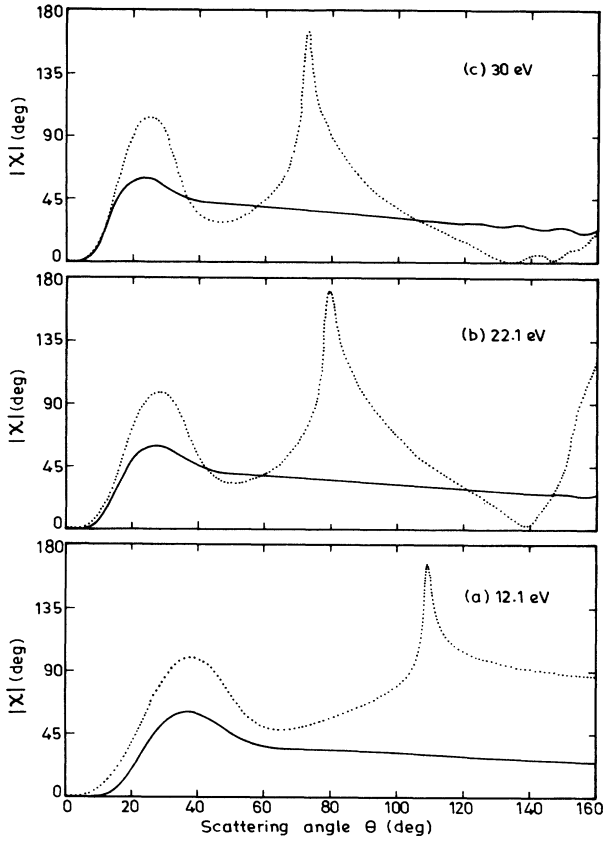

FIG. 3. $|\chi|$ parameter in positron- and electron-impact resonant excitation of sodium at (a) 12.1 eV, (b) 22.1 eV, and (c) 30 eV energy. Caption is the same as in Fig. 1.

cluded in the coefficients of the above equations. The coherence of excitation is measured by the reduced polarization

$$|\bar{P}|=\left[\left[\frac{P_1}{0.141}\right]^2+\left[\frac{P_2}{0.141}\right]^2+\left[\frac{P_3}{0.558}\right]^2\right]^{1/2}. \quad (19)$$

The angular distribution of the above parameters provides information about the shape and rotation of the excited state. λ measures the fraction of the $3p_0$ scattering probability. χ is the relative phase between $3p_1$ and $3p_0$ scattering amplitudes. $\langle L_y \rangle$ is the value of the angular momentum perpendicular to the scattering plane. $\langle L_y \rangle$ gives significant information about the way the angular momentum is transferred during the collision process. γ gives the alignment of the charge cloud with respect to the incident-beam direction. The coherence of excitation is implied by $|\bar{p}|=1$.

TABLE I. Integrated cross section (in πa_0^2) for $3s$-$3p$ excitation in e^+-Na scattering.

Energy (eV)	Present results	Four-state calculation[a]
10.0	60.6	65.8
12.1	53.9	
20.0	38.2	46.5
22.1	35.5	
30.0	28.2	38.7

[a]Sarkar, Basu, and Ghosh, Ref. 2.

III. RESULTS

We have used Eqs. (15)–(19) to obtain the differential and integrated cross sections, the angular correlation parameters λ, χ, $\langle L_y \rangle$, and the polarization parameters $|\bar{P}|$ and γ for the resonant excitation for sodium by positron impact at energies of 12.1, 22.1, and 30 eV. The results are presented in Figs. 1–8 where the positron results are compared with the corresponding electron results.[13]

In Table I we give the integrated $3s$-$3p$ excitation cross section for positrons and compare our results with the recent four-state close-coupling calculations of Sarkar *et al.*[2] We find that the two calculations are in reasonable accord at lower intermediate energies but differ at higher energies. This is expected since the close-coupling approximation would be more valid at lower energies close to the threshold and would be unsuitable at intermediate and higher energies where more and more chan-

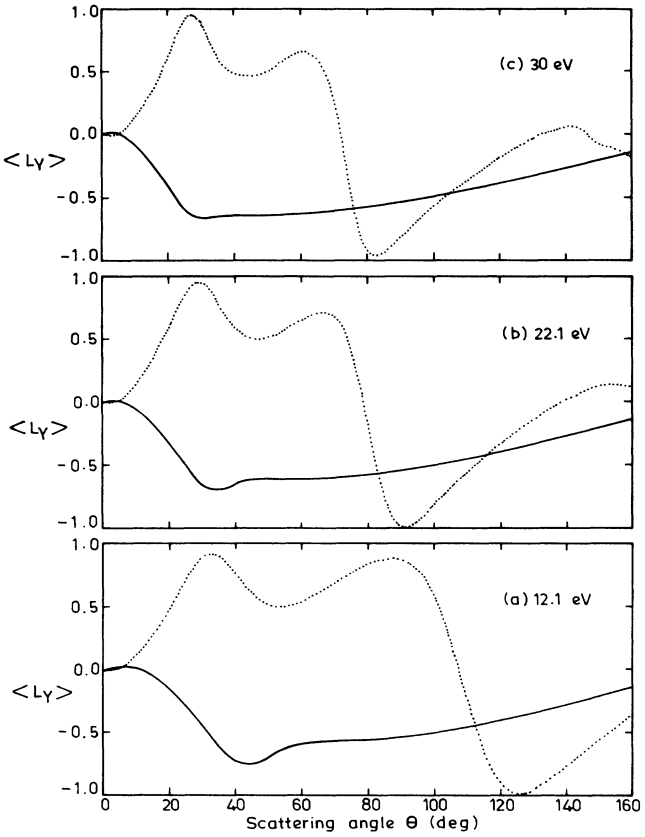

FIG. 4. $\langle L_y \rangle$ parameter in positron- and electron-impact resonant excitation of sodium at (a) 12.1 eV, (b) 22.1 eV, and (c) 30 eV energy. Caption is the same as in Fig. 1.

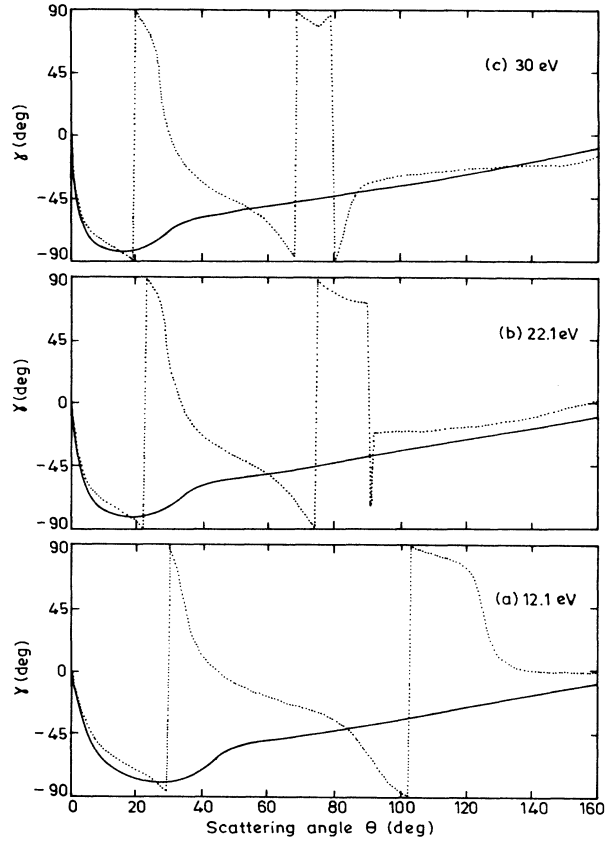

FIG. 5. Alignment angle γ, in positron- and electron-impact resonant excitation of sodium at (a) 12.1 eV, (b) 22.1 eV, and (c) 30 eV energy. Caption is the same as in Fig. 1.

nels become open. In the intermediate-energy region the present approach, which is based on the distorted-wave approximation with the proper account of the polarization effect, is expected to be more suitable.

Figure 1 gives the differential cross section for positron and electron resonant excitation. It is observed that at all energies the behavior of positron and electron differential cross sections is similar in nature at small angles. However, at intermediate and large scattering angles there are significant differences between the two cross sections. This is mainly due to the presence of the exchange in electron scattering and absence of the same in positron scattering.

Figures 2(a)–2(c) show a plot of the angular variation of λ. From the figure it is noticed that for all the energies the positron λ first acquires a minimum value from its initial value of unity and then shows a gradual increase towards its maximum value of unity. The position of the minimum shifts towards lower angles with the increase of energy. The comparison with electron scattering shows that, while in electron scattering two minimas are obtained, one at lower angle and the other at larger angle, only one minimum is obtained in positron scattering. Furthermore, the positions of the minimum in the positron scattering and the first minimum in electron scattering are nearly at the same scattering angle.

Figures 3(a)–3(c) show the variation of $|\chi|$ with scattering angle. The positron $|\chi|$ shows a gradual increase and acquires its maximum value beyond which it shows a slow decrease becoming almost constant at large scattering angles. On the other hand, the electron $|\chi|$ shows structures. The location of the first maximum in electron scattering is nearly at the same position as that of the maximum in positron scattering.

Figures 4(a)–4(c) show a plot of $\langle L_y \rangle$ with respect to the scattering angle. From the figure we observe that there is a significant difference between the positron and electron $\langle L_y \rangle$ at low and intermediate scattering angles. The positron $\langle L_y \rangle$ shows a negative value in the whole angular region, while the electron $\langle L_y \rangle$ shows a positive value for low and intermediate angles and becomes negative in the large angular region. This feature is similar to our earlier work on electron and positron scattering with the lithium atom.[6,14]

Figures 5(a)–5(c) show the variation of alignment angle γ with scattering angle. We find that for low scattering angles up to about 20° the variation of γ for positron and electron scattering remains identical at all energies. Beyond a scattering angle of 20° the positron γ shows a slow increase, whereas the electron γ shows rapid varia-

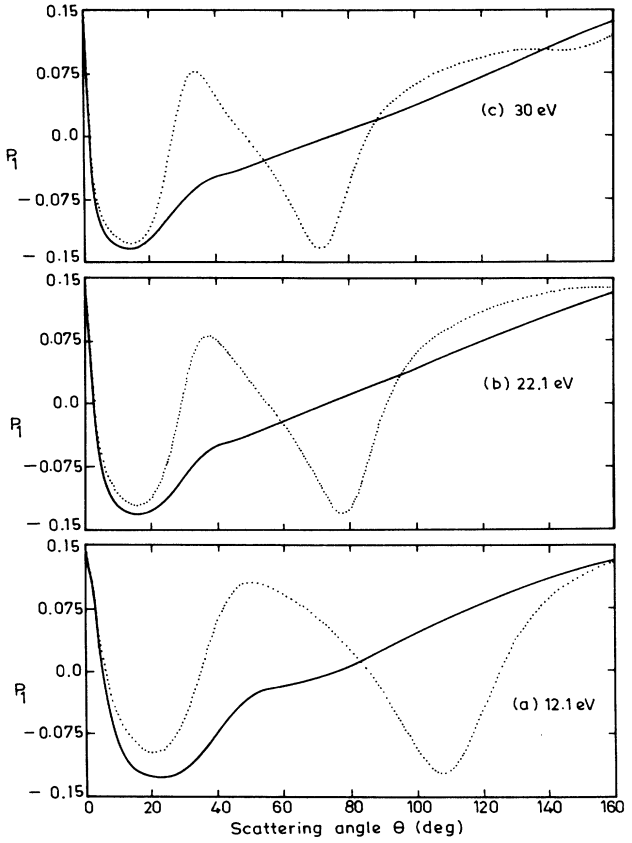

FIG. 6. Polarization parameter P_1 in positron- and electron-impact resonant excitation of sodium at (a) 12.1 eV, (b) 22.1 eV, and (c) 30 eV energy. Catpion is the same as in Fig. 1.

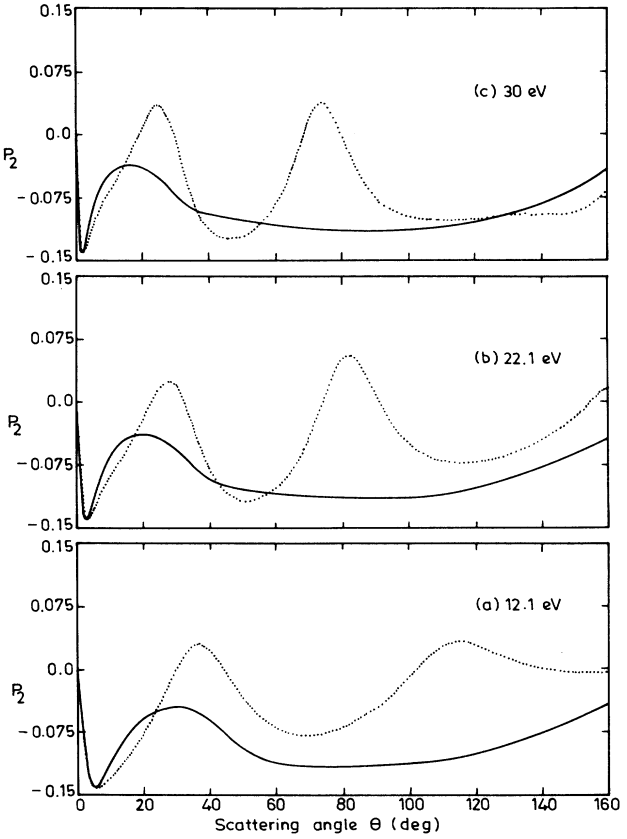

FIG. 7. Polarization parameter P_2 in positron- and electron-impact resonant excitation of sodium at (a) 12.1 eV, (b) 22.1 eV, and (c) 30 eV energy. Caption is the same as in Fig. 1.

tions. As the energy increases the behavior of γ for electron and positron scattering becomes nearly identical at large scattering angles also.

Since γ depends on the ratio of the components of polarization P_2 and P_1, respectively, we have also shown in Figs. (6) and (7) the angular variation of P_1 and P_2, for the sake of completeness.

Figure 8 gives a plot of reduced polarization $|\bar{P}|$ with scattering angle. The coherence of excitation is determined by the value of $|\bar{P}|$. For complete coherence, $|\bar{P}|=1$. From the figure it is noticed that while the excitation is coherent for positron scattering in the entire angular region, for electron impact it is limited to small angles below 20° and for large angles beyond 120°. The value of $|\bar{P}|$ in electron scattering deviates significantly from unity in the intermediate angular range. This deviation from coherence in electron scattering at intermediate angles is larger for lower energies as compared to higher energies.

From the above study we notice that there are considerable differences in the behavior of alignment and orientation parameters for positron and electron scattering.

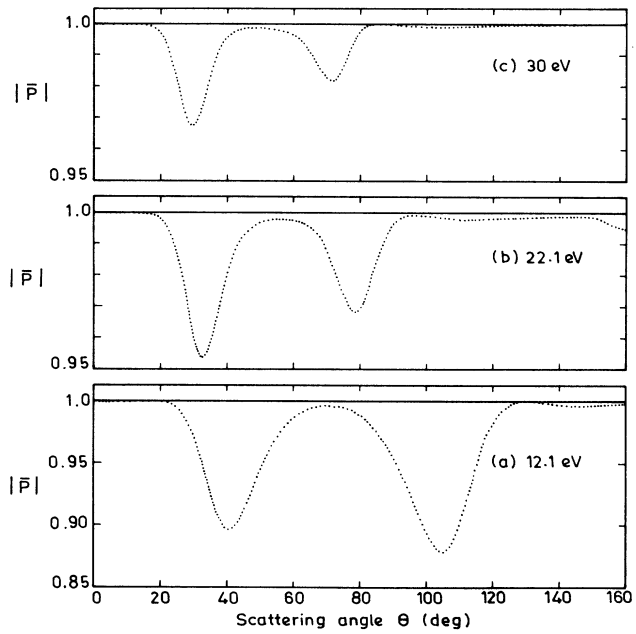

FIG. 8. Reduced polarization $|\bar{P}|$ in positron- and electron-impact resonant excitation of sodium at (a) 12.1 eV, (b) 22.1 eV, and (c) 30 eV energy. Caption is the same as in Fig. 1.

The reason for the same is due to the absence of exchange for positron scattering and is due to the different nature of distorting potentials in the positron and electron cases. While the static and polarization potentials are of opposite nature in positron scattering, they are of the same type (attractive) in electron scattering.

Kwan *et al.*[15] have started measurements on positron–alkali-atom scattering and we hope that measurements on differential-cross-section and angular correlation parameters will become available in the near future to compare with the present work. It may, however, be mentioned that the present approach provides reliable results for angular correlation parameters in electron-sodium scattering when compared with the measurements.[13]

ACKNOWLEDGMENTS

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[1]N. Andersen, J. W. Gallagher, and I. V. Hertel, Phys. Rep. **165**, 1 (1988).

[2]S. P. Khare and Vijayshri, J. Phys. B **16**, 3621 (1983); T. T. Gien, Phys. Rev. A **35**, 2026 (1987); K. P. Sarker, Madhumita Basu, and A. S. Ghosh, J. Phys. B **21**, 1649 (1988); T. S. Stein and W. E. Kaupilla, in *Electronic and Atomic Collisions,* edited by D. C. Lorentz, W. E. Meyerhof, and J. R. Paterson (North-Holland, Amsterdam, 1986); T. S. Stein, M. S. Debabneh, W. E, Kaupilla, C. K. Kwan, and Y. Y. J. Wan, in NATO Advanced Research Workshop on Atomic Physics with Positrons Abstracts, 1987 (unpublished), Pt. 2, and references therein.

[3]H. E. Fargher and M. J. Roberts, J. Phys. B **17**, L587 (1984).

[4]S. L. Willis, J. Hata, M. R. C. McDowell, C. J. Joachain, and F. W. Byron, J. Phys. B **14**, 2687 (1981).

[5]D. H. Madison and K. H. Winters, J. Phys. B **16**, 4437 (1983).

[6]S. Saxena and K. C. Mathur, J. Phys. B **19**, 3181 (1986).

[7]A. W. Pangantiwar and R. Srivastava, J. Phys. B **21**, 4007 (1988).

[8]S. Saxena and K. C. Mathur, J. Phys. B **18**, 509 (1985).

[9]K. Onda and D. G. Truhlar, Phys. Rev. A **22**, 86 (1980).

[10]D. Thirumalai, D. G. Truhlar, M. A. Brandt, R. A. Eades, and D. A. Dixon, Phys. Rev. A **25**, 2946 (1982).

[11]R. Danielle, J. Chem. Phys. **72**, 1276 (1980).

[12]U. Fano and J. H. Macek, Rev. Mod. Phys. **45**, 553 (1973).

[13]K. C. Mathur and S. P. Purohit, J. Phys. B **22**, L223 (1989).

[14]K. C. Mathur, in *Atomic and Molecular Physics,* edited by D. K. Rai and D. N. Tripathi (World Scientific, Singapore, 1987), p. 317.

[15]C. K. Kwan, Y. J. Wan, W. E. Kaupila, and T. S. Stein, in *Abstracts of the Fifteenth International Conference on the Physics of Electronic and Atomic Collisions, Brighton, 1987,* edited by J. Geddes, H. B. Gilbody, A. E. Kingston, C. J. Latimer, and H. J. R. Walters (Queen's University, Belfast, 1987).