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ELECTRON IMPACT POLARIZATION AND CORRELATION PROPERTIES
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**ELECTRON IMPACT POLARIZATION AND
CORRELATION PROPERTIES OF THE
INERT GASES**

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Abstract

For the heavier rare-gas targets, Ne, Ar, Kr, there is now a reasonable amount of experimental electron impact coherence parameter data available for excitation of the lowest $J = 1$ states. Theoretical results for those rare-gas targets, have been restricted to distorted-wave approximation (DWA) type theories.

We present a systemization of the experimental data and compare them with available theoretical results. In the case of the heavy rare gases, we compare the experimental and theoretical data available for the three species, Ne, Ar, Kr, in order to identify trends. We compare the experimental data with results from available theories (mainly DWA type) and discuss the importance of spin-orbit coupling effects and "shell" effects. We present our point-of-view as to the physical picture that is emerging from all collisional data, and conclude by recommending future experimental and theoretical activities that will, from our perspective, provide new insight into the physics of these processes.

I. INTRODUCTION

Electron-impact excitation studies on heavy rare-gas targets remain of interest even today. This is partially due to the great practical importance of these studies. Electron impact excitation of Ar and Kr atoms e.g. plays an important role in the modeling of the KrF laser-system (see articles in Cartwright [1]). The heavy rare-gas targets also provide an excellent testing ground for the study on the role of various physical effects in the electron collision process. In the case of neon target, for example, the spin-orbit coupling effect for the continuum electron can be neglected (Schackert [2], Walker [3]) while the spin-orbit coupling effect can be substantial in some of the excited states of neon (see Condon and Shortley [4]) such as the 1P_1 and 3P_1 states. This makes the heavy-rare gas targets excellent systems for the study of the role of target spin-orbit coupling in electron-impact excitation processes. It is important from the basic collision-physics point of view that for these targets not only electron impact integral cross sections (ICSs) and differential cross sections (DCSs), but also electron impact coherence parameters (EICPs) have been reported from electron-photon coincidence measurements (reviewed recently by Becker, Crowe, and McConkey [5]). Furthermore, the measurement of spin-asymmetry-functions (Hanne [6]) is scheduled in the near future (Gay [7]). This means that for the heavy rare-gas targets, very detailed electron-collision physics information is available or will soon be available, which will serve as a stringent test on collisional theories. The purpose of the present work is to supplement the information that was obtained previously on electron impact excitation of heavy rare gases from first-order many-body theory (FOMBT) calculations (Padial et al. [8], Machado et al. [9, 10], da Paixão et al. [11, 12], Meneses et al. [13, 14]). The plan of this paper is as follows: Sec. II describes the theoretical model and gives the formulas to be used and Sec. III discusses the results obtained.

II. Theoretical Model

The theoretical model used in this work is the same as the one used in our earlier works on electron impact excitation of argon (Padial et al. [8]), of neon (Machado et al. [9, 10] and of krypton (Meneses et al. [13, 14]). The scattering model used is that of first-order many-body theory (FOMBT) originally introduced for electron-atom inelastic scattering by Csanak et al. [15] and discussed in detail for its application for heavy rare-gas targets by Padial et al. [8]. The FOMBT has been shown to be one of many possible forms of a distorted wave approximation (DWA) by Rescigno et al. [16]. A special feature of the FOMBT as a DWA is that the distorted waves for both the incident and scattered electrons are calculated in the static-exchange field of the ground state of the target. Spin-orbit coupling effects in the continuum electron wave functions were neglected in our calculations. The representation of the target states in most cases is the same as in the earlier works quoted above. In this scheme the $1S_0$ ground state and the $ns'[1/2]_0^0$ ($3P_0$) and $ns[3/2]_2^0$ ($3P_2$) excited states are described in the LSJ coupling formalism, whereas the $ns'[1/2]_1^0$ ($1P_1$) and $ns[3/2]_1^0$ ($3P_1$) states are represented as linear combinations of LSJ coupled $1P_1$ and $3P_1$ states in the form

$$| ns'[1/2]_1^0; M_J \rangle = b | 1P_1; M_J \rangle + a | 3P_1; M_J \rangle \quad (1a)$$

$$| ns[3/2]_1^0; M_J \rangle = -a | 1P_1; M_J \rangle + b | 3P_1; M_J \rangle \quad (1b)$$

with $a = 0.266$ and $b = 0.964$ for neon ($n = 3$), with $a = 0.450$ and $b = 0.893$ for Argon ($n = 4$), and with $a = 0.730$ and $b = -0.683$ for Krypton ($n = 5$), obtained from Cowan [17]. Here we use the intermediate coupling notation of Moore [18] and put the closest LSJ coupled term in parentheses. (The same notation was used in our earlier works.) In other cases we used the CATS, ACE, and TAPS codes developed at Los Alamos National Laboratory (Abdallah et al. [19], Clark et al. [20-23]) that allowed a more accurate

representation of the wave-functions. The calculational procedure for the T-matrices for the various transitions is the same as in the earlier works of Padial et al. [8], Machado et al. [9, 10], and Clark et al [22, 23], thus it will not be given here.

In the present work we shall report electron impact coherence parameters for the excitation of the $3s'[1/2]_1^0$ and $3s[3/2]_1^0$ states of neon, and $5s'[1/2]_1^0$ and $5s[3/2]_1^0$ states of krypton using the FOMBT along with the representation of these wave-functions given by Eqs. (1a, b). In addition, we shall report spin-orbit coupling studies for neon and argon targets, and - dependence and Z-dependence studies via the use of the CATS, ACE, and TAPS codes. The relevant expressions for these physical quantities will be discussed now.

Following Bartschat [24], we shall define the electron scattering amplitude for the excitation of the J_1, M_1 excited state of the target by an incident electron of momentum $\vec{k}_1$ and spin m_0 and scattered electron of momentum $\vec{k}_1$ and spin m_1 as

$$f(M_1 m_1; m_0) = \left\langle J_1 M_1; \vec{k}_1 m_1 | T | S_0; \vec{k}_0 m_0 \right\rangle \quad (2)$$

where $|S_0; \vec{k}_0 m_0\rangle$ and $|J_1 M_1; \vec{k}_1 m_1\rangle$ refer to the state vectors of the electron plus atom system before and after the collision, respectively, and T is the electron scattering operator. If we denote by $\rho_{m'_0 m_0}$ the spin density matrix of the incident electron beam (for unpolarized electrons, $\rho_{m'_0 m_0} = 1/2 \delta_{m'_0 m_0}$) then the density matrix of the combined electron plus atom system after the collision can be given by the formula,

$$\rho_{m'_1 m_1}^{M'_1 M_1} = \sum_{m'_0 m_0} f(M'_1 m'_1; m'_0) f^*(M_1 m_1; m_0) \rho_{m'_0 m_0} \quad (3)$$

If the incident electron beam is unpolarized and if the spins of the scattered electrons are not detected, then we can define the reduced atomic density matrix in the form,

$$\rho_{M_1 M_1}^{at.} = \langle f(M_1) f^*(M_1) \rangle = \sum_{m_1} \rho_{m_1 m_1}^{M_1 M_1} = \frac{1}{2} \sum_{m_0 m_1} f(M_1 m_1; m_0) f^*(M_1 m_1; m_0) \quad . \quad (4)$$

The electron impact coherence parameters (EICP's) can now be defined conveniently in terms of the reduced atomic density matrix. One set of such parameters $\lambda, \Delta, \bar{\chi}, \epsilon$ was introduced by da Paixão et al. [11] via the equations,

$$\lambda = \frac{\sigma(0)}{\sigma(0) + 2\sigma(1)} \quad (5a)$$

$$\cos \Delta = \frac{|\langle f(1) f^*(0) \rangle|}{\sqrt{\sigma(0)\sigma(1)}} \quad (5b)$$

$$\bar{\chi} = \arg\{\langle f(1) f^*(0) \rangle\} \quad (5c)$$

$$\cos \epsilon = -\frac{\langle f(1) f^*(-1) \rangle}{\sigma(1)} \quad (5d)$$

where

$$\sigma(M) = \langle f(M) f^*(M) \rangle \quad (6)$$

is the electron impact excitation cross section for magnetic sub-level M, and

$$\sigma = \sum_M \sigma(M) \quad (7)$$

is the magnetic-sublevel summed differential cross section.

Another set of parameters that can be used in place of the above parameters are the Stokes parameters: P_1 , P_2 , P_3 , and P_4 . For a detailed discussion of these latter parameters see e.g. Andersen, Gallagher, Hertel [25] and Becker, Crowe and McConkey [5]. The P_1 , P_2 , P_3 Stokes parameters can be determined by an electron-photon coincidence experiment where the photon-detector is placed perpendicular to the collision plane, while P_4 can be measured in a similar experiment with the photon-detector being in the collision plane. The modulus $|P|$ of the total polarization vector $P = (P_1, P_2, P_3)$ gives the degree of polarization of the emitted radiation.

These Stokes parameters can be expressed in terms of the $\lambda, \bar{\chi}, \epsilon, \Delta$ parameters by the formulas, (Andersen, Gallagher, Hertel [25], Khakoo and McConkey [26]),

$$P_1 = \frac{\lambda(3+\cos \epsilon) - (1+\cos \epsilon)}{(1+\cos \epsilon) + \lambda(1-\cos \epsilon)} \quad (8a)$$

$$P_2 = \frac{-4[\lambda(1-\lambda)]^{1/2} \cos \Delta \cos \bar{\chi}}{(1+\cos \epsilon) + \lambda(1-\cos \epsilon)} \quad (8b)$$

$$P_3 = \frac{4[\lambda(1-\lambda)]^{1/2} \cos \Delta \sin \bar{\chi}}{(1+\cos \epsilon) + \lambda(1-\cos \epsilon)} \quad (8c)$$

$$P_4 = \frac{(\cos \epsilon - 1) + \lambda(3 - \cos \epsilon)}{(1 - \cos \epsilon) + \lambda(1 - \cos \epsilon)} \quad (8d)$$

Still another set of parameters, denoted by $(\gamma, L_{\perp}^+, P_L, \rho_{oo})$ was introduced by Hermann and Hertel [27]. These latter parameters can be expressed in terms of parameters already introduced by the formulas,

$$\gamma = \frac{1}{2} \arg(P_1 + iP_2) \quad (9a)$$

$$L_{\perp}^+ = -P_3 \quad (9b)$$

$$P_L = (P_1^2 + P_2^2)^{1/2} \quad (9c)$$

$$\rho_{oo} = \frac{1}{2}(1 - \lambda)(1 - \cos \epsilon) \quad . \quad (9d)$$

ρ_{oo} can also be expressed in terms of the P_1 and P_4 parameters in the form,

$$\rho_{oo} = \frac{(1+P_1)(1-P_4)}{4-(1-P_1)(1-P_4)} \quad . \quad (10)$$

III. Results and Discussion

A. Neon

First we shall discuss our FOMBT results for the neon $3s'[1/2]_1^0$ and $3s[3/2]_1^0$, EICPs. Fig. 1 shows our recent results for the DCSs for the excitation of the $3s[3/2]_1^0$, 2 and $3s'[1/2]_0^0$, 1 levels in neon, along with the experimental data of Register et al. [28]. This figure clearly shows the good agreement of the present calculation with the experimental data, especially for the excitation of the $J = 1$ levels. In Fig. 2 we compare our present FOMBT results for the P_1 , P_2 , and P_3 Stokes parameters and for the P_L and γ parameters in the case of the $J = 1$ levels excitation with the experimental data of Khakoo and McConkey [26].

This figure shows that FOMBT gives excellent agreement with experiment for the P_2 parameter practically for all angles measured and for the P_1 , P_3 and γ parameters for small scattering angles. The sign of the P_3 parameter agrees with that of the experiment for all scattering angles where comparison is possible. Fig. 3 shows the present results for the P_3 and P_4 parameters, for the excitation of both $J = 1$ levels in neon for incident electron energies $E = 20, 30, 50$, and 80 eV. It can be seen immediately that sometimes these parameters change drastically as a function of energy, especially from $E = 20$ eV to $E = 30$ eV.

Further discussion on the comparison of our results to other theoretical results, and experimental data, can be found in Zheng and Becker [35].

B. Krypton

Our present results for the DCS for the excitation of the $5s, 5s'$ levels of krypton at $E = 50$ eV incident electron energy are shown in Fig. 4 where they are compared with the experimental data of Trajmar, et al. [30]. It can be seen again that excellent agreement is obtained with the experiment, especially for the excitation of the $J = 1$ levels. The lowest panel of Fig. 12 shows our FOMBT results for the P_1 and P_2 parameters for incident electron energy $E = 50$ eV in the case of the excitation of the $5s'[1/2]_1^0$ level of krypton

where our present FOMBT results are compared with the distorted wave approximation (DWA) results of Bartschat and Madison [31] and with first-Born approximation (FBA) results as well as with the experimental data of Zheng and Becker [32]. From these figures it can be seen that for the quantities plotted at these energies, there is excellent agreement between the FOMBT results and experiment.

A more detailed discussion on the comparison of our results to other theories, and to the experimental data, can be found in Zheng and Becker [32].

C. Comparative Studies

In this section we report results from calculations using the CATS, ACE, and TAPS codes for some comparative studies.

1. Spin-orbit coupling effects

Fig. 5 shows the importance of spin-orbit-coupling effect in the excited state wave-function for the DCS in the case of the excitation of the " 3P_1 " and " 1P_1 " levels of neon. It can be seen immediately that the spin-orbit coupling has a drastic effect on the DCS for the excitation of the " 3P_1 " level of neon even though the mixing coefficient for the 1P_1 coefficient (see upper panel) is quite small. This is, of course, due to the fact that the 1P_1 component brings in the possibility of a direct excitation of the " 3P_1 " level.

Fig. 6 shows the importance of the spin-orbit coupling effect in the P_3 Stokes parameter for the electron impact excitation of the " 3P_1 " level of neon and argon. It can be immediately seen that the spin-orbit coupling effect has a very large effect on the P_3 parameter for " 3P_1 " excitation, in fact the spin-orbit coupled results for P_3 are practically identical for " 3P_1 " and " 1P_1 " excitations (especially for argon and for $\vartheta < 40^\circ$ scattering angles) showing a decisive influence of the 1P_1 component in the wave-function.

2. Principal quantum number dependence

Fig. 7 shows the principal quantum number (n) dependence of the P_1 , P_2 , and P_3 Stokes parameters in the case of the excitation of $ns'[1/2]_1^0$, $n = 3, 4, 5$, and 6 levels of neon by $E = 80$ eV energy incident electron. It can be seen immediately that the Stokes parameters are practically independent from the principal quantum number as was found to be the case for helium n^1P and n^3P excitations. (See Csanak and Cartwright [33,34].)

If n -independence of the EICP's is indeed true, then the measurement of the EICP's can be affected by detecting radiation from higher lying $ns'[1/2]_1^0$ or $ns'[3/2]_1^0$ levels to lower lying excited levels when infrared or visible photon detectors could be used which would be especially advantageous for the measurement of the P_3 parameter.

3. Atomic number dependence

Fig. 8 shows the DCS for the excitation of the 2^1P level of He and $ns'[1/2]_1^0$, ($n = 3, 4, 5$) levels of Ne, Ar, and Kr. We can immediately see, the increasingly pronounced diffraction (or interference) pattern with the increase of the atomic numbers due to the increasing number of partial waves with larger phase shifts that contribute to the DCS.

Fig. 9 shows identical studies for the γ and $L_\perp$ parameters and Fig. 10 for the P_3 parameter. It can be seen here also that with the increase of the atomic number the interference pattern becomes more complicated. It is important to point out that these latter quantities are ratios of two separate entities and interference effects appear in both the numerator and denominator, resulting in an even more complicated interference-effect in the ratio. Fig. 11 shows our results from identical studies for the ρ_{00} parameter. It can be immediately seen that the magnitude of this parameter, which characterizes the importance of angular momentum transfers to the target via a spin-flip process, increases with the increase of atomic numbers. This is obviously due to the increasing importance of the spin-orbit coupling effect in the final target state.

D. Conclusions

Our results show that FOMBT gives from good to excellent results for the EICP's in the case of the excitation of the $J=1$ levels of rare gases and that spin-orbit coupling effects in the target states are very important, even for neon. We found, as was the case for He, that the EICP's are practically independent of the principal quantum number and, for the heavier rare gases (argon, krypton), they are very similar for the " 1P_1 " and " 3P_1 " levels. These two theoretical predictions should be tested experimentally. The good FOMBT results for both DCS's and EICP's indicate that many-body perturbation theory (MBPT) is a rapidly convergent approach for the calculation of these quantities and that the next higher order MBPT (such as second order MBPT) might give experimentally accurate results.

The excellent detailed, and authoritative, review of Becker, Crowe, and McConkey [3] contains further conclusions and suggestions on this subject. However, experimental EICP data at larger scattering angles are needed (for several energies) and second order MBPT calculations need to be performed.

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Figure Captions

Fig. 1 Differential cross sections for electron impact excitation of neon for $E = 50$ eV incident electron energy.

Solid line: Present results.

Shaded regions: Experimental results (with error bars) of Register et al [28].

Fig. 2 Stokes parameters P_1 , P_2 , P_3 , and P_L and γ parameters for electron impact excitation of neon.

Solid lines with filled circles: FOMBT results for neon 1P_1 excitation at $E = 80$ eV incident electron energy.

Dashed lines with empty circles: FOMBT results for neon 3P_1 excitation at 80 eV incident electron energy.

Shaded regions: Experimental results of Khakoo and McConkey [26].

Fig. 3 FOMBT results of the P_3 and P_4 Stokes parameters for neon 1P_1 (denoted as sP1) and 3P_1 (denoted as tP1) excitation for $E = 20, 30, 50$, and 80 eV incident electron energies ($P_{\text{sub } 1}$ is P_1 and $P_{\text{sub } 2}$ is P_2). The notation for the various energies is given in the lower panel on the left side.

Fig. 4 Differential cross sections for the electron impact excitation of krypton for $E = 50$ eV incident electron energy.

Solid line: Present results

Shaded regions: Experimental results of Trajmar et al. [30].

Fig. 5 Spin-orbit coupling effect in neon DCS

Upper panel: a^2 and b^2 coefficients for rare gases [See Eqs. (1a, b)]

Lower panel: LS-coupled and spin-orbit coupled results for the Ne $J=1$ excitation DCS-s.

Heavy solid line: Spin-orbit coupled results.

Solid line with empty circles: LS-coupled results.

Shaded region: Experimental results of Register, et al. [28].

Fig. 6 Spin-orbit coupling effect in the P_3 Stokes parameter for neon and argon.

Solid line: Spin-orbit coupled results for 3P_1 excitation

Dotted line: LS-coupled results for 3P_1 excitation.

Dashed line: Spin-orbit coupled results for 1P_1 excitation

Upper panel: FOMBT results for neon

Lower panel: FOMBT results for argon

Fig. 7. Principal quantum number (n) dependence of the P_1 , P_2 , and P_3 Stokes parameters for the excitation of the $ns'[1/2]_1^0$ ($n = 3, 4, 5$, and 6) states of neon.

Fig. 8 Atomic number (Z) dependence of the DCS for the excitation of the $ns' [1/2]_1^0$ states of rare gases.

Fig. 9 Atomic number (Z) dependence of the γ (GAMMA) and $L_{\perp}$ (L-perp) EICP's for the $ns'[1/2]_1^0$ excitation of the rare gases.

Fig. 10 Atomic number (Z) dependence of the P_3 Stokes parameter for the $ns'[1/2]_1^0$ excitation of the rare gases.

Fig. 11 Atomic number (Z) dependence of the ρ_{00} (ρ_{00}) EICP for the $ns'[1/2]_1^0$ excitation of the rare gases.

Fig. 12 Atomic number (Z) dependence of the P_1 and P_2 Stokes parameters for the $ns'[1/2]_1^0$ excitation of the rare gases.

Solid line: DWA results of Bartschat and Madison [31]

Dashed line: FOMBT results from:

For He: Csanak and Cartwright [33, 34]

For Ne: presnet results

For Ar: da Paixão, et al. [12]

For Kr: Solid circles: Zheng and Becker [32]

Solid squares: Danjo, et al. [36]

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

spin-orbit coupling in Ne, triplet-P, E=50eV

spin-orbit coupling in Ar, triplet-P, E=50eV

Fig. 6

n-dependence of Stokes parameters
singlet-P states in Neon, 80eV

Fig. 7

Fig. 8

Fig. 9

Fig. 10

Fig. 11

$\angle$ -dependence at 50eV

Fig. 12

END

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