Excitation of the 6 $^{1,3}P_1$ states of mercury by spin-resolved electron impact

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Recent measurements have been made of the angle-integrated Stokes parameters for the spin-polarized electron impact excitation of the $6s6p$ $(J=1)$ states in mercury, resulting in the emission of 185 and 254 nm radiation to the ground state through the $^1P_1$-$^1S_0$ and $^3P_1$-$^1S_0$ transitions, respectively. These measurements give information on the electron exchange and spin-orbit coupling effects of the target and projectile electrons. We have evaluated the integrated Stokes parameters using our relativistic distorted-wave method which takes direct account of the fine structure of the excited atomic states as well as the spin of the incident electrons. We compare these results with the recent experimental and theoretical data. In general the agreement between our theoretical results and the experimental measurements is very good.

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I. INTRODUCTION

For electron scattering from a light atom such as helium, where the fine-structure splitting of the energy levels is insignificant, maximal information can be obtained using incident beams of electrons whose spins are unpolarized. However, for more complex targets, particularly heavy atoms with large nuclear charge, scattering of beams of spin-polarized electrons is required in order to determine all of the information available. Recently, Jüttemann *et al.* [1] carried out such experiments on mercury where they determined the angle-integrated Stokes parameters resulting from the excitation of the $^{1,3}P_1$ states. Since mercury is a heavy atom with nuclear charge $Z=80$, relativistic effects such as the fine-structure splitting of the energy levels of the target and the dependence of the scattering amplitudes on the spin of the incident electron are important. In fact, two of the three angle-integrated Stokes parameters would vanish if the incident beam were not spin polarized.

In this paper we have carried out relativistic calculations of the angle-integrated Stokes parameters to compare with the measurements and calculations reported in [1]. Theoretically, the most direct way of incorporating these relativistic effects is by using the Dirac equations to calculate the wave functions for both the atomic targets as well as the scattered electrons. Thus we have calculated Dirac-Fock wave functions for the mercury target by using the GRASP92 program of Parpia *et al.* [2]. The wave functions for the scattered electron are determined using our relativistic distorted-wave (RDW) method [3]. We have previously used our RDW method to calculate the differential scattering of unpolarized electrons from mercury [4,5]. Differential scattering of spin-polarized electrons was further considered in [6,7].

Section II briefly outlines the theory for the excitation of the 6 $^{1,3}P_1$ states of mercury from the ground 6 $^1S_0$ state and the calculation of integrated Stokes parameters. In Sec. III we describe the wave functions of the Hg target used in the calculation. Finally we present our results in Sec. IV and compare these with the measurements and other theoretical calculations.

II. THEORY

In the RDW method the T matrix for electron impact excitation from state a to state b of an atom having N electrons and nuclear charge Z can be written as

$$T_{a\to b}^{\mathrm{RDW}} = \langle \chi_b^-(1,2,\ldots,N+1)|V - U_b(N+1)|\chi_a^+(1,2,\ldots,N+1)\rangle, \quad (1)$$

where V is the projectile electron-atom interaction potential given by

$$V = -\frac{Z}{r_{N+1}} + \sum_{j=1}^{N} \frac{1}{|\mathbf{r}_j - \mathbf{r}_{N+1}|}. \quad (2)$$

Here $\mathbf{r}_j$ $(j=1,\ldots,N)$ represents the position coordinates of the target electrons and $\mathbf{r}_{N+1}$ is the position coordinate of the projectile electron with respect to the nucleus of the target. The distortion potential U_b is taken to be a function of only the radial coordinate of the projectile electron, r_{N+1}. We choose U_b to be the spherically averaged static potential of the excited state of the atom, which is the choice shown to yield most consistent results in the distorted-wave approximation.

In the RDW method, the wave functions $\chi_{a(b)}^{+(-)}$ in the initial state a and final state b are represented as a product of a relativistic multiconfiguration Dirac-Fock wave function $\Phi_{a(b)}^{rel}(1,2,\ldots,N)$ with total angular momentum $J_{a(b)}$ for the target atom and a relativistic distorted-wave for the projectile electron, i.e.,

$$\chi_{a(b)}^{+(-)}(1,2,\ldots,N+1) = A\Phi_{a(b)}^{rel}(1,2,\ldots,N)F_{a(b)\mu_{a(b)}}^{\mathrm{DW}+(-)}(k_{a(b)},N+1). \quad (3)$$

Here "+" indicates an outgoing wave, whereas "–" indicates an incoming wave and A is the antisymmetrizing operator which accounts for exchange of the incident electron with the bound electrons which is applied in the incident a channel only. The $F_{a(b)\mu_{a(b)}}^{\mathrm{DW}+(-)}$ are relativistic distorted waves for the projectile electron in the initial (final) state with linear momentum $\mathbf{k}_{a(b)}$, relativistic energy $E_{a(b)}=[\frac{1}{2}k_{a(b)}^2c^2+c^4]^{1/2}$, and

spin projection $\mu_{a(b)}$. The distorted waves are solutions of the Dirac equations including the distortion potential U_b and depend on the spin of the projectile electron. More details are given in [3].

In order to express the dependence of the T matrix on these angular momentum quantum numbers we write it in the following simplified form:

$$T_{a\to b}^{\mathrm{DW}} = \langle J_b M_b \mu_b | V - U_b | J_a M_a \mu_a \rangle = \frac{1}{(2\pi)^2} \sqrt{\frac{k_a}{k_b}} f(J_b M_b \mu_b, J_a M_a \mu_a), \quad (4)$$

where J and M represent the total angular momentum and its z component of the atomic state, μ is the spin projection of the free electron, and f is the scattering amplitude

We consider excitation of mercury atoms initially in the ground $6\ ^1S_0$ state with total angular momentum quantum numbers $J_a=0$, $M_a=0$ to the excited $6\ ^{1,3}P_1$ state with total angular momentum quantum numbers $J_b=1$, $M_b=0,\pm 1$ by an incident electron with linear momentum $\mathbf{k_a}$ and z component of spin $\mu_a=\pm 1/2$, where the projectile electron may be spin polarized but the target atom is unpolarized. The spin polarization of the incoming electron is described by the polarization vector $\boldsymbol{P}$ with Cartesian components P_x, P_y, and P_z. We take as our coordinate system the collision frame where the z axis is in the direction of the incident electron beam which is spin polarized in the direction of the y axis. Srivastava *et al.* [8] have given formulas for the angle-integrated Stokes parameters in the case when the scattered electron is not detected. The values of the hyperfine structure coupling coefficients $G_K(j)$ in these formulas are given by Wolcke *et al.* [9].

The three integrated Stokes parameters are given by

$$P_1 = \frac{I(0) - I(90)}{I(0) + I(90)},$$

$$P_2 = \frac{I(45) - I(135)}{I(45) + I(135)},$$

$$P_3 = \frac{I(\sigma^-) - I(\sigma^+)}{I(\sigma^-) + I(\sigma^+)}, \quad (5)$$

where $I(\theta)$ is the intensity of the emitted radiation measured in the y direction with a linear polarizer set at an angle θ to the z axis, while $I(\sigma^{+,-})$ are the intensities with circular polarization with positive or negative helicities, respectively.

III. ATOMIC WAVE FUNCTIONS

The ground state configuration of Hg ($Z=80$) is $1s^2 2s^2 2\bar{p}^2 2p^4 3s^2 3\bar{p}^2 3p^4 3\bar{d}^4 3d^6 4s^2 4\bar{p}^2 4p^4 4\bar{d}^4 4d^6 4\bar{f}^6 4f^8 5s^2 5\bar{p}^2 5p^4 5\bar{d}^4 5d^6 6s^2$ in the relativistic j-j coupling notation [10]. The total angular momentum J_a of the ground state is zero and thus in the LS-coupling scheme the ground state is represented as $6\ ^1S_0$. We consider excitations where the outer $6s$ electron is excited to the $6\bar{p}$ or $6p$ orbital and the excited state has total angular momentum $J_b=1$. In LS coupling such excited states are represented as $6\ ^1P_1$ and $6\ ^3P_1$.

TABLE I. Configuration mixing coefficients c_i corresponding to the SCGS wave functions for the $6\ ^{1,3}P_1$ excited states of mercury.

Excited state	c_1	c_2
$6\ ^3P_1$	0.8580	−0.5136
$6\ ^1P_1$	0.5136	0.8580

We performed two separate calculations using two different choices for the configurations included in the atomic wave functions. In the spectroscopic configuration ground state (SCGS) calculation we include only the basic spectroscopic configurations in the ground and excited states, while in the multiconfiguration ground state (MCGS) calculation we add additional configurations with the same J value and parity. Thus in our SCGS calculation, the ground state is represented by a single configuration $6s^2$ while the excited states are linear combinations of the configurations $6s6\bar{p}$ and $6s6p$ with $J=1$. In the MCGS calculations, $6\bar{p}^2$ and $6p^2$ configurations with $J=0$ are added to the ground state and as well, the configurations $6p6\bar{d}$, $6\bar{p}6\bar{d}$, and $6p6d$ with $J=1$ are included in the representation of excited states. Thus the wave functions for the ground state and excited states are expressed as the following:

(i) *SCGS.* For ground state

$$6\ ^1S_0: \quad (6s^2)_{J=0} \quad (6)$$

and for excited states

$$6\ ^{1,3}P_1: \quad c_1(6s6\bar{p})_{J=1} + c_2(6s6p)_{J=1}. \quad (7)$$

(ii) *MCGS.* For ground state

$$6\ ^1S_0: \quad a_1(6s^2)_{J=0} + a_2(6\bar{p}^2)_{J=0} + a_3(6p^2)_{J=0} \quad (8)$$

and for excited states

$$6\ ^{1,3}P_1: \quad c_1(6s6\bar{p})_{J=1} + c_2(6s6p)_{J=1} + c_3(6p6\bar{d})_{J=1} + c_4(6\bar{p}6\bar{d})_{J=1} + c_5(6p6d)_{J=1}, \quad (9)$$

where the c_i and a_i are the configuration mixing coefficients (CI coefficients). We used the GRASP92 code of Parpia *et al.* [2] to obtain the Dirac-Fock orbitals and CI coefficients. Table I lists the configuration mixing coefficients c_i for the SCGS wave functions of the excited states. The configuration mixing coefficients c_i for the MCGS wave functions of the excited states are given in Table II. The CI coefficients for the ground state MCGS wave function are $a_1=0.9834$, $a_2=0.1325$, and $a_3=0.1241$.

TABLE II. Configuration mixing coefficients c_i corresponding to the MCGS wave functions for the $6\ ^{1,3}P_1$ excited states of mercury.

Excited state	c_1	c_2	c_3	c_4	c_5
$6\ ^3P_1$	0.8582	−0.5132	0.0080	0.0062	−0.0023
$6\ ^1P_1$	0.5129	0.8581	0.0068	0.0205	0.0123

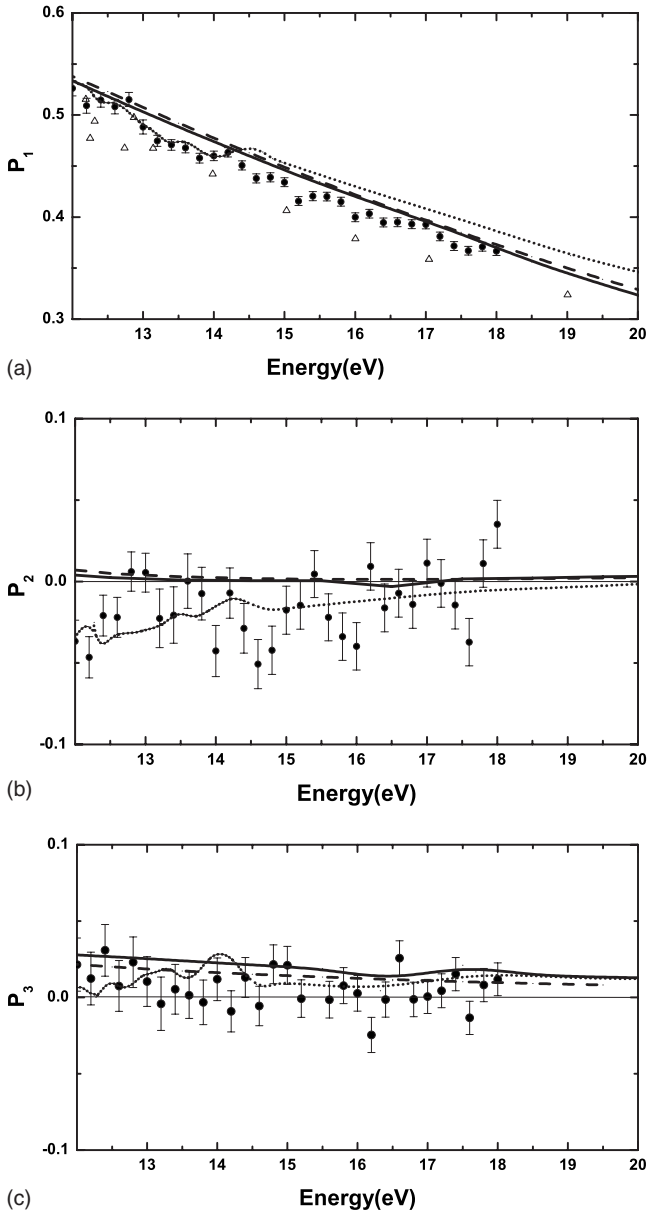

FIG. 1. Integrated Stokes parameters P_1, P_2, and P_3 for the excitation of the 6 $^1P_1$ state of Hg by electron impact: solid line, present MCGS results; dashed line present SCGS results; dotted line, DBSR results from [1]; solid circles with error bars, measurements of [1]; triangles, measurements of[11].

IV. RESULTS AND DISCUSSION

We performed RDW calculations for the excitation of 6 $^1P_1$ and 6 $^3P_1$ states of mercury from its ground state 6 $^1S_0$ using the two different representations for the atomic wave functions as outlined above and obtained the integrated Stokes parameters [Eq. (5)] for incident electron with energy above 12 eV where we expect our results to be reliable. The Stokes parameter P_1 can be nonzero for scattering of unpolarized electrons but P_2 and P_3 are zero unless the incident electron is spin polarized. P_2 is a measure of the strength of spin-dependent effects such as spin-orbit coupling in the scattering process while the magnitude of P_3 depends primarily on electron exchange taking place during scattering.

In Fig. 1 we show our results for the excitation of the singlet state for the three integrated Stokes parameters P_1, P_2, and P_3 along with the measurements of Jüttemann *et al.* [1], the earlier experimental results of Herting and Hanne [11] for P_1, and the DBSR-36 calculations from [1]. We note that the SCGS and MCGS results are very close for all three parameters. Above about 14 eV our results for P_1 are slightly above the measurements of [1] while the DBSR data are even higher. However, below 14 eV, the DBSR results are in better agreement with the measurements. For P_2 our results are small and positive while the DBSR results are slightly larger in magnitude but negative while the measured data exhibit significant variations taking both positive and negative values. All three theoretical results give similar values for P_3, especially for larger energies, which are small but positive, and in good agreement with the experimental data at most energies. Figure 2 presents similar results for the excitation of the triplet case. Here the Stokes parameters P_2

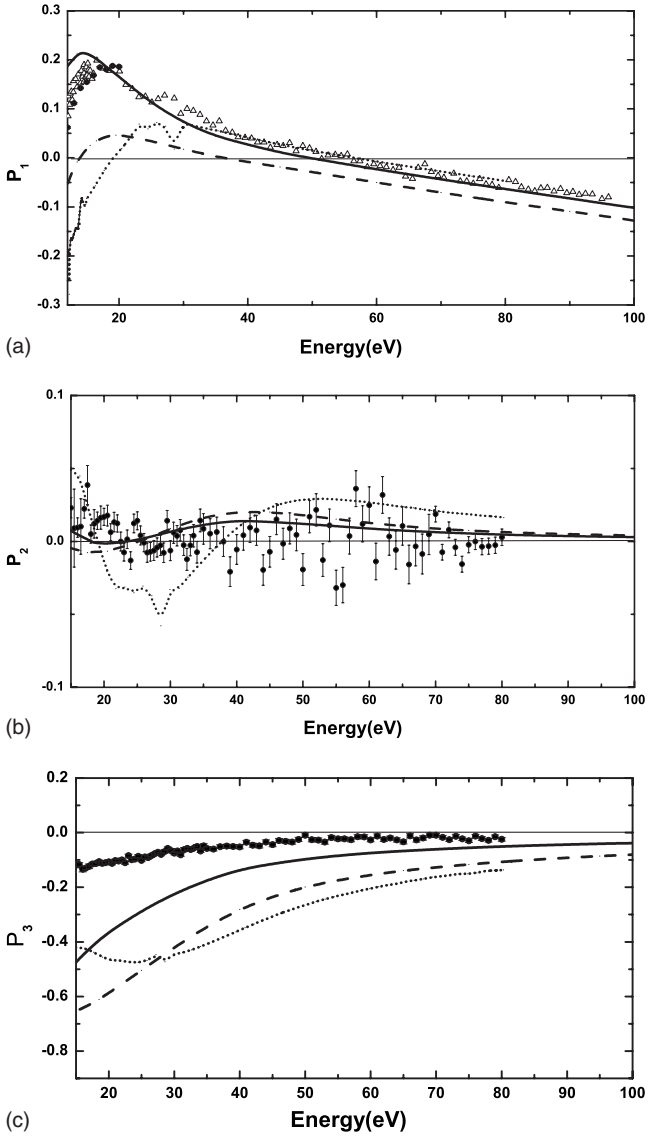

FIG. 2. As for Fig. 1 for the excitation of the 6 $^3P_1$ state of Hg.

and P_3 are larger in magnitude than for the singlet case and there are significant differences between our SCGS and MCGS results except in the case of P_2. Our MCGS results are in very good agreement with the measurements for P_1 especially above 15 eV while the SCGS results are distinctly lower. The DBSR calculations are close to our MCGS results and experiment above about 30 eV but fall much below both these sets of data for smaller energies. For P_2 our results are small and positive and in reasonable agreement with experiment at smaller energies. At larger energies there is significant variation in the measurements. The DBSR calculations show a rather different behavior with energy which does not reflect either our results or the measurements. The P_3 parameter is surprising large, indicating the importance of exchange for this transition and, while all four sets of data approach zero as the energy increases, there are significant differences in the magnitude of these results. Our MCGS calculations are closest to the measurements but there is still about a factor of 2 differences between the two sets of data. At these energies the experimental results can be affected by cascading from higher excited states to the $6\ ^3P_1$ state which may explain at least some of the discrepancy. However, the large differences among the three theoretical approaches indicate that this parameter is very sensitive to the approximations used.

V. CONCLUSIONS

We have calculated the angle-integrated Stokes parameters for excitation of the two lowest excited states of mercury with total angular momentum $J=1$ by applying our relativistic distorted-wave approximation which takes direct account of the fine-structure states of the target as well as the spin of the incident electron. The agreement we obtained with the recently measured values in [1] is further evidence that our model is capable of producing reliable scattering data at intermediate energies and is particularly suited to collisions with heavy atoms.

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