Effect of spin-orbit coupling on $2p_{1/2}$-$2p_{3/2}$ rotational transitions in heavy-ion collisions*

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We consider the effect of spin-orbit coupling between the molecular orbitals correlated to the united-atom $2p_{1/2}$ and $2p_{3/2}$ states on rotational-coupling transition probabilities in heavy-ion collisions. In low-Z, low-velocity encounters, where the splitting is small, calculations of the rotational-coupling cross section have been shown to be in agreement with experiment. We compute a correction factor to the previous calculations in terms of a general scaling parameter $\xi = \Delta E/(kv_1^2)^{1/3}$, where ΔE is the spin-orbit splitting in the united atom, v_1 is the ion velocity, and $k = Z_1Z_2(Z_1 + Z_2)^2/40$ a.u. The correction is generally small, but is observed in high-Z encounters at low velocities.

I. INTRODUCTION

In near-symmetric collisions with atomic charges $Z \leq 10$, $2p\sigma$-$2p\pi$ rotational coupling is responsible for the production of K vacancies in the lighter and, to a lesser extent, in the heavier collision partner.[1-4] In essence a vacancy in the $2p\pi$ molecular orbital (MO) correlates to the $2p_{\pm 1}$ orbital in the united atom (UA), where Coriolis coupling allows the vacancy to jump to the $2p\sigma$ MO and to correlate to the 1s levels of the separated atoms (SA) on the outgoing part of the collision (Fig. 1). Several calculations employing nonrelativistic molecular wave functions have been performed and generally have agreed very well with experimental data.[3-7] Most available data is for collisions with $Z \leq 10$ where nonrelativistic calculations are unquestionably appropriate.

Recently, in studying K-vacancy production in the lighter collision partner in collisions with $Z \geq 35$ using solid targets, we have found that a multiple collision process involving the rotational coupling mechanism can be very important.[8] Originally it was thought, because there are no $2p\pi$ vacancies initially present in these collisions, the Pauli exclusion principle would not allow $2p\sigma$ vacancy production to occur through the rotational coupling mechanism.[9] However, in solid targets, projectile L vacancies made in one collision can live long enough to enter the $2p\pi$ MO in a second collision, allowing $2p\sigma$ vacancy production to occur.[10]

Even in the absence of the multiple collision process (e.g., in monatomic gas targets), a two-step process involving $2p\sigma$-$2p\pi$ coupling may also take place.[2,8,11] In this process a $2p\pi$ electron would be either ionized or excited to an upper state early in the collision, allowing the $2p\sigma$-$2p\pi$ transition to occur later in the collision.

The Br + Br and I + I systems studied in Ref. 8 have UA charges 70 and 106, where the spin-orbit splitting between the $2p_{1/2}$ and $2p_{3/2}$ orbitals is approximately 1 and 8 keV, respectively. To our knowledge, the effect of such a large splitting has been considered only qualitatively to date.[12] We suspected that the splitting might inhibit $2p\sigma$-$2p\pi$ rotational coupling. In turn, this would affect calculated multiple collision and/or two-step contributions to the K-vacancy cross section.

The effect of spin-orbit coupling on outer-shell transitions has been considered previously. Many calculations have been made of fine-structure transition probabilities between SA states, e.g., Na and F $P_{1/2}$-$P_{3/2}$ transitions in collisions with inert gas atoms.[13,14] In those systems, transitions take place at large internuclear distances and the be-

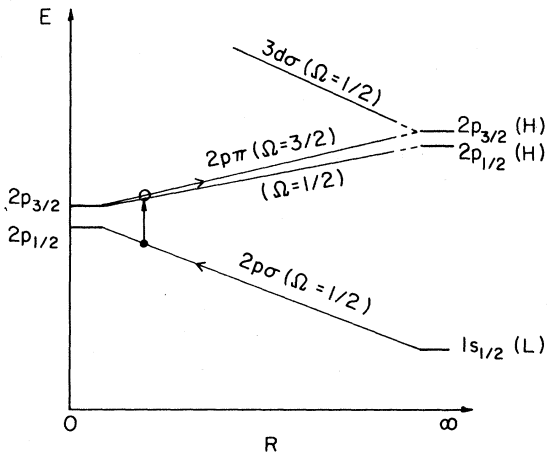

FIG. 1. Schematic correlation diagram for $2p$ and $3d$ MO's. Separated atom orbitals of the lower (L)- and higher (H)-Z collision partners are shown.

havior of the transition probabilities with increased spin-orbit coupling is liable to be fundamentally different from the present inner-shell cases.

Our calculations are described in Secs. II and III. We have performed approximate calculations which allow us to obtain a simple general correction factor in terms of a single dimensionless parameter ξ which involves the spin-orbit splitting, the ion velocity, and the projectile (Z_1) and target (Z_2) atomic numbers. The results are described in Sec. IV. Atomic units are used throughout the paper.

II. THEORY

In the impact-parameter approximation, we have to solve coupled differential equations for probability amplitudes[15,16]:

$$i\frac{db_i}{dt}=\sum_j\langle\psi_i|H-i\frac{\partial}{\partial t}|\psi_j\rangle b_j(t), \tag{1}$$

where H is taken as the sum of the molecular electrostatic Hamiltonian $H_{\rm elec}$ and of the spin-orbit Hamiltonian

$$H_{LS}=\zeta\vec{\mathrm{L}}\cdot\vec{\mathrm{S}}. \tag{2}$$

Here ζ is the spin-orbit coupling constant which is a function of internuclear distance R.

It is useful to consider the evolution of the total electronic wave function

$$\psi=\sum_j b_j(t)\psi_j[R(t),r]. \tag{3}$$

Here ψ_j contains spin as well as space variables and will be characterized by an angular momentum number Λ (L_z with z along the internuclear axis), as well as spin quantum numbers S, m_s, where $m_s=S_z$ and $S=\frac{1}{2}$. The sum $\Omega=\Lambda+m_s$ is the z component of the total spin and orbital momentum J. Since our Hamiltonian considers spin-orbit coupling as well as the electrostatic splitting between states of different Λ, Ω is the only good quantum number. At intermediate internuclear distances where $H_{\rm elec}\gg H_{LS}$ and $H_{\rm elec}\gg i\,\partial/\partial t$, the wave function will be adequately represented by the product $|L\Lambda\rangle|Sm_s\rangle$, i.e., by a pure $2p\sigma$ or $2p\pi$ MO multiplied by a spin wave function. At close distances, however, $H_{\rm elec}\approx 0$ so that $H_{LS}\gg H_{\rm elec}$ and $i\,\partial/\partial t\gg H_{\rm elec}$ and the total wave function can be a mixture of spin orbitals. The spin-orbit coupling mixes states of the same Ω quantum number and the Coriolis part of $i\,\partial/\partial t$ mixes states with Λ differing by ±1. In addition, Coriolis coupling will mix states with m_s differing by ±1. Finally, at large internuclear distances, coupling to other MO's (e.g., $3d_{1/2}$, $3d_{3/2}$, $2s_{1/2}$, etc.) will become important. Given the existence of one $2p_{3/2}$ vacancy initially, this coupling plays no role in producing K vacancies, and we can neglect coupling to these states.

We choose as basis states $\psi_j(t)$ the six spin MO's leading to the $2p$ levels in the UA:

$$|1\Lambda\rangle|\tfrac{1}{2}m_s\rangle\equiv|\Lambda m_s\rangle=|\pi^-\beta\rangle,\ |\pi^-\alpha\rangle,|\sigma\beta\rangle,$$

$$|\sigma\alpha\rangle,|\pi^+\beta\rangle,\text{ and }|\pi^+\alpha\rangle,$$

where σ, π^+, and π^- stand for $2p\sigma$, $2p\pi_{+1}$, and $2p\pi_{-1}$, respectively, and α and β are spin states $m_s=+\frac{1}{2}$ and $-\frac{1}{2}$, respectively. This basis diagonalizes $H_{\rm elec}$. The $2s_{1/2}$ state does not play a significant role in the rotational-coupling process.[5] Also it clearly does not spin-orbit couple to the $2p_{1/2}$ or $2p_{3/2}$ MO's. Therefore we have omitted it from the basis set. Masnou-Seeuws *et al.*[13] have discussed other possible basis sets. We have chosen the present set because of the relative simplicity of the calculations in this basis. A basis in which $H_{\rm elec}+H_{LS}$ is diagonal makes the calculations very difficult because the dynamical couplings in this basis involve extra radial coupling terms.

We now consider matrix elements. Since the basis states diagonalize $H_{\rm elec}$ we find

$$\langle\psi_i|H_{\rm elec}|\psi_j\rangle=\delta_{ij}\begin{cases}V_\sigma\\V_\pi\end{cases}, \tag{4}$$

depending on whether ψ_i is a σ or π state.

To simplify our calculations, we take the spin-orbit coupling constant ζ to be independent of the internuclear distance, and equal to the UA $2p$ value. The matrix element of H_{LS} is given by

$$\langle J\Omega|H_{LS}|J'\Omega'\rangle=\tfrac{1}{2}\zeta(J^2-L^2-S^2)\delta_{JJ'}\delta_{\Omega\Omega'}. \tag{5}$$

Thus if we set $E_{3/2}-E_{1/2}=\Delta$, we find $\zeta=\frac{2}{3}\Delta$. Using the usual vector coupling relationships[17]

$$|\Lambda m_s\rangle=\sum_J C(1,\tfrac{1}{2},J;\Lambda,\Omega-\Lambda)|J\Omega\rangle, \tag{6}$$

matrix elements between basis states $|\Lambda m_s\rangle$ may easily be determined. They are given in Table I.

Radial coupling does not operate between the $2p_{1/2}$ and $2p_{3/2}$ MO's, so the operator $\partial/\partial t$ in Eq. (1) is

$$\frac{\partial}{\partial t}=\dot\theta\frac{\partial}{\partial\theta}. \tag{7}$$

The angle θ is defined as the angle between the internuclear axis and the initial velocity of the projectile. Let $\psi_{\rm rot}$ be the wave function for a state defined in a rotating coordinate system linked to the internuclear axis and $\psi_{\rm fix}$ be the same wave function in a fixed coordinate frame linked to the initial beam direction. Then $\psi_{\rm rot}$ is obtained from $\psi_{\rm fix}$ by a rotation of θ.[16] As ψ contains both spin and space variables one must write[13]

TABLE I. Matrix elements of $H_{\rm elec}+H_{LS}-\dot\theta(L_y+S_y)$.

	$\pi^-\beta$	$\pi^-\alpha$	$\sigma\beta$	$\sigma\alpha$	$\pi^+\beta$	$\pi^+\alpha$
$\pi^-\beta$	$V_\pi+\Delta/3$	$-\frac{1}{2}i\dot\theta$	$-i\dot\theta/\sqrt{2}$	0	0	0
$\pi^-\alpha$	$i\dot\theta/2$	$V_\pi-\Delta/3$	$\sqrt{2}\Delta/3$	$-i\dot\theta/\sqrt{2}$	0	0
$\sigma\beta$	$i\dot\theta/\sqrt{2}$	$\sqrt{2}\Delta/3$	V_σ	$-i\dot\theta/2$	$-i\dot\theta/\sqrt{2}$	0
$\sigma\alpha$	0	$i\dot\theta/\sqrt{2}$	$i\dot\theta/2$	V_σ	$\sqrt{2}\Delta/3$	$-i\dot\theta/\sqrt{2}$
$\pi^+\beta$	0	0	$i\dot\theta/\sqrt{2}$	$\sqrt{2}\Delta/3$	$V_\pi-\Delta/3$	$-i\dot\theta/2$
$\pi^+\alpha$	0	0	0	$i\dot\theta/\sqrt{2}$	$i\dot\theta/2$	$V_\pi+\Delta/3$

$$\psi_{\rm rot}=e^{-i(L_y+S_y)\theta}\psi_{\rm fix}\ , \tag{8}$$

where L_y is the y component of the total electronic angular momentum and S_y is the total spin angular momentum along the axis perpendicular to the collision plane. We then have

$$\dot\theta\frac{\partial}{\partial\theta}\psi_{\rm rot}=-i(L_y+S_y)\dot\theta\psi_{\rm rot}\ , \tag{9}$$

since $(\partial/\partial\theta)\psi_{\rm fix}=0$. The rotation of the spin has not previously been considered.[3-6] We have verified that it produces no additional effect in the absence of spin-orbit coupling. When spin-orbit coupling is included, however, the rotation of the spin produces an effect that needs to be considered.

We now identify $|\Lambda m_s\rangle$ with $\psi_{\rm rot}$ and compute matrix elements of S_y and L_y in Eq. (9):

$$\begin{aligned}\langle\Lambda'\beta|-i\dot\theta S_y|\Lambda\alpha\rangle&=-\tfrac{1}{2}\dot\theta\delta_{\Lambda\Lambda'}\ ,\\ \langle\Lambda'\alpha|-i\dot\theta S_y|\Lambda\beta\rangle&=+\tfrac{1}{2}\dot\theta\delta_{\Lambda\Lambda'}\end{aligned} \tag{10}$$

and

$$\langle\Lambda'\ m_{s'}|-i\dot\theta L_y|\Lambda'\pm1\ m_s\rangle=\mp(\dot\theta/\sqrt{2})\delta_{m_s,m_{s'}}f(R)\ , \tag{11}$$

where $f(R)$ is given by Bates *et al.*[4] or Taulbjerg *et al.*[6] In our calculations we approximate $f(R)=1$. Matrix elements of $H-i\partial/\partial t$ are given in Table I.

To solve Eq. (1), we perform a unitary phase transform[5] to remove diagonal elements. Letting

$$a_i(t)=b_i(t)\exp\left(i\int^t H_{ii}(t')\,dt'\right), \tag{12}$$

we obtain

$$\frac{da_i}{dt}=\sum_{j\neq i}-iH_{ij}a_j(t)\exp[i\Phi_{ij}(t)]\ , \tag{13}$$

where

$$\Phi_{ij}(t)=\int^t[H_{ii}(t')-H_{jj}(t')]\,dt'\ .$$

We give values of H_{ij} and Φ_{ij} in Table II, where we have used the following abbreviations:

$$\begin{aligned}A\equiv A(t)&=\int^t[V_\pi(t')-V_\sigma(t')]\,dt'\ ,\\ B\equiv B(t)&=\tfrac{1}{3}t\Delta\ ,\\ T&=\tfrac{1}{2}\dot\theta\ ,\quad U=\tfrac{1}{3}\sqrt{2}\Delta\ .\end{aligned} \tag{14}$$

III. NUMERICAL CALCULATIONS—SCALING

It is appropriate here to summarize approximations which have been made to solve Eq. (1): (i) We take $\zeta=\frac{2}{3}\Delta$ to be constant and independent of R. (ii) We set the matrix element $\sqrt{2}\langle 2p\sigma|\partial/\partial\theta|2p\pi\rangle\equiv f(R)$ equal to unity. (iii) We neglect coupling between $2p_{1/2}$ and $2p_{3/2}$ and any other MO. (iv) We will integrate Eq. (13) along straight-line trajectories, neglecting the Coulomb deflection of the projectile. (v) We take the splitting $V_\pi-V_\sigma$ to be given by[6,18]

$$V_\pi(R)-V_\sigma(R)=kR^2\ , \tag{15}$$

where

$$k=Z_1^*Z_2^*(Z_1^*+Z_2^*)^2/40\ \text{a.u.}\ ,$$

TABLE II. Elements $-iH_{ij}$ and Φ_{ij} in Eq. (13).

	$-H_{ij}$						Φ_{ij}					
	$\pi^-\beta$	$\pi^-\alpha$	$\sigma\beta$	$\sigma\alpha$	$\pi^+\beta$	$\pi^+\alpha$	$\pi^-\beta$	$\pi^-\alpha$	$\sigma\beta$	$\sigma\alpha$	$\pi^+\beta$	$\pi^+\alpha$
$\pi^-\beta$	0	$-T$	$-\sqrt{2}T$	0	0	0	$\cdots$	$2B$	$A+B$	$\cdots$	$\cdots$	$\cdots$
$\pi^-\alpha$	T	0	$-iU$	$-\sqrt{2}T$	0	0	$-2B$	$\cdots$	$A-B$	$A-B$	$\cdots$	$\cdots$
$\sigma\beta$	$\sqrt{2}T$	$-iU$	0	$-T$	$-\sqrt{2}T$	0	$-A-B$	$-A+B$	$\cdots$	0	$-A+B$	$\cdots$
$\sigma\alpha$	0	$\sqrt{2}T$	T	0	$-iU$	$-\sqrt{2}T$	$\cdots$	$-A+B$	0	$\cdots$	$-A+B$	$-A-B$
$\pi^+\beta$	0	0	$\sqrt{2}T$	$-iU$	0	$-T$	$\cdots$	$\cdots$	$A-B$	$A-B$	$\cdots$	$-2B$
$\pi^+\alpha$	0	0	0	$\sqrt{2}T$	T	0	$\cdots$	$\cdots$	$\cdots$	$A+B$	$2B$	$\cdots$

TABLE III. Typical values of the reduced spin-orbit splitting parameter ξ and the spin-orbit correction function to the rotational cross section $f(\xi)$.

Z_1, Z_2	E_{lab} (MeV)	ξ	$f(\xi)$
H+H	500×10^{-6}	1.32×10^{-5}	1.00
Ne+Ne	500×10^{-3}	0.013	1.00
Cl+Ar	15	0.034	1.00
	30	0.027	1.00
Ni+Ni	15	0.170	1.00
	100	0.090	1.00
Br+Br	30	0.302	1.03
	100	0.225	1.01
Kr+Kr	200	0.178	1.00
I+I	15	1.940	0.23
	100	1.030	1.15
Xe+Xe	400	0.716	1.16
Pb+Pb	100	23.3	...

$Z_1^* = Z_1 - 1$, and $Z_2^* = Z_2 - 1$.

The effects of these approximations are twofold. First, along straight-line trajectories, the kinematic peak observed at small impact parameters b disappears.[3] This has a small effect on the total cross section. Second, the neglect of the dependence of $f(R)$ on R and the deviation of $V_\pi - V_\sigma$ from kR^2 at large distances produces cross sections in the limit $\zeta \to 0$ which are approximately 20% lower than the more accurate results of Taulbjerg *et al.*[6] Nevertheless, if we normalize by our $\zeta = 0$ cross sections, we expect our spin-orbit correction factor to be relatively more accurate.

We have basically two different terms in Eq. (13):

$$\frac{da_i}{dt} = a_j \gamma \frac{bv_1}{R^2} e^{i(\pm A \pm B)}, \qquad \frac{da_i}{dt} = a_j \left(\pm \frac{\sqrt{2}\Delta}{3}\right) e^{i(\pm A \pm B)}, \tag{16}$$

where $\gamma = \pm\frac{1}{2}$ or $\pm 1/\sqrt{2}$. If, instead of integrating along t, we integrate along $Z = v_1 t$ and define

$$z = (k/v_1)^{1/3} Z, \quad x = (k/v_1)^{1/3} b,$$

and

$$\xi = \Delta/(k^{1/3} v_1^{2/3}), \tag{17}$$

we obtain for A and B in Eq. (13):

$$A = x^2 z + \tfrac{1}{3} z^3 \quad \text{and} \quad B = \tfrac{1}{3}\xi z, \tag{18}$$

and for the two typical terms:

$$\frac{da_i}{dz} = a_j \gamma \frac{x}{x^2 + z^2} e^{i(\pm A \pm B)}, \qquad \frac{da_i}{dz} = a_j \left(\pm \frac{\sqrt{2}\,\xi}{3}\right) e^{i(\pm A \pm B)}. \tag{19}$$

Hence we can replace T and U in Eq. (14) and Table II with

$$T = \tfrac{1}{2} x/(x^2 + z^2) \quad \text{and} \quad U = \tfrac{1}{3}\sqrt{2}\,\xi. \tag{20}$$

Equation (13) is solved with the condition for one initial electron in the $2p\sigma$ MO $[a_{|\sigma\alpha\rangle}(-\infty) = 1]$ coupling to fully empty $2p\pi$ MO's. The cross section is related to the probability for one initial SA $2p$ vacancy to couple to the $2p\sigma$ MO by the Briggs and Macek statistical factors.[3] Equation (13) was numerically integrated using a Zonneveld-Adams-Moulton differential equation solver.[19] The transition probability $P(x, \xi)$ is defined as

$$P(x, \xi) = \sum_{\Lambda = \pm 1} \sum_{m_s = \pm\frac{1}{2}} |a_{|\Lambda m_s\rangle}|^2. \tag{21}$$

The cross section is obtained from

$$\sigma_K = \left(\frac{v_1}{k}\right)^{2/3} \int_0^\infty 2\pi x\, dx\, P(x, \xi) = \sigma_0 f(\xi), \tag{22}$$

where σ_0 is approximately equal to $2(v_1/k)^{2/3}$ and can be taken to be the nonrelativistic cross section. The correction function $f(\xi)$ is defined so that $f(0) = 1$. To obtain a more accurate evaluation of σ_K, $f(\xi)$ can be applied to calculated cross sections of Taulbjerg *et al.*[6]

Table III gives typical values of the reduced spin-

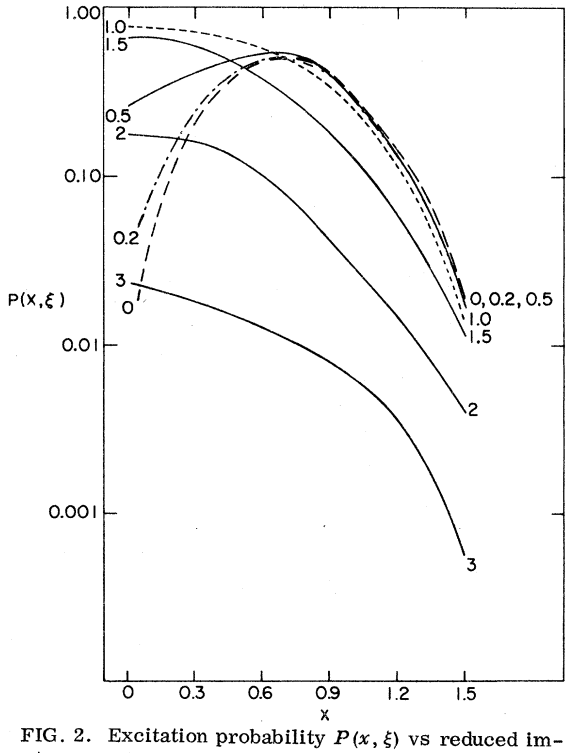

FIG. 2. Excitation probability $P(x, \xi)$ vs reduced impact parameter x [Eq. (24)] for various values of the reduced spin-orbit splitting parameter ξ [Eq. (23)] denoted by numbers to the left and right of curves.

orbit splitting parameter ξ for systems of interest. The parameter is dimensionless and can be calculated in different ways. In atomic units ξ is obtained from

$$\xi = \Delta[(Z_1^* Z_2^* Z_u^2/40)v_1^2]^{-1/3}, \quad (23)$$

where Δ is the experimental $2p_{3/2}$-$2p_{1/2}$ splitting in the UA, and $Z_u = Z_1^* + Z_2^*$. For later reference we also give the reduced impact parameter x using atomic units

$$x = (Z_1^* Z_2^* Z_u^2/40\, v_1)^{1/3} b. \quad (24)$$

IV. RESULTS

Figure 2 shows $P(x, \xi)$ vs x for various values of ξ. For $\xi < 1$, the main effect is an increase in $P(x, \xi)$ for small values of x as ξ increases. For large values of x, $P(x, \xi)$ remains unchanged. Once $\xi = 1$ is reached, the entire $P(x, \xi)$ curve decreases rapidly in magnitude with larger ξ.

To explain this behavior partially it is helpful to examine Fig. 3 where we have made additional calculations without Coriolis coupling ($J_y = L_y + S_y = 0$) for $\xi = 0.5$, 1.0, and 2.0. For comparison we also show the curve without spin-orbit coupling and the full results. With $J_y = 0$, $P(x, \xi)$ increases up to $\xi = 1$ because the off-diagonal matrix elements increase in magnitude, increasing the strength of the coupling. For $\xi > 1$, the increase in the matrix elements does not lead to greater transition probabilities. The increased energy gap [B factors in Eq. (14)] becomes important, and $P(x, \xi)$ falls for larger values of ξ. Crudely speaking then, for $\xi < 1$, Coriolis coupling dominates for large x values, and spin-orbit coupling dominates for small x values. For large ξ values, however, the spin-orbit energy gap dominates $P(x, \xi)$.

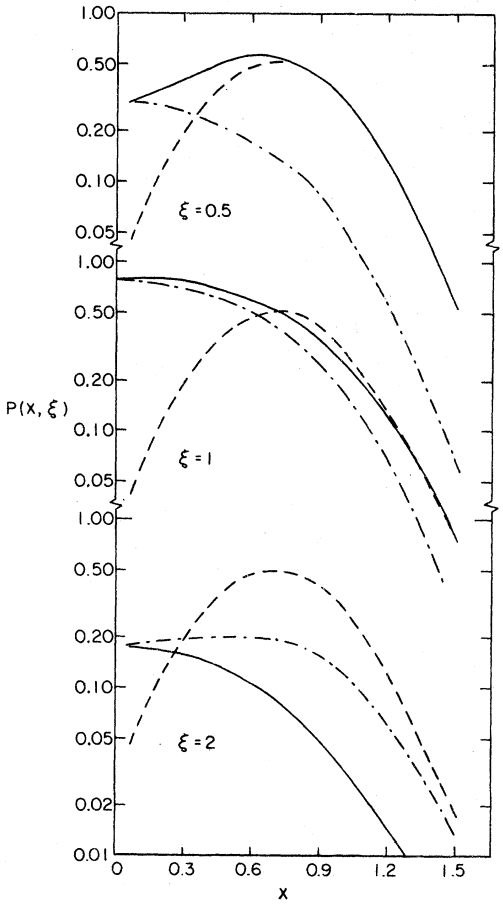

FIG. 3. Same as Fig. 2 for $\xi = 0.5$, 1.0, and 2.0 (solid line). In each case $P(x, 0)$ (dashed line) is given for reference. The dash-dot line is a calculation with all Coriolis matrix elements set equal to zero.

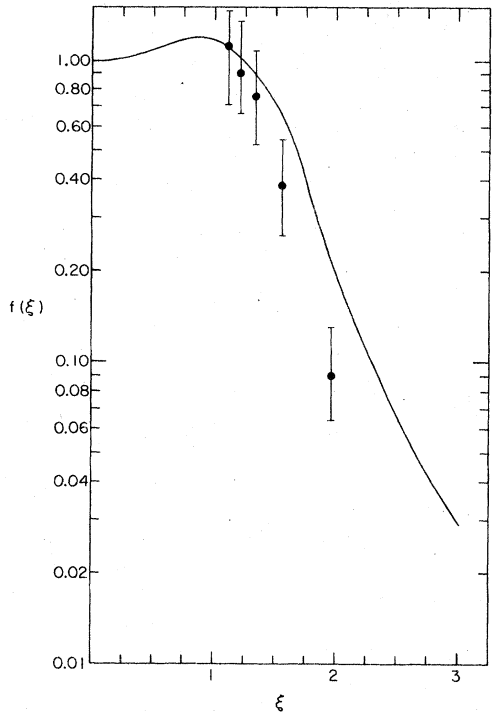

FIG. 4. Cross-section correction function $f(\xi)$ vs the reduced spin-orbit splitting parameter ξ [Eq. (23)]. Experimental points are for 15–80-MeV I+I collisions (Ref. 8).

In Fig. 4 we show results for the correction factor $f(\xi)$ to the cross section [Eq. (22)]. We see that the effects of spin-orbit coupling for $\xi < 1$ lead to an approximate 15% increase in $f(\xi)$ while for $\xi > 1$, $f(\xi)$ falls off rapidly. Experimental errors in the vacancy production cross sections typically are at least 10%. Table III indicates that most experiments done so far have had $\xi \lesssim 0.5$. The experiments have given results for the rotational cross section in agreement with Taulbjerg *et al.*[6]

$[f(\xi)=1]$ within experimental error. Clearly it will be difficult to determine this effect experimentally unless one studies cross sections for $Z>50$ collisions at very low velocities.

We have measured the K-vacancy production in I+NaI collisions,[8] which is expected to occur mainly by the multiple collision mechanism described in the introduction. The K-vacancy cross section is proportional to the projectile $2p$ vacancy production as well as to the rotational-coupling cross section. By measuring the projectile $2p$ x-ray production cross section (as well as the K-vacancy cross section), we were able to obtain an experimental estimate of the rotational-coupling cross section. Dividing the latter by the value of Taulbjerg *et al.*,[6] we obtained experimental estimate of $f(\xi)$, shown in Fig. 4. The points show that the calculated value of $f(\xi)$ has the correct trend. There is the possibility of systematic experimental errors, as well as a possible overestimate of the calculated value of $f(\xi)$ in the low-velocity high-Z region because of the various approximations made.

The only other system that has been studied where $f(\xi)<1$ is a system of 100-MeV Pb+Pb collisions.[20] There ξ is equal to 23 and we found it impossible to calculate $f(\xi)$ accurately. In addition, it is doubtful whether our approximations i, ii, iv, and v are valid for this very high-Z encounter. We can draw the following conclusions, however. In all probability $f(\xi)$ is very small for this case. This should be the case anyway since the energy transfer needed to promote the $2p_{1/2}$ electron to the $2p_{3/2}$ orbital is 280 keV at the united atom, compared to 340 keV needed to ionize the electron there. Hence, the rotational-coupling cross section should not differ from the ionization cross section by more than one to two orders of magnitude. In this case, there would be no particular advantage for $2p\sigma$-vacancy production to occur through multiple collision or two-step processes, since the number of $2p\pi$ vacancies brought into the collision by these two processes must be much less than unity. Therefore, the observed Pb+Pb cross section probably represents the $2p\sigma$ impact ionization cross section, in agreement with the assumptions made by the authors of that work.[20]

Studies of $P(b)$ might confirm the deviation at the low impact parameters for larger ξ values. Unfortunately the presence of the kinematic peak at small impact parameters will tend to obscure this behavior. Thus far impact-parameter studies have been done for systems as high in Z as Cl+Ar.[11] There $\xi=0.03$ and one cannot expect to see any spin-orbit effects. Studies have also been made in 45-MeV Ni+Mn encounters,[21] in solid targets where the multiple collision mechanism probably dominates. There too ξ is only about 0.1, which does not produce a sufficiently large change in $P(b)$ (Fig. 2).

V. CONCLUSIONS

The effects of spin-orbit coupling on $2p_{1/2}$-$2p_{3/2}$ rotational-coupling transitions have been calculated. For low-velocity high-Z systems such as 15-MeV I+I, significant effects are predicted and observed. For low-Z systems ($\xi<1$) the rotational cross section is only at most 15% higher than the nonrelativistic results of Taulbjerg *et al.*[6] Significant deviations in the impact-parameter dependence for low b values are predicted, but measurements are not yet available to confirm these deviations.

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