Electron Spin Exchange in Atomic Collisions*

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We consider electron spin-exchange collisions between an atom with an electron spin of $\frac{1}{2}$ and a target atom with an arbitrary electron spin. The cross sections that describe the collision are expressed in terms of generalized direct and exchange amplitudes and are shown to depend only on the electron spin, polarization, and alignment of the target atom. We include the effects of an external magnetic field and the nuclear spin of the spin-$\frac{1}{2}$ atom on the collision. We calculate the cross sections connecting the initial and final states of the free Hamiltonian describing the spin-$\frac{1}{2}$ atom, with analytic results being displayed for the two limiting cases of the external magnetic field. For the general case, graphical results are presented for several common values of nuclear spin that allow the cross sections to be evaluated for arbitrary magnetic fields. The results are applied to several situations of current interest.

I. INTRODUCTION

Spin exchange is an essentially elastic process that can occur in any collision between partners having nonzero electron spins. By measuring differential cross sections in each of the available spin states, one can obtain detailed information on the spin dependence of interatomic potentials. Such experiments have been carried out by Pritchard *et al.*[1] and Beck *et al.*[2] and Höh *et al.*[2] for the case of alkali-alkali scattering at thermal energies. The technique can be extended to more complicated systems with total spin angular momentum greater than unity. We present in this paper an analysis of spin-exchange scattering for an incident atom of spin $\frac{1}{2}$ on a target of arbitrary spin. Our analysis also takes into account the effect of nuclear spin of the incident atom. We allow for the effects of an applied magnetic field since many experiments are carried out in an intermediate-field region.

Although the effects of nuclear spin and magnetic field are not fundamental, they must be taken into account accurately in analyzing experimental results. In this paper we attempt to treat these effects so as to permit their easy calculation in situations of current interest.

A number of workers have treated various aspects of the problems considered here. Glassgold[3] first treated the effects of nuclear spin at zero magnetic field. These results were extended by Burnham[4] to include effects of a polarized spin-$\frac{1}{2}$ target and were applied to experiments in which the scattered atom is polarized and analyzed in a high magnetic field, but in which the collision occurs at zero magnetic field. The effects of intermediate magnetic field have been considered by Rubin[5] and Glassgold,[6] and more recently by Glassgold and Walker.[7] All of these works dealt with targets with electron spin of $\frac{1}{2}$. The present work generalizes all these results by including them simultaneously, and generalizing them to a case of a target with arbitrary electron spin (in which case the alignment of the target must also be considered).

Our presentation is divided into several sections. In Secs. II and III we find the scattering matrix for spin exchange between a spin-$\frac{1}{2}$ system and a target of arbitrary spin. In Sec. IV we introduce the additional formalism necessary to include nuclear spin in an arbitrary magnetic field. In Sec. V these results are applied to find the full scattering matrix. In Sec. VI we use these results to calculate cross sections of current experimental interest.

We have also solved this problem using density-matrix techniques.[8] In this article we forgo this formalism for a more "old-fashioned" approach in which the effects of the collision on the electrons of colliding atoms may be considered in some detail before adding the complications of nuclear spin and hyperfine coupling.

II. EXCHANGE AND DIRECT AMPLITUDES FOR TARGET SPIN L

Let us now consider the effects of a collision between an atom with an electron spin of $\frac{1}{2}$ and a target of electron spin L. We assume that both atom and target are in S states so that all interactions are spherically symmetric. If the target spin is composed of several electrons coupled together (e.g., the $^3\Sigma$ ground state of O_2 or the ^4S ground state[9] of N), then there must not be any nearby excited states that would permit the target to "come apart" or to assume different spin during the collision. If we assume, in addition, that the collision is slow enough (KE less than a few eV) that no electronic excitation processes are possible, and fast enough (KE > 0.001 eV) that the spins couple insignificantly to anything (the orbital motion, rotational motion, nuclear moments, etc.) but themselves, then there is an interaction potential of the form

$$V_{\rm int} = P_- V_-(R) + P_+ V_+(R) , \tag{1}$$

where P_- is the projection operator for the coupled state with spin $L-\frac{1}{2}$ and P_+ is the projection operator for the coupled state with spin $L+\frac{1}{2}$ (R is the internuclear separation).

These assumptions mean that the two coupled spin states scatter independently during the collision, and thus the scattering matrix for the collision may be written in the form

$$F(\theta) = P_- f_-(\theta) + P_+ f_+(\theta) , \tag{2}$$

where $f_-(\theta)$ and $f_+(\theta)$ are the scattering amplitudes for the two states, and may be found from the corresponding potentials by the usual methods. This formulation reflects the fact that the nuclear spin and the external magnetic field have no effect on the collision process itself. They cause observable effects only by coupling to the electron spin in the time intervals before and after collision.

We now consider the simple case of a ^2S atom with $I=0$ colliding with a target whose electron spin is L. (The only effect of the magnetic field is to fix the axis of quantization.) This discussion will illustrate how the scattering amplitude in Eq. (2) causes spin exchange, and it will result in a simple expression for the collision matrix.

We consider the scattering of an atom with a spin-up electron and a target whose z component of angular momentum is m_L. It is more convenient to express the Clebsch-Gordan coefficients (see Table I) in terms of m_L rather than m_J, and therefore we have the identities

$$\begin{aligned} |L+\tfrac{1}{2}, m_L+\tfrac{1}{2}\rangle &= \left(\frac{L+m_L+1}{2L+1}\right)^{1/2} |m_L, \uparrow\rangle + \left(\frac{L-m_L}{2L+1}\right)^{1/2} |m_L+1, \downarrow\rangle , \\ |L-\tfrac{1}{2}, m_L+\tfrac{1}{2}\rangle &= -\left(\frac{L-m_L}{2L+1}\right)^{1/2} |m_L, \uparrow\rangle + \left(\frac{L+m_L+1}{2L+1}\right)^{1/2} |m_L+1, \downarrow\rangle , \end{aligned} \tag{3}$$

which express the states with coupled spin in terms of states with independent spin. The incident spin state prior to the collision may now be written

$$|\chi_i\rangle = |m_L, \uparrow\rangle = \left(\frac{L+m_L+1}{2L+1}\right)^{1/2} |L+\tfrac{1}{2}, m_L+\tfrac{1}{2}\rangle - \left(\frac{L-m_L}{2L+1}\right)^{1/2} |L-\tfrac{1}{2}, m_L+\tfrac{1}{2}\rangle , \tag{4}$$

where the last step follows from Eq. (3). Expressed in this form, it is easy to find the scattered state since the two coupled spin states are explicitly displayed.

$$\begin{aligned} |\chi_f\rangle = F(\theta)|\chi_i\rangle &= \left(\frac{L+m_L+1}{2L+1}\right)^{1/2} f_+(\theta)|L+\tfrac{1}{2}, m_L+\tfrac{1}{2}\rangle - \left(\frac{L-m_L}{2L+1}\right)^{1/2} f_-(\theta)|L-\tfrac{1}{2}, m_L+\tfrac{1}{2}\rangle \\ &= \left[\left(\frac{L+m_L+1}{2L+1}\right) f_+(\theta) + \left(\frac{L-m_L}{2L+1}\right) f_-(\theta)\right] |m_L, \uparrow\rangle \\ &\quad + \left(\frac{(L+m_L+1)^{1/2}(L-m_L)^{1/2}}{2L+1}\right) \times [f_+(\theta) - f_-(\theta)]\, |m_L+1, \downarrow\rangle . \end{aligned} \tag{5}$$

In the last step we have used Eq. (3) to express the result in the independent-spin representation. The amplitudes for scattering with and without spin exchange are obvious. If the initial electron spin is down, rather than up, we can find the amplitudes for scattering with and without exchange by a similar procedure with the result

$$\begin{aligned} |\chi_f\rangle &= F(\theta)|m_L, \downarrow\rangle \\ &= \left[\left(\frac{L-m_L+1}{2L+1}\right) f_+(\theta) + \left(\frac{L+m_L}{2L+1}\right) f_-(\theta)\right] |m_L, \downarrow\rangle \end{aligned}$$

TABLE I. Notation and convention.

Name	Spin	z projection
Electron	S $(=\frac{1}{2})$	$\uparrow$ or $\downarrow$
Target	L	m_L
Nuclear	I	m_I
Electron plus target	J	m_J
Electron plus nuclear	F	m_F
Convention in kets:		
Independent representation		
for collision		$\|m_L, \uparrow\rangle$
for atom		$\|\uparrow, m_I\rangle$
Coupled representation		
for collision		$\|J, m_J\rangle$
for atom		$\|F, m_F\rangle$
Clebsch-Gordan Coefficients:		

$$\begin{aligned} |L+\tfrac{1}{2}, m_J\rangle &= \left(\frac{L+m_J+1/2}{2L+1}\right)^{1/2} |m_J-\tfrac{1}{2}, \uparrow\rangle + \left(\frac{L-m_J+1/2}{2L+1}\right)^{1/2} |m_J+\tfrac{1}{2}, \downarrow\rangle \\ |L-\tfrac{1}{2}, m_J\rangle &= -\left(\frac{L-m_J+1/2}{2L+1}\right)^{1/2} |m_J-\tfrac{1}{2}, \uparrow\rangle + \left(\frac{L+m_J+1/2}{2L+1}\right)^{1/2} |m_J+\tfrac{1}{2}, \downarrow\rangle \end{aligned}$$

$$+\left(\frac{(L-m_L+1)^{1/2}(L+m_L)^{1/2}}{2L+1}\right)\times[f_+(\theta)-f_-(\theta)]\;|m_L-1,\uparrow\rangle\;. \quad (6)$$

It is convenient to represent the effects of the collision on the electron spin by defining a 2×2 matrix that operates on the incident electron state ($|m_L,\uparrow\rangle$ or $|m_L,\downarrow\rangle$) and produces the scattered state. This matrix depends on the scattering angle and the initial z projection of the target spin. The first column is obtained from Eq. (5), while the second may be obtained by finding the corresponding amplitudes for initial electron spin down:

$$\overleftrightarrow{c}(m_L,\theta)=\begin{pmatrix} \frac{L+1}{2L+1}f_+ + \frac{L}{2L+1}f_- + \frac{m_L}{2L+1}(f_+-f_-) & \left(\frac{L^2+L-(m_L^2-m_L)}{2L+1}\right)^{1/2}(f_+-f_-) \\ \left(\frac{L^2+L-(m_L^2+m_L)}{2L+1}\right)^{1/2}(f_+-f_-) & \frac{L+1}{2L+1}f_+ + \frac{L}{2L+1}f_- - \frac{m_L}{2L+1}(f_+-f_-) \end{pmatrix}\;. \quad (7)$$

The off-diagonal elements of $\overleftrightarrow{c}(m_L,\theta)$ are responsible for spin exchange, and since they are so similar it is convenient to define the exchange amplitude as

$$F_x(\theta)=\frac{f_+(\theta)-f_-(\theta)}{2L+1}\;. \quad (8)$$

This differs by a factor of 2 from Glassgold's definition,[3] which was chosen for special convenience with $L=\frac{1}{2}$. We also define

$$F_d(\theta)=\frac{(L+1)f_+(\theta)+Lf_-(\theta)}{2L+1}\;, \quad (9)$$

so that the collision matrix becomes

$$\overleftrightarrow{c}(m_L,\theta)=\begin{pmatrix} F_d+m_LF_x & [(L+\frac{1}{2})^2-(m_L-\frac{1}{2})^2]^{1/2}F_x \\ [(L+\frac{1}{2})^2-(m_L+\frac{1}{2})^2]^{1/2}F_x & F_d-m_LF_x \end{pmatrix}\;. \quad (10)$$

III. CROSS SECTIONS WITH NO NUCLEAR SPIN

The cross sections for scattering with and without spin exchange may be obtained simply by squaring the magnitudes of the appropriate amplitudes:

$$\begin{aligned}\sigma(\uparrow m_L\to\uparrow m_L)&=|F_d|^2+m_L(F_d^*F_x+F_x^*F_d)+m_L^2|F_x|^2\;,\\ \sigma(\uparrow m_L\to\downarrow m_L+1)&=[(L+\tfrac{1}{2})^2-(m_L+\tfrac{1}{2})^2]\,|F_x|^2\;,\\ \sigma(\downarrow m_L\to\uparrow m_L-1)&=[(L+\tfrac{1}{2})^2-(m_L-\tfrac{1}{2})^2]\,|F_x|^2\;,\\ \sigma(\downarrow m_L\to\downarrow m_L)&=|F_d|^2-m_L(F_d^*F_x+F_x^*F_d)+m_L^2|F_x|^2\;.\end{aligned} \quad (11)$$

Note that the amplitudes for unphysical processes are zero, so that

$$\sigma(\uparrow,L\to\downarrow,L+1)=\sigma(\downarrow,-L\to\uparrow,-L-1)=0\;.$$

High-Field Limit

Effects of the nuclear spin of the primary atom have been neglected so far, and thus the results [Eq. (11)] apply only for atoms with $I=0$. However, cross sections for atoms with $I\neq 0$ will approach these cross sections [Eq. (11)] when the external magnetic field in the collision region is large enough that the nuclear and electron spins of the primary atom are decoupled [but still small enough that the assumptions underlying Eq. (1) are not violated]. Thus we call the cross sections in Eq. (11) the "high-field limit."

In general the target will not be in a pure state of specified m_L, and we will have to average the cross sections in Eq. (11) over the distribution of target m_L. The cross sections that result are sensitive to only two features of the distribution of target m_L: the polarization and the alignment (for spin-$\frac{1}{2}$ targets the alignment is always zero).

When we sum the cross sections in Eq. (11) we will get weighted averages of m_L and m_L^2, but no higher moments. If p_m is the probability that the z component of the target atom's angular momentum is m_L, then we define the excess probability ρ_m as

$$\rho_m=p_m-1/(2L+1)\;. \quad (12)$$

This quantity is zero for atoms which are in spin equilibrium at some high temperature. If we define polarization and alignment as

$$P=\sum_{m=-L}^{L}m\rho_m \text{ for polarization}\;,\qquad Q=\sum_{m=-L}^{L}m^2\rho_m \text{ for alignment}\;, \quad (13)$$

respectively, then it may be shown that

$$\sum_{m=-L}^{L} m p_m = P , \qquad \sum_{m=-L}^{L} m^2 p_m = Q + \tfrac{1}{3} L(L+1) . \tag{14}$$

Using these equations we can find all of the spin-dependent cross sections for collisions (which occur at high magnetic field) between ^2S atoms and targets of arbitrary electron spin, polarization, and alignment:

$$\begin{aligned}
\sigma(\uparrow \to \uparrow) &= \sum_{m=-L}^{L} p_m \sigma(\uparrow m \to \uparrow m) \\
&= |F_d|^2 + P(F_d^* F_x + F_x^* F_d) \\
&\qquad + [\tfrac{1}{3}L(L+1) + Q]\, |F_x|^2 , \\
\sigma(\uparrow \to \downarrow) &= \{(L+\tfrac{1}{2})^2 - [\tfrac{1}{3}L(L+1) + Q] - P\}\, |F_x|^2 \\
&= [\tfrac{2}{3}L(L+1) - Q - P]\, |F_x|^2 , \qquad (15) \\
\sigma(\downarrow \to \uparrow) &= [\tfrac{2}{3}L(L+1) - Q + P]\, |F_x|^2 , \\
\sigma(\downarrow \to \downarrow) &= |F_d|^2 - P(F_d F_x^* + F_x F_d^*) \\
&\qquad + [\tfrac{1}{3}L(L+1) + Q]\, |F_x|^2 .
\end{aligned}$$

IV. MAGNETIC FIELD STATES

We have shown how the spin-dependent cross sections are determined if the primary atoms do not possess any nuclear spin, or if the external magnetic field in the scattering region is large enough to decouple the nuclear spins.

In general the magnetic field is not large, and the nuclear spin is not zero (especially for ^2S atoms); consequently the electron spin couples to the combined external and nuclear magnetic field. Under these circumstances it is not possible to measure changes in m_S; rather, changes in the states of the atom in an intermediate magnetic field are observed.

The intermediate field states for an isolated ^2S atom are $|f, m_F\rangle$ with $f = f^{\pm} = I \pm \frac{1}{2}$. The capital subscript (on m_F) stresses that the z component of the total angular momentum m_F is a good quantum number at all magnetic fields. f has no physical significance except at zero field (the low-field limit), where $f \to F$, the total spin of the atom, and then we have the ordinary hyperfine states $|F, m_F\rangle$ [see Eq. (A8)]. Since there are only two intermediate field states with a given m_F, the transformation between the $|f, m_F\rangle$ states and the $|m_S, m_I\rangle$ representation may be represented by a unitary 2×2 matrix $\overleftrightarrow{\mathrm{m}}(m_F)$, operating on the appropriate spinor:

$$\begin{pmatrix} |f^+, m_F\rangle \\ |f^-, m_F\rangle \end{pmatrix} = \overleftrightarrow{\mathrm{m}}(m_F) \begin{pmatrix} |\downarrow, m_F + \frac{1}{2}\rangle \\ |\uparrow, m_F - \frac{1}{2}\rangle \end{pmatrix} , \tag{16}$$

where

$$\overleftrightarrow{\mathrm{m}}(m_F) = \begin{pmatrix} \beta_+(m_F) & \alpha_+(m_F) \\ \beta_-(m_F) & \alpha_-(m_F) \end{pmatrix} . \tag{17}$$

$\alpha_\pm(m_F)$ and $\beta_\pm(m_F)$ are functions of magnetic field and are calculated in the Appendix (see Fig. 1). They obey the relationships

$$\begin{aligned}
\beta_-(M) &= \alpha_+(M) , \\
\beta_+(M) &= -\alpha_-(M)
\end{aligned} \tag{18}$$

and

$$\begin{aligned}
\alpha_\pm^2(M) + \beta_\pm^2(M) &= 1 , \\
\alpha_+(M)\alpha_-(M) + \beta_+(M)\beta_-(M) &= 0 .
\end{aligned} \tag{19}$$

It is clear from these relationships that $\overleftrightarrow{\mathrm{m}}$ is a unitary matrix, so that

$$\begin{pmatrix} |\downarrow, m_F + \frac{1}{2}\rangle \\ |\uparrow, m_F - \frac{1}{2}\rangle \end{pmatrix} = \overleftrightarrow{\mathrm{m}}^\dagger(m_F) \begin{pmatrix} |f^+, m_F\rangle \\ |f^-, m_F\rangle \end{pmatrix} . \tag{20}$$

In Sec. V we will need to transform states that are combinations of several $|f, m_F\rangle$ states, so we need to define a larger matrix

$$\overleftrightarrow{\mathrm{M}} = \begin{pmatrix} \overleftrightarrow{\mathrm{m}}(I+\frac{1}{2}) & 0 & \cdot & \cdot & \cdot \\ 0 & \overleftrightarrow{\mathrm{m}}(I-\frac{1}{2}) & & & \cdot \\ \cdot & & \cdot & & \cdot \\ \cdot & & & \cdot & \cdot \\ 0 & & \cdot & \cdot & \overleftrightarrow{\mathrm{m}}(-I-\frac{1}{2}) \end{pmatrix} , \tag{21}$$

whose only nonzero elements are the 2×2 matrices $\overleftrightarrow{\mathrm{m}}(m_F)$ on the diagonal.

The definition of $\overleftrightarrow{\mathrm{m}}$ and $\overleftrightarrow{\mathrm{M}}$ contain implicitly a specific ordering of both $|f, m_F\rangle$ and $|m_S, m_I\rangle$ states, which is displayed in Table II. In order to preserve the orderly arrangement of states necessary to facilitate formal calculations, we have in-

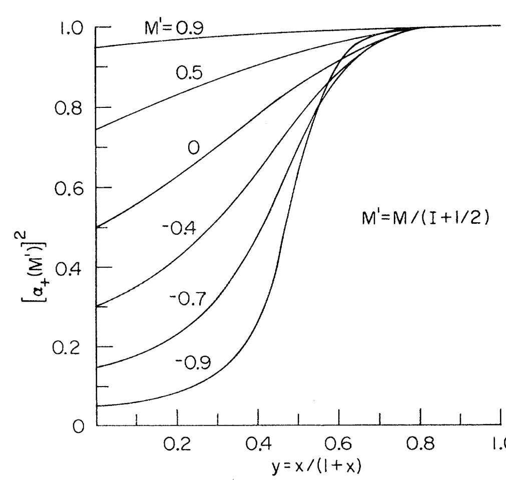

FIG. 1. $\alpha_+^2(M')$ vs magnetic field showing the fraction of states with electron spin up in upper intermediate field state for several values of alignment parameter $M' = M/(I+\frac{1}{2})$.

troduced two unphysical states in both sets of states. The coefficients [$\alpha_\pm$ or $\beta_\pm$, Eq. (A6) and (A7)] that mix these unphysical states with the real states when changing representation are always zero [as may be seen from the Appendix, Eq. (A7)], i.e., for $|m_F| = I + \frac{1}{2}$,

$$\overleftrightarrow{m}(I+\tfrac{1}{2}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \overleftrightarrow{m}(-I-\tfrac{1}{2}) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \qquad (22)$$

Consequently, the extra states never affect the answer.

V. CROSS SECTION $\sigma(f, m_F \to f', m_F')$

In this section we find the differential cross sections for all of the spin-dependent processes that occur when an atom in an intermediate-field state collides with a target of spin L, polarization P, and alignment Q. The approach is straightforward, if tedious, and follows the following prescription: The initial intermediate-field state is expressed as a linear combination of $|m_S, m_I\rangle$ states by means of the $\overleftrightarrow{M}^\dagger$ matrix discussed in Sec. IV. Under the assumption that m_I is unaffected by the collision, the effect of the collision is simply to multiply the electron spinor associated with *each* m_I by $\overleftrightarrow{c}(m_L, \theta)$ [see Eq. (10)]. Since the individual $|f, m_F\rangle$ states evolve independently after the collision, we use the $\overleftrightarrow{M}$ matrix to express the final $|m_S, m_I\rangle$ states in terms of $|f, m_F\rangle$ states. This procedure yields the amplitudes for all relevant spin-dependent collision processes, and the associated cross sections may be found by squaring the amplitudes and averaging over target spin.

The assumption that the nuclear spin state is unaffected by the collision is justified when the total collision time is much shorter than the hyperfine period. This situation obtains for thermal collisions at temperatures down to a few degrees kelvin. Formally the assumption means that the collision matrix $\overleftrightarrow{C}$ for the whole atom is a direct product of $\overleftrightarrow{c}$ and the identity matrix for the nuclear spin; $\overleftrightarrow{c}(m_L, \theta) \otimes I_{2I+1}$. Since we have added two unphysical states to preserve the systematic arrangement of the states, we have

$$\overleftrightarrow{C}(m_L, \theta) = \begin{pmatrix} U & 0 & \cdot & \cdot & 0 \\ 0 & \overleftrightarrow{c}(m_L, \theta) & & & \cdot \\ \cdot & & \cdot & & \cdot \\ \cdot & & & \overleftrightarrow{c}(m_L, \theta) & \cdot \\ 0 & \cdot & \cdot & \cdot & U \end{pmatrix}, \qquad (23)$$

where there are $2I+1$ 2×2 matrices down the diagonal, and the two U's designate single unphysical states.

The arrangement of states in this collision matrix is consistent with our ordering of the $|m_I, m_S\rangle$ states (Table II), so we can easily write the final $|f, m_F\rangle$ state in terms of the incident one,

$$(f) = \overleftrightarrow{M}\,\overleftrightarrow{C}\,\overleftrightarrow{M}^\dagger (i) . \qquad (24)$$

If the initial state is $|f^+, m_F\rangle$, then it is straightforward to show that [using relations among the α's and β's, Eq. (23)]

$$(f) = \overleftrightarrow{M}\overleftrightarrow{C}\,\overleftrightarrow{M}^\dagger \begin{pmatrix} 0 \\ 0 \\ \cdots \\ \cdots \\ \cdots \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \cdots \\ \cdots \\ \cdots \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \cdots \\ \cdots \\ \cdots \\ [(L+\frac{1}{2})^2 - (m_L - \frac{1}{2})^2]^{1/2}\, \alpha_+(m_F+1)\beta_+(m_F) F_x \\ [(L+\frac{1}{2})^2 - (m_L - \frac{1}{2})^2]^{1/2}\, \alpha_-(m_F+1)\beta_+(m_F) F_x \\ F_d + m_L(2\alpha_+^2(m_F) - 1) F_x \\ 2m_L[\alpha_-(m_F)\,\alpha_+(m_F)]\, F_x \\ [(L+\frac{1}{2})^2 - (m_L + \frac{1}{2})^2]^{1/2}\, \beta_+(m_F-1)\,\alpha_+(m_F)\, F_x \\ [(L+\frac{1}{2})^2 - (m_L + \frac{1}{2})^2]^{1/2}\, \beta_-(m_F-1)\,\alpha_+(m_F)\, F_x \\ \cdots \\ \cdots \\ \cdots \\ 0 \\ 0 \end{pmatrix} \qquad (25)$$

TABLE II. Arrangement of states in matrix notation.

$m_S\, m_I$	Transforms $\|m_S m_I\rangle$ to $\|f m_F\rangle$	f	m_F
U ↓ $I+1$	$\overleftrightarrow{\mathrm{m}}(I+\frac{1}{2})$	$I+\frac{1}{2}$	$I+\frac{1}{2}$
↑ I		$I-\frac{1}{2}$	$I+\frac{1}{2}$ U
↓ I	$\overleftrightarrow{\mathrm{m}}(I-\frac{1}{2})$	$I+\frac{1}{2}$	$I-\frac{1}{2}$
↑ $I-1$		$I-\frac{1}{2}$	$I-\frac{1}{2}$
⋮		⋮	
		$I-\frac{1}{2}$	$-I+\frac{1}{2}$
↓ $-I$	$\overleftrightarrow{\mathrm{m}}(-I-\frac{1}{2})$	$I+\frac{1}{2}$	$-I-\frac{1}{2}$
U ↑ $-I-1$		$I-\frac{1}{2}$	$-I-\frac{1}{2}$ U

Unphysical states labeled U

Although we have not chosen m_F close to $\pm(I+\frac{1}{2})$, this result is valid even for $|m_F|=I+\frac{1}{2}$, since the α's and β's involved in all unphysical processes will always be zero [see Eq. (A7)]. The amplitudes for the case with initial state $|f^-, m_F\rangle$ may be obtained by the same technique.

There are several significant features about this result. The first is that F_d appears in only one amplitude—the amplitude for scattering with no change of f, m_F. This is reasonable, since no change of the $|f, m_F\rangle$ state should result if the electron spin is unchanged by the collision. The amplitude for no change of $|f, m_F\rangle$ also contains a term in $m_L F_x$, reflecting the fact that F_x, which causes *all* of the change in electron spin, also causes *some* scattering with no spin change [cf. Eq. (7)]. All other amplitudes, even the one for change in f with no change in m_F, contain only F_x.

We square these amplitudes to obtain the cross sections for the processes $\sigma(f m_F m_L \to f' m'_F m'_L)$. These are for targets in a state with definite m_L, just like the cross sections in Eq. (11):

$$\sigma(f^\pm, m_F \to f^\pm, m_F) = |F_d|^2 + m_L[F_d^* F_x + F_d F_x^*][2\alpha_\pm^2(m_F) - 1] + m_L^2 |F_x|^2 [2\alpha_\pm^2(m_F) - 1]^2 ,$$

$$\sigma(f^\pm, m_F \to f^\mp, m_F) = 4|F_x|^2 m_L^2 [\alpha_+(m_F)\alpha_-(m_F)]^2 ,$$

$$\sigma(f^\pm, m_F \to f^\pm, m_F+1) = |F_x|^2[(L+\tfrac{1}{2})^2 - (m_L - \tfrac{1}{2})^2]\, \alpha_\pm^2(m_F+1)\beta_\pm^2(m_F) ,$$

$$\sigma(f^\pm m_F \to f^\mp, m_F+1) = |F_x|^2[(L+\tfrac{1}{2})^2 - (m_L - \tfrac{1}{2})^2]\, \alpha_\mp^2(m_F+1)\beta_\pm^2(m_F) ,$$

$$\sigma(f^\pm m_F \to f^\pm, m_F-1) = |F_x|^2[(L+\tfrac{1}{2})^2 - (m_L + \tfrac{1}{2})^2]\, \beta_\pm^2(m_F-1)\,\alpha_\pm^2(m_F) ,$$

$$\sigma(f^\pm m_F \to f^\mp, m_F-1) = |F_x|^2[(L+\tfrac{1}{2})^2 - (m_L + \tfrac{1}{2})^2]\, \beta_\mp^2(m_F-1)\alpha_\pm^2(m_F) . \tag{26}$$

It is clear from this equation that the effect of nuclear spin is simply to multiply the various terms in the cross sections found for no nuclear spin [Eq. (11)] by different combinations of $\alpha_\pm$ and $\beta_\pm$. Only one such function is required for each cross section [except for the $\sigma(fm_F \to fm_F)$, which requires a different one for each distinct combination of F_d and F_x], and none of the functions depend on the target spin. Since the effects of nuclear spin are independent of m_L, the averaging and summing over possible m_L values in the target is exactly the same as in Sec. III. The cross sections obtained for targets of spin L, polarization P, and alignment Q are given in Table III.

We stress that the parameters L, P, and Q completely determine the results of the collision (assuming that no off-diagonal density-matrix elements exist in the target) even if more information is known about the target (for instance, its precise distribution p_m for $-L \le m \le L$).

In the high-field limit we regain Eq. (15) if we use the adiabatic correspondence [Eq. (A9)]. In the low-field limit $\alpha_\pm$ and $\beta_\pm$ become Clebsch-Gordan coefficients, so that these equations contain only integral powers of m_F.

VI. CROSS SECTIONS OF CURRENT INTEREST

The preparation or detection of an atom in a particular $|f, m_F\rangle$ state is quite difficult, and the cross sections which we have calculated thus far have slight application. Studies of scattering, optical pumping, or hyperfine radiation depend on various sums and averages of the $\sigma(f, m_F \to f' m'_F)$ cross sections, rather than on the individual cross sections. For this reason we have performed the sums and averages appropriate to several situations of current interest. These include scattering with high-field state selectors (e.g., Stern-Gerlach type magnets), scattering with no state selection, collisions which change the hyperfine level f, and collisions which change m_F (and consequently the polarization). Some of these cross sections depend on the magnetic field, and we have calculated and plotted several new field-dependent functions that permit the easy calculation of these special cross sections for arbitrary field and for several selected values of $I(\frac{1}{2}, 1, \frac{3}{2}, \frac{5}{2}$, and $\frac{7}{2})$.

Magnetic State Selectors

There are several scattering experiments[1,2,10] that measure the differential spin-exchange cross sections using an alkali primary beam and a target

TABLE III. Individual cross sections.

Initial state	Final state	$\sigma(I \to F)$
$\lvert f^{\pm} m_F\rangle$	$\lvert f^{\pm} m_F\rangle$	$\lvert F_d\rvert^2 + P(F_x F_d^* + F_d F_x^*)[2\alpha_\pm^2(m_F) - 1]$
		$+ \lvert F_x\rvert^2[\frac{1}{3}L(L+1) + Q][2\alpha_\pm^2(m_F) - 1]^2$
$\lvert f^{\pm} m_F\rangle$	$\lvert f^{\mp} m_F\rangle$	$\lvert F_x\rvert^2[\frac{1}{3}L(L+1) + Q]4\alpha_+^2(m_F)\alpha_-^2(m_F)$
$\lvert f^{\pm} m_F\rangle$	$\lvert f^{\pm}, m_F+1\rangle$	$\lvert F_x\rvert^2[\frac{2}{3}L(L+1) + P - Q]\alpha_\pm^2(m_F+1)\beta_\pm^2(m_F)$
$\lvert f^{\pm} m_F\rangle$	$\lvert f^{\pm} m_F-1\rangle$	$\lvert F_x\rvert^2[\frac{2}{3}L(L+1) - P - Q]\beta_\pm^2(m_F-1)\alpha_\pm^2(m_F)$
$\lvert f^{\pm} m_F\rangle$	$\lvert f^{\mp} m_F+1\rangle$	$\lvert F_x\rvert^2[\frac{2}{3}L(L+1) + P - Q]\alpha_\mp^2(m_F+1)\beta_\pm^2(m_F)$
$\lvert f^{\pm} m_F\rangle$	$\lvert f^{\mp} m_F-1$	$\lvert F_x\rvert^2[\frac{2}{3}L(L+1) - P - Q]\beta_\mp^2(m_F-1)\alpha_\pm^2(m_F)$

atom with spin. These experiments use high magnetic field [$x \to \infty$, Eq. (A4)] polarizers and analyzers that create and select the states according to m_S in the high-field limit [see Eq. (A9)]. Great care is taken in these experiments to assume that the transitions between the selectors and analyzers and the scattering region are adiabatic (and corrections are made to the data when they are not). Since the selectors are insensitive to m_I, an equal statistical mixture of the $\lvert f, m_F\rangle$ states that correspond to the selected m_S [via Eq. (A9)] appear in the scattering region. The analyzers are equally sensitive to the $\lvert f, m_F\rangle$ states corresponding to the analyzed m_S, and insensitive to those that correspond to the opposite m_S state. Thus the measured cross section is found by averaging the cross sections in Table III over the initial $\lvert f, m_F\rangle$ values connected to the initial m_S value and summing over the final $\lvert f, m_F\rangle$ values connected to the final m_S value. We label these cross sections by the initial m_S value and the final m_S value, [$\sigma(i, f)$, i is initial, f is final), noting that there are $2I+1$ initial (and final) states in each category. There are four cross sections that can be measured:

$$\bar{\sigma}(+\tfrac{1}{2}, +\tfrac{1}{2}) = \frac{1}{2I+1} \sum_{m_F=-I+1/2}^{I+1/2} \sum_{m_F'=-I+1/2}^{I+1/2} \sigma(f^+ m_F, f^+ m_F') , \tag{27}$$

$$\bar{\sigma}(-\tfrac{1}{2}, -\tfrac{1}{2}) = \frac{1}{2I+1} \sum_{m_F=-I+1/2}^{I-1/2} \sum_{m_F'=-I+1/2}^{I-1/2} \sigma(f^- m_F, f^- m_F') + \frac{1}{2I+1} \sum_{m_F'=-I+1/2}^{I-1/2} \sigma(f^+ - I - \tfrac{1}{2}, f^- m_F')$$
$$+ \frac{1}{2I+1} \sum_{m_F=-I+1/2}^{I-1/2} \sigma(f^- m_F, f^+ - I - \tfrac{1}{2}) + \frac{1}{2I+1}\sigma(f^+ - I - \tfrac{1}{2}, f^+ - I - \tfrac{1}{2}) , \tag{28}$$

$$\bar{\sigma}(+\tfrac{1}{2}, -\tfrac{1}{2}) = \frac{1}{2I+1} \left(\sum_{m_F=-I+1/2}^{I+1/2} \sum_{m_F'=-I+1/2}^{I-1/2} \sigma(f^+ m_F, f^- m_F') + \sum_{m_F=-I+1/2}^{I+1/2} \sigma(f^+ m_F, f^+ - I - \tfrac{1}{2}) \right), \tag{29}$$

$$\bar{\sigma}(-\tfrac{1}{2}, +\tfrac{1}{2}) = \frac{1}{2I+1} \left(\sum_{m_F=-I+1/2}^{I-1/2} \sum_{m_F'=-I+1/2}^{I+1/2} \sigma(f^- m_F, f^+ m_F') + \sum_{m_F'=-I+1/2}^{I+1/2} \sigma(f^+ - I - \tfrac{1}{2}, f^+ m_F') \right) . \tag{30}$$

At arbitrary magnetic field these cross sections contain sums of $\alpha_\pm^2$ and $\beta_\pm^2$ that can not be evaluated analytically because of the square roots in Eq. (A4). Fortunately, the relationships among the α's and β's is such that there are only three distinctly different sums of the α's and β's in Eqs. (27)–(30). These have been calculated by computer for many values of magnetic field with $I = \frac{1}{2}$, 1, $\frac{3}{2}$, $\frac{5}{2}$, and $\frac{7}{2}$. Table IV shows which coefficient applies to each important function of the scattering amplitudes and target variables. Thus, for example,

$$\bar{\sigma}(-\tfrac{1}{2}, -\tfrac{1}{2}) = \lvert F_d\rvert^2 - (F_x F_d^* + F_d F_x^*) P A_P(x)$$
$$+ \lvert F_x\rvert^2 [\tfrac{1}{3}L(L+1) A(x) + Q A_Q(x)] , \tag{31}$$

where A, A_P, and A_Q may be determined graphically from Figs. 2–4.

In high magnetic field all the field-dependent functions approach unity. Hence, the cross sections approach the cross sections in Eq. (15) for the "high-field limit." A decrease in magnetic field affects the terms A, A_P, and A_Q quite differently. A, for example, never changes by more than 50% (see Fig. 2), so that the cross sections $\bar{\sigma}(+\frac{1}{2}, -\frac{1}{2})$ and $\bar{\sigma}(-\frac{1}{2}, +\frac{1}{2})$ for unpolarized, unaligned targets do not depend strongly on magnetic fields. We can write for $P = Q = 0$

$$\bar{\sigma}(\pm\tfrac{1}{2}, \mp\tfrac{1}{2}, x, I) = R(x, I)\,\sigma(+\tfrac{1}{2}, -\tfrac{1}{2}, x \to \infty) , \tag{32}$$

with

$$R = \tfrac{1}{2}[3 - A(x)] , \tag{33}$$

and $R(x, I)$ will always be between 0.75 (for $I = \frac{1}{2}$, $x = 0$) and 1.0. When $x = 0$, this R function is the same as $m(I)$ in Ref. 1.

The polarization-dependent terms in the cross section contain A_P (see Fig. 3), which decreases markedly as x decreases, approaching $1/(2I+1)$ as $x \to 0$. The field dependence of the functions

TABLE IV. Field-dependent coefficients of various terms in average cross sections.

Cross section	$\|F_d\|^2$	$\|F_x\|^2 \frac{1}{3} L(L+1)$	$P(F_x F_d^* + F_x^* F_d)$	$P\|F_x\|^2$	$Q\|F_x\|^2$
$\bar{\sigma}(+\frac{1}{2}, +\frac{1}{2})$	1.0	$A(x)$	$A_P(x)$	0	$A_Q(x)$
$\bar{\sigma}(-\frac{1}{2}, -\frac{1}{2})$	1.0	$A(x)$	$-A_P(x)$	0	$A_Q(x)$
$\bar{\sigma}(+\frac{1}{2}, -\frac{1}{2})$	0	$3-A(x)$	0	$-A_P(x)$	$-A_Q(x)$
$\bar{\sigma}(-\frac{1}{2}, +\frac{1}{2})$	0	$3-A(x)$	0	$A_P(x)$	$-A_Q(x)$
$\bar{\sigma}(\Delta f=+1)$	0	$B(x)$	0	$B_P(x)$	$-B_Q(x)$
$\bar{\sigma}(\Delta f=-1)$	0	$\frac{2I}{2I+2} B(x)$	0	$\frac{-2I}{2I+2} B_P(x)$	$\frac{-2I}{2I+2} B_Q(x)$

$A_P(I)$ closely resembles that of the function $\alpha_+(I)$ (see Fig. 1) because both are related to the expectation value for m_S.

The alignment-dependent term has the most complicated dependence on magnetic field. For $I=0$, $A_Q=1$ for all x, as discussed earlier. For $I=\frac{1}{2}$, $A_Q \to 0$ as $x \to 0$, and for $I>\frac{1}{2}$, A_Q is negative at small values of magnetic field.

In the limit of zero magnetic field, $\alpha_\pm^2$ and $\beta_\pm^2$ become simple functions of m_F and I that may be summed algebraically. This has been done before for A, and A_P, but not for A_Q.[4] The cross sections at zero field are presented in Table V in a similar manner to Table IV, except that $A(I, x)$ has been replaced by its limiting value as $x \to 0$, which is an analytic function of I. Note that these expressions reproduce the high-field limit for $I=0$ [cf. Eq. (15)].

The computer program was checked against both the low- and high-field limits.

Δf Collisions

Spin-exchange collisions can excite a ground-state atom to the upper hyperfine level, from which it may radiate spontaneously. This process is important in astronomy,[11] and we calculate its dependence on magnetic field.

We find the cross sections for collisions that change f by averaging the individual f, m_F cross sections (Table III) over all initial m_F states and summing over all final m_F states. We have (neglecting identity effects)

$$\bar{\sigma}(\Delta f=+1)=\frac{1}{2I}\sum_{m_F=-I+1/2}^{I-1/2}\;\sum_{m_F'=-I-1/2}^{I+1/2}\sigma(f^-m_F, f^+m_F'), \tag{34}$$

$$\bar{\sigma}(\Delta f=-1)=\frac{1}{2I+2}\sum_{m_F=-I-1/2}^{I+1/2}\;\sum_{m_F'=-I+1/2}^{I-1/2}\sigma(f^+m_F, f^-m_F'), \tag{35}$$

where $\Delta f=+1$ means that the initial state is $|f^-, m_F\rangle$ and the final state $|f^+m_F\rangle$, and $\Delta f=-1$ transitions mean that the initial state is $|f^+, m_F\rangle$ and the

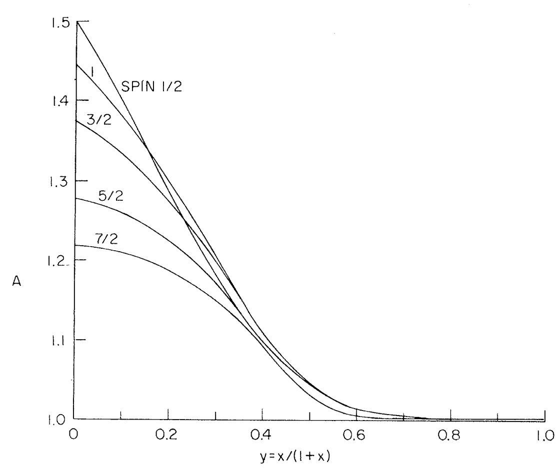

FIG. 2. The function $A(x)$, which determines the amount of spin exchange seen as no exchange for various values of I using high-field selectors.

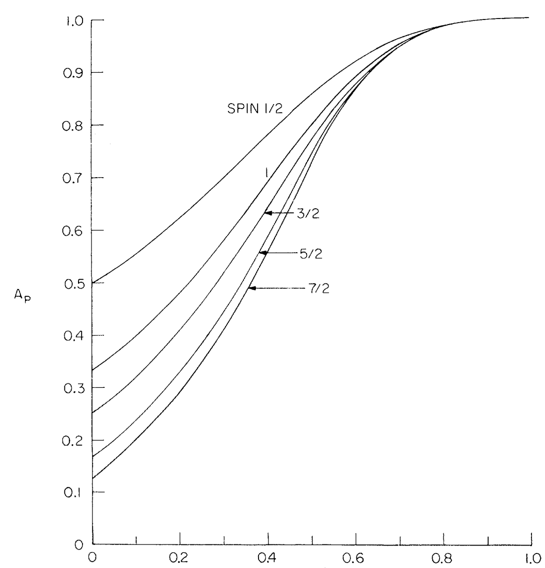

FIG. 3. The function $A_P(x)$, which equals the fraction of polarization-dependent terms observed with high-field selectors for different I.

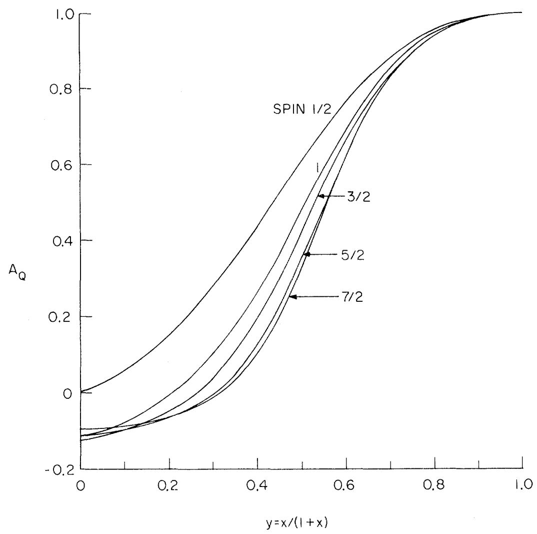

FIG. 4. The function $A_Q(x)$, which is the coefficient of alignment for various values of I (using high-field selectors).

final state is $|f^- m_F'\rangle$.

The magnetic field dependence of the Δf cross sections may be parametrized like the cross sections for high-field selectors. Tables IV and V include parameters for the Δf cross sections in intermediate fields and zero field, respectively. $B(I, x)$ is shown in Fig. 5 (B_p and B_Q may be found in Ref. 8). Note that the magnetic field dependence of $B(I, x)$ is quadratic at low fields.

Δm_F Collisions

One technique for measuring the total spin-exchange cross section is to pump a sample of gas into the $|f^+, m_F = f^+\rangle$ state with circularly polarized resonance radiation and then measure the rate of depolarization due to collisions with a second species (the target).[12] Under suitable conditions the measurement is sensitive only to changes in m_F, and one measures $\sigma(f^+, f^+, \Delta m = -1)$, where

$$\sigma(f^\pm, m, \Delta m = -1) = \int [\sigma(f^\pm, m \to f^\pm, m-1) + \sigma(f^\pm, m \to f^\mp, m-1)]\, d\Omega$$

TABLE V. High- and low-magnetic-field limits of coefficients in the average cross section.

Cross section	$\|F_d\|^2$	$\|F_x\|^2 \frac{1}{3} L(L+1)$	$Q\|F_x\|^2$	$P(F_x F_d^* + F_d F_x^*)$	$P\|F_x\|^2$
$\bar\sigma\ (+\frac{1}{2}, +\frac{1}{2})$					
$x=0$	1.0	$1+\frac{4I}{(2I+1)^2}$	$-\frac{(2I-1)}{(2I+1)^2}$	$\frac{1}{(2I+1)}$	0
$x=\infty$	1.0	1.0	1.0	1.0	0
$\bar\sigma\ (-\frac{1}{2}, -\frac{1}{2})$					
$x=0$	1.0	$1+\frac{4I}{(2I+1)^2}$	$-\frac{(2I-1)}{(2I+1)^2}$	$-\frac{1}{2I+1}$	0
$x=\infty$	1.0	1.0	1.0	-1.0	0
$\bar\sigma\ (+\frac{1}{2}, -\frac{1}{2})$					
$x=0$	0	$2-\frac{4I}{(2I+1)^2}$	$\frac{(2I-1)}{(2I+1)^2}$	0	$-\frac{1}{2I+1}$
$x=\infty$	0	2	-1.0	0	-1.0
$\bar\sigma\ (-\frac{1}{2}, +\frac{1}{2})$					
$x=0$	0	$2-\frac{4I}{(2I+1)^2}$	$\frac{2I-1}{(2I+1)^2}$	0	$\frac{1}{2I+1}$
$x=\infty$	0	2	-1.0	0	1.0
$\bar\sigma\ (\Delta f=+1)$					
$x=0$	0	$\frac{2(2I+2)}{2I+1}$	0	0	0
$x=\infty$	0	2	-1.0	0	1.0
$\bar\sigma\ (\Delta f=-1)$					
$x=0$	0	$2\frac{2I}{(2I+1)}$	0	0	0
$x=\infty$	0	$2\frac{2I}{(2I+2)}$	$\frac{-2I}{2I+2}$	0	$\frac{-2I}{2I+2}$

$$= \int d\Omega \left| F_x(\theta) \right|^2 \left[\tfrac{2}{3} L(L+1) - P - Q \right] \alpha_\pm^2(m) \; . \qquad (36)$$

If P and Q are both zero, then $\sigma(f^+, f^+, \Delta m = -1)$ reduces to $\frac{1}{2}$ the usual expression for the total spin-exchange cross section for spin-$\frac{1}{2}$ targets. This is because σ_{ex} is usually defined as the cross section for scattering with spin exchange when the incident spins are known to be oppositely aligned, in which case $[\frac{2}{3}L(L+1) - P - Q] = \frac{2}{3}L(L+1) + L - L^2 + \frac{1}{3}L(L+1) = 2L$, rather than $\frac{2}{3}L(L+1)$ (for $P = Q = 0$). For $L = \frac{1}{2}$, $2L = 1$ and $\frac{2}{3}L(L+1) = \frac{1}{2}$, so the ratio is 2 : 1. This factor of $\frac{1}{2}$ has caused some difficulty in comparing values of the total spin-exchange cross section.[13] Note that for $L > 2$, less exchange occurs for an oppositely polarized, completely aligned target than for one with $P = Q = 0$. This may be understood by noting that a large target spin behaves like a magnetic field (with interaction $\vec{S} \cdot \vec{L}$ instead of $\vec{S} \cdot \vec{H}$), which is less effective in changing m_S if it is along the axis of quantization rather than perpendicular to it.

Sum Cross Section

Several experiments[14] have been performed on atom-atom systems where incident and target beams both had spin $\frac{1}{2}$, but where no attempt was made to measure the spin dependence of the cross section. These experiments measure the cross sections in Table III averaged over all initial f, m_F values and summed over all final ones. This cross section may be found most easily by combining terms in Table IV, where most of the summing has been done:

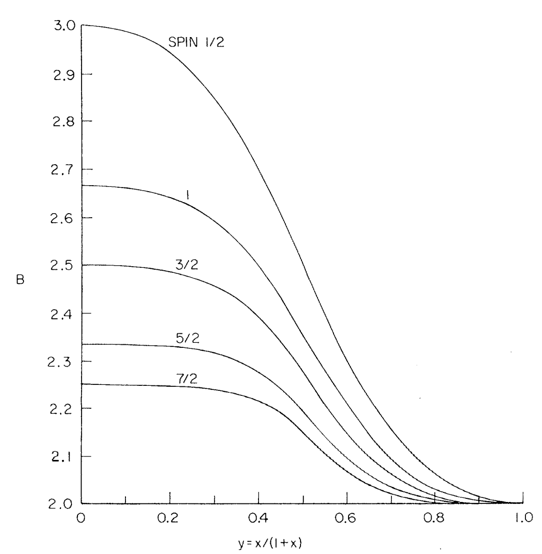

FIG. 5. The function $B(x)$, which determines the effectiveness of spin exchange as a mechanism to raise F from $I - \frac{1}{2}$ to $I + \frac{1}{2}$.

$$\sigma_{\text{sum}} = \tfrac{1}{2} [\bar{\sigma}(+\tfrac{1}{2}, +\tfrac{1}{2}) + \bar{\sigma}(-\tfrac{1}{2}, -\tfrac{1}{2}) + \bar{\sigma}(-\tfrac{1}{2}, +\tfrac{1}{2}) + \bar{\sigma}(+\tfrac{1}{2}, -\tfrac{1}{2})] = |F_d|^2 + L(L+1) |F_x|^2 \; . \qquad (37)$$

Using the definition of F_d and F_x [Eqs. (8) and (9)], we find

$$\sigma_{\text{sum}} = \frac{L+1}{2L+1} |f_+|^2 + \frac{L}{2L+1} |f_-|^2 \; , \qquad (38)$$

which shows that the sum cross section contains no interference terms between the scattering with $J = L + \frac{1}{2}$ and $J = L - \frac{1}{2}$. The cross section is simply a statistical average of the cross sections for scattering from the two potentials in Eq. (1). This is a generalization of Glassgold's result to the case with arbitrary target spin, and it is true for all magnetic fields, as one would expect.

If the incident beam is selected by high-field analyzers the sum cross section may be obtained simply by summing over final spins if the polarization of the target is zero, as may be seen from Table IV. In an experiment which measures $\bar{\sigma}(+\frac{1}{2}, +\frac{1}{2})$ and $\bar{\sigma}(+\frac{1}{2}, -\frac{1}{2})$, it may be easier to analyze σ_{sum}, rather than $\bar{\sigma}(+\frac{1}{2}, +\frac{1}{2})$ [in addition to $\bar{\sigma}(+\frac{1}{2}, -\frac{1}{2})$], because it contains sums of single-channel cross sections which have been analyzed extensively.[15]

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APPENDIX

In this appendix we discuss the problem of a ^2S atom with nuclear spin I in a magnetic field, giving the eigenvectors for intermediate magnetic field. To begin, the Hamiltonian is written in standard form,

$$\mathcal{H} = [\Delta W / (I + \tfrac{1}{2})] \vec{I} \cdot \vec{J} + \mu_B g_I I_3 H + \mu_B g_J J_3 H \; . \qquad (A1)$$

ΔW is the separation of the hyperfine components in the absence of an external magnetic field, μ_B is the Bohr magneton, and g_I and g_J are the Landé g factors for the nuclear and electronic configurations, respectively. The $z(3)$ axis is along the external magnetic field H. Torrey[16] has evaluated the diagonal states $|f, M\rangle$ of (A1) in terms of the hyperfine states $|F, M\rangle$. He obtains

$$|f^\pm, M\rangle = A_M^\pm |F^+, M\rangle + B_M^\pm |F^-, M\rangle \; , \qquad (A2)$$

where $F^+ = I + \frac{1}{2}$ and $F^- = I - \frac{1}{2}$ The coefficients A and B are

TABLE VI. Nuclear spin and characteristic field for some common ^2S atoms.

Atoms (abundance)	I	B_0 [magnetic field in gauss for which $x=1$ in Eq. (A4)]
H	$\frac{1}{2}$	507
D	1	117
Li^6 (7%)	1	82
Li^7 (93%)	$\frac{3}{2}$	288
Na^{23}	$\frac{3}{2}$	634
K^{39}	$\frac{3}{2}$	164
Rb^{85} (72%)	$\frac{5}{2}$	1080
Rb^{87} (28%)	$\frac{3}{2}$	2420
Cs^{133}	$\frac{7}{2}$	3260

$$A_M^{\pm}=\frac{1}{\sqrt{2}}\left[1\pm\left(1+\frac{2Mx}{2I+1}\right)R_M^{-1}\right]^{1/2},$$

$$B_M^{\pm}=\mp\frac{1}{\sqrt{2}}\left[1\mp\left(1+\frac{2Mx}{2I+1}\right)R_M^{-1}\right]^{1/2},\quad M\neq\pm(I+\tfrac{1}{2})$$

$$A^{+}_{(I+1/2)}=A^{-}_{-(I+1/2)=1},\qquad \text{(A3)}$$

$$B^{+}_{(I+1/2)}=B^{-}_{-(I+1/2)}=0,$$

where

$$R_M=\left(1+\frac{4Mx}{2I+1}+x^2\right)^{1/2},\quad x=\frac{(g_J-g_I)\mu_B H}{\Delta W}.\qquad \text{(A4)}$$

Using Clebsch-Gordan coefficients (Table I) to express (A2) in the $|m_S, m_I\rangle$ basis we obtain

$$|f^{\pm}, M\rangle=\alpha_{\pm}(M)|\tfrac{1}{2}, M-\tfrac{1}{2}\rangle+\beta_{\pm}(M)|-\tfrac{1}{2}, M+\tfrac{1}{2}\rangle,\qquad \text{(A5)}$$

with

$$\alpha_{\pm}^2(M)=\tfrac{1}{2}\{1\pm[x+2M/(2I+1)]R_M^{-1}\},$$

$$\beta_{-}(M)=\alpha_{+}(M),\qquad \beta_{+}(M)=-\alpha_{-}(M),\quad M\neq\pm(I+\tfrac{1}{2}).\qquad \text{(A6)}$$

If we use the − sign in the square root in R_M when $M=-(I+\frac{1}{2})$, then we find that

$$\alpha_{+}(I+\tfrac{1}{2})=\beta_{+}(-I-\tfrac{1}{2})=1,$$

$$\alpha_{+}(-I-\tfrac{1}{2})=\beta_{+}(+I+\tfrac{1}{2})=0.\qquad \text{(A7)}$$

The α's and β's depend on x and I as well as on M, but we make explicit only the M dependence because it alone is critical to the manipulations in Secs. IV and V.

The coefficients in Eq. (A6) do not depend fundamentally on I, but only on the fractional projection $M'=M/(I+\frac{1}{2})$. The function $\alpha_{+}^2(x)$ is shown in Fig. 1 for several values of M'. In the low-field limit, defined by $x\to 0$ [Eq. (A4)], the coefficients in Eq. (A6) become Clebsch-Gordan coefficients, so that

$$|f^{\pm}, M_F\rangle \underset{x\to 0}{\to} |F^{\pm}, M_F\rangle.\qquad \text{(A8)}$$

In the high-field limit, defined by $x\to\infty$, we find that

$$|f^{+}, m_F\rangle\to|m_S=+\tfrac{1}{2}\rangle,\quad m_F=I+\tfrac{1}{2},\ \ldots,\ -I+\tfrac{1}{2},$$

$$|f^{+}, -I-\tfrac{1}{2}\rangle\to|m_S=-\tfrac{1}{2}\rangle,\qquad \text{(A9)}$$

$$|f^{-}, m_F\rangle\to|m_S=-\tfrac{1}{2}\rangle,\ m_F=I-\tfrac{1}{2},\ \ldots,\ -I+\tfrac{1}{2}.$$

(It is understood that the states $|m_S\rangle$ are really $|m_S, m_I\rangle$, where $m_I=m_F-m_S$.)

Negative Hyperfine Interaction

The discussion so far has assumed that the hyperfine separation is positive [$\Delta W>0$ in Eq. (A1)]. If ΔW is negative, x, the magnetic field parameter, will also be negative (if the magnetic field points along the positive z direction). In order to apply the results of this paper, it is necessary to choose the z axis oppositely, so that x will still be positive. This procedure reverses the signs of all quantities that depend on the direction of the z axis. This includes m_F, m_S [Eq. (15)], the $\pm\frac{1}{2}$ in the cross sections for high-field selectors [Eqs. (34)–(37)], the target spin m_L, and the target polarization P.

In Table VI we list the magnetic fields at which $x=1$ for some common ^2S atoms, along with their nuclear spin. When a mixture of isotopes with different I and B_0 is present, the functions $\alpha_{\pm}^2$ in Eq. (A6), as well as the field-dependent functions in Table V, must be replaced by the appropriate weighted averages.

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Calculation of Energies and Widths of Resonances in Inelastic Scattering: Stabilization Method*

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In previous work, the stabilization method of calculating resonance parameters was applied to potential scattering and to elastic scattering from a target. The method is here extended to compound-state resonances in inelastic scattering and its application to a model problem for a target with three bound states is examined. The eigenfunctions associated with eigenvalues ϵ_j obtained from the diagonalization of the exact Hamiltonian in appropriately chosen sets of square-integrable basis functions are good approximations, in the inner region, to particular linear combinations of the degenerate exact scattering solutions at $E=\epsilon_j$ (above inelastic threshold). The partial widths are calculated from a Fermi's-"Golden-Rule"-like formula involving the matrix elements of the exact Hamiltonian between the square-integrable eigenfunctions representing the resonance state and potential-scattering solutions at the same energy. The slowly varying (as a function of E) potential-scattering S matrix, knowledge of which is required in the calculation of the decay widths, is determined using the criterion that several good approximations to the resonance state yield exactly the same widths. For the exactly soluble model problem studied here, the resonance parameters obtained with the stabilization method compare well with the exact values, especially for narrow resonances. The theoretical limitations of the method are discussed.

I. INTRODUCTION

For collision processes which involve the formation and decay of a quasidiscrete resonance state, the energy dependence of the cross section can be expressed in terms of a few physically meaningful parameters, such as the resonance energy E_r, the width Γ (or the decay lifetime $\hbar/\Gamma$), and the slowly varying potential-scattering S matrix. In recent years, several methods[1,2] have been proposed for the direct calculation of these parameters from approximations to the exact resonance wave function, without recourse to solution of the complete energy-dependent cross section. One example is the stabilization method[3-5] which, until now, has been applied only to resonances occurring in elastic scattering. Since many processes of interest involve excitation of the target, we investigate here the extension of the method to inelastic scattering.

In Paper I,[3] the stabilization method was applied to scattering from a one-dimensional model potential whose barrier gave rise to so-called single-particle resonances. Later in II,[4] we extended the method to elastic scattering from a target and studied its application to a model problem in which compound resonances occurred. In III,[5] we proposed a new method for the calculation of all the resonance parameters including the potential-scattering or background phase shift. This method utilizes approximate resonance wave functions obtained from the stabilization procedure, together with a Fermi's-"Golden-Rule"-like formula originally proposed by Miller.[6] In this paper, we shall extend the stabilization method to inelastic scattering and study its application to a model problem in which compound resonances decay into two open channels. Also, we shall generalize the method proposed in III for the calculation of the resonance parameters, so that, in principle, the stabilization method may be applied to problems with an arbitrary number of open channels.

In order to establish the framework for the discussion that follows, we summarize briefly the stabilization method as applied to elastic scattering.[4,5] For scattering from a target, the complete (no-exchange) wave function may be written in the form

$$\Psi_E=\sum_{t=1}^{\infty}\phi_t(\vec{r}_0)\,F_t(\vec{r}) , \tag{1.1}$$