

## Polarization and Correlation of Electron Spin in Low-Energy Elastic Electron-Hydrogen Collisions\*

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The polarization and correlation of electron spin in low-energy electron-hydrogen scattering are investigated. The physical basis of such phenomena is discussed and quantities in terms of which they may be measured are defined. Expressions relating these quantities before and after collision are given in terms of the singlet and triplet amplitudes for electron-hydrogen scattering. These expressions are plotted as functions of scattering angle for incident electron energies below threshold for excitation of the second quantum level in hydrogen, using the results of an approximate close-coupling solution of the associated scattering problem.

SINCE the earliest days of quantum mechanics the scattering of electrons by atomic hydrogen has been the subject of intensive investigation, and recent years have witnessed an upsurge of activity in this field.<sup>1</sup> Almost all the research on electron-hydrogen collisions has been aimed at a determination of total cross section as a function of incident electron energy. In this paper we wish to describe a quite different aspect of the problem: the polarization phenomena which can accompany the scattering of electrons by hydrogen.<sup>2</sup>

Polarization is not often treated within the context of atomic scattering problems; modern research on this topic has been done almost exclusively in nuclear physics.<sup>3</sup> This is so, no doubt, because of the explicit spin dependence in nuclear interactions—a dependence certainly not present in the simple, static Coulomb forces appropriate to the low energy electrons we deal with here. That polarization is possible at all under these circumstances is due to the requirements of the Pauli principle which demand that the wave function of the electron-hydrogen system be antisymmetric in the coordinates of the bound and free electrons. Remembering that the spin function of the two electrons is symmetric in the triplet state and antisymmetric in the singlet, we see at once that the *spatial* part of the total wave function must be antisymmetric in the triplet state and symmetric in the singlet. For this

reason the electrons will, on the average, move in different regions of the potentials in the different spin states, and there results an *effective* (though not explicit) spin dependence in the forces. Thus the mechanism for polarization in electron-hydrogen collisions can ultimately be traced back, through the Pauli principle, to the indistinguishability of the bound and free electrons.

To carry through the details of our analysis we assume the proton to be infinitely massive and therefore stationary during the collision; hence, we deal with a two-electron system. We shall distinguish the two electrons by labeling them 1 and 2. In the representation in which the spin of each electron and its  $z$  component are good quantum numbers, any operator in the composite spin space of the two electrons can be written in the form  $\omega^{(1)} \times \nu^{(2)}$  where  $\omega^{(1)}$  and  $\nu^{(2)}$  are operators in the separate spin spaces of the two electrons, and  $\times$  denotes the matrix outer product. We define two sets of operators of this form; they are

$$\begin{aligned}\alpha_i &= \sigma_i^{(1)} \times 1, & (i=x,y,z), \\ \beta_i &= 1 \times \sigma_i^{(2)}, & (i=x,y,z),\end{aligned}$$

where  $\sigma_i^{(1)}$  and  $\sigma_i^{(2)}$  are components of the Pauli spin matrices for the two electrons and 1 is the two-by-two unit matrix.<sup>4</sup> With these matters established we are now ready to define the quantities which are the subject of this discussion.

The polarization,  $\mathbf{P}^{(1)}$ , of electron 1 (which may be either electron) is defined as the expectation value of the spin of electron 1, there being no measurement made of the spin of electron 2. In symbols

$$P_i^{(1)} = \langle \alpha_i \rangle, \quad (i=x,y,z).$$

A completely analogous definition holds for the polariza-

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<sup>1</sup> P. G. Burke and H. M. Schey, preceding paper [Phys. Rev. **126**, 147 (1962)]. References are given here to earlier work.

<sup>2</sup> The words "polarization" and "correlation" are sometimes used in discussing electron-hydrogen collisions, as well as in other branches of physics, with meanings different from those intended here. Explicit definitions will be given later; for the present, to avoid confusion, we remark that in this paper they refer to expectation values of certain electron spin operators.

<sup>3</sup> See, for example, C. R. Schumacher and H. A. Bethe, Phys. Rev. **121**, 1534 (1961). The present work is, to some extent, an atomic version of the analysis made in this reference. Because of the simplicity of the electron-hydrogen Hamiltonian, containing, as it does, no spin-orbit interaction, the analysis can be carried further here than in the nuclear case.

<sup>4</sup> The coordinates  $x, y, z$ , referred to here and elsewhere in dealing with spin, constitute an arbitrary orthogonal triad. Because of the absence of spin-orbit forces, there is no preferred direction in space as far as spin-dependent quantities are concerned.

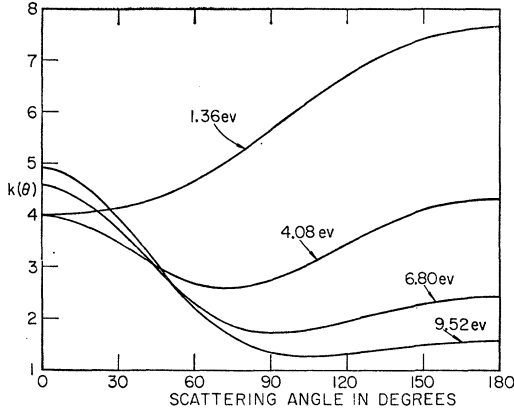


FIG. 1.  $k(\theta)$  in units of  $a_0^2$  as a function of scattering angle for four incident electron energies.

zation,  $\mathbf{P}^{(2)}$ , of the second electron; we have

$$P_i^{(2)} = \langle \beta_i \rangle, \quad (i = x, y, z).$$

Finally, we define a tensor  $Q$  with elements

$$Q_{ij} = \langle \alpha_i \beta_j \rangle, \quad (i, j = x, y, z),$$

which refers to a measurement of the spins of both electrons.  $Q$  is called the correlation tensor.

To proceed, it is convenient to introduce the density matrix for the two-electron system prior to collision. If the spin state of the system is described by  $\mathbf{P}^{(1)}$ ,  $\mathbf{P}^{(2)}$ , and  $Q$  then the density matrix is

$$\rho = \frac{1}{4} [1 + \sum_i P_i^{(1)} \alpha_i + \sum_i P_i^{(2)} \beta_i + \sum_{ij} Q_{ij} \alpha_i \beta_j],$$

where 1 is now the four-by-four unit matrix. This expression is established in Appendix I, where certain useful relations among the components of the polarization vectors and the elements of the correlation tensor are also derived. The density matrix after scattering is given by

$$\rho' = M(\theta) \rho M(\theta)^\dagger,$$

where  $M(\theta)$ , a function of the scattering angle  $\theta$ , is the scattering matrix for the two-electron system. In Appendix II we show that

$$M(\theta) = \frac{1}{4} [3F(\theta) + G(\theta)] + \frac{1}{4} [F(\theta) - G(\theta)] \sum_i \alpha_i \beta_i,$$

where  $F(\theta)$  and  $G(\theta)$  are, respectively, the triplet and singlet scattering amplitudes, determined as described below. The polarizations and the correlation tensor after scattering are given by

$$\begin{aligned} P_i^{(1)}(\theta)' &= \text{Tr}(\rho' \alpha_i) / \text{Tr} \rho', \\ P_i^{(2)}(\theta)' &= \text{Tr}(\rho' \beta_i) / \text{Tr} \rho', \quad (i, j = x, y, z) \\ Q_{ij}(\theta)' &= \text{Tr}(\rho' \alpha_i \beta_j) / \text{Tr} \rho', \end{aligned}$$

while the differential scattering cross section is

$$\sigma(\theta) = \text{Tr} \rho'.$$

The algebra involved in carrying through the operations

implied in these equations is straightforward but tedious, and we omit all details. The results are

$$\begin{aligned} \sigma(\theta) P_k^{(1)}(\theta)' &= n(\theta) P_k^{(1)} + p(\theta) P_k^{(2)} + q(\theta) \sum_j \epsilon_{ijk} Q_{ij}, \\ \sigma(\theta) P_k^{(2)}(\theta)' &= p(\theta) P_k^{(1)} + n(\theta) P_k^{(2)} - q(\theta) \sum_j \epsilon_{ijk} Q_{ij}, \\ \sigma(\theta) Q_{ij}(\theta)' &= m(\theta) \delta_{ij} [1 - \sum_l Q_{ll}] + n(\theta) Q_{ij} + p(\theta) Q_{ji} \\ &\quad - q(\theta) \sum_k \epsilon_{ijk} [P_k^{(1)} - P_k^{(2)}], \\ \sigma(\theta) &= k(\theta) + m(\theta) \sum_l Q_{ll}, \end{aligned}$$

where the functions  $k$ ,  $m$ ,  $n$ ,  $p$ , and  $q$  are given in terms of the triplet and singlet scattering amplitudes as follows:

$$\begin{aligned} k(\theta) &= \frac{1}{4} [3F(\theta)F^*(\theta) + G(\theta)G^*(\theta)], \\ m(\theta) &= \frac{1}{4} [F(\theta)F^*(\theta) - G(\theta)G^*(\theta)], \\ n(\theta) &= \frac{1}{4} [2F(\theta)F^*(\theta) + F(\theta)G^*(\theta) + F^*(\theta)G(\theta)], \\ p(\theta) &= \frac{1}{4} [2F(\theta)F^*(\theta) - F(\theta)G^*(\theta) - F^*(\theta)G(\theta)], \\ q(\theta) &= (i/4) [F^*(\theta)G(\theta) - F(\theta)G^*(\theta)]. \end{aligned}$$

Of these five functions only three may be chosen independently (see later). The indices  $i$ ,  $j$ ,  $k$ , and  $l$  appearing throughout range over the coordinates  $x$ ,  $y$ , and  $z$ .  $\delta_{ij}$  and  $\epsilon_{ijk}$  are the standard Kronecker delta and epsilon.

In these equations we have related the polarizations and the correlation after scattering to their counterparts before scattering; the two sets of quantities are connected by functions of the singlet and triplet scattering amplitudes  $G(\theta)$  and  $F(\theta)$ . In the case for which we give numerical results in this paper, i.e., that in which the incident electron energy is too low to excite the target atom, we have for these amplitudes the conventional expressions

$$\begin{aligned} F(\theta) &= \frac{1}{2iK} \sum_l (2l+1) [\exp(2i\delta_l^{(1)}) - 1] P_l(\cos\theta), \\ G(\theta) &= \frac{1}{2iK} \sum_l (2l+1) [\exp(2i\delta_l^{(0)}) - 1] P_l(\cos\theta). \end{aligned}$$

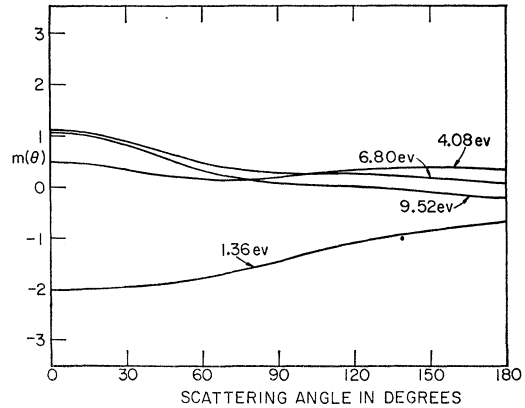


FIG. 2.  $m(\theta)$  in units of  $a_0^2$  as a function of scattering angle for four incident electron energies.

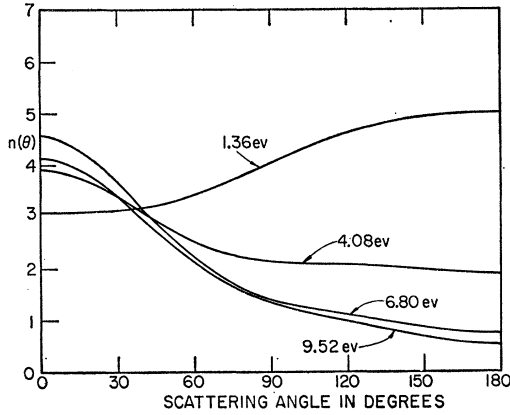


FIG. 3.  $n(\theta)$  in units of  $a_0^2$  as a function of scattering angle for four incident electron energies.

Here  $K$  is the incident wave number and  $\delta_l^{(1)}$  and  $\delta_l^{(0)}$  are the triplet and singlet phase shifts determined from the asymptotic form of the solution of the Schrödinger equation which describes the collision. The formalism established here for dealing with polarization in electron-hydrogen collisions is, however, completely general; thus in the case of an atomic transition from  $n'l_1'm'K_n'$  to  $nl_1mK_n$ , we need only replace the amplitudes  $F(\theta)$  and  $G(\theta)$  by

$$A_S(\theta, \phi) = \frac{1}{2iK_n' l_2 l_2' L} \sum i^{(l_2' - l_2)} [4\pi(2l_2' + 1)]^{\frac{1}{2}} \\ \times C_{l_1' l_2'}(Lm'; m'0) C_{l_1 l_2}(Lm; m, m' - m) \\ \times [S^{LS}_{nK_n l_1 l_2, n'K_n' l_1' l_2'} - \delta_{nK_n l_1 l_2, n'K_n' l_1' l_2'}] \\ \times Y_{l_2}^{m' - m}(\theta, \phi),$$

with  $S=0$  for the singlet case and  $S=1$  for the triplet. The functions  $Y_l^m(\theta, \phi)$  are standard spherical harmonics while the quantities  $C_{l_1 l_2}(LM; M_1 M_2)$  are Clebsch-Gordan coefficients in the notation of Blatt and Weisskopf.<sup>5</sup> The elements of the  $S$  matrix as defined by Blatt and Biedenharn<sup>6</sup> are determined from the asymptotic form of the wave function just as are the phase shifts in the simple case described above.

Since the functions  $\mathbf{P}^{(1)}(\theta)'$ ,  $\mathbf{P}^{(2)}(\theta)'$ , and  $Q(\theta)'$  depend upon initial conditions, i.e., upon  $\mathbf{P}^{(1)}$ ,  $\mathbf{P}^{(2)}$ , and  $Q$ , our results are most cogently given in terms of the five functions  $k(\theta)$ ,  $m(\theta)$ ,  $n(\theta)$ ,  $p(\theta)$ , and  $q(\theta)$  defined earlier. In Figs. 1-5 we plot each of these as a function of scattering angle  $\theta$  for several energies in the range considered. The phase shifts required for this calculation are taken from the treatment of elastic scattering given by Burke and Schey.<sup>1</sup>

Most of the quantities arising in this discussion are

<sup>5</sup> J. M. Blatt and V. F. Weisskopf, *Revs. Modern Phys.* **24**, 258 (1952).

<sup>6</sup> J. M. Blatt and L. C. Biedenharn, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952), p. 790ff.

probably beyond the reach of present experimental techniques. One exception may be the polarization of the bound electron. For this reason we define the depolarization ratio

$$d(\theta) = P_k^{(2)}(\theta)' / P_k^{(2)} = n(\theta) / \sigma(\theta),$$

a measure of the extent to which the bound electron loses its polarization as a result of the collision. The expression given above results from assuming an unpolarized beam impinges upon a polarized target, there being no correlation between the two; that is, we have the initial conditions  $\mathbf{P}^{(1)}=0$ ,  $\mathbf{P}^{(2)} \neq 0$ ,  $Q=0$ . The depolarization ratio may be rewritten directly in terms of the scattering amplitudes:

$$d(\theta) = 1 - \frac{|F(\theta) - G(\theta)|^2}{3|F(\theta)|^2 + |G(\theta)|^2}.$$

We point out that the same expression obtains for the case of a polarized beam scattering on an unpolarized target, in which case it measures the extent to which the projectile loses its polarization as a result of the collision. In Fig. 6 we plot the depolarization ratio as a function of scattering angle for several energies in the range considered.

A quantity closely related to the depolarization ratio is the so-called spin-flip cross section, defined as the cross section for scattering in which the initial and final spins of the scattered electron are oppositely oriented. The amplitude for such a process is given by

$$\langle \frac{1}{2}, -\frac{1}{2} | M(\theta) | -\frac{1}{2}, \frac{1}{2} \rangle = \langle -\frac{1}{2}, \frac{1}{2} | M(\theta) | \frac{1}{2}, -\frac{1}{2} \rangle \\ = \frac{1}{2} [F(\theta) - G(\theta)],$$

where the elements of the scattering matrix are labeled by the  $z$  components of the spins of the two electrons. The spin-flip cross section is therefore

$$\sigma_{\text{SF}}(\theta) = \frac{1}{4} |F(\theta) - G(\theta)|^2.$$

What we might term the "ordinary" cross section,

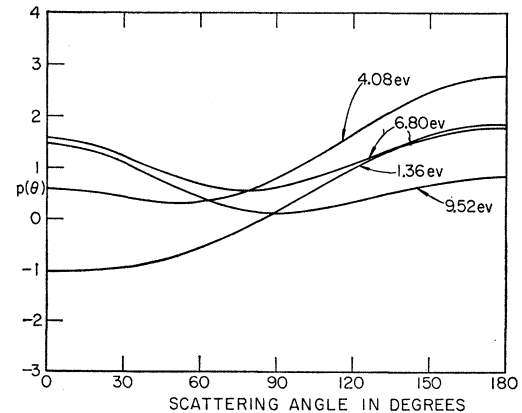


FIG. 4.  $p(\theta)$  in units of  $a_0^2$  as a function of scattering angle for four incident electron energies.

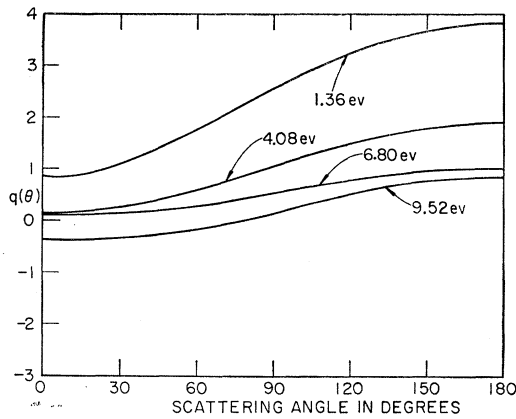


FIG. 5.  $q(\theta)$  in units of  $a_0^2$  as a function of scattering angle for four incident electron energies.

which describes a simple scattering experiment involving unpolarized, uncorrelated electrons and targets, is given by the celebrated expression

$$\sigma_0(\theta) = \frac{3}{4} |F(\theta)|^2 + \frac{1}{4} |G(\theta)|^2.$$

[This can be derived from our general expression for the differential cross section given earlier simply by putting  $Q_{II}=0$ . Thus  $\sigma_0(\theta) = k(\theta)$ .] The depolarization ratio is now easily written in terms of these two cross sections:

$$d(\theta) = 1 - \sigma_{\text{SF}}(\theta) / \sigma_0(\theta).$$

Rearranging this equation we find

$$\sigma_{\text{SF}}(\theta) = \sigma_0(\theta) [1 - d(\theta)].$$

Thus a measurement of the ordinary cross section and the depolarization ratio will provide the spin-flip cross section. The computed values of the spin-flip cross section are given as functions of the scattering angle for various energies in Fig. 7. Figure 8 is a plot of  $\sigma_{\text{SF}}(\theta) / \sigma_0(\theta) = 1 - d(\theta)$ , i.e., the ratio of the spin-flip to the ordinary cross section.

The zero-energy values of all quantities calculated here are given in Table I.

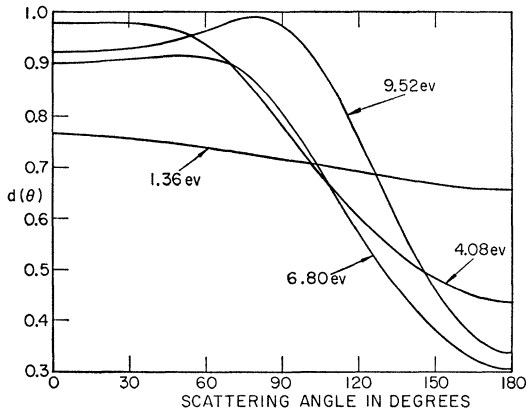


FIG. 6. The depolarization ratio  $d(\theta)$  as a function of scattering angle for four incident electron energies.

TABLE I. Zero-energy values;  $a_0$  is the Bohr radius  $\hbar^2/me^2$ .

Function	Value at zero energy	
	Burke-Schey <sup>a</sup>	Schwartz <sup>b</sup>
$k(\theta)$	$14.05a_0^2$	$11.24a_0^2$
$m(\theta)$	$-10.5a_0^2$	$-8.11a_0^2$
$n(\theta)$	$8.17a_0^2$	$6.06a_0^2$
$p(\theta)$	$-4.59a_0^2$	$-4.49a_0^2$
$q(\theta)$	$0.00a_0^2$	$0.00a_0^2$
$d(\theta)$	0.582	0.392
Spin-flip cross section	$5.87a_0^2$	$6.84a_0^2$
Ratio of spin-flip to ordinary differential cross section	0.418	0.608

<sup>a</sup> See reference 1.

<sup>b</sup> See reference 7.

In addition to the calculations presented here, we have carried out others in which the Burke-Schey singlet- $S$  phase shifts are replaced by those of Schwartz<sup>7</sup> which are probably more accurate. Away from zero energy the results differ negligibly from those obtained using the Burke-Schey data. At and near zero energy there are non-negligible differences and the Schwartz values are therefore included in Table I for purposes of comparison.

It is to be hoped that in the not too distant future means will be devised to measure other quantities involved in polarization phenomena. Apart from their intrinsic interest they would provide useful information. As an example if one could polarize both electrons completely and align them so that  $\mathbf{P}^{(1)} = \mathbf{P}^{(2)} = \hat{e}_z$ , say, then  $Q_{zz} = 1$  (see Appendix I) and  $\sigma(\theta) = |F(\theta)|^2$ . This result, combined with the ordinary cross section discussed above, would then permit a determination of the triplet and singlet cross sections separately rather than in combination as is usually the case. Other experiments would yield further information such as

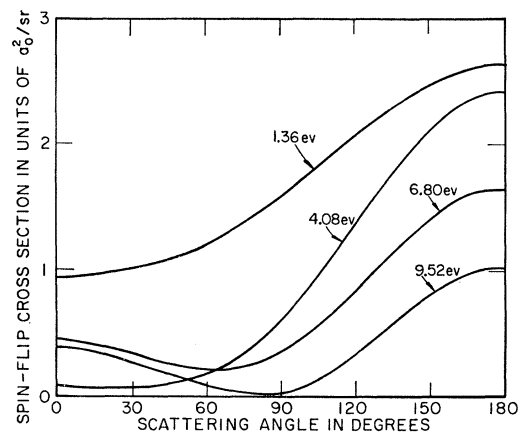


FIG. 7. The spin-flip cross section in units of  $a_0^2/\text{sr}$  as a function of scattering angle for four incident electron energies.

<sup>7</sup> C. Schwartz, in *Second International Conference on the Physics of Electronic and Atomic Collisions*, University of Colorado, Boulder, Colorado, June 1961 (W. A. Benjamin, Inc., New York, 1961), Paper II; and also C. Schwartz, *Phys. Rev.* **124**, 1468 (1961).

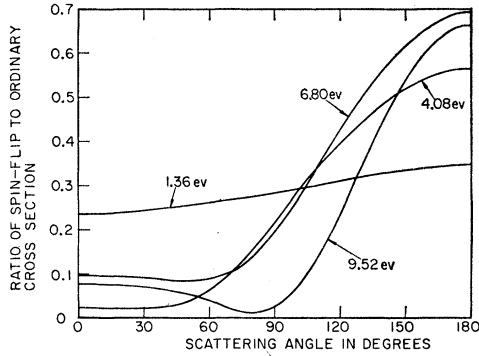


FIG. 8. The ratio of spin-flip cross section to ordinary differential cross section as a function of scattering angle for four incident electron energies.

the relative phase of the singlet and triplet amplitudes; in fact, at any scattering angle and incident electron energy, the singlet and triplet amplitudes and their relative phase completely characterize the collision, so that, in principle, three measurements at each angle and energy would yield all possible information.

The experimental difficulties encountered with hydrogen targets are expected to be considerably less formidable when alkali atoms are used instead.<sup>8</sup> It is not unlikely that the scattering of electrons by alkali atom targets can be treated reasonably well theoretically without much change in the methods being used for hydrogen,<sup>1</sup> while the polarization formalism given here goes over without any change whatever. Hence alkali atom targets may furnish common ground for theorist and experimentalist and provide a means of checking polarization calculations.

Finally, in concluding, we remark that work now in progress on electron-hydrogen collisions in energy ranges different from that considered here will make possible further polarization calculations to be reported on at a later date.

#### ACKNOWLEDGMENT

We extend our thanks to Mr. Samuel F. Mendicino for his helpful and most important collaboration in the numerical aspects of this work.

#### APPENDIX I

We shall establish here the form of the density matrix given in the main body of the paper. The 16 matrices  $\alpha_i$ ,  $\beta_j$ ,  $\alpha_i\beta_j$  ( $i, j = x, y, z$ ) and the four-by-four unit matrix 1 comprise a linearly independent set which spans the space of all four-by-four Hermitian matrices. It follows from this that the density matrix can be expanded in the form

$$\rho = \lambda 1 + \sum_i a_i \alpha_i + \sum_i b_i \beta_i + \sum_{ij} c_{ij} \alpha_i \beta_j.$$

The constant  $\lambda$  is fixed by the normalization condition

$$\text{Tr} \rho = 1 = 4\lambda.$$

<sup>8</sup> G. Brink (private communication).

Remembering that the expectation value of any operator in the spin space of the two-electron system is given by the trace of the product of that operator with the density matrix, we determine the remaining constants by means of the relations

$$P_i^{(1)} = \text{Tr} \rho \alpha_i = 4a_i,$$

$$P_i^{(2)} = \text{Tr} \rho \beta_i = 4b_i,$$

$$Q_{ij} = \text{Tr} \rho \alpha_i \beta_j = 4c_{ij}.$$

The form of  $\rho$  given in the text now follows at once.

The density matrix for the two-electron system may be used to derive certain relations connecting  $\mathbf{P}^{(1)}$ ,  $\mathbf{P}^{(2)}$ , and  $Q$ . The general theory of the density matrix<sup>9</sup> establishes, among others, two inequalities satisfied by any density matrix  $\rho$ . They are

$$\text{Tr}(\rho^2) \leq 1,$$

and

$$\rho_{kk} \geq 0.$$

The first of these is independent of the representation in which  $\rho$  is written. Not so the second: The elements of  $\rho$  (and in particular here, the diagonal elements) differ from representation to representation. In the most general case (for two electrons) we may put

$$\mathbf{P}^{(1)} = P_1 \hat{e}_z,$$

and

$$\mathbf{P}^{(2)} = P_2 (\hat{e}_x \sin \xi + \hat{e}_z \cos \xi),$$

where  $\xi$  is the angle between the two polarization vectors. The density matrix in this situation is given by

$$\rho = \frac{1}{4} [1 + P_1 \alpha_z + P_2 (\beta_x \sin \xi + \beta_z \cos \xi)] + \frac{1}{4} \sum_{ij} Q_{ij} \alpha_i \beta_j,$$

and the unitary transformation

$$U = \cos(\xi/2) + i\beta_y \sin(\xi/2),$$

will be found to diagonalize the part of  $\rho$  in square brackets. Thus

$$\rho' = U \rho U^\dagger = \frac{1}{4} [1 + P_1 \alpha_z + P_2 \beta_z] + \frac{1}{4} \sum_{ij} Q_{ij} U \alpha_i \beta_j U^\dagger.$$

Further, it proves possible to write

$$\sum_{ij} Q_{ij} U \alpha_i \beta_j U^\dagger = \sum_{ij} Q'_{ij} \alpha_i \beta_j,$$

with

$$Q'_{ij} = \sum_{kl} Q_{kl} \text{Tr}(\alpha_i \beta_j U \alpha_k \beta_l U^\dagger),$$

and the new density matrix therefore becomes

$$\rho' = \frac{1}{4} [1 + P_1 \alpha_z + P_2 \beta_z + \sum_{ij} Q'_{ij} \alpha_i \beta_j].$$

The condition that the diagonal elements of the density matrix be positive definite leads now to the

<sup>9</sup> U. Fano, *Revs. Modern Phys.* **29**, 74 (1957).

four relations

$$\begin{aligned} 1+P_1+P_2+Q_{zz}' &\geq 0, \\ 1+P_1-P_2-Q_{zz}' &\geq 0, \\ 1-P_1+P_2-Q_{zz}' &\geq 0, \\ 1-P_1-P_2+Q_{zz}' &\geq 0, \end{aligned}$$

where

$$Q_{zz}' = Q_{zz} \cos \xi + Q_{zx} \sin \xi.$$

If both electrons are completely polarized,  $P_1 = P_2 = 1$ , these inequalities give  $Q_{zz}' = 1$ . The condition  $\text{Tr}(\rho^2) \leq 1$  written out for a two-electron system has the general form

$$1 + \mathbf{P}^{(1)} \cdot \mathbf{P}^{(1)} + \mathbf{P}^{(2)} \cdot \mathbf{P}^{(2)} + \sum_{ij} Q_{ij}^2 \leq 4,$$

but in the special case of complete polarization it becomes

$$\sum_{ij} (Q_{ij}')^2 \leq 1.$$

Taking out the term  $Q_{zz}' = 1$ , we get

$$\sum_{i \neq z} \sum_{j \neq z} (Q_{ij}')^2 \leq 1 - (Q_{zz}')^2 = 0,$$

whence  $Q_{ij}' = 0$ ,  $i, j \neq z$ . Thus the pair of equations

$$\begin{aligned} Q_{zz}' &= Q_{zz} \cos \xi + Q_{zx} \sin \xi = 1, \\ Q_{zx}' &= Q_{zx} \cos \xi - Q_{zz} \sin \xi = 0, \end{aligned}$$

may be solved to give

$$\begin{aligned} Q_{zx} &= \sin \xi, \\ Q_{zz} &= \cos \xi. \end{aligned}$$

These are the only elements of the correlation tensor in the unprimed representation which can be different from zero. Thus in the special case in which both electrons are completely polarized we have

$$Q_{ij} = P_i^{(1)} P_j^{(2)}.$$

It is not to be expected, however, that any such simple relation exists under other circumstances, and, in fact, generally  $\mathbf{P}^{(1)}$ ,  $\mathbf{P}^{(2)}$ , and  $Q$  satisfy only the weaker conditions expressed by the four inequalities given above in terms of  $P_1$ ,  $P_2$ , and  $Q_{zz}'$ .

## APPENDIX II

The derivation of the scattering matrix given in the main body of the paper is an exercise in quantum-mechanical transformation theory. Consider a representation in which the total spin  $S$  of the two electrons and its  $z$  component  $M$  are good quantum numbers. In such a representation the scattering matrix takes on an especially simple and well-known form,<sup>10</sup> namely

$$\bar{M}(\theta) = \begin{bmatrix} F(\theta) & 0 & 0 & 0 \\ 0 & F(\theta) & 0 & 0 \\ 0 & 0 & F(\theta) & 0 \\ 0 & 0 & 0 & G(\theta) \end{bmatrix}.$$

To transform this into the representation used in the paper, we use the familiar equations which relate the wave functions in the two representations:

$$\begin{aligned} \chi_{11} &= \alpha(1)\alpha(2), \\ \chi_{10} &= [\alpha(1)\beta(2) + \beta(1)\alpha(2)]/\sqrt{2}, \\ \chi_{1,-1} &= \beta(1)\beta(2), \\ \chi_{00} &= [\alpha(1)\beta(2) - \beta(1)\alpha(2)]/\sqrt{2}. \end{aligned}$$

Here the  $\chi_{SM}$  are the wave functions in the  $SM$  representation and  $\alpha(i)$  and  $\beta(i)$ , which are combined to give the wave functions in the single-particle representation, are the conventional Pauli spinors for particles of spin  $\frac{1}{2}$ . From these equations we read off the unitary transformation  $U$  which connects the two representations:

$$U = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \end{bmatrix}.$$

Thus using standard quantum-mechanical transformation theory we find

$$M(\theta) = U^\dagger \bar{M}(\theta) U = \begin{bmatrix} F(\theta) & 0 & 0 & 0 \\ 0 & \frac{1}{2}(F+G) & \frac{1}{2}(F-G) & 0 \\ 0 & \frac{1}{2}(F-G) & \frac{1}{2}(F+G) & 0 \\ 0 & 0 & 0 & F(\theta) \end{bmatrix}.$$

From this explicit form and the definitions of the matrices  $\alpha_i$  and  $\beta_i$ , the expression for  $M(\theta)$  given in the main body of the paper can easily be determined.

<sup>10</sup> See, for example, I. C. Percival and M. J. Seaton, Proc. Cambridge Phil. Soc. **53**, 654 (1957).