Entanglement and Bell Correlation in Electron-Exchange Collisions

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Elastic collisions between initially unpolarized electrons and hydrogenlike atoms are discussed, aiming to analyze the entanglement properties of the correlated final spin system. Explicit spin-dependent interactions are neglected and electron exchange only is taken into account. We show the final spin system to be completely characterized by a single spin correlation parameter depending on scattering angle and energy. Its numerical value identifies the final spins of the collision partners to be either in the separable, entangled, or Bell correlated regions. We emphasize explicit examples for the mixed spin system in order to illustrate the abstract concepts. The analysis of published experimental and numerical data reveals the possibility to create tunable pairs of collision partners with any desired degree of spin entanglement.

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Quantum entanglement is one of the most intriguing phenomena in nature. It plays a crucial role in quantum information and quantum computation and its determination in combined quantum systems is a basic task. Most investigations so far utilized pairs of polarized photons, giving key insights into fundamental quantum mechanics [1,2]. More recently, entanglement properties between electronic spins in photon-induced ionization have been reported [3], while dissipative studies of the entanglement dynamics give even rise to sudden death of entanglement [4]. On the other hand, spin-dependent collisions between electrons and atoms have been studied for many years with increasing precision and efficiency, aiming to obtain information on the scattering dynamics [5,6]. We suggest supplementing these investigations by exploring entanglement properties of the collision partners after the interation and study the interrelation between scattering dynamics and the creation of nonlocal correlations.

It is useful to start with a simple collision system that allows for a most direct and transparent discussion of the basic concepts. We therefore analyze collisions between initially unpolarized electrons and unpolarized hydrogenlike atoms having electronic spin-$1/2$. It is assumed that all explicit spin-dependent forces can be neglected and only electron exchange is taken into account. We investigate under which conditions nonlocal spin correlations between the scattering partners can be generated during the collision, starting from a maximally chaotic initial spin state. It turns out that the spin-spin correlations of the final system are completely characterized by a single dynamical parameter, while its numerical value determines whether the final spin system is separable, entangled, or even Bell correlated; i.e. it violates any of the Bell inequalities [7,8]. This allows for the construction of explicit expressions of the final state density matrix for the various outcomes, which is one of the main aims of this research. Such studies unveil new fundamental aspects of collisions, e.g., the completely different nature of spin correlations for separable and entangled states. Furthermore, our analysis of published experimental and numerical data exhibits that Coulomb plus exchange forces are even capable of generating Bell correlated pairs out of an initially completely uncorrelated system. This should allow creation of tunable pairs of collision partners with any desired degree of spin entanglement.

We describe the initial unpolarized state by the density matrix $\rho_{\rm in}$ being an incoherent superposition of the equally distributed spins of the first (electrons) and second particle (atoms), respectively. The density matrix, characterizing the final state after the scattering is given by $\rho = T\rho_{\rm in}T^{+}$, where T is the transition operator. Assuming scattering angle and energy as fixed, and denoting the final state spin components of the two particles by M and m, we obtain the 4×4 spin density matrix $\langle M'm'|\rho|Mm\rangle$ in the explicit form

$$\rho = \frac{1}{8\sigma}\begin{pmatrix} 2|f^{(1)}|^2 & 0 & 0 & 0 \\ 0 & |f^{(1)}|^2+|f^{(0)}|^2 & |f^{(1)}|^2-|f^{(0)}|^2 & 0 \\ 0 & |f^{(1)}|^2-|f^{(0)}|^2 & |f^{(1)}|^2+|f^{(0)}|^2 & 0 \\ 0 & 0 & 0 & 2|f^{(1)}|^2 \end{pmatrix}, \tag{1}$$

where $f^{(S)}$ denote the triplet ($S=1$) and singlet ($S=0$) scattering amplitudes, respectively. Here, ρ is normalized by the differential cross section $\sigma = \frac{1}{4}(3|f^{(1)}|^2 + |f^{(0)}|^2)$, and $\mathrm{tr}\rho = 1$. The spin density matrix Eq. (1) can be completely characterized in terms of the two individually measured polarization vectors $\mathbf{P}^{(1)}$ and $\mathbf{P}^{(2)}$, referring to particles 1 and 2 [9], and the nine direct product components $P_i^{(1)} \times P_j^{(2)}$ of the spin-spin correlation tensor $(i,j = x,y,z)$, defined by the expression [10]

$$P_i^{(1)} \times P_j^{(2)} = \mathrm{tr}\rho(\sigma_i \times \sigma_j). \tag{2}$$

The correlation parameters refer to experiments where both scattered particles are measured in coincidence by two observers. For example, $P_z^{(1)} \times P_z^{(2)}$ gives the outcome of an experiment where both detectors are oriented along the z direction [11]. The simple structure of the density matrix Eq. (1) allows for quickly calculating the relevant parameters. The individual polarization vectors of the two subsystems cancel, and the only nonvanishing spin correlation parameters are

$$P = P_i^{(1)} \times P_i^{(2)} = \frac{|f^{(1)}|^2 - |f^{(0)}|^2}{3|f^{(1)}|^2 + |f^{(0)}|^2}, \qquad i = x, y, z, \quad (3)$$

where we introduced the parameter $P = P(\theta, E)$, which is a function of scattering angle and energy. It is related to the spin asymmetry A_{ex} [12], via $P = -A_{\mathrm{ex}}$, as follows from the general equations [13]. Applying the tensorial properties of $P_i^{(1)} \times P_i^{(2)}$ one obtains for general directions **a** and **b** of the two detectors $P_a^{(1)} \times P_b^{(2)} = P\cos\beta$, where β is the angle between **a** and **b** [10]. This and Eq. (3) exhibit the rotational symmetry of the spin-spin system. A scheme of an e-H spin correlation experiment is depicted in the Supplemental Material [14]. Expressing the density matrix Eq. (1) in terms of the spin correlation parameter Eq. (3), we obtain

$$\rho = \frac{1}{4}\begin{pmatrix} 1+P & 0 & 0 & 0 \\ 0 & 1-P & 2P & 0 \\ 0 & 2P & 1-P & 0 \\ 0 & 0 & 0 & 1+P \end{pmatrix}. \quad (4)$$

From its structure, Eq. (4) represents a so-called X matrix, with only diagonal and antidiagonal elements, which has been used in the analyses of two-qubit quantum systems [4,15].

For a general scattering experiment, e.g., including spin-orbit interaction and more general initial conditions, the density matrix can depend on up to 15 independent parameters. In contrast, for our system with unpolarized initial particles, ρ only depends on the single parameter P as shown in Eq. (4). In general, the values of the correlation parameter are restricted to the region $[-1, 1]$. From Eq. (3) we get the further restriction $-1 \le P \le \frac{1}{3}$ for our present case of interest.

We now discuss under which conditions the mixed spin state Eq. (4) is separable or entangled, or a combination of both. Generally, a density matrix of a bipartite mixed state is called separable if and only if it is possible to express it in the form

$$\rho = \sum_{i=1}^{n} p_i |a_i\rangle\langle a_i| \times |b_i\rangle\langle b_i|, \quad (5)$$

where the pure one-particle states $|a_i\rangle$ and $|b_i\rangle$ refer to the first (electron) and second (atom) particle, respectively. The parameters $p_i \ge 0$ denote the relevant probabilities. If no transformation of a given density matrix ρ to the form Eq. (5) can be given, the system is said to be nonseparable or entangled. Peres [16] and Horodecki *et al.* [17] derived a convenient criterion which, in the case of a 4×4 density matrix, yields a necessary and sufficient condition for separability. For this, we construct the partial transpose density matrix ρ^{PT}, where only the variables of one subsystem are transposed: $\langle M'm'|\rho^{\mathrm{PT}}|Mm\rangle = \langle Mm'|\rho|M'm\rangle$. A given density matrix ρ describes a separable state if *all* eigenvalues of ρ^{PT} are positive. In contrast, ρ describes an entangled system if at least one eigenvalue is negative [16,17]. Calculating the eigenvalues λ_i of ρ^{PT} yields

$$\lambda_{1,2,3} = \frac{1}{4}(1-P) \quad \text{and} \quad \lambda_4 = \frac{1}{4}(1+3P). \quad (6)$$

Equation (6) indicates that all eigenvalues are positive for P values in the range $-\frac{1}{3} \le P \le \frac{1}{3}$, and that the scattering matrix ρ is separable in this region. The density matrix ρ describes an entangled system in the range $-1 \le P < -\frac{1}{3}$, where λ_4 becomes negative. The system is maximally entangled for $P = -1$, as depicted in Fig. 1.

Illustrating our somewhat abstract results by explicit examples gives further insight. Decomposition of mixed states is not unique. However, if it is possible to transform the scattering matrix to the form of Eq. (5), then ρ is separable. In general, this task is very cumbersome. In our case of interest, though, it is simple, since the results Eq. (3) provide the essential hint. We derive the results for positive and negative values of P separately.

Inserting explicitly $P = |P|$, we rewrite the spin density matrix Eq. (4) by subtracting a term proportional to the four-dimensional unit matrix. The remaining matrix can then be expressed in terms of the three triplet states $|S = 1M_s\rangle$, with $M_s = -1$, 0, 1, respectively. We obtain

$$\rho = \frac{1-3|P|}{4}\mathbb{1} + |P|\sum_{M_s}|1M_s\rangle\langle 1M_s|. \quad (7)$$

The unit matrix $\mathbb{1}$ describes a completely uncorrelated mixture of states, e.g.,

$$\mathbb{1} = \sum_i |a_i b_i\rangle\langle a_i b_i|, \quad \text{with} \quad a_i, b_i \in \{\uparrow, \downarrow\}, \quad (8)$$

where the two particles can be found in any of the four separable states with equal probability $\frac{1}{4}$. The four states occurring in Eq. (8) and the states $|11\rangle = |\uparrow\uparrow\rangle$ and $|1-1\rangle = |\downarrow\downarrow\rangle$ in Eq. (7) are clearly separable, but the Bell state $|10\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ is maximally entangled. One might assume that ρ is at least partially entangled, but

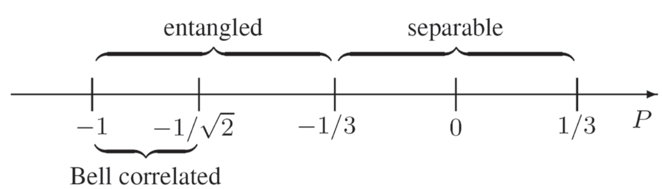

FIG. 1. Separable, entangled, and Bell correlated areas (see text).

Fig. 1 shows that ρ is separable for all allowed positive values of P. We will now construct such a representation. Guided by the results Eq. (3) for the correlation parameter, we start by considering the spin density matrix

$$\rho_1 = \frac{1}{6}\sum_i |\uparrow_i\rangle\langle\uparrow_i| \times |\uparrow_i\rangle\langle\uparrow_i| + |\downarrow_i\rangle\langle\downarrow_i| \times |\downarrow_i\rangle\langle\downarrow_i|, \quad (9)$$

where $|\uparrow_i\rangle$ and $|\downarrow_i\rangle$ denote particle states with *spin-up* $(\uparrow)$ and *spin-down* $(\downarrow)$ with respect to the i axis $(i = x, y, z)$ [18]. The state Eq. (9) is of the general form of Eq. (5) and clearly separable. It can be prepared by two spatially separated observers, commonly called Alice and Bob, in an entirely classical way, i.e., by agreeing over the phone on the local preparation of their respective states. For instance, Alice prepares a subset of electrons locally in the state $|\uparrow_x\rangle$. She communicates this to Bob via a classical channel, e.g., phone. Then, Bob will prepare the corresponding subset of his particles, hydrogenlike atoms, in the same spin state. This operation is repeated for the other five states in Eq. (9). The beams created by Alice and Bob remain spatially separated without interaction. The total final spin system is then described by the matrix ρ_1, which contains the full information on the system. Any mixed state that is prepared in this way by local operations and classical communication (LOCC) contains correlated spins, but these correlations are created entirely by classical means. By contrast, LOCC cannot be used to create entangled states [2]. Calculation of the correlation parameters for ρ_1 by means of Eq. (2) yields the results $P_i \times P_i = \frac{1}{3}$ and $P_i \times P_j = 0$, for $i \neq j$, with $(i, j = x, y, z)$. The individual polarization vectors vanish. In particular, we get $P_a \times P_a = \frac{1}{3}$, for any direction **a** of the two spin detector systems. Comparing this with Eq. (3), we see that the two spin systems have the same rotational symmetry. Only the magnitudes of the correlation parameters differ ($P_i \times P_i = \frac{1}{3}$ in the case of ρ_1 and $0 \leq P_i \times P_i = P \leq \frac{1}{3}$ for ρ). The correlations contained in ρ_1 can be reduced by mixing ρ_1 with a completely uncorrelated system, described by the 4×4 unit matrix Eq. (8), until this mixture contains the same amount of correlations as ρ. We obtain for the spin scattering matrix Eq. (7) the expression

$$\rho = \frac{1 - 3|P|}{4}\mathbb{1} + 3|P|\rho_1. \quad (10)$$

The mixing parameters follow from the condition that the spin matrix Eq. (7) and the mixture on the right-hand side of Eq. (10), both, must have the same trace and correlation parameters. Remembering Eq. (5), we obtain from Eq. (10) that the spin matrix ρ is separable if $|P| \leq \frac{1}{3}$ (see Fig. 1), which is in accordance with the Peres-Horodecki criterion. The essential point is that, on the left-hand side of Eq. (10), we have the spin matrix Eq. (7) describing the spin correlations between colliding pairs of spin-1/2 particles. On the right-hand side, we have a mixture of $\mathbb{1}$ and ρ_1, which can be prepared by LOCC. Both systems, ρ and the mixture, coincide in all measurable polarization and correlation parameters and are therefore physically indistinguishable. Of course, there are many different ways of preparing the same state ρ. But produced in a collision, the important point is that the spin correlations of separable systems can be reproduced entirely by a classical mechanism. Hence, it is quite reasonable to state that separable states contain no entanglement.

Now, we consider anticorrelated spins. Inserting $P = -|P|$ in Eq. (4) we can write the scattering matrix ρ in the form of a Werner state [19],

$$\rho = \frac{1 - |P|}{4}\mathbb{1} + |P||00\rangle\langle 00|, \quad (11)$$

where $|00\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ is the singlet state. The Werner state Eq. (11) represents a mixture of the completely uncorrelated state Eq. (8) $\sim\mathbb{1}$ (with amount $1 - |P|$) and the maximally entangled singlet state. The magnitude $|P|$ of the correlation parameter plays the role of a mixing parameter in the Werner state. From the Peres-Horodecki criterion, it follows that the state Eq. (11) is separable for $0 \geq P \geq -\frac{1}{3}$ (see Fig. 1). We illustrate this result by explicit construction, following essentially the same procedure as in the preceding case. Since the correlations are negative, we consider the density matrix ρ_2 with anticorrelated spins,

$$\rho_2 = \frac{1}{6}\sum_i |\uparrow_i\rangle\langle\uparrow_i| \times |\downarrow_i\rangle\langle\downarrow_i| + |\downarrow_i\rangle\langle\downarrow_i| \times |\uparrow_i\rangle\langle\uparrow_i| \quad (12)$$

$(i = x, y, z)$. As ρ_2 is of the form of Eq. (5), it is separable and hence can be prepared by LOCC. The only nonvanishing components of the correlation tensor are given by $P_i \times P_i = -\frac{1}{3}$ $(i = x, y, z)$. Repeating the steps from Eq. (9) to Eq. (10) we can rewrite the Werner state Eq. (11) in the explicit separable form $(0 \geq P \geq -\frac{1}{3})$

$$\rho = \frac{1 - 3|P|}{4}\mathbb{1} + 3|P|\rho_2. \quad (13)$$

Both sides of Eq. (13) are normalized and are characterized by the same set [Eq. (3)] of correlation parameters. They are therefore physically indistinguishable. The discussion following Eq. (10) applies directly to Eq. (13).

We now focus on the state Eq. (11) in the region $-\frac{1}{3} > P \geq -1$, where the spin scattering matrix is nonseparable or entangled. The amount of entanglement, produced in the system ρ during the collision, can be quantified using the concept of negativity [20,21], which is based directly on the Peres-Horodecki criterion. The negativity is defined as $N(\rho) = -2\sum_i n_i$, where the n_i are the negative eigenvalues of the partial transpose density matrix ρ^{PT}. If all eigenvalues are positive, the corresponding density matrix is separable, and $N(\rho)$ vanishes. Thus, $N(\rho)$ "measures" the amount by which ρ^{PT} fails to be positive definite, and it is intuitively sensible to use $N(\rho)$ as a measure for the entanglement present in the system ρ [21]. In our case of interest, only the eigenvalue λ_4 in Eq. (6) can become negative for $P < -\frac{1}{3}$. Hence, $N(\rho) = -2\lambda_4 = \frac{1}{2}(3|P| - 1)$. $N(\rho)$ is one for maximal entanglement ($P = -1$), and equals zero for zero entanglement ($P = -\frac{1}{3}$). The negativity is proportional to P, which in turn depends on the collision dynamics. We can illustrate these results by rewriting the Werner state Eq. (11) in the form $(-\frac{1}{3} > P \geq -1)$

$$\rho = (1 - N)\rho_2 + N|00\rangle\langle 00|, \tag{14}$$

where the contribution of the maximally entangled singlet state is given by the negativity.

The representation of the spin density matrix ρ in terms of Werner states [Eq. (11)] for negative correlation parameters $P = -|P|$ is related to Bell's theorem [7]. Whereas pure entangled spin-1/2 states are necessarily Bell correlated [22], surprisingly, this is in general not the case for mixed entangled states. Werner [19] proved that a state of the form Eq. (11) is Bell correlated if the condition $P < -\frac{1}{\sqrt{2}}$ is satisfied for the mixing parameter. Thus, as depicted in Fig. 1, the spin density matrix is entangled in the range $-\frac{1}{3} > P > -\frac{1}{\sqrt{2}}$ but does not violate any Bell inequalities since the spin correlation in this region is not sufficiently strong.

In order to get some insight into the relation between collision dynamics and entanglement properties, we analyze published numerical and experimental data for the spin asymmetry A_{ex}, which we reinterpret in terms of spin correlations ($P = -A_{\mathrm{ex}}$). Several groups investigated spin-dependent elastic e-H scattering; e.g., see Refs. [23–27]. In the energy region studied (0.14–300 eV), however, the data indicate that practically no entanglement can be created, except at the lowest energies [26]; see the multipseudostate close coupling (MPCC) data in Fig. 2 at $E = 0.14$ ev. Remarkable measurements have been performed on spin-dependent elastic e-Na scattering by the NIST group [28–32]. We have selected experimental data at 4.1 and 10 eV (see Fig. 2). For $E = 4.1$ eV, the data reveal pronounced entanglement effects between about 80° and 105° with a sharp minimum around $\theta = 90°$, with $P \simeq -0.87$ and negativity $N(\rho) \simeq 0.81$. These data are well in the Bell correlated area. Even more striking are the results for $E = 10$ eV, where P decreases rapidly around $\theta = 60°$ to values near $P = -1$. Here, the spins of the colliding pairs form intermediately the maximally entangled singlet state, and the Werner state Eq. (14) is dominated by the singlet contribution with negativity $N(\rho) = 1$. It is remarkable that the values of P vary over the full allowed range from $P = \frac{1}{3}$ to $P = -1$. These data are in excellent agreement with convergence close coupling (CCC) [33–35] and coupled channel optical (CCO) calculations [36], respectively (Fig. 2). For energies around the $3p$ threshold (2.1 eV) or higher, close coupling (CC) data are available [37]. Considerable degrees of entanglement can be generated;

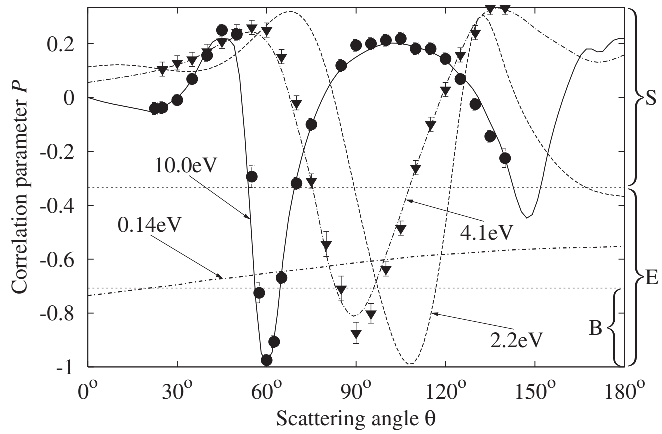

FIG. 2. Correlation parameter P versus scattering angle θ for different scattering energies and elements. Experimental data: Na 4.1 eV (triangle), Na 10 eV (circle), NIST group [31]. Numerical data: H 0.14 eV, (MPCC) van Wyngaarden and Walters [26]; Na 2.2 eV, (CC) Moores and Norcross [37]; Na 4.1 and 10 eV, (CCC) Bray [33,34]. Horizontal lines divide separable (S), entangled (E), and Bell correlated (B) regions.

e.g., for $E = 2.2$ eV, we obtain $P \simeq -1$ at $\theta \simeq 107.5°$. Interestingly, similar behavior is observed in experimental data on elastic e-Li scattering [38]. Here, the asymmetry was measured as a function of the collision energy at fixed scattering angles. For $\theta = 107.5°$, the correlation parameter decreases rapidly to $P = -1$ at $2p$ threshold (1.84 eV) and remains low up to $E \simeq 4$ eV. These data are in generally good agreement with CCO calculations [39]. On the other hand, for elastic e-Na scattering the NIST data reveal that for $E = 1.0$ and 1.6 eV, as well as for $E \geq 20$ eV, practically no entanglement can be produced. The Li data show a similar behavior.

In conclusion, we have discussed under which conditions entanglement can be generated in collisions between electrons and light, pseudo- (or truly) one-electron atoms, both initially unpolarized. The areas where the spins of the collision partners remain separable, or are entangled, or Bell correlated have been identified and the entanglement properties of the final spin system in the various regions have been discussed and interpreted. Our analysis of published numerical and experimental data on spin asymmetries exhibits the remarkable result that Coulomb forces plus electron exchange are capable of generating entangled beams of spin-1/2 particles in the full entangled range between $P = -\frac{1}{3}$ and $P = -1$ out of initially totally chaotic states. In particular, mixed collision states can be experimentally produced which violate the Bell inequalities. By studying asymmetry data, one can tune to a particular scattering energy and angle and create pairs of collision partners with any desired degree of spin entanglement, which can then be used for further experiments. This might be of interest for quantum communication or teleportation studies.

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