Spin exchange in hydrogen–antihydrogen collisions

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Received 15 January 2009, in final form 30 April 2009
Published 1 June 2009
Online at stacks.iop.org/JPhysB/42/125204

Abstract
We consider spin exchange in ultracold collisions of hydrogen (H) and antihydrogen (\(\bar{\text{H}}\)) atoms. The cross sections for transitions between various hyperfine states are calculated. We show that the process of spin exchange in \(\bar{\text{H}}–\text{H}\) collisions is basically driven by the strong force between a proton and an antiproton.

1. Introduction
The successful production of low energy antihydrogen atoms \([1, 2]\) and current experiments on their trapping \([3, 4]\) have stimulated interest in the interaction of antiatoms with ordinary matter. The simplest example of matter–antimatter interaction is given by collisions between antihydrogen and hydrogen atoms \([5–12]\). Collisions between antihydrogen and helium atoms have also been studied \([13]\). These investigations revealed that cold collisions between atoms and antiatoms do not necessarily result in annihilation, but may lead to elastic scattering or rearrangement reactions. Interestingly, it was shown that the cross sections for processes that do not result in annihilation (e.g., elastic scattering) are sensitive to the strong interaction between particles and antiparticles \([12–17]\). This presents an interesting perspective for investigating the details of strong interactions between matter and antimatter in low energy collisions of atoms and antiatoms.

In this work, we investigate spin exchange in hydrogen–antihydrogen collisions. The incoming atoms are assumed to be asymptotically in the well-defined hyperfine states which can be changed as a result of collisions. This can happen with or without changing the internal energy of the individual atoms so that some of these collisions appear elastic, apart from spin flip. We find that in the case of \(\text{H}–\bar{\text{H}}\) scattering, the main source of such spin-exchange transitions is the strong force. This is in contrast to spin exchange in atom–atom collisions (see \([18, 19]\) and the references therein), where the strong-force effects are usually negligible. At the same time the leptonic contribution to spin exchange in \(\text{H}–\bar{\text{H}}\) collisions is found to be negligibly small, in spite of the fact that the magnetic moments of the leptons (electron (e) and positron (\(\bar{e}\))) are on the order of \(10^3\) times larger than those of the hadrons (proton (p) and antiproton (\(\bar{p}\))). We will show that long-range van der Waals interactions between atoms and antiatoms play the role of a magnifying glass that exposes the strong-force effects on the molecular scale. Another unique feature of the spin-exchange cross sections is their sensitivity to the equality of the hyperfine energy levels in \(\text{H}\) and \(\bar{\text{H}}\), ensured by the CPT invariance. Violation of this invariance results in a radical change of certain cross sections for spin exchange.

This paper is organized as follows. In section 2, we present the formalism used in calculating spin-exchange cross sections. Section 3 discusses the main results. The physical sense of these results is analysed in terms of a transparent zero-range potential model of strong forces. Section 4 contains the conclusions and the appendix gives the details of certain derivations.

2. Formalism
We assume the following four-body Hamiltonian for the \(\text{H}–\bar{\text{H}}\) system:
\[ \hat{H} = \hat{H}_\text{nr} + \sum_\alpha \hat{W}_\alpha(s_\alpha, r_\alpha). \] (1)

Here \(\hat{H}_\text{nr}\) is the nonrelativistic spin-independent Hamiltonian, which includes the kinetic and Coulomb interaction energy for all particles. The subscript \(\alpha\) labels the pairs of interacting particles: (pp), (p\(\bar{e}\)), (\(\bar{p}\)e), (\(\bar{p}\bar{e}\)) or (ee). \(\hat{W}_\alpha(s_\alpha, r_\alpha)\) is the spin-dependent pair interaction, arising from low-order relativistic corrections to the nonrelativistic Hamiltonian; \(\hat{W}_\alpha(s_\alpha, r_\alpha)\) acts on the spin \(s_\alpha\) and the relative coordinates \(r_\alpha\) of the particle pair \(\alpha\).

The forthcoming analysis can be greatly simplified by taking into account the characteristic spatial and energy scales of the interactions involved in \(\text{H}–\bar{\text{H}}\) scattering. As pointed out in \([5–7, 20–25]\), the rearrangement transitions...
to protonium (Pn) and positronium (Ps) occur mainly at internuclear distances smaller than the rearrangement radius $R_0 \approx 1$ au. For internuclear distances above $R_0$ the adiabatic approximation, leading to the separation of leptonic and hadronic motion, is well justified. This allows the description of ultralow energy H–H scattering within a one-channel model based on a nonrelativistic Hamiltonian \([8, 23, 24]\):

$$\hat{H}_{ad} \approx \hat{T}_{kin} + \hat{V}_{opt} + V_{ad}(R). \tag{2}$$

The above Hamiltonian describes the interatomic motion in a fixed adiabatic leptonic state, where $\hat{T}_{kin}$ is the operator of kinetic energy of internuclear motion, $V_{ad}(R)$ is the adiabatic potential in a given leptonic state and $\hat{V}_{opt}$ is the effective complex optical potential that accounts for the inelastic rearrangement and vanishes for internuclear distances $R > R_0$.

In the following, we will discuss the ultralow energy collisions of H and H in the ground leptonic state. We will use the adiabatic interaction potential $V_{ad}(R)$ obtained in \([26]\). It is worth noting that since the Pauli principle does not forbid an electron and a positron to occupy identical spin-space states, the adiabatic potential $V_{ad}(R)$ is independent of the leptonic spin state. This is in contrast to the case of HH, where due to the Pauli principle the adiabatic potential is different in singlet and triplet electronic states. This difference is important for our considerations. In fact, the spin-exchange transitions in H–H collisions can occur only when the (relativistic) spin-dependent terms $\hat{W}_{s}(s_a, r_a)$ are taken into account. At the same time in the HH case, the main contribution to such transition rates comes from the above-mentioned effective spin dependence of the nonrelativistic adiabatic potential, while the explicitly spin-dependent interaction appears as a perturbation. We will show in the following that the spin-exchange reactions in H–H collisions are particularly sensitive to the spin-dependent strong force between a proton and antiproton.

The general form of the spin-dependent interaction is

$$\hat{W}_{s} = W_{0}^{0}(r_a) + W_{1}^{0}(r_a)(\mathbf{L}_{a}\mathbf{S}_{a}) + W_{2}^{0}(r_a)(\mathbf{r}_{a}\mathbf{S}_{a})^{2} + W_{2}^{1}(r_a)\mathbf{S}_{a}^{2}. \tag{3}$$

In the above formula, $r_a, L_a, S_a$ are relative coordinate, angular momentum and spin operators for the particle pair $a$ respectively.

The particular form of the leptonic–leptonic and leptonic–hadron pair interactions can be obtained within the QED \([27]\). In the case of $(pe)$ and $(\bar{p}\bar{e})$, they are responsible for the hyperfine splitting of the ground state of hydrogen and antihydrogen. In this work, we will approximate the nonrelativistic pair interactions for $(pe)$ and $(\bar{p}\bar{e})$ by the following effective terms \([18]\):

$$\hat{W}_{(pe), (\bar{p}\bar{e})} = a_{HF}(s_c, s_{p}, p_{p}) = \frac{a_{HF}}{2}(\mathbf{F}^{2} - 3/2). \tag{4}$$

Here $a_{HF} = 2.15710^{-7}$ au is the hyperfine constant, $s_c, s_{p}$ is the electron (positron) spin, $p_{p}$ is the proton (antiproton) spin and $\mathbf{F} = s + i$ is the total spin of the $(pe)$ or $(\bar{p}\bar{e})$ pair. The above interaction correctly reproduces the ground-state hyperfine splitting of separated H and $\bar{H}$ atoms.

The influence of the $(pe)$ or $(\bar{p}\bar{e})$ spin-dependent terms on the spin-exchange reaction rate is expected to be small due to the Coulomb repulsion that prevents the involved particles from approaching each other. We will neglect such terms in our study.

In the case of $(ee)$, the spin-dependent interaction is responsible for the fine structure and annihilation in positronium \([27]\). Due to the CP invariance, this interaction conserves spin in positronium. In our treatment, we will use the following simplified model of the $(ee)$ spin-dependent term:

$$\hat{W}_{(ee)} = a^{0}\delta(r_{ps})\hat{P}_{0} + a^{1}\delta(r_{ps})\hat{P}_{1}. \tag{5}$$

Here, $a^{0}$ and $a^{1}$ are the singlet and triplet interaction constants respectively:

$$a^{0} = -4.3 \times 10^{-4} - i 4.9 \times 10^{-6} \text{ au}, \tag{6}$$

$$a^{1} = 3.3 \times 10^{-4} - i 4.3 \times 10^{-9} \text{ au}. \tag{7}$$

Here, $\hat{P}_{0} = |S_{ps} = 0, 0\rangle\langle S_{ps} = 0, 0\rangle$ and $\hat{P}_{1} = \sum_{R} |S_{ps} = 1, \bar{M}\rangle\langle S_{ps} = 1, M\rangle$ are the projection operators on the subspace of singlet or triplet states of positronium. The suggested form of interaction conserves spin and correctly reproduces the energy shift and annihilation lifetime of para- and ortho-positronium. The spin–orbit coupling terms are neglected; we will show below that such terms are not important for the spin-exchange transition rates in the H–$\bar{H}$ system.

The leading contribution to the spin-dependent component of the $(pp)$ interaction arises from the strong force. Strong interaction is CP invariant and conserves the spin $S_{pp}$ of protonium. Furthermore, this interaction is attractive and localized to distances within $R < R_s$ with $R_s \approx 1$ fm ($1.88 \times 10^{-5}$ au). It also includes an absorptive component that is responsible for coupling to the $(pp)$ annihilation channels.

There are several models of low energy pp interaction (see \([28]\) and references therein) that differ in the detailed behaviour of spin-dependent potentials. These models, however, give close values for the p$\bar{p}$ strong-force singlet and triplet scattering lengths $a^{0,1}_{sc}$. Since the range of strong forces is much shorter compared to that of atomic interaction, it is possible to take into account the strong-force effect through an appropriate modification of the boundary condition for the scattering wavefunction. Such a procedure is based only on the knowledge of the strong-force scattering lengths \([11, 16]\). Indeed, at distances such that $R_s \ll R \ll R_f$ the interaction is dominated by the Coulomb p$\bar{p}$ potential. The wavefunction of internuclear motion at such distances behaves as a superposition of regular $F_{0}(pR)$ and irregular $G_{0}(pR)$ Coulomb solutions, with momentum $p \to 0$ \([16]\). The coefficient that mixes these two solutions, the $K$-matrix element $k$, is determined by the strong-force scattering length according to \([16, 29]\):

$$k = \tan (\delta_{sc}^{0,1}) = -2\pi M a^{0,1}_{sc}, \tag{8}$$

where $M$ stands for the reduced mass of p$\bar{p}$. We will use the following values of the $S$-state strong-force scattering length \([28, 30]\):

$$a^{0}_{sc} = (1.07 - i 1.45) \times 10^{-5} \text{ au}, \tag{9}$$

$$a^{1}_{sc} = 1.07 \times 10^{-5} \text{ au}. \tag{10}$$
\[
a_{sc} = (1.68 - i 1.06) \times 10^{-5} \text{ au.} \tag{10}
\]

The corresponding nuclear \( k \)-matrix elements become
\[
\tan (\delta_{sc}^0) = -0.06 + i 0.08, \tag{11}
\]
\[
\tan (\delta_{sc}^1) = -0.1 + i 0.06. \tag{12}
\]

In terms of state vectors \(| f(R), S_{pn} \rangle\), \( R_s < R \ll R_t \), this result can be formulated as follows:
\[
| f(R), S_{pn} \rangle \sim | F_0(pR), S_{pn} \rangle + \hat{K} | G_0(pR), S_{pn} \rangle \tag{13}
\]
\[
\hat{K} = -2\pi M \left( a_{sc}^0 \pi_0 + a_{sc}^1 \pi_1 \right). \tag{14}
\]

Here, \( \pi_{0,1} \) are projection operators on the subspaces of singlet and triplet protonium states. In this way, the effect of strong forces could be taken into account by introducing the \( K \)-matrix (14). The latter determines the boundary condition that can be imposed on the wavefunction in the range \( R_s < R \ll R_t \). The effect of the strong-force-induced boundary condition (14) is equivalent to the action of the zero-range potential [31]:
\[
\hat{V}_s = \frac{2\pi}{M} \left( a_{sc}^0 \pi_0 + a_{sc}^1 \pi_1 \right) \delta(R) \left( \frac{\partial}{\partial R} \right). \tag{15}
\]

To proceed with the calculation of spin-exchange rates within the effective adiabatic model, one needs to find the contribution of all spin-dependent terms (3) to the effective internuclear interaction. We will accommodate these terms to the first order of perturbation theory. To do so, we average the spin-dependent interactions that depend on leptonic coordinates over the unperturbed leptonic potentials for the singlet and triplet states. In this way, the effect of strong forces could be taken into account by introducing the effective internuclear interaction. We will accommodate these terms to the first order of perturbation theory. To do so, we average the spin-dependent interactions that depend on leptonic coordinates over the unperturbed leptonic wavefunction \( \Psi_{\eta, \mu}(R, r_x, r_t) \) (calculated without taking spin-dependent interactions into account). Taking into account our assumptions about the spin-dependent terms and their radial dependence, such averaging will involve only the \( (e\bar{e}) \) interaction:
\[
\hat{V}_{ee}(R) = \int |\Psi_{e\bar{e}}(R, r_x, r_t)|^2 \tilde{W}_{ee} \text{d}r_x \text{d}r_t \tag{16}
\]
\[
\hat{V}_{ee}(R) = A(R) (\alpha^0 \bar{P}_0 + \alpha^1 \bar{P}_1), \tag{17}
\]
where \( A(R) = \int |\Psi_{e\bar{e}}(R, r_x, r_t)|^2 \) is the leptonic coalescence probability. We use the values of the coalescence probability calculated in [11]. The corresponding spin-dependent leptonic potentials for the singlet and triplet states are shown in figure 1. We note that the spin-dependent interactions (3) also modify the final states of \( P_n \) and \( P_s \) in the rearrangement channels, so that the latter may contribute to the effective optical potential \( \hat{V}_{opt} \). Such a contribution only arises at the level of second-order perturbation theory and will not be taken into account here.

We may now formulate the scattering problem for spin-exchange transitions. The spin state of the colliding \( H\bar{H} \) system can be described in different representations, in terms of 16 spin-basis vectors. Since the spin-dependent terms for \((p\bar{p})\) and \((e\bar{e})\) interactions conserve the spin of the corresponding pairs, they will be diagonal in the basis set with given \((p\bar{p})\) and \((e\bar{e})\) spins. Such a basis set will be denoted as \(|S_{p,p}, M_{p,p}, S_{e,e}, M_{e,e}\rangle\). We will hereafter refer to this basis as the \( S \)-representation.

![Figure 1. Real part of the spin-dependent leptonic potentials for the singlet (dashed line) and triplet (solid line) states.](image)

The asymptotic Hamiltonian, which describes the separated \( H \) and \( \bar{H} \) atoms and includes the hyperfine terms \( \hat{W}_{pe} \) and \( \hat{W}_{p\bar{p}} \), is diagonal in the basis with given \((pe)\) and \((p\bar{p})\) spins \( F_H \) and \( F_{\bar{H}} \), respectively. Such a basis set will be denoted as \(|F_H, M_{F_H}, F_{\bar{H}}, M_{F_{\bar{H}}}\rangle\) and will be called the \( F \)-representation. The scattering state vector \(|\psi\rangle\) is a superposition of basis spin states:
\[
|\psi\rangle = \sum_{F_H, M_{F_H}, F_{\bar{H}}, M_{F_{\bar{H}}}} f(R)_{F_H, M_{F_H}, F_{\bar{H}}, M_{F_{\bar{H}}}} |F_H, M_{F_H}, F_{\bar{H}}, M_{F_{\bar{H}}}\rangle. \tag{18}
\]

The \( R \)-dependent expansion coefficients play the role of hadronic wavefunctions for the \( HH \) system in a given spin state of four particles. The asymptotic form of functions \( f(R) \) at large \( R \) gives in a standard way the \( S \)-matrix in the given spin-state representation. The desired wavefunctions are found from the solution to the coupled equation system:
\[
\sum_{\mu} (|\mu\rangle \hat{H} - E|\mu\rangle) F(R)_{\mu, \eta} = 0, \quad \eta = 1, 2, \ldots, 16. \tag{19}
\]

Here, \( F(R)_{\mu, \eta} \) is a 16×16 solution matrix whose indices label the outgoing \((\mu')\) and incoming \((\mu)\) channels, respectively, and \( \eta \) labels the sets of spin quantum numbers \( F_{\bar{H}}, M_{F_{\bar{H}}}, F_H, M_{F_H} \).

While solving the coupled channel equations we utilize the fact that for interatomic distances \( R \sim 1 \) au and below the characteristic values of the local adiabatic potential they are much greater than the hyperfine splitting. Thus even in the zero-energy limit, the hyperfine terms may be neglected in solution (19) at short and intermediate internuclear distances. At such distances, the equation system can be decoupled in the \(|S_{p,p}, M_{p,p}, S_{e,e}, M_{e,e}\rangle\) basis:
\[
\left( -\frac{1}{2M} \frac{\text{d}^2}{\text{d}R^2} + \hat{V}_{opt} + V_{ad}(R) + A(R) \alpha^S_{\eta} - E \right) F(R)_{\mu, \mu'} = 0, \tag{20}
\]
where \( \mu \) denotes a set of quantum numbers \( S_{p,p}, M_{p,p}, S_{e,e}, M_{e,e} \). Such an equation system should be supplied with boundary conditions, imposed at arbitrary \( R_0 \) within the range \( R_s < R_0 < R_t \), and specified by the strong-force \( K \)-matrix (14):
\[
F(R_0)_{\mu, \mu'} = \delta_{\mu, \mu'} \left( F_0(pR_0) - 2\pi a_{sc}^{(opt)} G_0(pR_0) \right). \tag{21}
\]
\[ F'(R_0)_{\mu,\nu} = \delta_{\mu,\nu} \left( F'(pR_0) - 2\pi a_{\delta}^2 S_{\delta} p R_0 \right). \] (22)

Instead of solving the equation system (20) with the boundary conditions (21) and (22), we use the more practical method developed in [16]. It amounts to introducing specially fitted boundary conditions at the rearrangement radius \( R = R_c \):

\[ (F'(R_c) F^{-1}(R_c))_{\mu,\nu} = \delta_{\mu,\nu} \left( p(R_c) \cot (\delta + \delta_0) \right), \] (23)

where \( p(R_c) = \sqrt{2MV_{\text{ad}}(R_c)} \) is a classical local momentum given at the internuclear separation \( R_c \). The phase shift \( \delta \) takes into account the effect of the optical and adiabatic potentials accumulated at distances below \( R_c \). Strong forces are taken into account by adding to the phase shift \( \delta \) the spin-dependent strong-force phase shift \( \delta_{\text{sff}} \). The additivity of phases is explained by the fact that the contribution of the optical potential to the phase shift vanishes in the region \( R < R_c \), characteristic for strong forces. The phase shift \( \delta \) is calculated using the model nonlocal optical potential [16] and is given by

\[ \delta = 0.74 + i0.32. \] (24)

The advantage of the above method is that once the phase shift \( \delta \) is calculated, the effect of rearrangement transitions is incorporated through the boundary condition (23) obviating cumbersome calculations with nonlocal potentials. The phase-shift approach gives a useful universal tool for the treatment and analysis of rearrangement transitions.

Once the (decoupled) equation system is solved in the \( S \)-representation, the solutions (valid in the limited range below \( R \sim 1 \text{ au} \)) should be transformed back to the asymptotically correct \( F \)-representation. This is done by means of a unitary transformation [19]:

\[ \tilde{F}(R) = U^* F(R) U \] (25)

\[ U = (S_p, M_p, S_e, M_e, M_1, M_2, M_3, M_4) \] (26)

The so-obtained solution \( \tilde{F}(R) \) should be matched at some point \( R_0 \sim 1 \text{ au} \) with a solution \( \Phi \), in which the hyperfine energy splitting is now taken into account:

\[ \sum_{\mu} \left[ \left( -\frac{1}{2M} \frac{d^2}{dR^2} + V_{\text{ad}}(R) \right) \delta_{\mu',\mu} + \left[ U^* \tilde{V}_{\text{ad}}(R) U \right]_{\mu',\mu} + Q_{\mu',\mu} \right] \times \Phi_{\mu',\mu}(R) = E \Phi_{\mu',\mu}(R) \] (27)

\[ \left( F'(R_0) \tilde{F}^{-1}(R_0) \right)_{\mu',\mu} = \left[ \Phi(R_0) \Phi^{-1}(R_0) \right]_{\mu',\mu}. \] (28)

Here \( Q_{\mu',\mu} \) is a diagonal (16 \times 16) hyperfine energy matrix, which gives the threshold energies in channels with different combinations of total spin \( F_H \) and \( F_\text{f} \). Its diagonal values are

\[ Q_{\mu,\mu} = \begin{cases} a_{\text{HF}} & \text{if } (F_H = 0, F_\text{f} = 0) \\ 0 & \text{if } (F_H = 1, F_\text{f} = 0) \text{ or } (F_H = 0, F_\text{f} = 1) \\ 2 & \text{if } (F_H = 1, F_\text{f} = 1) \end{cases} \] (29)

From the conservation of the projection of total spin \( (M_{\text{HF}} = M_H + M_\text{f}) \) it follows that the \( \Phi \)-matrix has a block structure, consisting of a \( 6 \times 6 \) matrix \( (M = 0) \), two \( 4 \times 4 \) matrices \( (M_{\text{HF}} = 1 \text{ and } M_{\text{HF}} = -1) \) and two \( 1 \times 1 \) matrices \( (M_{\text{HF}} = 2 \text{ and } M_{\text{HF}} = -2) \).

Figure 2. The spin-exchange cross sections \( \sigma_{d\bar{a} \rightarrow \bar{a}d} \) (solid line) and \( \sigma_{d\bar{a} \rightarrow \bar{a}d} \) (dashed line).

The solution matrix \( \Phi \) has the following asymptotic form as \( R \rightarrow \infty \):

\[ \Phi(R) \rightarrow \exp(-ipR) - \exp(ipR)p^{1/2}S^{1/2}. \] (30)

Here \( p \) is a diagonal matrix whose elements are \( p_{\mu,\mu} = \sqrt{2M(E - Q_{\mu,\mu})} \), and \( \exp(\mp i\vec{p}R) \) is a diagonal matrix with elements \( \exp(\mp i\vec{p}_\mu R) \) and \( \vec{S} \) is the desired \( S \)-matrix.

3. Results and discussion

We consider the \( H - \bar{H} \) collisions in the absence of an external magnetic field \( (B = 0) \). We follow the usual notation for the hyperfine states, i.e., the \( H \) state \( |F_H = 0, M_H = 0 \rangle \) is denoted as \( a \), the state \( |F_H = 1, M_H = -1 \rangle \) is denoted as \( b \), the state \( |F_H = 1, M_H = 0 \rangle \) is denoted as \( c \) and the state \( |F_H = 1, M_H = 1 \rangle \) is denoted as \( d \). The corresponding spin states of \( \bar{H} \) are denoted by \( \bar{a}, \bar{b}, \bar{c} \) and \( \bar{d} \). We present three types of the typical behaviour of spin-exchange cross sections as a function of collision energy. The spin-exchange cross sections \( \sigma_{d\bar{a} \rightarrow \bar{a}d} \) and \( \sigma_{d\bar{a} \rightarrow \bar{a}d} \) are shown in figure 2; the cross section \( \sigma_{\bar{a}d \rightarrow \bar{a}d} \) is shown in figure 3.

According to the CPT invariance, the energies of the \( d \bar{a} \) and \( a \bar{d} \) states are equal and so the reaction \( d \bar{a} \rightarrow a \bar{d} \) takes place even in the limit of vanishing collision energy, \( E \rightarrow 0 \). In this limit, the cross section tends to a constant value, \( \sigma_{d\bar{a} \rightarrow \bar{a}d}(E) \rightarrow 0.04 \text{ au}^{-2} \).

The reaction \( d \bar{a} \rightarrow c \bar{d} \) can only occur above the threshold energy \( Q_{d\bar{a} \rightarrow \bar{a}d} = a_{\text{HF}} \). The threshold behaviour of the associated cross section is clearly seen in figure 2. Again, according to the CPT invariance, the cross sections for conjugated reactions are the same, giving \( \sigma_{d\bar{a} \rightarrow \bar{a}d} = \sigma_{a\bar{d} \rightarrow \bar{a}d} \).

The inverse reaction \( c \bar{d} \rightarrow d \bar{a} \) is exothermic (in our case, the energies of the final states for exothermic reactions are smaller than the energies of the initial states by \( a_{\text{HF}} \) or \( 2a_{\text{HF}} \)) so that the cross section varies as \( 1/\nu \), where \( \nu \) is the incident channel velocity. Such behaviour is shown in figure 3. Hence, for collisional energies \( E < a_{\text{HF}} \), the cross sections of exothermic reactions are the largest among spin-exchange cross sections.
Let us mention that a hypothetical violation of CPT invariance would manifest itself in a radical change of the spin-exchange cross sections. In particular, the energy difference between the hyperfine levels of H and $\bar{H}$ (induced by the CPT violation) would follow the above-mentioned ($v$ and $1/v$) threshold pattern, instead of tending to the established constant value $E_{\text{th}}$.

Consequently, the cross sections of the reactions $d\bar{a} \rightarrow a\bar{d}$ would follow the above-mentioned ($v$ and $1/v$) threshold pattern, instead of tending to the established constant value in the limit $E \rightarrow 0$.

For increasing collision energies, i.e. when $E \gg \alpha_{\text{eff}}$, all spin-exchange cross sections tend to the same limit. In such a case, the hyperfine splitting can be neglected even in the asymptotic states. Therefore, the $S$-matrix is diagonal in the $S$-representation. The $S$-matrix in the $F$-representation (needed in our calculation of cross sections) is obtained by the transformation specified in equation (26). One can show (using the explicit form of the transformation matrix $U$ [19]) that the $S$-matrix elements in the $F$-representation for the reactions $d\bar{a} \rightarrow a\bar{d}$ and $d\bar{a} \rightarrow \bar{c}d$ are connected to the matrix elements in the $S$-representation in the following way:

$$S_{d\bar{a} \rightarrow a\bar{d}} = \frac{\langle 0, 1 | S | 0, 1 \rangle + \langle 1, 0 | S | 1, 0 \rangle}{4},$$  \hspace{1cm} (31)

$$S_{d\bar{a} \rightarrow \bar{c}d} = \frac{\langle 0, 1 | S | 0, 1 \rangle - \langle 1, 0 | S | 1, 0 \rangle}{4}.\hspace{1cm} (32)$$

Here $\langle i, j | S | i, j \rangle$ is the $S$-matrix element in the $S$-representation, with $S_{pp} = i$ and $S_{ee} = j (i, j = 0, 1)$. It follows from (31) and (32) that the equality of cross sections $\sigma_{d\bar{a} \rightarrow a\bar{d}} = \sigma_{d\bar{a} \rightarrow \bar{c}d}$ requires

$$\langle 0, 1 | S | 0, 1 \rangle + \langle 1, 0 | S | 1, 0 \rangle = 0.\hspace{1cm} (33)$$

The above equality means that the elastic scattering in the state $|S_{pp} = 1, S_{ee} = 0\rangle$ is the same as in the state $|S_{pp} = 1, S_{ee} = 1\rangle$. This can hold if the contribution of the (ee) spin-dependent potential (17) is negligible. A calculation made without the inclusion of the potential (17) confirmed this assertion. The scattering lengths $a_{10}$ and $a_{11}$ in the states $|S_{pp} = 1, S_{ee} = 0\rangle$ and $|S_{pp} = 1, S_{ee} = 1\rangle$ turned out to be

$$a_{10} = 5.665 - i2.216 \text{ au}\hspace{1cm} \text{while the scattering length } a_{11},\text{ calculated without the inclusion of the potential (17) turned out to be }$$

$$a_{11} = 5.677 - i2.216 \text{ au}\hspace{1cm} \text{while the scattering length } a_{11},\text{ calculated without the inclusion of the potential (17) turned out to be }$$

$$a_{11} = 5.666 - i2.216 \text{ au}.\hspace{1cm} \text{The small difference between these scattering lengths proves that the role of spin-dependent e}\bar{e}\text{ interaction is negligible. To understand this, we note that the ratio } |V_{ee}(R)/V_{\bar{c}\bar{d}}(R)| \text{ never exceeds } 10^{-3} \text{ and reaches a maximum in the range } 3 \text{ au} \ll R < 5 \text{ au}.\hspace{1cm} \text{At these distances, the WKB approximation is still justified. The semiclassical phase accumulated at these distances by the wavefunction (without taking } V_{ee}(R) \text{ into account) is}$$

$$\delta_{\text{WKB}} = \int_{R_{1}}^{R_{2}} \sqrt{2M(|V_{ee}(R)|)} \, dr.$$

The change of this phase due to the spin-dependent leptonic potential $V_{ee}(R)$ is

$$\Delta \delta_{\text{WKB}} = \int_{R_{1}}^{R_{2}} \sqrt{2M(|V_{ee}(R)|)} \, dr < 10^{-3} \frac{\delta_{\text{WKB}}}{2},$$

which explains why the contribution of the leptonic spin-dependent interaction to the phase of the wavefunction, and therefore to the $S$-matrix, is small [16]. Thus, we come to the conclusion that the role of spin exchange in H$-$H collisions is determined by the pp strong interaction.

The short-range character of strong forces enables the factorization of nuclear and atomic interactions and simplifies the study of the energy dependence of the spin-exchange cross sections. At short distances, where spin transitions take place, the energy difference between the final states can be totally neglected. Using the explicit form of the transition matrix $U$ (26) and the zero-range pseudo-potential (15), one can get the transition amplitude between different spin states in the distorted wave approximation:

$$f_{\alpha\beta} = \frac{a_{\alpha\beta}^{i} - a_{\alpha\beta}^{0}}{4} \int \Psi_{\alpha}(R)\delta(\mathbf{R}) \left( \frac{\partial}{\partial R} \right) \Psi_{\beta}^{*}(R) \, d^{3}R \hspace{1cm} (36)$$

Here $\Psi_{\alpha}^{0}(R)\text{ is the wavefunction corresponding to the initial (final) spin state } \alpha(\beta),\text{ calculated without taking strong forces into account}.\hspace{1cm} \text{(Note that the exact expression for the transition amplitude can be obtained from (36) upon replacing } \Psi_{\alpha\beta}^{0}(R)\text{ by the wavefunction calculated by taking strong forces into account). The only contribution to the spin-exchange amplitude arises from the S-wave, since the higher partial wavefunctions tend to zero at the origin. The spin-exchange cross section is then given by the following expression:}$$

$$\sigma_{\alpha\beta} = \frac{P_{\alpha\beta}}{P_{\alpha}} |a_{\alpha\beta}^{i} - a_{\alpha\beta}^{0}|^{2} |\Psi_{\alpha}(0)|^{2} |\Psi_{\beta}(0)|^{2},$$

where $p_{\alpha\beta}$ is the channel momentum. It is convenient to perform a further analysis in terms of the Jost function $f_{1}$. Following the definition of the S-wave Jost function [32], we may for our case write

$$\Psi_{\alpha}(R) = \frac{\phi_{\alpha}^{0}(R)}{Rf_{1}(p_{\alpha})}.$$
where $\phi_0^\alpha(R)$ is the regular 5-wave radial solution of the Schrödinger equation (neglecting strong forces) in spin state $\alpha$. The behaviour of the regular solution at the origin is

$$\phi_0^\alpha(R \rightarrow 0) = R$$

so that

$$\Psi_0^\alpha(0) = \frac{1}{f_j(p_\alpha)}. \quad (39)$$

Equation (37) now takes the form

$$\sigma_{\alpha\beta} = \pi \frac{p_\beta}{p_\alpha} \left| \frac{a_{\alpha^0} - a_{\alpha^0}}{2 f_j(p_\beta) f_j(p_\alpha)} \right|^2. \quad (40)$$

Near the threshold, the momentum dependence of the Jost function is known to be [32]

$$f_j(p_\alpha) = f_j(0) \exp(-ip_\alpha a), \quad (41)$$

where $a$ is the atom–antiatom scattering length (without taking the strong forces into account). Numerical calculations give the following values for $a$ and $1/|f_j(0)|^2$:

$$a = 5.2 - i1.8 \text{ au} \quad (42)$$

$$1/|f_j(0)|^2 = 29067. \quad (43)$$

We can exploit the smallness of the energy thresholds (determined by the hyperfine constant $\alpha_{HF}$) in different spin states, and get for the near-threshold behaviour of the spin-exchange cross section

$$\sigma_{\alpha\beta} = \pi \frac{p_\beta}{p_\alpha} \exp(2 \text{Im} a(p_\alpha + p_\beta)) \left| \frac{a_{\alpha^0} - a_{\alpha^0}}{2 f_j^2(0)} \right|^2. \quad (44)$$

It follows from the above formula that, in the case $p_\alpha = p_\beta$, the cross section in the zero-energy limit tends to the constant value

$$\sigma_0 = \pi \left| \frac{a_{\alpha^0} - a_{\alpha^0}}{2 f_j^2(0)} \right|^2 = 0.04 \text{ au} \quad (45)$$

while in the presence of the energy threshold the behaviour of the cross section is determined by the imaginary part $\text{Im} a$ of the atom–antiatom scattering length:

$$\sigma_{\alpha\beta} = \frac{P_\beta}{P_\alpha} \exp(2 \text{Im} a(p_\alpha + p_\beta)) \sigma_0. \quad (46)$$

Comparison of the above expression, obtained in the distorted wave approximation, with the results of numerical calculations shows that formula (46) is accurate to within a few percent for collision energies below $10^{-5}$ au.

The behaviour of the cross section (46) near the threshold has a clear physical meaning. Spin exchange can only occur when the nuclei approach distances characteristic for strong forces, i.e., 1 fm. Due to inelastic rearrangement transitions into the $Pn+Ps$ channels, the flux of H–H at such distances is damped by the factor $\exp(2 \text{Im} a(p_\alpha + p_\beta))$. The damping rate is given by the imaginary part of scattering length for H–H collisions. We note that the imaginary part of the scattering length can be extracted from the energy dependence of the spin-exchange cross sections [33].

In the case of exothermic reactions (e.g., $c \tilde{a} \rightarrow \tilde{d}a$ or $bd \rightarrow aa$), there is an energy excess in the final channel: $\Delta E_\beta = n\alpha_{HF}, n = 1, 2$. It follows from (46) that the cross sections for such reactions behave like $d_{\alpha}/v$ in the limit $E \rightarrow 0$. Taking into account that as $E \rightarrow 0 p_\beta \rightarrow \sqrt{2M\alpha_{HF}}$, we obtain for $d_{\alpha}$

$$d_{\alpha} = \frac{2M\alpha_{HF}}{\sqrt{2}} \exp(2 \text{Im} a\alpha_{HF}) \sigma_0. \quad (47)$$

which gives

$$d_1 = 8.0 \times 10^{-7} \text{ au}^2 \quad (48)$$

$$d_2 = 1.1 \times 10^{-6} \text{ au}^2. \quad (49)$$

The ratio of the near-threshold spin-exchange reaction rates $bd \rightarrow aa$ and $c \tilde{d} \rightarrow \tilde{d}a$ is given by

$$d_2/d_1 = \frac{2\sqrt{2}(\sqrt{2} - 1) \text{Im} a\alpha_{HF}}{\sqrt{2}M\alpha_{HF}} = 1.375. \quad (50)$$

As one can see, this ratio is determined by the product $\text{Im} a\alpha_{HF}$. The cross sections of the inverse reactions ($d\tilde{a} \rightarrow \tilde{c}a$ or $aa \rightarrow bd$) show characteristic threshold behaviour. In the vicinity of the threshold, they behave like $pd_{\alpha}/\sqrt{2M\alpha_{HF}}$.

It was already mentioned that for $E \gg \alpha_{HF}$, all the spin-exchange cross sections tend to the same limit. Within the zero-range potential model of strong forces, this limit is given by

$$\sigma = \exp(4 \text{Im} ap)\sigma_0. \quad (51)$$

A remarkable feature of the obtained results is the factorization of the spin-dependent strong-force effect and the effect of long-range atomic interaction (44). While the first appears through the difference between singlet and triplet strong-force scattering lengths, the second is given by the Jost function for the interatomic motion of the H–H pair. This latter factor ($1/|f_j(0)|^4$) strongly enhances (approximately $10^9$ times!) the effect of strong forces, due to focusing of the flux of p–p towards the centre by the molecular potential. The large value of the enhancement factor is determined by the large ratio of atomic to nuclear scales.

Under certain conditions, the enhancement factor $1/|f_j(0)|^4$ could become even larger. This additional enhancement is due to the existence of the near-threshold quasi-molecular H–H states [16]. Indeed, such quasi-bound states manifest themselves as zeros of the Jost function $f_j(p)$ in the complex momentum plane. The presence of these zeros in the threshold vicinity leads to a small value for $f_j(0)$. To study the question in more detail, we will use the analytical expression for the Jost function based on the WKB approximation for interatomic motion at distances 1 au < R < 5 au (see the appendix):

$$\frac{1}{|f_j(0)|^2} = \frac{2\pi M a_0}{\sin^2(\pi/8 + \Omega + \delta)}. \quad (52)$$

In the above equation, $a_0$ is the characteristic scale for the van der Waals interaction between H and H [16]:

$$a_0 = \sqrt{2M C_6 / 2\sqrt{2} \Gamma(3/4)} \simeq 4.99 \text{ au}. \quad (53)$$

$C_6 = 6.5$ is the van der Waals constant for H–H interaction, $\Omega$ is the semiclassical phase, accumulated in the distance range $R > R_T$

$$\Omega = \int_{R_T}^{\infty} \sqrt{2MV_{\alpha}(R)} dR = 19.38. \quad (54)$$
and $\delta = 0.74 + i0.32$ is the complex phase shift (24) accumulated at distances less than $R_{v}$. The value of expression (52), obtained within the WKB approximation, turns out to be

$$\frac{1}{|J_{f}^{\text{WKB}}(0)|^2} = 24830$$

and is comparatively close to the exact value (43).

Following the method developed in [16], we will vary the total phase of the wavefunction $\varphi = \pi/8 + \delta + \Omega$. The physical sense of such a procedure is as follows. It is known that interatomic interactions can be modified by means of external magnetic or electric fields (see [34, 35] and references therein). Without specifying the physical method of such modification, we may describe the resulting effect as a variation of the magnetic or electric fields (see [34, 35] and references therein).

Without specifying the physical method of such modification, we may describe the resulting effect as a variation of the magnetic or electric fields (see [34, 35] and references therein).

In figure 4, we present the zero-energy limit of the $c\tilde{d} \rightarrow \tilde{d}c$ cross section as a function of the phase variation that expresses a modification of the interatomic interaction due to the presence of an external field.

$$\varphi = \pi k, k = 0, 1, 2, \ldots$$

As long as there is an imaginary component of the total phase $\varphi$ (which represents the absorption of the $H-H$ flux into rearrangement channels), such a condition cannot be satisfied exactly; however, the enhancement factor will show maxima corresponding to values of the total phase satisfying $\text{Re} \varphi = \pi k$. As was shown in [16], this condition corresponds to the appearance of a decaying quasi-bound state in the spectrum of the $H-H$ system close to the dissociation threshold.

In figure 4, we present the zero-energy limit of the cross section for the reaction $c\tilde{d} \rightarrow \tilde{d}c$ as a function of phase variation. For certain values of the total phase $\varphi$, the spin-exchange cross section increases more than 50 times in comparison with its ‘unbiased’ value ($\varphi = 20.51 + i3.2$) obtained in the absence of any external perturbation. Strictly speaking, in such a resonant case the distorted wave approximation (36) is not justified and one should substitute the approximate value of $\Psi_{1,0}(0)$ by the wavefunction calculated by taking strong forces into account. Nevertheless, this result indicates that the modification of the interatomic $H-H$ interaction by external fields could in principle strongly increase the spin-exchange cross sections, exposing the effect of strong forces. Such additional enhancement might also occur in collisions with other atoms, due to the sensitivity of the cross sections to the reduced mass of the colliding nuclei [16].

4. Conclusions

We found that the spin-exchange transitions in $H-H$ collisions are caused mainly by the strong force. This mechanism of spin exchange is a unique feature of atom–antiatom interaction, with no counterpart in atom–atom collisions. The corresponding transition amplitudes are proportional to the difference between singlet and triplet strong-force scattering lengths. Meanwhile, the cross sections acquire molecular dimensions due to the large enhancement of the strong-force effect; this enhancement originates from the presence of long-range, atom–antiatom interaction. We have shown that the enhancement factor is on the order of $10^9$.

The energy behaviour of the spin-exchange cross sections turns to be sensitive to the difference between hyperfine energy levels in $H$ and $\tilde{H}$ (which might occur due to CPT violation). If such violation were to occur, the threshold behaviour of the spin-exchange cross sections would be radically different from the CPT-invariant case. We present a universal description of the influence of external fields on the $H-H$ scattering, which suggests that field-induced modification of the interatomic interaction can additionally enhance (up to 50 times) the spin-exchange cross sections, exposing the strong-force effects.

Acknowledgments

We would like to acknowledge the support from the Swedish Research council, from the Wenner-Gren Foundations and the Royal Swedish Academy of Sciences. One of the authors (AV) would like to thank E Shulgina for very useful discussions and comments.

Appendix

This appendix outlines the derivation of the analytical expression for the Jost function $f_1(0)$ for a zero collision energy of the $H-H$ system. We start with the expression for the $S$-wave scattering length for $H-H$, obtained in [16] under the following assumptions. At distances $R > R_{h} \sim 1$ au the $H-H$ interaction is well described by the one-channel, adiabatic potential $V_{ad}(R)$. At distances $R > R_{b} \sim 5$ au this potential can be accurately reproduced by the van der Waals interaction $-C_{6}/R^{6}$, with $C_{6} = 6.5$. There exists a domain $R_{t} < R < R_{b} \ll R_{vdW}$, with $R_{vdW} = \sqrt{2M/C_{6}} \approx 10.5$ au, where the WKB approximation is well justified.

Matching the WKB wavefunction to the exactly known asymptotic zero-energy solution of the Schrödinger equation with the $-C_{6}/R^{6}$ potential, one gets the following expression for the scattering length in $H-H$ collisions:

$$a = a_{0} \left(1 + \cot \left(\frac{\pi}{8} + \Omega + \delta\right)\right).$$

(A.1)
where $a_0$ is
\[ a_0 = R_{\text{eff}} \Gamma(3/4) / 2\sqrt{2} \Gamma(5/4) \approx 4.99 \text{ au} \] (A.2)
and $\Omega = 19.38$ is the WKB phase (54), accumulated in the domain $R_t < R < \infty$.

To calculate the Jost function, we determine the variation of the scattering length (A.1) with the small variation of phase $\Delta \delta$:
\[ \Delta a = -a_0 \frac{\Delta \delta}{\sin^2 \left( \frac{\pi}{2} + \Omega + \delta \right)} . \] (A.3)
In the case of the zero-range potential
\[ V_{\text{ZRP}} = \frac{2\pi}{M} a \delta(R) \left( \frac{\partial}{\partial R} R \right) , \] (A.4)
the variation of phase is given by (8)
\[ \Delta \delta = -2\pi M a \delta_c . \] (A.5)
The corresponding variation of the scattering amplitude, induced by the zero-range potential (A.4), can be obtained within the distorted wave approximation:
\[ \Delta f = -a |\Psi_0(R)|^2 V_{\text{ZRP}} \Psi_0(R) \mathrm{d}^3 R = -a_0 |\Psi_0(0)|^2 , \] (A.6)
where $\Psi_0(R)$ is the wavefunction calculated without taking potential (A.4) into account. We now use equation (39) to express the wavefunction in terms of the Jost function and obtain
\[ \Delta f = -\frac{a_0}{|f_1(0)|^2} . \] (A.7)
The S-wave scattering length is connected to the zero-energy scattering amplitude by the relation $a = -f(0)$. Inserting this relation into equation (A.7) and comparing (A.7) with (A.3), we finally obtain the following expression for $1/|f_1(0)|^2$:
\[ 1/|f_1(0)|^2 = \frac{2\pi M a_0}{\sin^2(\pi/2 + \Omega + \delta)} . \] (A.8)

References

[1] Gabrielse G et al 2002 Phys. Rev. Lett. 89 233401
[2] Amoretti M et al 2002 Nature 419 456
[3] Gabrielse G et al 2008 Phys. Rev. Lett. 100 113001
[4] Andersen G B et al 2008 J. Phys. B: At. Mol. Opt. Phys. 41 011001
[5] Froelich P 2002 Quantum chemistry of antimatter Adv. Quantum Chem. 41 185 and the references therein
[6] Froelich P et al 2000 Phys. Rev. Lett. 84 4577
[7] Jonsell S, Saenz A, Froelich P, Dalgaro A and Zygelman B 2001 Phys. Rev. A 64 052712
[8] Voronin A and Carbonell J 2001 Nucl. Phys. A 689 5292
[9] Armour E and Chamberlain C W 2002 J. Phys. B: At. Mol. Opt. Phys. 35 L489
[10] Sinha P K, Chaudhuri P and Ghosh A S 2003 J. Phys. B: At. Mol. Opt. Phys. 67 052509
[11] Froelich P et al 2004 Phys. Rev. A 70 022509
[12] Armore E, Lin Y and Vigier A 2005 J. Phys. B: At. Mol. Opt. Phys. 38 L47
[13] Jonsell S, Saenz A, Froelich P, Zygelman B and Dalgaro A 2005 Can. J. Phys. 83 435
[14] Jonsell S, Saenz A, Froelich P, Zygelman B and Dalgaro A 2004 J. Phys. B: At. Mol. Opt. Phys. 37 1195
[15] Jonsell S, Froelich P, Eriksson S and Strasburger K 2004 Phys. Rev. A 70 062708
[16] Voronin A and Froelich P 2008 Phys. Rev. A 77 022505
[17] Berggren P, Stegeby H, Voronin A and Froelich P 2008 J. Phys. B: At. Mol. Opt. Phys. 41 L55202
[18] Stoof H T C, Koelman J M V A and Verhaar B J 1988 Phys. Rev. B 38 4688
[19] Zygelman B, Dalgaro A, Jamieson M J and Stancil P C 2003 Phys. Rev. A 67 042715
[20] Kolos W, Morgan D L, Schrader D M and Wolniewicz L 1975 Phys. Rev. A 11 1792
[21] Shlyapnikov G V, Walraven J T M and Surkov E L 1993 Hyperfine Interact. 76 31
[22] Voronin A and Carbonell J 1998 Hyperfine Interact. 115 143
[23] Voronin A and Carbonell J 2004 Nucl. Instrum. Methods B 214 139
[24] Zygelman B et al 2004 Phys. Rev. A 69 042715
[25] Armore E A G, Chamberlain C W, Liu Y and Martin G D R 2004 Nucl. Instrum. Methods B 221 1
[26] Strasburger K 2004 J. Phys. B: At. Mol. Opt. Phys. 37 4483
[27] Berestetskii V B, Pitaevskii L P and Lifshitz E M 1982 Quantum Electrodynamics: Landau and Lifshitz Course of Theoretical Physics vol 4 (Portsmouth, NH: Butterworth-Heinemann)
[28] Carbonell J, Richard J M and Wycech S 1998 Z. Phys. A 343 325
[29] Froelich P et al 2004 Few-Body Syst. 72 63
[30] Kohno M and Weise W 1986 Nucl. Phys. A 454 429
[31] Demkov Yu N and Ostrovskii V N 1988 Zero-Range Potentials and Their Applications in Atomic Physics (New York: Plenum)
[32] Newton R G 1982 Scattering Theory of Waves and Particles (New York: Springer)
[33] Dalkarov O D and Protasov K V 1992 Phys. Lett. B 280 117
[34] Marinescu M and You L 1998 Phys. Rev. Lett. 81 4596
[35] Tiesinga E, Verhaar B J and Stoof H T C 1993 Phys. Rev. A 47 4114