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Hyperfine transitions in ultracold hydrogen-antihydrogen collisions

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We consider the hyperfine transitions in ultracold collisions of hydrogen (H) and antihydrogen ($\overline{\mathrm{H}}$) atoms. The cross sections for transitions between various spin states are calculated. We show that hyperfine transitions in $\overline{\mathrm{H}}-\mathrm{H}$ collisions are basically driven by the strong force between proton and antiproton.

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I. INTRODUCTION

The synthesis of low-energy antihydrogen atoms [1,2] and the on-going experiments on their trapping [3,4] have stimulated interest in the interaction of antiatoms with ordinary matter [5–12].

In the present work we investigate hyperfine transitions in hydrogen-antihydrogen collisions. We find that the main source of such transitions is the *strong force*, whereas the leptonic contribution is negligibly small. This is in contrast to spin exchange in atom-atom collisions (see [13,14], and references therein) where the strong-force effects are usually negligible. We show that the long-range van der Waals interaction between atoms and antiatoms greatly enhances the strong-force effects. The standard model extension theories indicate that the hyperfine structure of antihydrogen should be rather sensitive to possible *CPT* violation [15], which motivates projects of spectroscopic measurements of that structure [16]. Studies of cross sections for spin exchange might provide another, collisional way to compare the hyperfine structures of hydrogen and antihydrogen. We show that possible differences could be inferred from the *trends in energy dependence* of the cross sections.

II. FORMALISM

The spin state of the colliding $\mathrm{H}-\overline{\mathrm{H}}$ system can be described in terms of 16 spin basis vectors. The basis set which conserves spin of $(p\bar{p})$ and $(e\bar{e})$ pairs will be denoted $|S_{(p,\bar{p})},M_{(p,\bar{p})},S_{(e,\bar{e})},M_{(e,\bar{e})}\rangle$ and will be called as the S representation. The asymptotic Hamiltonian that describes the separated H and $\overline{\mathrm{H}}$ atoms is diagonal in the basis with given (pe) and $(\bar{p}\bar{e})$ spins F_{H} and $F_{\overline{\mathrm{H}}}$, respectively. Such basis set will be denoted $|F_{\mathrm{H}},M_{\mathrm{H}},F_{\overline{\mathrm{H}}},M_{\overline{\mathrm{H}}}\rangle$ and will be called the F representation. We follow the usual notation for the hyperfine states of the H atom, i.e., $|F_{\mathrm{H}}=0,M_{\mathrm{H}}=0\rangle\equiv a$, $|F_{\mathrm{H}}=1,M_{\mathrm{H}}=-1\rangle\equiv b$, $|F_{\mathrm{H}}=1,M_{\mathrm{H}}=0\rangle\equiv c$, and $|F_{\mathrm{H}}=1,M_{\mathrm{H}}=1\rangle\equiv d$. The corresponding spin states of $\overline{\mathrm{H}}$ are denoted $\bar{a}$, $\bar{b}$, $\bar{c}$, and $\bar{d}$. The colliding $\mathrm{H}-\mathrm{H}$ system is described by the four-body Hamiltonian,

$$\hat{H}=\hat{H}_{nr}+\sum_{\alpha}\hat{W}_{\alpha}(\mathbf{s}_{\alpha},\mathbf{r}_{\alpha}), \tag{1}$$

where $\hat{H}_{nr}$ is the nonrelativistic spin-independent Hamiltonian which includes kinetic energy and Coulomb interaction energy of all particles. $\hat{W}_{\alpha}(\mathbf{s}_{\alpha},\mathbf{r}_{\alpha})$ are the spin-dependent pair interactions for the particle-pair $\alpha\equiv p\bar{p}$, pe, $p\bar{e}$, $\bar{p}e$, $\bar{p}\bar{e}$, or $e\bar{e}$, arising from the account of lowest-order relativistic corrections to the nonrelativistic Hamiltonian.

As pointed out in [6,7,17–19], the rearrangement transitions to protonium (Pn) and positronium (Ps) occur mainly at internuclear distances smaller than the rearrangement radius $R_r\simeq 1$ a.u.. For internuclear distances above R_r the adiabatic approximation, leading to separation of leptonic and hadronic motion, is well justified. This allows the description of ultralow energy $\mathrm{H}-\overline{\mathrm{H}}$ scattering within the one-channel model based on the nonrelativistic Hamiltonian [17,18]

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

The above Hamiltonian describes the interatomic motion in a fixed adiabatic leptonic state, $\hat{T}_{kin}$ 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 potential that accounts for inelastic rearrangement [18].

In the following we will discuss the ultralow energy collisions of H and $\overline{\mathrm{H}}$ in the ground leptonic state. We will use the adiabatic interaction potential $V_{ad}(R)$ obtained in Ref. [20]. We note that $V_{ad}(R)$ is independent of the leptonic spin state. Hence, the spin-exchange transitions in $\mathrm{H}-\overline{\mathrm{H}}$ collisions can occur only when the (*relativistic*) spin-dependent terms $\hat{W}_{\alpha}(\mathbf{s}_{\alpha},\mathbf{r}_{\alpha})$ are taken into account. 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, so that the main contribution to spin transition rates comes from the effective spin dependence of the *nonrelativistic* adiabatic potential, while the explicitly spin-dependent interaction appears as a perturbation. We will show that the spin-exchange reactions in $\mathrm{H}-\overline{\mathrm{H}}$ collisions are particularly sensitive to the spin-dependent strong force between proton and antiproton.

For (pe) and $(\bar{p}\bar{e})$ spin-dependent pair interactions $\hat{W}_{\alpha}$ we adopt the effective form [13]

$$\hat{W}_{(ep),(\bar{e}\bar{p})}=a_{HF}(\mathbf{s}_{e,\bar{e}}\cdot\mathbf{i}_{p,\bar{p}})=\frac{a_{HF}}{2}(\mathbf{F}^2-3/2), \tag{3}$$

where $a_{HF}=2.157\times10^{-7}$ a.u. is the hyperfine constant, $\mathbf{s}_{e,\bar{e}}$ is the electron (positron) spin, $\mathbf{i}_{p,\bar{p}}$ is the proton (antiproton) spin, and $\mathbf{F}=\mathbf{s}+\mathbf{i}$ 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 $\overline{\mathrm{H}}$ atoms.

The influence of the $\hat{W}_{(\bar{p}e)}$ or $\hat{W}_{(p\bar{e})}$ terms is expected to be small due to the Coulomb repulsion that prevents the involved particles from approaching each other. These terms are neglected in our Rapid Communication.

The spin-dependent interaction $\hat{W}_{(e\bar{e})}$ is responsible for the fine structure and annihilation in positronium [21]. Here we use

$$\hat{W}_{(e\bar{e})} = \alpha^0 \delta(\mathbf{r}_{\mathrm{Ps}})\hat{P}_0 + \alpha^1 \delta(\mathbf{r}_{\mathrm{Ps}})\hat{P}_1, \tag{4}$$

where $\alpha^0 = -4.3\times10^{-4} - i4.9\times10^{-6}$ a.u. and $\alpha^1 = 3.3\times10^{-4} - i4.3\times10^{-9}$ a.u. are the singlet and triplet interaction constants and $\hat{P}_0 = |S_{\mathrm{Ps}}=0,0\rangle\langle S_{\mathrm{Ps}}=0,0|$ and $\hat{P}_1 = \Sigma_M |S_{\mathrm{Ps}}=1,M\rangle\langle S_{\mathrm{Ps}}=1,M|$ are the projection operators on the subspace of singlet or triplet states of positronium. The above effective form of interaction conserves spin (as required by the *CP* invariance of Ps) and correctly reproduces the energy shift and annihilation lifetimes of parapositronium and orthopositronium.

The leading contribution to the interaction $\hat{W}_{(p\bar{p})}$ is given by the strong force, localized within $R < R_s \simeq 1$ fm. Its influence on $\bar{\mathrm{H}}-\mathrm{H}$ scattering can be accounted for through the imposition of strong-force boundary condition on the wave function of interhadronic motion $F(R)$, at distances $R_s \ll R \ll R_r$ [22]. Such a boundary condition is equivalent to the action of the zero-range pseudopotential [23]:

$$\hat{V}_s = \frac{2\pi}{M}(a^0_{sc}\hat{\pi}_0 + a^1_{sc}\hat{\pi}_1)\delta(\mathbf{R})\left(\frac{\partial}{\partial R}R\right), \tag{5}$$

where M stands for the reduced mass of $p\bar{p}$, $\hat{\pi}_{0,1}$ are the projection operators on the subspaces of singlet and triplet protonium states, and $a^{0,1}_{sc}$ are the S state, strong-force scattering lengths $a^0_{sc} = (1.73 - i1.24)\times10^{-5}$ a.u. and $a^1_{sc} = (1.55 - i0.94)\times10^{-5}$ a.u. We use the model predictions [24], which take into account the full set of existing $N\bar{N}$ data [25].

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 in Eq. (1) to the effective internuclear interaction. We will accommodate these terms to the first order of perturbation theory. To do so we need to average the spin-dependent interactions that depend on leptonic coordinates over the unperturbed leptonic wave function $\Psi_{e,\bar{e}}(R,\mathbf{r}_e,\mathbf{r}_{\bar{e}})$ (calculated without the account of spin-dependent interactions). Such averaging will involve only the $(e\bar{e})$ interaction [Eq. (4)]

$$\hat{V}_{e\bar{e}}(R) = \int |\Psi_{e,\bar{e}}(R,\mathbf{r}_e,\mathbf{r}_{\bar{e}})|^2 \hat{W}_{e\bar{e}} d\mathbf{r}_e d\mathbf{r}_{\bar{e}}, \tag{6}$$

$$\hat{V}_{e\bar{e}}(R) = A(R)(\alpha_0\hat{P}_0 + \alpha_1\hat{P}_1). \tag{7}$$

We use the values of coalescence probability $A(R) = |\Psi_{e,\bar{e}}(R,\mathbf{r}_e=\mathbf{r}_{\bar{e}})|^2$ from Ref. [11].

The scattering state vector $|\phi\rangle$ is a superposition of basis spin states:

$$|\phi\rangle = \sum_\mu F_\mu(R)|\mu\rangle; \quad \mu \equiv F_{\mathrm{H}}, M_{\mathrm{H}}, F_{\bar{\mathrm{H}}}, M_{\bar{\mathrm{H}}}. \tag{8}$$

The R-dependent expansion coefficients play role of hadronic wave functions of $\mathrm{H}\bar{\mathrm{H}}$ in a given spin state of four particles. These wave functions can be found from the solution of the coupled equation system:

$$\sum_\mu \langle\mu'|\hat{H} - E|\mu\rangle \hat{F}(R)_{\mu,\eta} = 0, \quad \eta = 1,2,\ldots,16. \tag{9}$$

Here $\hat{F}(R)_{\mu',\mu}$ is a 16×16 solution matrix whose first index labels the outgoing channel, second index labels the incoming channel, μ', μ, and η stand for the sets of spin quantum numbers $F_{\mathrm{H}}, M_{\mathrm{H}}, F_{\bar{\mathrm{H}}}, M_{\bar{\mathrm{H}}}$.

We utilize the fact that, for interatomic distances $R \sim 1$ a.u. and below, the characteristic values of the local adiabatic potential are much greater than the hyperfine splitting. At these distances, the hyperfine terms may be neglected in solution (9) even at the zero-energy limit. The equation system can be decoupled in the $|S_{(p,\bar{p})}, M_{(p,\bar{p})}, S_{(e,\bar{e})}, M_{(e,\bar{e})}\rangle$ representation. The uncoupled solutions $F_{\mu,\mu}(R)$ are subject to the following boundary conditions at the *rearrangement radius* $R = R_r$ [26]:

$$[\hat{F}'(R_r)\hat{F}^{-1}(R_r)]_{\mu,\mu'} = \delta_{\mu,\mu'} p(R_r)\cot[\delta + \delta^{S_{(p\bar{p})}}_{sc}], \tag{10}$$

where $p(R_r) = \sqrt{2MV_{ad}(R_r)}$ is a classical local momentum given at the internuclear separation R_r. The phase shift δ takes into account the effect of the optical and adiabatic potentials accumulated at distances below R_r. The account of strong forces is achieved by adding to the phase shift δ the spin-dependent strong-force phase shift $\delta^{S_{(p\bar{p})}}_{sc} = -2\pi M a^{S_{(p\bar{p})}}_{sc}$ [26]. The additivity of phases is explained by vanishing contribution of the optical potential to the phase shift at distances $R < R_s$, a characteristic for strong forces. The phase shift δ is calculated using the model nonlocal optical potential [26] and is taken to be $\delta = 0.7 + i0.3$.

Boundary condition (10) for the (decoupled) equation system is suitable in the S representation. The equivalent boundary condition for the asymptotically correct solution $\hat{\Phi}$ in the F representation can be obtained by means of a unitary transformation $\hat{U} = \langle S_{(p,\bar{p})}, M_{(p,\bar{p})}, S_{(e,\bar{e})}, M_{(e,\bar{e})} | F_{\mathrm{H}}, M_{\mathrm{H}}, F_{\bar{\mathrm{H}}}, M_{\bar{\mathrm{H}}}\rangle$ [14] and becomes $\hat{\Phi}'(R_r)\hat{\Phi}^{-1}(R_r) = \hat{U}^+\hat{F}'(R_r)\hat{F}^{-1}(R_r)\hat{U}$. The solution matrix $\hat{\Phi}$, in which now the hyperfine energy splitting is taken into account, satisfies the equation system:

$$\left[\left(\frac{-1}{2M}\frac{d^2}{dR^2} + V_{ad}(R) - E\right)\hat{I} + \hat{U}^+\hat{V}_{(e\bar{e})}\hat{U} + \hat{Q}\right]\hat{\Phi}(R) = 0, \tag{11}$$

where $\hat{I}$ is an identity matrix and $\hat{Q}$ is a diagonal (16×16) hyperfine energy matrix which gives the threshold energies $(0, \alpha_{HF}$ or $2\alpha_{HF})$ in channels with different combinations of quantum numbers F_{H} and $F_{\bar{\mathrm{H}}}$.

The solution matrix obtained in this way gives access to the S matrix (and so far to the cross sections) of interest.

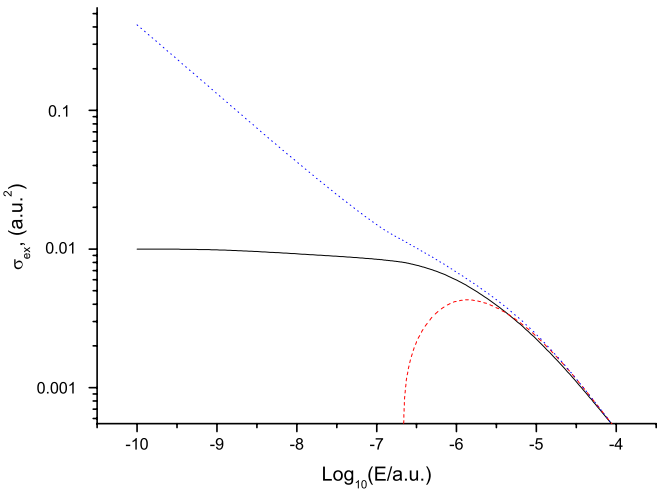

FIG. 1. (Color online) The spin-exchange cross-sections $\sigma_{d\bar{a}\to a\bar{d}}$ (solid line), $\sigma_{d\bar{a}\to c\bar{d}}$ (dashed line), and $\sigma_{c\bar{d}\to d\bar{a}}$ (dotted line).

III. RESULTS AND DISCUSSION

We present three types of typical behavior of spin-exchange cross sections as function of collision energy. The results for spin-exchange cross sections $\sigma_{d\bar{a}\to a\bar{d}}$, and $\sigma_{d\bar{a}\to c\bar{d}}$ and $\sigma_{c\bar{d}\to d\bar{a}}$ are shown on Fig. 1.

According to the *CPT* invariance the energies of the $d\bar{a}$ and $a\bar{d}$ states are equal and so the reaction $d\bar{a}\to a\bar{d}$ takes place even in the limit of vanishing collision energy, $E\to 0$. In that limit the cross section tends to constant value, $\sigma_{d\bar{a}\to a\bar{d}}(E)\to 0.01$ a.u.^{2} (solid line on Fig. 1). The spin averaged elastic cross section is much larger $\sigma_{el}=466$ a.u.^{2} [26]. Reaction $d\bar{a}\to c\bar{d}$ can only occur above the threshold energy $Q_{d\bar{a}\to c\bar{d}}=\alpha_{HF}$ (see Fig. 1, dashed line). The cross sections for conjugated reactions are the same so that $\sigma_{d\bar{a}\to c\bar{d}}=\sigma_{a\bar{d}\to d\bar{c}}$. The inverse reaction $c\bar{d}\to d\bar{a}$ is exothermic (the released energy is α_{HF} or $2\alpha_{HF}$) so it behaves like $1/v$, where v is the incident channel velocity. Such behavior is presented by dotted line on Fig. 1. We mention that the violation of *CPT* invariance, if it were to come about, would manifest itself in the radical change in the spin-exchange cross sections. In particular, the energy difference between hyperfine levels of H and $\bar{\mathrm{H}}$ (induced by the *CPT* violation) would result in the appearance of new reaction thresholds. Consequently, the cross sections of reactions $d\bar{a}\leftrightarrows a\bar{d}$ would demonstrate the above mentioned (v and $1/v$) threshold behavior, instead of tending to the established constant value in the limit $E\to 0$.

For the increasing collisional energies, i.e., in the case $E\gg\alpha_{HF}$, 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 S representation. This suggests that the contribution of the $(e\bar{e})$ spin-dependent potential [Eq. (7)] is negligible. Indeed we found that the scattering lengths $a_{10}=5.665-i2.216$ a.u. and $a_{11}=5.677-i2.216$ a.u. in the states $|S_{p\bar{p}}=1,S_{e\bar{e}}=0\rangle$ and $|S_{p\bar{p}}=1,S_{e\bar{e}}=1\rangle$ are almost identical to the scattering length $a_1=5.666-i2.216$ a.u. calculated without inclusion of the potential [Eq. (7)]. Thus we come to the conclusion that the rate of spin exchange in $\mathrm{H}-\bar{\mathrm{H}}$ collisions is determined by the $p\bar{p}$ *strong interaction*. To demonstrate the sensitivity of the spin-exchange cross sections to the strong forces we calculated the mentioned cross sections for another set of Coulomb corrected $p\bar{p}$ strong-force scattering lengths obtained in earlier $N\bar{N}$ potential models [27,28] $a_{sc}^0=(1.07-i1.45)\times 10^{-5}$ a.u. and $a_{sc}^1=(1.68-i1.06)\times 10^{-5}$ a.u.. The corresponding cross sections turned to be approximately four times greater, in particular, $\sigma_{d\bar{a}\to a\bar{d}}(E\to 0)\to 0.04$ a.u.^{2}

The short-range character of strong forces enables the factorization of nuclear and atomic interactions. At short distances, where spin transitions take place, the energy difference between various hyperfine states can be neglected. Using the explicit form of the transformation matrix $\hat{U}$ and the zero-range pseudopotential [Eq. (5)], one can get the transition amplitude between different spin states in the distorted wave approximation:

$$f_{\alpha\beta}=\frac{a_{sc}^1-a_{sc}^0}{4}\Psi_\beta^{0*}(0)\Psi_\alpha^0(0). \tag{12}$$

Here $\Psi_{\alpha,\beta}^0(\mathbf{R})$ is the wave function (calculated without taking into account the strong interaction) corresponding to the initial (final) spin state α (β). Since the higher partial wave functions tend to zero at the origin, the spin exchange cross section is then

$$\sigma_{\alpha\beta}=\pi\frac{p_\beta}{p_\alpha}\frac{|a_{sc}^1-a_{sc}^0|^2}{4}|\Psi_\beta^0(0)\Psi_\alpha^0(0)|^2, \tag{13}$$

where $p_{\alpha,\beta}$ is the channel momentum. Introducing the S-wave Jost function $\Psi_\alpha^0(0)=1/f_J(p_\alpha)$, taking into account its near-threshold relation to the HH scattering length a, $f_J(p_\alpha)\to f_J(0)\exp(-ip_\alpha a)$ [29], and exploiting small difference (α_{HF}) between energy in spin states α and β, one obtains

$$\sigma_{\alpha\beta}=\pi\frac{p_\beta}{p_\alpha}\exp[2\ \mathrm{Im}\ a(p_\alpha+p_\beta)]\left|\frac{a_{sc}^1-a_{sc}^0}{2f_J^2(0)}\right|^2. \tag{14}$$

Numerical calculations [17,26] give $a=5.2-i1.8$ a.u. and $1/|f_J(0)|^2=29\,067$. In the case $p_\alpha=p_\beta$, the cross section in the zero-energy limit tends to the constant value: $\sigma_0=\pi|(a_{sc}^1-a_{sc}^0)/2f_J^2(0)|^2$. For collision energies below 10^{-5} a.u. formula (14) obtained in the distorted wave approximation is accurate within few percent with the results of our coupled channel numerical calculation [Eq. (11)].

In case of the exothermic reaction (such as $c\bar{d}\to d\bar{a}$ or $b\bar{d}\to a\bar{a}$) there is an energy excess in the final channel: $\Delta E_\beta=n\alpha_{HF}$ and $n=1,2$. It follows from Eq. (14) that the cross sections for such reactions behave like d_n/v in the limit $E\to 0$, with $d_n=(\sqrt{2Mn\alpha_{HF}}/M)\exp(2\ \mathrm{Im}\ a\sqrt{2Mn\alpha_{HF}})\sigma_0$. The cross sections of inverse reactions ($d\bar{a}\to c\bar{d}$ or $a\bar{a}\to b\bar{d}$) show a characteristic threshold behavior of type $pd_n/\sqrt{2Mn\alpha_{HF}}$. For increasing energies $E\gg\alpha_{HF}$ all spin-exchange cross sections tend to the same limit. Within the zero-range potential model of strong forces, this limit is given by $\sigma=\exp(4\ \mathrm{Im}\ ap)\sigma_0$.

The remarkable feature of the obtained results is the factorization of the spin-dependent strong-force effect and the long-range atomic interaction [Eq. (14)]. While the first appears through the difference of singlet and triplet *strong-force* scattering lengths, the second is given by the Jost function for the interatomic motion of the $H-\bar{H}$ pair. This later factor $[|1/f_J(0)|^4]$ strongly enhances (approximately 10^9 times) the effect of strong forces, due to focusing of the flux of $p-\bar{p}$ toward each other by the attractive adiabatic potential V_{ad}, whose long range is determined by the tail of the van der Waals interaction.

IV. CONCLUSIONS

In conclusion we found that spin-exchange transitions in $H-\bar{H}$ collisions are caused mainly by the strong force. This mechanism of spin exchange is a unique feature of atom-antiatom interaction, without counterpart in atom-atom collisions. The corresponding transition amplitudes are proportional to the difference between singlet and triplet strong-force scattering lengths, but the cross sections have the molecular scale due to the large enhancement of the strong-force effect; this enhancement (approximately 10^9) originates from the presence of the long-range atom-antiatom interaction. This opens the perspective to study strong force effects in $H\bar{H}$ spin-exchange collisions. The energy behavior of the spin-exchange cross sections turns out to be sensitive to the difference between hyperfine energy levels in H and $\bar{H}$ (which might occur due to *CPT* violation). If such a violation takes place the threshold behavior of the spin-exchange cross sections is radically different in comparison to the *CPT* invariant case. This suggests alternative experimental way of comparing H and $\bar{H}$ hyperfine structures.

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