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Nonadiabatic treatment of hydrogen-antihydrogen collisions

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We present a nonadiabatic treatment of the hydrogen-antihydrogen system. The technique used to describe H-$\bar{\text{H}}$ collisions is based on the coupled-rearrangement-channel method. Within this approach the total, nonadiabatic wave function of the system is divided into two parts: an inner and an outer one. To describe the inner part a set of square-integrable four-body functions is used. These functions are obtained by a diagonalization of the total Hamiltonian projected on a chosen L^2 subspace; they explicitly contain components of various arrangement channels expressed in terms of corresponding Jacobi coordinates. The outer part of the total wave function reflects its asymptotic character. Our procedure leads to a system of nonlocal integrodifferential equations that are solved iteratively and simultaneously determine the outer part of the solution and the coefficients in the four-body expansion of the inner part. To solve these equations the compact fine difference method was applied. Using this formalism we perform a one-channel calculation of the elastic scattering to obtain the S matrix, the nonadiabatic scattering length, and the cross section for the low-energy elastic scattering in the H-$\bar{\text{H}}$ channel.

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I. INTRODUCTION

The studies of interaction of antiatoms with ordinary matter have become possible thanks to the spectacular progress in the production and trapping of cold antihydrogen. In 2011 antihydrogen atoms were trapped for more than 1000 s [1]; this allowed the first spectroscopic measurements for antiatoms in 2012 [2]. In 2013 the first test of the gravitational properties of antiatoms was presented [3] and very recently [4] one has succeeded to demonstrate the prototype of the antihydrogen beam. Experiments with antiatoms can provide us with the information crucial for testing the fundamental symmetries underlying the standard model of physics [3]. The theoretical description of antimatter interacting with matter is centered around the simplest but not yet fully understood benchmark system consisting of hydrogen and antihydrogen atoms [5]. The H-$\bar{\text{H}}$ pair is the simplest neutral atomic system containing both ordinary matter and antimatter. A very important and difficult feature of this system is that unlike H_2 it cannot form a stable molecular structure even at the Coulombic level of description; instead various decay processes are possible. The most important Coulombic process, which competes with processes driven by leptonic and nuclear annihilation, is the rearrangement into protonium and positronium atoms:

$$\text{H} + \bar{\text{H}} \rightarrow \text{Pn(N)} + \text{Ps(n)}. \tag{1}$$

The competing processes include "on the flight" annihilation of hadrons:

$$\text{H} + \bar{\text{H}} \rightarrow e + \bar{e} + \text{annihilation products (photons, pions, etc.)}, \tag{2}$$

leptonic annihilation:

$$\text{H} + \bar{\text{H}} \rightarrow \bar{\text{p}} + \text{p} + 2\gamma \ \text{(or } 3\gamma), \tag{3}$$

and formation of metastable molecular resonances:

$$\text{H} + \bar{\text{H}} \rightarrow \text{H}\bar{\text{H}} + \gamma. \tag{4}$$

Leptonic annihilation (3) is less probable than the hadronic one by three orders of magnitude [6], in spite of the apparently large interleptonic correlation leading to the rearrangement reactions (1). The cross sections for radiative association (4) are also very small [7]. However, the molecular H$\bar{\text{H}}$ resonances can play an important role as the intermediate states during the rearrangement collisions (1). The intermediate H$\bar{\text{H}}$ molecule decays further to positronium and protonium, or via intramolecular annihilation of the proton and antiproton:

$$\text{H} + \bar{\text{H}} \rightarrow \text{H}\bar{\text{H}} \rightarrow \text{Pn(N)} + \text{Ps(n)} \quad \text{or} \quad \text{p} + \bar{\text{p}} + 2\gamma. \tag{5}$$

The four-body H-$\bar{\text{H}}$ system has in the past been treated by means of approximate methods. The first theoretical description was given by means of the Born-Oppenheimer (BO) approximation [8]. In more recent publications the ultracold H-$\bar{\text{H}}$ collisions have been studied by means of the adiabatic distorted-wave approximation [9–11], the optical-potential method [12], the Kohn variational method [13,14], the close-coupling method [15], and the coupled-channel method [16,17].

Though the H-$\bar{\text{H}}$ interaction at interatomic distances exceeding few bohrs could be very precisely described by the adiabatic potential, the description of rearrangement collisions, which occur at distances smaller then ~ 1 a.u. is a nontrivial problem. Below the critical proton-antiproton distance $r_c \approx 0.7$ a.u. [18] the leptons are no longer bound by the proton-antiproton dipole and the rearrangement takes

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place. The existence of the critical distance causes serious problems in the BO-based methods. The BO-based techniques require a choice of the interaction potential for distances smaller than the critical distance. More disturbing is that one cannot systematically improve this description by including adiabatic and off-diagonal corrections, because, as was shown by Strasburger [18] the adiabatic correction to the BO potential is not well defined for this system. So far, the interaction in this region was treated approximatively, using Born-Oppenheimer or optical potentials. One has also attempted the Kohn variational method, which is not based on the BO separation. However, the results previously presented within this approach [13] were obtained in a relatively small basis set.

In the present paper we are trying to overcome these obstacles by employing the fully nonadiabatic description of the four-body system, namely, the coupled-rearrangement-channel method (CRCM). This technique allows one to include different possible arrangement channels of the system under consideration. Moreover the proper asymptotic form of the continuum wave function is ensured, while the inner part of the wave function can still be described with square-integrable basis functions, as in the bound state calculations. The CRCM does not involve any presumptions concerning the adiabaticity of the collision process. In particular, it does not suffer from the presence of the critical distance characteristic for the BO approach and it allows a proper description of the four-body system for any interatomic distance and for any arrangement configuration.

II. NONADIABATIC COUPLED-REARRANGEMENT-CHANNEL METHOD

The system under consideration can, for a given energy, undergo rearrangement to different physical channels which have distinct asymptotic features, i.e., the system can "dissociate" into pairs of different atoms. The two main rearrangement channels which are possible are hydrogen-antihydrogen and protonium-positronium channels. Depending on the total energy of the system in each rearrangement channel several physical channels can be opened, which correspond to various excited states of the fragments and different dissociation limits.

Following [19,20] we represent the total wave function as a sum of two terms. The first term is aimed to describe correctly the asymptotic behavior of the wave functions in all physical channels; the second term is used to describe the inner region of the wave function:

$$\Psi = \sum_{c} \phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)\frac{\chi_c(R_c)}{R_c} + \sum_{v}^{v_{\max}} b_v \Phi_v, \tag{6}$$

where c numbers open physical channels (possibly in different rearrangement channels), $\phi_x^{(c)}$ is a wave function of an isolated atom x in channel c, and $\mathbf{r}_c$ and $\mathbf{q}_c$ are the internal coordinates of the atoms. The yet unknown functions χ_c satisfying the appropriate boundary conditions are added to describe the relative motion of the atoms in each open channel c, and $\mathbf{R}_c$ is the interatomic Jacobi coordinate for this channel.

To facilitate the description of the inner (nonasymptotic) part of the total wave function Ψ a set of auxiliary functions Φ_v is added. It is important to emphasize that functions χ_c are not requested to vanish in the inner region (except for $R_c = 0$). In that way they can contribute to the description of the inner region spanned by functions Φ_v, and at the same time facilitate a smooth transition between the inner and outer regions. As will be seen in following, expansion coefficients b_v and functions χ_c are determined simultaneously via a self-consistent, integrodifferential procedure.

The Φ_v functions are square-integrable and are chosen to be solutions of the following eigenvalue problem of the total Hamiltonian projected onto the subspace P:

$$H_P \Phi_v = E_v \Phi_v. \tag{7}$$

The H_P Hamiltonian is defined as

$$H_P = PHP, \tag{8}$$

where H is the total four-body Hamiltonian of the system and P is a projector operator on some subspace $\mathcal{H}'$ of the total Hilbert space $\mathcal{H}$. $\mathcal{H}'$ is spanned by $L^2(\mathbb{R})$ basis functions and these functions are of the finite range (i.e., they can be considered to vanish at some distance). Since they are used to provide a proper description of the inner part of the wave function, it is not intended to extend the spatial range of these functions when the dimension of P is enlarged. The enlargement of the basis leads to a more complete span of the inner region and gives a procedure allowing the systematic improvement of the accuracy of the obtained solutions Ψ.

The total function (6) must fulfill the time-independent Schrödinger equation with the full four-body Hamiltonian H:

$$(H - E)\Psi = 0. \tag{9}$$

To find both functions χ_c and expansion parameters b_v one is now projecting Eq. (9) onto the atoms' functions in each channel

$$\big\langle \phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)\big|H - E\big|\Psi\big\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c} = 0, \quad \text{for } c = 1,\ldots,N_c, \tag{10}$$

where the subscript in the bracketed notation means that the integration goes over vectors $\mathbf{r}_c,\mathbf{q}_c$ and angular coordinates of the $\mathbf{R}_c$ vector. Similarly one can project (9) onto the Φ_v functions:

$$\langle \Phi_v|H - E|\Psi\rangle = 0, \quad \text{for } v = 1,\ldots,v_{\max}. \tag{11}$$

Using (11) together with (6) and the fact that functions Φ_v are chosen to diagonalize the Hamiltonian H in the subspace P,

$$\langle \Phi_v|H|\Phi_{v'}\rangle = \langle \Phi_v|H_P|\Phi_{v'}\rangle = E_v\delta_{vv'}, \tag{12}$$

we can write the following explicit expression for the expansion parameters b_v:

$$b_v = -\frac{1}{E_v - E}\left\langle \Phi_v \middle| H - E \middle| \sum_{c} \phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)\frac{\chi_c(R_c)}{R_c}\right\rangle. \tag{13}$$

Similarly using (6), (10), and (13) we may write

$$\left\langle \phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)\middle| H - E \middle| \phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)\frac{\chi_c(R_c)}{R_c}\right\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c} + \sum_{c'\neq c}\left\langle \phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)\middle| H - E\middle|\phi_a^{(c')}(\mathbf{r}_{c'})\phi_b^{(c')}(\mathbf{q}_{c'})Y^{(c')}(\hat{R}_{c'})\frac{\chi_{c'}(R_{c'})}{R_{c'}}\right\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c} + \sum_v^{v_{\max}}\left\langle \phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)\middle| H - E\middle| b_v\Phi_v\right\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c} = 0. \tag{14}$$

By representing the total Hamiltonian as a sum of atomic Hamiltonians h_a, h_b, kinetic energy operator of the relative motion $T_{\mathbf{R}}$ and the interaction part $V_{ab}^{\text{int}} = H - T_{\mathbf{R}} - h_a - h_b$ the integration in the first term in (14) can be performed explicitly which leads to the following expression:

$$\left\langle \phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)\middle| H - E\middle|\phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)\frac{\chi_c(R_c)}{R_c}\right\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c} = -\frac{1}{2\mu_c R_c}\left[\frac{d^2}{dR_c^2} - \frac{J(J+1)}{R_c^2} + k_c^2 - U^{(c)}(R_c)\right]\chi_c(R_c), \tag{15}$$

where $k_c^2 = 2\mu_c(E - e_a^{(c)} - e_b^{(c)})$, with μ_c being the reduced mass of the atoms in channel c, and $e_x^{(c)}$ being the energies of the isolated atoms in this channel. The function U in Eq. (18) is given by

$$U^{(c)}(R_c) = 2\mu_c\,\langle\phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)|V_{ab}^{\text{int}}|\phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c}, \tag{16}$$

where h_x stands for a monomer's Hamiltonian, i.e., a Hamiltonian for a two-body Jacobi fragment, which in our case might be hydrogen, antihydrogen, protonium, or positronium atom. One can easily recognize that $U^{(c)}$ is the first-order interaction potential between monomers a and b.

The last term in Eq. (14) is evaluated by inserting (13) which, after additional algebraic manipulations, leads to the following expression:

$$\sum_v^{v_{\max}}\langle\phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)|H - E|b_v\Phi_v\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c} = \sum_{c'}\int_0^\infty R_{c'}\sum_v^{v_{\max}}\langle\phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)|H - E|\Phi_v\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c}\frac{1}{E - E_v} \times\langle\Phi_v|H - E|\phi_a^{(c')}(\mathbf{r}_{c'})\phi_b^{(c')}(\mathbf{q}_{c'})Y^{(c')}(\hat{R}_{c'})\rangle_{\mathbf{r}_{c'}\mathbf{q}_{c'}\hat{R}_{c'}}\,\chi_{c'}(R_{c'})dR_{c'}. \tag{17}$$

Using (15) and (17) in (14) and introducing some new notation we can write the equation for the χ_c function in the following form:

$$\left[\frac{d^2}{dR_c^2} - \frac{J(J+1)}{R_c^2} + k_c^2 - U^{(c)}(R_c)\right]\chi_c(R_c) + \int_0^\infty W^{(cc)}(R_c,R_c')\chi_c(R_c')dR_c' + \sum_{c'\neq c}\int_0^\infty W^{(cc')}(R_c,R_{c'})\chi_{c'}(R_{c'})dR_{c'} = 0. \tag{18}$$

The second term in (18) represents the diagonal ($c = c'$) part of (17), whereas the off-diagonal term of (18) stems from the second term in (14) and the of-diagonal part of (17). The nonlocal kernels $W^{(cc)}$ and $W^{(cc')}$ are responsible for introducing higher order corrections to potential $U^{(c)}$. Equation (18) is the main equation of the nonadiabatic coupled-rearrangement-channel (NACRC) method, which will be used in a later part of the present work. For more detailed derivation and definitions see Appendix A.

III. BOUNDARY CONDITIONS

To solve Eq. (18) one needs to apply the proper boundary conditions for the functions χ_c. Since the second term on the right-hand side of (6) is always finite, and the total wave function Ψ has to be finite at each point, it means that the functions $\chi_c(R_c)$ must vanish at $R_c = 0$. This gives us the boundary conditions at zero

$$\chi_c(0) = 0. \tag{19}$$

The other boundary condition we can use is given by the asymptotic form of the wave functions for large separations between monomers:

$$\lim_{R_c\to\infty}\chi_c(R_c) = u^{(-)}(k_cR_c)\delta_{cc_0} - \sqrt{\frac{v_{c_0}}{v_c}}S_{cc_0}u^{(+)}(k_cR_c), \tag{20}$$

where c_0 denotes the initial channel, and

$$u^{(\pm)}(kR) = Rh_0^{(\pm)}(kR), \tag{21}$$

with $h_J^{(\pm)}$ being the Riccati-Hankel functions [21]. The condition given by (20) is valid for R_c large enough, so the interaction between monomers is negligible. In practice, the boundary condition is implemented by matching the function χ_c to the combination of Hankel functions given on the right-hand side of (20) at a given channel radius $R_c^{\max}$. This combination is, however, given in terms of the unknown (and sought after) S-matrix element. Hence, while the boundary condition (19) can be used explicitly in the numerical procedure, the condition (20) must be rewritten in another form that temporarily eliminates S. To do this, we are assuming that Eq. (20) is fulfilled for some large $R_c^{\max}$

$$\chi_c\left(R_c^{\max}\right) = u^{(-)}\left(k_cR_c^{\max}\right)\delta_{cc_0} - \sqrt{\frac{v_{c_0}}{v_c}}S_{cc_0}u^{(+)}\left(k_cR_c^{\max}\right). \tag{22}$$

The condition (22) is written as a condition at some chosen point $R_c^{\max}$, but the initial condition (20) is given as a functions equality. This means that the analog relation can be written for the first derivative of χ_c,

$$\chi_c'\left(R_c^{\max}\right) = u^{(-)'}\left(k_c R_c^{\max}\right)\delta_{cc_0} - \sqrt{\frac{v_{c_0}}{v_c}} S_{cc_0} u^{(+)'}\left(k_c R_c^{\max}\right). \tag{23}$$

Both conditions (22) and (23) involve the yet unknown scattering matrix element S_{cc_0}; for practical reasons we need to temporarily eliminate it from our equations by combining both boundary conditions (for the function and for the first derivative) together. For $c = c_0$ the resultant condition can be written as

$$\frac{\chi_{c_0}\left(R_{c_0}^{\max}\right) - u^{(-)}\left(k_{c_0} R_{c_0}^{\max}\right)}{u^{(+)}\left(k_{c_0} R_{c_0}^{\max}\right)} = \frac{\chi_{c_0}'\left(R_{c_0}^{\max}\right) - u^{(-)'}\left(k_{c_0} R_{c_0}^{\max}\right)}{u^{(+)'}\left(k_{c_0} R_{c_0}^{\max}\right)} \tag{24}$$

and a similar condition can be written for the $c \neq c_0$ case,

$$\frac{\chi_c\left(R_c^{\max}\right)}{u^{(+)}\left(k_c R_c^{\max}\right)} = \frac{\chi_c'\left(R_c^{\max}\right)}{u^{(+)'}\left(k_c R_c^{\max}\right)}. \tag{25}$$

In the case of the H-$\bar{\text{H}}$ system we can introduce a modification of the boundary condition (20). For the distances much larger than the critical distance r_c the H$\bar{\text{H}}$ system is supposed to be well described within the adiabatic (or Born-Oppenheimer) approximation. This should allow us to impose the boundary conditions at much smaller distances. Since the adiabatic functions possess the correct asymptotic shape it is possible to use them instead of functions h_0 in (20), which will ensure the proper description of the interatomic interaction (including dispersion) at medium and larger distances. In this case the functions $u^{\pm}$ for H-$\bar{\text{H}}$ in (20) need to be replaced by functions $\xi^{\pm}$ defined as

$$\xi^{\pm}(R) = R\varphi^{\pm}(R), \tag{26}$$

where $\varphi^{\pm}(R)$ denotes the Born-Oppenheimer nuclear wave function obtained with the following boundary conditions:

$$\begin{aligned} &\lim_{R\to\infty} \varphi^{\pm}(R) = h_0^{\pm}(kR), \\ &\lim_{R\to\infty} \frac{\mathrm{d}}{\mathrm{dR}}\varphi^{\pm}(R) = \frac{\mathrm{d}}{\mathrm{dR}} h_0^{\pm}(kR). \end{aligned} \tag{27}$$

The $\varphi^{\pm}$ functions were obtained by means of numerical integration of the nuclear Schrödinger equation with the mass-scaled Born-Oppenheimer potential [22]. Since functions $\varphi^{\pm}$ fulfill the condition (27) Eqs. (22) and (23) must be valid for functions $\xi^{\pm}$ in place of $u^{\pm}$, with the same S, but for smaller $R_c^{\max}$.

IV. NUMERICAL RESULTS

We have performed one-channel computations for the elastic scattering in the H-$\bar{\text{H}}$ channel with $J = 0$. Our aim in this paper is to describe the scattering of hydrogen and antihydrogen ground state atoms at low energies. For the collisions at very low energies only the S-wave scattering is contributing to the cross section and scattering length. For this reason in our calculations we only consider zero angular momentum for the relative motion of the atoms. Moreover, since the orbital angular momenta for the ground state atoms is also zero, due to the conservation law the total angular momentum of the four-body system must be $J = 0$. For the calculation of the scattering length (which determines the low-energy limit of the elastic cross section) the collision energy was chosen to be 10^{-9} hartree. For this energy several calculations were done with different lengths of the expansion in (6). The functions used in this expansion are the solutions of the four-body problem that explicitly contain components of the Pn + Ps and H + $\bar{\text{H}}$ arrangement channels. The solution of the four-body problem is described in Appendix B. The value of the scattering matrix element S is obtained by fitting the calculated χ function to the form given by (22) in an asymptotic region. Function χ is obtained as the solution to the integrodifferential equation (18); the method of solving this equation is described in Appendix C. After the iterative procedure of solving the integrodifferential equations (C13) has converged the nonunitarity of S is smaller than one part in 10^8. From the S value, the phase shift δ can be easily computed as

$$\delta = \frac{\ln S}{2i}. \tag{28}$$

Using δ the value of the scattering length can be estimated as

$$a = -\frac{\tan\delta}{k}, \tag{29}$$

where k is a momentum of the relative motion of the monomers.

In the present calculations the boundary condition radius $R^{\max}$ was chosen to be 14 bohrs. In principle we are aiming to make the value of $R^{\max}$ as small as possible so that the proper asymptotic shape of the wave function, which includes dispersion, is "switched on" as soon as possible (i.e., at the smallest distance where its correct form is known). Of course $R^{\max}$ has to be chosen such that the overlap of the leptonic charges can be considered negligible at this distance. Then the total interaction potential is well represented by the asymptotic form of the dispersion energy. To achieve that for the H-$\bar{\text{H}}$ system, $R^{\max}$ must not be smaller than ~12 a.u.

Shrinking of the matching radius to such a small value is possible thanks to the use of modified boundary conditions (24) and (25), where the nuclear Born-Oppenheimer functions $\xi^{\pm}$ replace the Hankel functions $u^{\pm}$. This has two important effects. First, it shrinks the internal configuration space described by the projector P. Therefore, given the number of basis functions, one obtains a much more complete description of the inner rearrangement region. Second, it allows for the correct description of the dispersion interaction in the entire region where the latter occurs.

Let us stress here, that proper asymptotic behavior of the wave function is crucial in the calculations of the scattering length. Since the potential U_c in Eq. (18) is the first-order interaction energy between monomers, it does not, by itself, possess the asymptotic form of the dispersion forces. The dispersion interaction, governed by the well-known $-C_6/R^6$ term, is generated by the integral part of Eq. (18), i.e., by the nonlocal potentials W. However, the pseudostates Φ_v, which constitute integral kernels W, are expanded in the L^2

TABLE I. Scattering length as a function of the expansion size $v_{\max}$.

$v_{\max}$	a (a.u.)
0	3.691
1	5.768
2	6.324
5	7.112
10	7.225
15	7.242
20	7.266
30	7.267
44	7.267

basis set, and this means that information about higher order contribution to the interaction energy is included at most to the distance at which functions Φ_v die out. Therefore, to facilitate the description of dispersion interaction, we move in the boundary conditions point $R^{\max}$ as close as possible to the range of the functions Φ_v, i.e., we have chosen the $R^{\max}$ value to be the same as the spatial extent of the Φ_v functions. In our case this is ∼14–15 bohrs.

Table I presents the convergence of the calculated scattering length a with the size $v_{\max}$ of the four-body expansion used in (6). The value of the scattering length obtained in the present work, $a = 7.3$ bohr, can be compared with the previous result obtained within the Born-Oppenheimer approximation, $a = 8.1$ bohr [10]. This gives an approximately 10% difference between nonadiabatic and BO calculations. The results of the previous calculations which aimed to somehow go beyond the Born-Oppenheimer approximation [12,17] suggested that the value of the scattering length obtained within the BO scheme is overestimated and our present calculations support this observation. The smaller value of the scattering length also implies that the value of the scattering cross section for the elastic collisions should be smaller than in the BO case. Since our result was obtained in one-channel calculations, but with the wave function that explicitly contains the Pn-Ps component, one can draw the conclusion that the presence of closed channels plays a significant role in elastic H-$\bar{\text{H}}$ scattering.

Knowing the value of the scattering matrix S one cannot only calculate the scattering length, which characterizes the zero energy collisions, but also the scattering cross section σ, which is a function of collision energy. For a given J the cross section for scattering from channel c_0 to c is given as

$$\sigma^J_{cc_0} = \frac{\pi}{k^2_{c_0}}(2J+1)\left|\delta_{cc_0} - S^J_{cc_0}\right|^2, \tag{30}$$

where k_{c_0} is a relative momentum of the atoms in the initial channel. In our case we are considering the elastic collisions for $J = 0$, which simplifies the above formula to

$$\sigma^0_{\text{elast}} = \frac{\pi}{k^2_{c_0}}\left|1 - S^0_{c_0c_0}\right|^2. \tag{31}$$

The results for the cross section for the elastic H-$\bar{\text{H}}$ collisions are presented in Fig. 1.

Similarly the cross section for the rearrangement process can be obtained from the scattering matrix elements S_{cc_0} that are explicitly present in our scheme of integrodifferential equations (18); however, this kind of calculation is much more demanding from the numerical point of view.

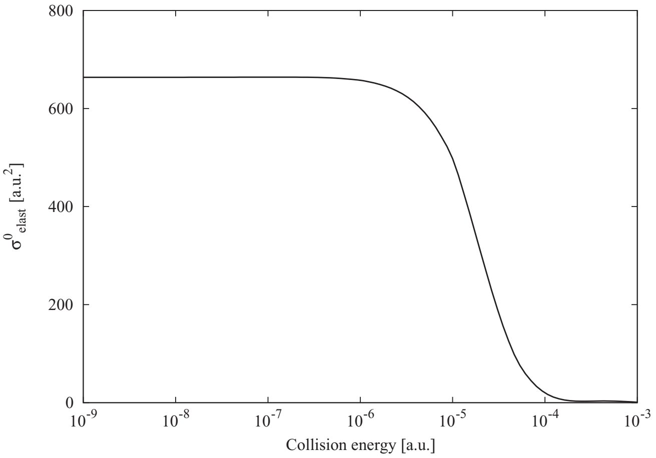

FIG. 1. The cross section for the elastic H-$\bar{\text{H}}$ scattering as a function of the collision energy.

One notices that the elastic cross section shows the correct behavior expected from the general theory of scattering for slow particles, i.e., it tends to the constant value in the low-energy limit. It is also interesting to see what are the contributions of different Φ_v functions to the total wave function Ψ in Eq. (6). For this, in Table II we collected the absolute values of the complex expansion parameters b_v together with the energy differences $E_v - E$. It should be stressed that b_v does not necessarily decrease as $|E_v - E|$ increase. It can be seen that $|E - E_v|$ is one of the factors

TABLE II. Expansion parameters b_v for $R^{\max} = 14$ a.u. and $v_{\max} = 44$.

v	$E_v - E$ (a.u.)	$\lvert b_v \rvert$	v	$E_v - E$ (a.u.)	$\lvert b_v \rvert$
1	0.0002648	2.0581016	23	0.0186578	0.0039995
2	0.0005100	1.9558148	24	0.0213473	0.0225094
3	0.0008304	0.9120635	25	0.0214303	0.0066594
4	0.0012221	0.0057262	26	0.0235457	0.0004833
5	0.0017036	0.4609114	27	0.0248763	0.0110494
6	0.0020820	0.0008963	28	0.0274537	0.0148000
7	0.0022992	0.5510484	29	0.0286673	0.0008758
8	0.0030274	0.4592296	30	0.0300451	0.0023895
9	0.0034076	0.0009672	31	−0.0012953	0.0007571
10	0.0036412	0.0009671	32	−0.0042211	0.0001288
11	0.0038913	0.3267039	33	−0.0050323	0.0000850
12	0.0048078	0.2327922	34	−0.0074774	0.0000151
13	0.0059240	0.1719270	35	−0.0085173	0.0000006
14	0.0064491	0.0078132	36	−0.0107979	0.0000435
15	0.0072433	0.1209706	37	−0.0137106	0.0002640
16	0.0087856	0.0932506	38	−0.0158440	0.0000161
17	0.0100517	0.0020057	39	−0.0185291	0.0000658
18	0.0109006	0.0680535	40	−0.0213553	0.0000434
19	0.0136014	0.0485956	41	−0.0226220	0.0000576
20	0.0140060	0.0069673	42	−0.0229332	0.0000071
21	0.0158479	0.0052012	43	−0.0238608	0.0000094
22	0.0170979	0.0334709	44	−0.0273824	0.0000144

determining the value of b_v, as can be seen in (13), but it is not the only one. The other important factor which determines the value of b_v is the "nature" of the Φ_v function. Functions with "adiabatic nature", whose main contribution has the form of a product of an adiabatic nuclear function and monomers' ground state functions, seem to be of the highest importance.

V. CONCLUSIONS

We have presented the nonadiabatic description of the elastic hydrogen-antihydrogen scattering. The method used here allowed us to provide the proper description of the rearrangement region, i.e., the inner part of the wave function, which caused the main difficulties in the previous calculations. The improvement was possible due to the use of the four-body technique, where the inner part of the wave function is described by explicitly coupling the two most important arrangement channels (i.e., hydrogen-antihydrogen and protonium-positronium channels). At the same time our approach is tailored to assure the proper description of the *outer* part of the wave function. This is achieved by the matching procedure, whereby the inner part is matched to the asymptotically correct wave functions. These functions were obtained within the Born-Oppenheimer approximation so as to properly account for the dispersion interactions in the asymptotic region. It should be stressed that the Born-Oppenheimer functions were used only in the region where the nonadiabaticity of the system under consideration can be neglected, and the total calculation is nonadiabatic in its nature.

The nonadiabaticity in the system under consideration can be seen as originating from different sources. First of all the rearrangement process ($\mathrm{H}+\bar{\mathrm{H}} \to \mathrm{Pn}+\mathrm{Ps}$) by itself is strictly nonadiabatic, since the nuclear motion cannot be decoupled here from the leptonic motion. Of course the many-channel calculations are needed in order to fully describe this process, however, the rearrangement process is not the only source of the nonadiabaticity in the H-$\bar{\mathrm{H}}$ system. In the normal molecular systems, the nonadiabaticity usually occurs when at least two electronic energy levels come close to each other for a given nuclear geometry. In the case of the hydrogen molecule the electronic ground state is well isolated from all other electronic states and the rovibrational levels of the ground state do not overlap with rovibrational levels of excited states. For this reason the H_2 molecule can be considered as an adiabatic system. On the other hand, the situation for the $\mathrm{H}\bar{\mathrm{H}}$ quasimolecule is essentially different. The Born-Oppenheimer potential energy curve for the leptonic ground state as well as the energy curves for the leptonic excited states are attractive for all internuclear distances and tend to minus infinity when the distance between hadrons tends to zero. Because of this feature of the adiabats, the ground leptonic state is not isolated from other (excited) leptonic states and the corresponding rovibrational spectra do overlap to some extent. Therefore the hydrogen-antihydrogen system should be considered nonadiabatic even when the rearrangement process is not explicitly present in the calculations.

One of the benefits of our method is a possibility to improve the accuracy of the four-body calculations for the S matrix in a self-consistent way. We would also like to stress that our method provides a better description of the inner (below ~1 bohr) region than that in the Born-Oppenheimer picture, where a simple Coulombic interaction between nuclei has been adapted below the critical distance. In our procedure no assumptions of this kind are made and forces between all particles are explicitly taken into account.

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APPENDIX A: DERIVATION OF THE NACRC METHOD EQUATIONS

We will discuss here the derivation of Eq. (18) in a more detailed way. The nonlocal kernels $W^{(cc')}$ introduced in (18) can be conveniently written with the help of auxiliary functions V given as

$$V_{cv}(R_c) = \big\langle \phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c)Y^{(c)}(\hat{R}_c)\big| H - E \big|\Phi_v(\mathbf{r}_c,\mathbf{q}_c,\mathbf{R}_c)\big\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c}. \qquad \text{(A1)}$$

Using the above quantity we can write the "diagonal" function $W^{(cc)}$ as

$$W^{(cc)}(R_c,R'_c) = 2\mu_c R_c R'_c \sum_v V_{cv}(R_c)\frac{1}{E-E_v}V_{cv}(R'_c). \qquad \text{(A2)}$$

This quantity is obtained from (17) for $c'=c$. Let us remark that $W^{(cc)}$ can be also written in a form which resembles the expression for the second-order correction in the perturbation theory

$$W^{(cc)} = 2\mu_c R_c R'_c \big\langle \phi_a^{(c)}\phi_b^{(c)}Y^{(c)}\big|(H-E)\mathcal{R}(H-E) \times \big|\phi_a^{(c)}\phi_b^{(c)}Y^{(c)}\big\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c}, \qquad \text{(A3)}$$

where

$$\mathcal{R} = \sum_v \frac{|\Phi_v\rangle\,\langle\Phi_v|}{E-E_v}. \qquad \text{(A4)}$$

Therefore $W^{(cc)}$ can be interpreted as a term which introduces the higher order corrections to the U^c potential.

Functions $W^{(cc')}$, which are responsible for the coupling between different physical channels, consist of two parts

$$W^{(cc')}(R_c,R_{c'}) = W_1^{(cc')}(R_c,R'_c) + W_2^{(cc')}(R_c,R_{c'}), \quad c' \neq c. \qquad \text{(A5)}$$

The first part is defined in a similar way to $W^{(cc)}$ in Eq. (A2), and is obtained from (17) for $c' \neq c$:

$$W_1^{(cc')}(R_c,R_{c'}) = 2\mu_c R_c R'_c \sum_v V_{cv}(R_c)\frac{1}{E-E_v}V_{c'v}(R_{c'}), \quad c' \neq c. \qquad \text{(A6)}$$

The second part, i.e., $W_2^{(cc')}$, is derived from the middle term in (14). When c and c' are different physical channels and they belong to different arrangement channels, the $W_2^{(cc')}$ function is given as

$$\begin{aligned} W_2^{(cc')} &= 2\mu_c R_c R_{c'} \big\langle \phi_a^{(c)}(\mathbf{s},\mathbf{R}_{c'},\mathbf{R}_c)\phi_b^{(c)}(\mathbf{s},\mathbf{R}_{c'},\mathbf{R}_c) Y(\hat{R}_c) \big| H \\ &\quad - E \big| J_{cc'}\phi_a^{(c')}(\mathbf{s},\mathbf{R}_{c'},\mathbf{R}_c)\phi_b^{(c')}(\mathbf{s},\mathbf{R}_{c'},\mathbf{R}_c) Y(\hat{R}_{c'}) \big\rangle_{\mathbf{s}\hat{R}_{c'}\hat{R}_c}, \\ &\quad c' \neq c, \end{aligned} \tag{A7}$$

where $\mathbf{s}$ is $\mathbf{r}_c$ or $\mathbf{q}_c$ and $J_{cc'}$ is a Jacobian of the coordinates transformation connecting channels c and c',

$$d\mathbf{r}_c\, d\mathbf{q}_c\, d\hat{R}_c = J_{cc'}\, d\mathbf{s}\, d\mathbf{R}_{c'}\, d\hat{R}_c. \tag{A8}$$

The explicit form of the transformation (A8) depends on the particular choice of the coordinates used. Two of the new coordinates need to be $\mathbf{R}_c$ and $\mathbf{R}_{c'}$; as for the third vector $\mathbf{s}$ we are free to choose one of the remaining coordinates, namely, $\mathbf{r}_c$, $\mathbf{q}_c$, $\mathbf{r}_{c'}$, or $\mathbf{q}_{c'}$. For the case when c corresponds to the H-$\bar{\text{H}}$ channel and c' to the Pn-Ps channel the most convenient transformations are

$$d\mathbf{r}_{\text{ep}}\, d\mathbf{r}_{\bar{e}\bar{p}}\, d\mathbf{r}_{\text{H}\bar{\text{H}}} = 8\, d\mathbf{r}_{ep}\, d\mathbf{r}_{\text{PnPs}}\, d\mathbf{r}_{\text{H}\bar{\text{H}}} \tag{A9}$$

and

$$d\mathbf{r}_{ep}\, d\mathbf{r}_{\bar{e}\bar{p}}\, d\mathbf{r}_{\text{H}\bar{\text{H}}} = 8\, d\mathbf{r}_{\bar{e}\bar{p}}\, d\mathbf{r}_{\text{PnPs}}\, d\mathbf{r}_{\text{H}\bar{\text{H}}}. \tag{A10}$$

Similarly for the case with c corresponding to the Pn-Ps channel and c' to the H-$\bar{\text{H}}$ the most convenient coordinate transformations are

$$d\mathbf{r}_{e\bar{e}}\, d\mathbf{r}_{p\bar{p}}\, d\mathbf{r}_{\text{PnPs}} = \left(\frac{m_{\text{H}}}{m_p}\right)^3 d\mathbf{r}_{e\bar{e}}\, d\mathbf{r}_{\text{H}\bar{\text{H}}}\, d\mathbf{r}_{\text{PnPs}} \tag{A11}$$

and

$$d\mathbf{r}_{e\bar{e}}\, d\mathbf{r}_{p\bar{p}}\, d\mathbf{r}_{\text{PnPs}} = m_{\text{H}}^3\, d\mathbf{r}_{p\bar{p}}\, d\mathbf{r}_{\text{H}\bar{\text{H}}}\, d\mathbf{r}_{\text{PnPs}}, \tag{A12}$$

where m_{H} and m_p denote hydrogen and proton masses, respectively.

If two different physical channels ($c \neq c'$) belong to the same arrangement channel, then $(\mathbf{r}_c,\mathbf{q}_c,\mathbf{R}_c)$ and $(\mathbf{r}_{c'},\mathbf{q}_{c'},\mathbf{R}_{c'})$ are the same coordinates and the derivations of Eq. (A7) must be changed, leading to the following, somewhat simpler expression:

$$\begin{aligned} W_2^{(cc')}(R_c,R_{c'}) &= 2\mu_c R_{c'} \big\langle \phi_a^{(c)}(\mathbf{r}_c)\phi_b^{(c)}(\mathbf{q}_c) Y(\hat{R}_c) \big| H \\ &\quad - h_a^{(c)} - h_b^{(c)} \big| \phi_a^{(c')}(\mathbf{r}_c)\phi_b^{(c')}(\mathbf{q}_c) Y(\hat{R}_c) \big\rangle_{\mathbf{r}_c\mathbf{q}_c\hat{R}_c} \\ &\quad \times \delta(R_c - R_{c'}). \end{aligned} \tag{A13}$$

APPENDIX B: CALCULATIONS OF THE FOUR-BODY FUNCTIONS

To calculate the four-body functions Φ_v the square-integrable basis functions, constructed with the triple products of the wave functions describing the Jacobi fragments and their relative motions, were used. Let us denote a single basis function used in the expansion of Φ_v by

$$\zeta^{\mathfrak{c}JM}_{\{n\}\{l\}} = \big[\phi^{n_\alpha l_\alpha}_{\mathfrak{c}\alpha}(\mathbf{r}_{\mathfrak{c}\alpha})\phi^{n_\beta l_\beta}_{\mathfrak{c}\beta}(\mathbf{r}_{\mathfrak{c}\beta})\phi^{n_\gamma l_\gamma}_{\mathfrak{c}\gamma}(\mathbf{r}_{\mathfrak{c}\gamma})\big]_{JM}, \tag{B1}$$

where $\mathfrak{c}$ numbers the arrangement channels (H-$\bar{\text{H}}$ or Pn-Ps), and $\mathbf{r}_{\mathfrak{c}x}$ ($x = \alpha,\beta,\gamma$) denotes the Jacobi coordinates for a given channel $\mathfrak{c}$. Symbols $\{n\}$ and $\{l\}$ stand for $\{n_\alpha,n_\beta,n_\gamma\}$ and $\{l_\alpha,l_\beta,l_\gamma\}$, where n_x and l_x denote a "principal" quantum number and angular momentum for coordinate $\mathbf{r}_{\mathfrak{c}x}$. The choice of the functions entering expansions of functions ϕ is described at the end of this section. Here it is sufficient to say that they are constructed by means of expansion in Gaussian and/or oscillating Gaussian functions. Note, however, that since square-integrable functions are used to describe motion in each Jacobi coordinate, all functions ϕ are characterized by a discreet principal quantum number n, even when they correspond to a scattering state.

Symbol $[\cdots]_{JM}$ in (B1) denotes that angular momenta of the functions constituting a triple product are coupled to a total angular momentum J and its projection M. In the present work we are considering states with $J = 0$, so (B1) can be written explicitly as

$$\begin{aligned} \zeta^{\mathfrak{c}00}_{\{n\}\{l\}} &= \big[\phi^{n_\alpha l_\alpha}_{\mathfrak{c}\alpha}(\mathbf{r}_{\mathfrak{c}\alpha})\phi^{n_\beta l_\beta}_{\mathfrak{c}\beta}(\mathbf{r}_{\mathfrak{c}\beta})\phi^{n_\gamma l_\gamma}_{\mathfrak{c}\gamma}(\mathbf{r}_{\mathfrak{c}\gamma})\big]_{00} \\ &= \sum_{\lambda=|l_\alpha-l_\beta|}^{l_\alpha+l_\beta} \sum_{\mu\, m_\gamma} \sum_{m_\alpha\, m_\beta} (l_\alpha m_\alpha, l_\beta m_\beta|\lambda\mu)(\lambda\mu, l_\gamma m_\gamma|00) \\ &\quad \times \phi^{n_\alpha l_\alpha}_{\mathfrak{c}\alpha}(\mathbf{r}_{\mathfrak{c}\alpha})\phi^{n_\beta l_\beta}_{\mathfrak{c}\beta}(\mathbf{r}_{\mathfrak{c}\beta})\phi^{n_\gamma l_\gamma}_{\mathfrak{c}\gamma}(\mathbf{r}_{\mathfrak{c}\gamma}), \end{aligned} \tag{B2}$$

where $(l_\alpha m_\alpha, l_\beta m_\beta|\lambda\mu)$ are Clebsch-Gordan coefficients.

Additionally the four-body basis functions (B2) for the H-$\bar{\text{H}}$ channel were symmetrized using operator $\mathscr{S}$:

$$\begin{aligned} &\mathscr{S}\big[\phi^{n_1 l_1}_{\text{H}}(\mathbf{r}_{ep})\phi^{n_2 l_2}_{\bar{\text{H}}}(\mathbf{r}_{\bar{e}\bar{p}})\phi^{n_3 l_3}_{\text{H}\bar{\text{H}}}(\mathbf{r}_{\text{H}\bar{\text{H}}})\big]_{00} \\ &\quad = \frac{1}{\sqrt{2}}\Big(\big[\phi^{n_1 l_1}_{\text{H}}(\mathbf{r}_{ep})\phi^{n_2 l_2}_{\bar{\text{H}}}(\mathbf{r}_{\bar{e}\bar{p}})\phi^{n_3 l_3}_{\text{H}\bar{\text{H}}}(\mathbf{r}_{\text{H}\bar{\text{H}}})\big]_{00} \\ &\qquad + \big[\phi^{n_2 l_2}_{\text{H}}(\mathbf{r}_{ep})\phi^{n_1 l_1}_{\bar{\text{H}}}(\mathbf{r}_{\bar{e}\bar{p}})\phi^{n_3 l_3}_{\text{H}\bar{\text{H}}}(\mathbf{r}_{\text{H}\bar{\text{H}}})\big]_{00}\Big), \end{aligned} \tag{B3}$$

for $\{l_1,l_2,l_3\} = \{0,0,0\}$ or $\{1,1,0\}$. This symmetrization is done due to the fact that the system under consideration can be symmetric or antisymmetric with respect to the electric charge conjugation operation. Since the symmetric and antisymmetric states do not couple, we are allowed to choose one type and do not include the other. The symmetrization in the Pn-Ps channel is easier to perform; the basis functions with $\{l_1,l_2,l_3\} = \{0,0,0\}$ and $\{1,1,0\}$ are already symmetric, whereas the functions with $\{l_1,l_2,l_3\} = \{1,0,1\}$ and $\{0,1,1\}$ are antisymmetric with respect to the considered transformation. This means that, in this case, the symmetrization is automatically ensured upon the choice of the proper angular momenta configurations. After the symmetrization the total size of the basis set used in the present calculations was 16 320 functions of the form given by (B2).

Finally the four-body wave function Φ is written as an explicit sum of contributions from different rearrangement channels:

$$\Phi = \Phi^{\text{H}\bar{\text{H}}}(\mathbf{r}_{ep},\mathbf{r}_{\bar{e}\bar{p}},\mathbf{r}_{\text{H}\bar{\text{H}}}) + \Phi^{\text{PnPs}}(\mathbf{r}_{e\bar{e}},\mathbf{r}_{p\bar{p}},\mathbf{r}_{\text{PnPs}}), \tag{B4}$$

where each part on the right-hand side of (B4) is represented as a linear combination of symmetrized functions of the form given by (B2):

$$\Phi^{\mathfrak{c}} = \sum_{\{n\}\{l\}} A^{\mathfrak{c}}_{\{n\}\{l\}} \mathscr{S}\zeta^{\mathfrak{c}00}_{\{n\}\{l\}}, \tag{B5}$$

where $\mathscr{S}$ is the symmetrization operator given by (B3) for functions from the H-H̄ channel and by identity for functions from the Pn-Ps channel. The expansion coefficients $A^{\mathrm{c}}_{\{n\}\{l\}}$ are determined by solving the eigenvalue problem for the H_P Hamiltonian:

$$H_P(\Phi^{\mathrm{H\bar{H}}} + \Phi^{\mathrm{PnPs}}) = E(\Phi^{\mathrm{H\bar{H}}} + \Phi^{\mathrm{PnPs}}). \tag{B6}$$

Since both parts of the wave function (B4) are expressed in different Jacobi coordinate systems, one needs to be able to transform between them in order to solve (B6). The explicit transformation between the H-H̄ and Pn-Ps channels is given as

$$\begin{pmatrix} \mathbf{r_{ep}} \\ \mathbf{r}_{\bar{e}\bar{p}} \\ \mathbf{r}_{\mathrm{H\bar{H}}} \end{pmatrix} = \underbrace{\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 1 \\ -\frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{m_{\mathrm{H}}} & \frac{m_p}{m_{\mathrm{H}}} & 0 \end{pmatrix}}_{\mathbb{R}} \begin{pmatrix} \mathbf{r_{e\bar{e}}} \\ \mathbf{r}_{p\bar{p}} \\ \mathbf{r}_{\mathrm{PnPs}} \end{pmatrix}. \tag{B7}$$

Due to this transformation a function which has a form of a product of three Gaussians in coordinates from the H-H̄ channel can be rewritten in the coordinates from the Pn-Ps channel in the following manner:

$$\begin{aligned} &\exp\left(-\alpha r_{ep}^2 - \beta r_{\bar{e}\bar{p}}^2 - \gamma r_{\mathrm{H\bar{H}}}^2\right) \\ &\quad = \exp\left(-a r_{e\bar{e}}^2 - b r_{p\bar{p}}^2 - c r_{\mathrm{PnPs}}^2 - 2f\mathbf{r}_{e\bar{e}}\mathbf{r}_{p\bar{p}} - 2g\mathbf{r}_{e\bar{e}}\mathbf{r}_{\mathrm{PnPs}} \right. \\ &\qquad \left. - 2h\mathbf{r}_{p\bar{p}}\mathbf{r}_{\mathrm{PnPs}}\right), \end{aligned} \tag{B8}$$

where

$$\begin{aligned} a &= \alpha\mathbb{R}_{11}^2 + \beta\mathbb{R}_{21}^2 + \gamma\mathbb{R}_{31}^2, \\ b &= \alpha\mathbb{R}_{21}^2 + \beta\mathbb{R}_{22}^2 + \gamma\mathbb{R}_{32}^2, \\ c &= \alpha\mathbb{R}_{31}^2 + \beta\mathbb{R}_{32}^2 + \gamma\mathbb{R}_{33}^2, \\ f &= \alpha\mathbb{R}_{11}\mathbb{R}_{12} + \beta\mathbb{R}_{21}\mathbb{R}_{22} + \gamma\mathbb{R}_{31}\mathbb{R}_{32}, \\ g &= \alpha\mathbb{R}_{11}\mathbb{R}_{13} + \beta\mathbb{R}_{21}\mathbb{R}_{23} + \gamma\mathbb{R}_{31}\mathbb{R}_{33}, \\ h &= \alpha\mathbb{R}_{12}\mathbb{R}_{13} + \beta\mathbb{R}_{22}\mathbb{R}_{23} + \gamma\mathbb{R}_{32}\mathbb{R}_{33}. \end{aligned} \tag{B9}$$

Of course the transformation (B7) can be reverted and the product of three functions in the Pn-Ps channel can be represented in the H-H̄ channel.

1. Construction of basis functions for Jacobi fragments

The ϕ_{cx}^{nl} functions, constituting the basis functions (B2), are obtained in the prediagonalization procedure as contracts of the primitive Gaussian functions or oscillating Gaussian functions [22]. To expand functions describing hydrogen and positronium atoms, as well as the relative Pn-Ps motion the primitive Gaussian functions of the following form were used:

$$g_{nlm}(\mathbf{r}) = N_{nl} r^l e^{-\nu_n r^2} Y_{lm}(\hat{r}), \tag{B10}$$

where N_{nl} is a normalization constant, Y_{lm} is a spherical harmonics, and ν_n is calculated as

$$\nu_n = \frac{1}{r_{\min}^2}\left(\frac{r_{\min}}{r_{\max}}\right)^{2(n-1)/(n_{\max}-1)} \tag{B11}$$

with $n_{\max}$ being the total number of the primitive Gaussian functions and $r_{\min}, r_{\max}$ being free parameters defining the basis set (see Table III). These parameters are chosen independently for each degree of freedom for each physical channel.

TABLE III. Basis sets used to expand the four-body Φ_v functions.

Channel	$\mathbf{r}_\alpha$	$\mathbf{r}_\beta$	$\mathbf{r}_\gamma$	l_α	l_β	l_γ	$n_\alpha^{\max}$	$n_\beta^{\max}$	$n_\gamma^{\max}$
HH̄	$\mathbf{r}_{pe}$	$\mathbf{r}_{\bar{p}\bar{e}}$	$\mathbf{r}_{\mathrm{H\bar{H}}}$	0	0	0	8	8	120
H-H̄	$\mathbf{r}_{pe}$	$\mathbf{r}_{\bar{p}\bar{e}}$	$\mathbf{r}_{\mathrm{H\bar{H}}}$	1	1	0	8	8	120
Pn-Ps	$\mathbf{r}_{e\bar{e}}$	$\mathbf{r}_{p\bar{p}}$	$\mathbf{r}_{\mathrm{PnPs}}$	0	0	0	8	8	120

Since both protonium wave functions and the wave functions describing the relative motion of the H and H̄ atoms oscillate rapidly for small interparticle distances, it was necessary to use the oscillating Gaussian functions instead of the plain Gaussians for the expansion purpose:

$$\begin{aligned} g_{nlm}^{\mathrm{c}}(\mathbf{r}) &= N_{nl}^{\mathrm{c}} r^l e^{-\nu_n r^2} \cos(\alpha\nu_n r^2) Y_{lm}(\hat{r}), \\ g_{nlm}^{\mathrm{s}}(\mathbf{r}) &= N_{nl}^{\mathrm{s}} r^l e^{-\nu_n r^2} \sin(\alpha\nu_n r^2) Y_{lm}(\hat{r}), \end{aligned} \tag{B12}$$

with $\alpha = \frac{\pi}{2}$. The geometric progression (B11) of the nonlinear parameter of the Gaussian functions (both standard and oscillating) facilitates the "elasticity" of the description of the inner part of the total wave function. The basis set parameters for the primitive Gaussians are collected in Table IV. With these parameters the accuracy in the description of the excited states of protonium with $N = 24$ was better than one part in 10^6. It should also be stressed that the prediagonalized functions span the same space as the original Gaussian functions.

APPENDIX C: SOLVING NACRC METHOD EQUATIONS

To solve Eq. (18) together with conditions (19) and (20) the compact finite difference method (CFDM) is used [23]. To obtain numerical solutions of Eq. (18) we are using a nonuniform grid $\{r_k^{(c)}\}$ in each coordinate R_c and the flowing fifth-order finite difference scheme

$$p^{(k)}v_{k-1}'' + q^{(k)}v_k'' + r^{(k)}v_{k+1}'' = a^{(k)}v_{k-1} + b^{(k)}v_k + c^{(k)}v_{k+1}, \tag{C1}$$

where $v_k = \chi(r_k)$, $v_k'' = \chi''(r_k)$, and parameters a, b, c, p, q, and r are given in terms of the nearest grid steps $h_1 = r_k - r_{k-1}$

TABLE IV. The basis set parameters defining Gaussian functions used in the expansion of the four-body wave functions ($\gamma_{1/2}^{\max}$ is the half width at half maximum of the broadest Gaussian in the given basis set).

Coordinate	Angular momentum	$r_{\min}$ (a.u.)	$r_{\max}$ (a.u.)	$n_{\max}$	$\gamma_{1/2}^{\max}$ (a.u.)
r_{ep} and $r_{\bar{e}\bar{p}}$	0	0.13000	7.2	8	5.99
r_{ep} and $r_{\bar{e}\bar{p}}$	1	0.80000	14.0	8	11.66
$r_{e\bar{e}}$	0	0.35000	20.0	8	16.65
$r_{p\bar{p}}$	0	0.00003	1.7	120	1.42
$r_{\mathrm{H\bar{H}}}$	0	0.00007	6.0	120	5.00
r_{PnPs}	0	1.00000	6.6	8	5.49

and $h_2 = r_{k+1} - r_k$:

$$\begin{aligned} a &= 1, \quad b = -1 - \frac{h_1}{h_2}, \quad c = \frac{h_1}{h_2}, \\ p &= \frac{1}{12}\left(h_1^2 + h_1 h_2 - h_2^2\right), \\ q &= \frac{1}{12h_2}\left(h_1^3 + 4h_1h_2 + 4h_1h_2^2 + h_2^3\right), \\ r &= \frac{1}{12h_2}\left(-h_1^3 + h_1^2 h_2 + h_1 h_2^2\right). \end{aligned} \tag{C2}$$

If the grid steps are uniform ($h_1 = h_2$) one is obtaining a sixth-order CFDM scheme. In order to deal with the boundary conditions the CFDM equations need to be modified. To impose boundary conditions at $R = 0$ we are using the following sixth-order formula with uniform grid around $R = 0$:

$$\frac{h}{12}\left(14v_1'' - 5v_2'' + 4v_3'' - v_4''\right) = v_0 - 2v_1 + v_2, \tag{C3}$$

where $v_0 = \chi(0)$. The boundary conditions for $R^{\max}$ are a bit more cumbersome. First we express $v_N' = \chi'(R^{\max})$ in terms of v_k (on a uniform grid):

$$v_N' = \sum_{k=0}^{5} c_k v_{N-k} + O(h^6), \tag{C4}$$

where

$$\begin{aligned} c_0 &= \frac{137}{60h}, \quad c_1 = -\frac{5}{h}, \quad c_2 = \frac{5}{h}, \\ c_3 &= -\frac{10}{3h}, \quad c_4 = \frac{5}{4h}, \quad c_5 = \frac{1}{5h}. \end{aligned} \tag{C5}$$

Now let us rewrite Eq. (24) as

$$\frac{1}{\beta}v_N - \frac{1}{\beta'}v_N' = \frac{\alpha}{\beta} - \frac{\alpha'}{\beta'}, \tag{C6}$$

where $\alpha = u^{(-)}(R^{\max})$, $\beta = u^{(+)}(R^{\max})$, $\alpha' = u^{(-)'}(R^{\max})$, and $\beta' = u^{(+)'}(R^{\max})$. Including (C4) into (C6) one obtains the following relation:

$$v_N = \sum_{k=1}^{5} \frac{\beta c_k}{\beta' - \beta c_0} v_{N-k} + \frac{\alpha\beta' - \alpha'\beta}{\beta' - \beta c_0}. \tag{C7}$$

A similar relation for boundary condition (25) can be easily obtained from (C7) simply by setting $\alpha = 0$ and $\alpha' = 0$. Now we can use (C7) in the sixth-order CFDM scheme:

$$\begin{aligned} &\frac{h}{12}\left(-v_{N-4}'' + 4v_{N-3}'' - 5v_{N-2}'' + 14v_{N-1}''\right) \\ &\quad = v_{N-2} - 2v_{N-1} + v_N, \end{aligned} \tag{C8}$$

which leads to the following relation:

$$\frac{h}{12}\left(-v_{N-4}'' + 4v_{N-3}'' - 5v_{N-2}'' + 14v_{N-1}''\right) = \sum_{k=1}^{5} d_k v_{N-k} + \gamma, \tag{C9}$$

where

$$d_k = \frac{\beta c_k}{\beta' - \beta c_0} - 2\delta_{k,1} + \delta_{k,2} \tag{C10}$$

and

$$\gamma = \frac{\alpha\beta' - \alpha'\beta}{\beta' - \beta c_0}. \tag{C11}$$

Using Eqs. (C1), (C3), and (C9) we can write

$$\mathbb{M}V'' = \mathbb{A}V + H, \tag{C12}$$

where $V = (v_1, v_2, \ldots, v_{N-1})^T$, $V'' = (v_1'', v_2'', \ldots, v_{N-1}'')^T$, $H = (v_0, 0, \ldots, 0, \gamma)^T$, and $\mathbb{M}, \mathbb{A}$ are $(N-1) \times (N-1)$ matrices of CFDM coefficients. Now let us rewrite Eq. (18) in the following discretized way:

$$V^{(c)''} + \mathbb{F}^{(c)}V^{(c)} + \sum_{c'} G^{(cc')}[V^{(c')}] = 0, \tag{C13}$$

where

$$F^{(c)}_{kk'} = 2\mu_c\left(k_c^2 - \frac{J(J+1)}{r_k^{(c)}} - U^{(c)}\left(r_k^{(c)}\right)\right)\delta_{k,k'} \tag{C14}$$

and

$$G^{(cc')}[V^{(c)}]_k = \int_0^\infty W^{cc'}\left(r_k^{(c)}, P\right)\chi_{c'}(P)\,dP. \tag{C15}$$

Applying (C12) to (C13) one obtains the final expression for $V^{(c)}$:

$$V^{(c)} = -(\mathbb{A} + \mathbb{M}\mathbb{F}^{(c)})^{-1}\left(H + \mathbb{M}\sum_{c'} G^{(cc')}[V^{(c')}]\right). \tag{C16}$$

Since the right-hand side of Eq. (C16) depends on $V^{(c)}$ it needs to be solved iteratively. Functions χ_c obtained in the previous iteration are used to calculate vectors $G^{(cc')}$ for the next step.

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