

Four-body calculations of elastic scattering in H– $\bar{\text{H}}$ collisions

Konrad Piszczatowski · Alexei Voronin · Piotr Froelich

Published online: 29 May 2014

© The Author(s) 2014. This article is published with open access at Springerlink.com

Abstract 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 channels 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 4-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 the system of non-local integro-differential equations that are solved iteratively and simultaneously determine both the shape of the outer part of the wave function and the coefficients in the four-body expansion of the inner part. Using this formalism we perform the one-channel calculation of the elastic scattering to obtain the S-matrix and nonadiabatic scattering length.

Keywords Hydrogen-antihydrogen interaction · Hydrogen-antihydrogen collisions · Nonadiabatic scattering theory

Proceedings of the 11th International Conference on Low Energy Antiproton Physics (LEAP 2013) held in Uppsala, Sweden, 10–15 June, 2013

K. Piszczatowski (✉) · P. Froelich
Department of Chemistry – Ångström Laboratory,
Uppsala University, Box 518,
751-20 Uppsala, Sweden
e-mail: konrad.piszczatowski@gmail.com

P. Froelich
e-mail: piotr.froelich@kemi.uu.se

A. Voronin
P. N. Lebedev Physical Institute,
53 Leninsky prospect, 117924 Moscow, Russia

1 Introduction

The studies of interaction of antiatoms with ordinary matter have become possible thanks to the spectacular progress in the productions and trapping of cold antihydrogen. In 2011 antihydrogen atoms were trapped for ca. 1000 s [1], this in consequence allowed the first spectroscopic measurements for antiatoms, which were performed in 2012 [2]. Experiments with antiatoms can provide us with the information crucial for testing the fundamental symmetries underlying the modern physical [3].

The theoretical description of antimatter interacting with matter is centered around the simplest but not yet fully understood bench-mark system consisting of hydrogen and anti-hydrogen atoms [4]. The $\bar{\text{H}} - \text{H}$ pair is the simplest neutral atomic system containing both the ordinary matter and antimatter. The 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.

This four body system has in the past been treated by means of approximate methods. The first theoretical description of the hydrogen-antihydrogen scattering was given by means of the Born-Oppenheimer approximation [5]. In the more recent publications the ultra-cold $\bar{\text{H}} - \text{H}$ collisions have been studied by means of the adiabatic distorted-wave approximation [6–8], the optical-potential method [9], Kohn variational method [10, 11], close-coupling method [12], and coupled channel method [13, 14].

In the present paper we are trying to improve on the previous treatment by employing the fully nonadiabatic description of the 4-body system, namely the Coupled Rearrangement Channel Method (CRCM). This technique allows to include different possible arrangement channels of the system under consideration.

2 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 monomers. Depending on the total energy of the system, in each rearrangement channel several physical channels can be opened, which correspond to different dissociation limits. The wave function should possess this channel structure, and therefore, following [5, 6] we are representing the total wave function as a sum of two terms.

$$\Psi = \sum_c \phi_a^{(c)}(\mathbf{r}_c) \phi_b^{(c)}(\mathbf{q}_c) Y^{(c)}(\hat{R}_c) \frac{\chi_c(R_c)}{R_c} + \sum_v b_v \Phi_v, \quad (1)$$

where c labels open physical channels (possibly in different rearrangement channels), $\phi_x^{(c)}$ is a wave function of an isolated monomer x in channel c , \mathbf{r}_c and \mathbf{q}_c are the internal coordinates of the monomers, the yet unknown functions χ_c satisfying the appropriate boundary conditions are added to describe the relative motion of the monomers in each open channel c . The Φ_v functions are square-integrable and are chosen to be solutions of the eigenvalue problem of the total 4-body Hamiltonian projected onto subspace P that is spanned by the L^2 basis functions

$$H_P \Phi_v = E_v \Phi_v. \quad (2)$$

The H_P Hamiltonian is defined as $H_P = P H P$.

Function (1) must fulfill the time-independent Schrödinger equation with the total 4-body Hamiltonian H

$$(H - E)\Psi = 0 \tag{3}$$

By projecting (3) onto the monomers' functions in each channel and onto the Φ_v functions one can find the equations for the functions χ , which in the case when only one channel is opened take form of the following integro-differential equation

$$\left[-\frac{d^2}{dR^2} + \frac{J(J+1)}{R^2} - k^2 + U(R) \right] \chi(R) = \int_0^\infty W(R, R') \chi(R') dR' \tag{4}$$

where $k^2 = 2\mu(E - e_a - e_b)$. The function U in equation (4) is given by

$$U(R) = 2\mu \langle \phi_a(\mathbf{r}) \phi_b(\mathbf{q}) | H - h_a - h_b | \phi_a(\mathbf{r}) \phi_b(\mathbf{q}) \rangle_{\mathbf{r}\mathbf{q}\hat{R}}, \tag{5}$$

where h_x stands for a monomer's Hamiltonian. One can easily recognize that U is the first order interaction potential between monomers a and b . The non-local integral kernel W can be written in a form which resembles the expression for the second order correction in the perturbation theory

$$W = \langle \phi_a(\mathbf{r}) \phi_b(\mathbf{q}) Y(\hat{R}) | (H - E) \mathcal{R} (H - E) | \phi_a(\mathbf{r}) \phi_b(\mathbf{q}) Y(\hat{R}) \rangle_{\mathbf{r}\mathbf{q}\hat{R}}, \quad \text{where } \mathcal{R} = \sum_v \frac{|\Phi_v\rangle \langle \Phi_v|}{E - E_v}. \tag{6}$$

The scattering boundary condition can be imposed on the asymptotic form of the wave function:

$$\lim_{R \rightarrow \infty} \chi(R) = u^{(-)}(kR) - S u^{(+)}(kR), \tag{7}$$

where $u^{(\pm)}(kR) = R h_0^{(\pm)}(kR)$, with $h_j^{(\pm)}$ being the Ricatti-Hankel functions.

3 Results

We have performed one-channel computations for the elastic scattering in the H- $\bar{\text{H}}$ channel with $J = 0$. To obtain the scattering length the collision energy was chosen to be 10^{-9} hartree. For this energy several calculations were done with different length of the expansion in (1). Functions Φ_v entering this expression have been obtained by diagonalizing the 4-body matrix eigenvalue problem in the basis of 16 320 functions. The value of the scattering matrix element S is obtained by matching the calculated χ function to the form given by (7) in an asymptotic region. The integro-differential (4) was solved by means of the compact finite difference method [15]. From the S value, the phase shift δ can be easily computed as

$$\delta = \frac{\ln S}{2i}. \tag{8}$$

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

$$a = -\frac{\tan \delta}{k}, \tag{9}$$

where k is a momentum of the relative motion of the monomers. 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 [7]. This gives approximately 10 % difference between nonadiabatic and BO calculations.

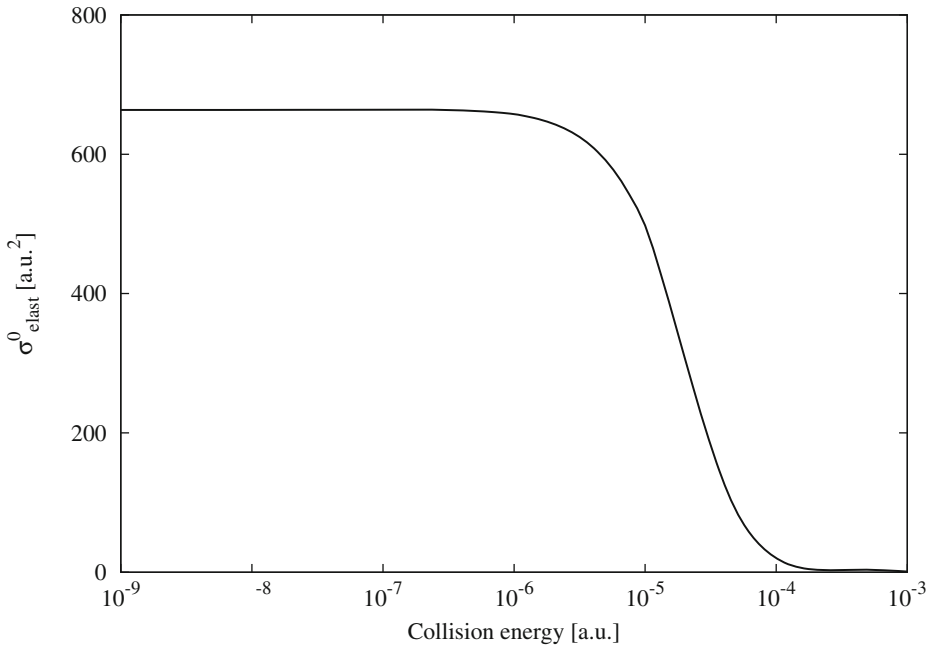


Fig. 1 The cross-section for the elastic H- $\bar{\text{H}}$ scattering as a function of the collision energy

Knowing the value of the scattering matrix S one can not only calculate the scattering length, which characterizes the zero energy collisions, but also the scattering cross-section σ , which is a function of the collision energy. In our case we are considering the elastic collisions for $J = 0$, and the cross-section for the elastic scattering is given by

$$\sigma_{\text{elast}}^0 = \frac{\pi}{k^2} |1 - S|^2. \quad (10)$$

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

4 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 of the two most important arrangement channels (i.e., hydrogen–antihydrogen and protonium–positronium). One of the benefits of our method is a possibility to improve the accuracy of the 4-body calculations for the S-matrix in a self-consistent way. The present method provides much better description of the inner (below ca. 1 bohr) region than it is done in the Born-Oppenheimer picture, where simple Coulombic interaction between nuclei has been adapted to described the nuclear motion below the critical distance (i.e., the distance below

which the leptons are no longer bound by the proton-antiproton dipole). In our procedure no assumptions of this kind are made and forces between all particles are explicitly taken into account.

Open Access This article is distributed under the terms of the Creative Commons Attribution License which permits any use, distribution, and reproduction in any medium, provided the original author(s) and the source are credited.

References

1. The ALPHA Collaboration: *Nat. Phys.* **7**, 558 (2011)
2. Amole, C., Ashkezari, M.D., Baquero-Ruiz, M., Bertsche, W., Bowe, P.D., Butler, E., Capra, A., Cesar, C.L., Charlton, M., Deller, A., et al.: *Nature* **483**, 439 (2012)
3. The ALPHA Collaboration, Charman, A.E.: *Nat. Commun.* **4**, 1785 (2013)
4. Froelich, P.: *Adv. Quantum Chem.* **41**, 185 (2002)
5. Kołos, W., Morgan, D.L., Schrader, D.M., Wolniewicz, L.: *Phys. Rev. A* **11**, 1792 (1975)
6. Froelich, P., Jonsell, S., Saenz, A., Zygelman, B., Dalgarno, A.: *Phys. Rev. Lett.* **84**, 4577 (2000)
7. Jonsell, S., Saenz, A., Froelich, P., Zygelman, B., Dalgarno, A.: *Phys. Rev. A* **64**, 052712 (2001)
8. Froelich, P., Jonsell, S., Saenz, A., Eriksson, S., Zygelman, B., Dalgarno, A.: *Phys. Rev. A* **70**, 022509 (2004)
9. Zygelman, B., Saenz, A., Froelich, P., Jonsell, S.: *Phys. Rev. A* **69**, 042715 (2004)
10. Armour, E., Chamberlain, C.: *Few-Body Syst.* **31**, 101 (2002)
11. Liu, Y., Martin, G.D.R., Armour, E.A.D., Chamberlain, C.W.: *Nucl. Instr. Meth. B* **221**, 1 (2004)
12. Sinha, P., Ghosh, A.: *Europhys. Lett.* **49**, 558 (2000)
13. Voronin, A., Carbonell, J.: *Hyperfine Interact* **115**, 143 (1998)
14. Voronin, A., Carbonell, J.: *Nucl. Inst. Methods B* **214**, 139 (2004)
15. Zhao, J., Corless, R.M.: *App. Math. Comput.* **177**, 271 (2006)