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Quantum-semiclassical approach for treating excitation and ionization of hydrogen-like atoms and ions in collisions with heavy particles

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Abstract. We have developed a quantum-semiclassical approach for treating dynamics of few-dimensional quantum systems. In this approach the problem is reduced to Schrödinger-like equations for some degrees of freedom which integrated symphoniously with the classical equations describing the remaining part. This approach was successfully applied for treating self-ionization of hydrogen-like ions in magnetic fields, break-up of some halo nuclei and for excitation and ionization of helium ions by protons. Here we present the method application to calculation of ionization and excitation/deexcitation of helium ions by slow antiprotons. The calculated cross sections are important for experimental investigations in antiproton physics and provide a strong challenge to theory. The method can be applied for other actual problems in few body physics.

Keywords: computational methods, transition probabilities.

1. Introduction

The idea to simultaneously treat quantum and classical degrees of freedom goes back to Refs. [1, 2] where it was applied to the collisional dynamics of molecular processes. One can also note the similar self-consistent classical-quantal treatment of muon capture by the hydrogen atoms [3] and time-dependent calculations of the atomic hydrogen ionization by antiproton impact [4].

Following this idea we have developed quantum-semiclassical approach for treating different quantum dynamics in three-body collisions and two-body charged systems in magnetic fields [5, 6]. Key element of the approach is the integration of the arising time-dependent 3D Schrödinger equation for which we have developed an efficient computational split-operator scheme with non-direct product discrete-variable approximation (npDVR) for angular variables [7–9]. Here, we apply this scheme to calculation of ionization and excitation/deexcitation of helium ions by slow antiprotons - an actual problem of antiproton physics.

2. Computational scheme

We present here the key elements of the computational scheme in application to the reactions

$$(\mathrm{He}^+)_{n_i l_i} + \overline{p} \rightarrow e + He^{++} + \overline{p},$$

and

$$(\mathrm{He}^+)_{n_i l_i} + \overline{p} \rightarrow (\mathrm{He}^+)_{n_f l_f} + \overline{p}.$$

These transitions are effected by the time-dependent Coulomb field between the He^+ and the antiproton.

We describe the collisions by the 3D time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = \left[H_0(\boldsymbol{r}) + V(\boldsymbol{r},\boldsymbol{R}(t))\right]\,\psi(\boldsymbol{r},t) \tag{1}$$

coupled with the classical Hamiltonian equations for the antiproton degrees of freedom $\boldsymbol{R}(t)$. Here, the wave packet $\psi(\boldsymbol{r},t)$ corresponds to the relative motion of the electron and the helium nucleus. In the above expression,

$$H_0 = -\frac{1}{2\mu}\triangle_{\boldsymbol{r}} - \frac{2}{r}$$

is the internal Hamiltonian of He^+ with reduced mass $\mu = m_e m_{\mathrm{He}}/M$, where m_e and m_{He} are the masses of the electron and helium nucleus, respectively, and $M = m_e + m_{\mathrm{He}}$. The interaction of the projectile $\overline{p}$ with the target He^+ is given by

$$V(\boldsymbol{r},t) = -\frac{2}{\mid \boldsymbol{R}(t) + m_e\boldsymbol{r}/M \mid} + \frac{1}{\mid \boldsymbol{R}(t) - m_{\mathrm{He}}\boldsymbol{r}/M \mid}, \tag{2}$$

where $\boldsymbol{R}(t)$ is the relative coordinate between the projectile and the center-of-mass of the target. The Schrödinger equation (1) is integrated simultaneously with the classical Hamilton equations

$$\frac{d}{dt}\boldsymbol{P}(t) = -\frac{\partial}{\partial \boldsymbol{R}} H_{cl}(\boldsymbol{P}(t),\boldsymbol{R}(t)),$$

$$\frac{d}{dt}\boldsymbol{R}(t) = \frac{\partial}{\partial \boldsymbol{P}} H_{cl}(\boldsymbol{P}(t),\boldsymbol{R}(t)),$$

where

$$H_{cl}(\boldsymbol{P},\boldsymbol{R}) = \frac{1}{2M_0}\boldsymbol{P}^2 + H_0(\boldsymbol{p},\boldsymbol{r}) + \langle\psi(\boldsymbol{r},t) \mid V(\boldsymbol{r},\boldsymbol{R}) \mid \psi(\boldsymbol{r},t)\rangle,$$

with $M_0 = m_p M/(m_p + M)$. The computational scheme includes the coupling $\langle \psi(\boldsymbol{r}, t) \mid V(\boldsymbol{r}, \boldsymbol{R}) \mid \psi(\boldsymbol{r}, t) \rangle$ between the electron and antiproton variables and conserves the total energy of the system.

We use npDVR on the subspace grid (θ_i, ϕ_i) for the angular variables of the electron coordinate $\boldsymbol{r}$ [9]. This yields a diagonal representation for the interaction $V(r, \theta_i, \phi_i, t)$ between the projectile and the target. As a consequence, the problem is reduced to the Schrödinger-type time-dependent radial equations coupled only through the nondiagonal angular part of the kinetic energy operator. This equation is propagated using a split-operator method, which permits fast diagonalization of the remaining nondiagonal part [8, 9]. For discretizing with respect to the radial variable r, a sixth-order finite-difference approximation on a quasi-uniform grid is used. The scheme is unconditionally stable, maintains unitarity, and has the same order of accuracy as the conventional Crank-Nickolson algorithm [9]. It allows a full 3D quantal treatment of the electronic motion during the collisions. The only additional simplification is the use of the classical approximation for the relative projectile-target trajectory $\boldsymbol{R}(t)$, which is

Table 1
Excitation/deexcitation $\sigma_{ex}(n_i l_i, n_f)$ and ionization $\sigma_{ion}(n_i l_i)$ cross sections from the initial states $n_i l_i = 1s, 2s, 2p$ of the He^+ for a few antiproton energies $E_{\overline{p}}$ (in units of 10^{-18} cm^2). The cross sections are calculated for final $n_f = 1, ..., 10$ and summed over final quantum numbers l_f and m_f of the He^+.

$E_{\overline{p}}$	100 keV			10 keV			1 keV		
	1s	2s	2p	1s	2s	2p	1s	2s	2p
1		0.68	2.46		0.67	1.07		1.18	0.16
2	8.03			3.99			1.65		
3	1.59	186.	233.	0.927	190.	202.	0.451	144.	122.
4	0.580	34.4	41.0	0.370	57.8	59.9	0.155	41.4	35.8
5	0.279	12.8	15.1	0.188	24.0	24.1	0.120	29.8	24.9
6	0.156	6.37	7.42	0.108	12.6	12.5	0.066	15.3	13.0
7	0.096	3.67	4.27	0.067	7.53	7.42	0.045	9.88	8.47
8	0.064	2.35	2.73	0.045	4.90	4.82	0.031	6.55	5.61
9	0.044	1.58	1.82	0.031	3.34	3.28	0.023	4.55	3.89
10	0.032	1.12	1.30	0.023	2.40	2.35	0.016	3.26	2.77
ion	9.76	93.6	103.	4.73	180.	162.	1.64	90.0	73.1

physically well-justified for the range of the velocities considered in the present work.

Our scheme has principal advantage as compared with the previous classical-quantal approaches [1–4]. In previous calculations, the Schrödinger equation was solved with an expansion in spherical harmonics. Therefore it requires analytical treatment of the angular part of the necessary integrals. In such a scheme, the matrix elements H_{cl} can be calculated only with a multipole expansion of the time-dependent potential (2) [1,2], which in some kinematical regions can be a challenging computational problem. Our approach is free from this drawback since in npDVR the matrix (2) is diagonal, and the diagonal elements are simply the values of the potential $V(\boldsymbol{r}, t)$ at the angular grid points.

3. Ionization and excitation/deexcitation of hydrogen and helium in slow collisions of antiprotons

We apply here our scheme for computation of the ionization and excitation/deexcitation cross sections of He^+ in slow collisions with antiprotons: see Table 1. Particularly, we have calculated for the first time the excitation cross sections from the initial states $n_i = 1, 2$ to all possible excitations up to n_f=10.

There has been done a large number of theoretical studies of the $\overline{p}$-H and $\overline{p}$-He^+. However, more or less convergent results were obtained only for ionization in the collisions $\overline{p}$-H(1s) and $\overline{p}$-He^+(1s) from the ground states and also some attempts were done for collisions $\overline{p}$-He^+(2s) from $2s$ excited state (see [10–12] and Refs. therein).

4. Conclusions

We have calculated cross sections of ionization and excitation/deexcitation of helium ions by slow antiprotons. The cross sections are in demand in experimental investigations in antiproton physics. The developed quantum-semiclassical approach opens, thanks to its efficiency and flexibility, unique possibilities for treating different cascade processes and other actual problems of few-body physics.

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