Quantum scattering problem without partial-wave analysis

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We have suggested a method for treating different quantum few-body dynamics without usual partial-wave analysis. With this approach new results were obtained in the physics of ultracold atom-atom collisions and ionization and excitation/deexcitation of helium ions. The developed computational scheme opens new possibilities for analysis the actual problem of ultracold atom wave-packets collisions in strong laser or magnetic confinement.

I. INTRODUCTION

In our papers [1, 2] an alternative approach to the conventional partial-wave analysis was suggested to represent the few-dimensional Schrödinger equation on the basis constructed from the eigenfunctions of the angular momentum square operator defined on the angular grid in the spirit of the discrete variable representation (DVR) [3] or the Lagrange-mesh method [4].

To construct the basis orthogonal on the angular grid for one angular variable is a solvable problem if to chose the grid points coinciding with the nodes of the Gauss quadrature. Different kinds of the one-dimensional DVR or Lagrange-meshes are broadly applied for quantum computations[3, 4] due to the simplicity and efficiency of this approach. However, an extension of this representation to the two-dimensional case (two angles $\theta$ and $\phi$ of the unit sphere) is a nontrivial problem. Actually, the simple idea to construct the two-dimensional DVR as a direct product of two one-dimensional DVRs leads to essential complication of the matrix of the angular part of the kinetic energy operator. As a result, the advantages of the one-dimensional DVR, its simplicity and efficiency, are loosing [3]. Another way to construct two-dimensional DVR on an unit sphere is to use the spherical harmonics defined on the two-dimensional grid. However, at that it becomes not possible to satisfy the orthogonality conditions for all the elements of the fixed set of this basis on the chosen grid. To overcome this difficulty we have suggested [5, 9] to use the basis of the orthogonalized combinations of the spherical harmonics on the two-dimensional grid over $\theta$ and $\phi$ variables. It happened that this idea was very efficient for the time-dependent Schrödinger equation with three nonseparable spatial variables [5]. Particularly, it has permitted to get with this approach a few important results in problems of the atomic interaction with strong external electric and magnetic fields[2, 5, 6], the Coulomb breakup of halo nuclei [7–9].

Recently, we have extended this method to the problem of the stripping and excitation of helium ions by protons[10] and antiprotons. We also analysed for the first time the three-dimensional anisotropic scattering in the problem of ultracold atom-atom collisions in a laser field [11, 12].

II. BREAKUP PROCESSES AND ULTRACOLD COLLISIONS

A. Ionization and excitation/deexcitation of helium ions in slow collisions with antiprotons

Experimental investigation of the collisions for slow antiprotons ($\overline{p}$) with hydrogen and helium becomes an actual problem for antiproton physics. It provides a strong challenge to the-
ory. Actually, there has been done a large number of theoretical studies of the $\bar{p}$-H and $\bar{p}$-He$^+$ recently. However, more or less convergent results were obtained only for ionization in the collisions $\bar{p}$-H(1s) and $\bar{p}$-He$^+$(1s) from the ground states (where there is an agreement within about 20% between the existing calculations) and also some attempts were done for $\bar{p}$-He$^+$(2s) (see [13] and Refs. therein).

We have obtained new theoretical results for ionization and excitation/deexcitation processes in slow collisions ($100 \text{ keV} \geq E_\bar{p} \geq 0.1 \text{ keV}$) of $\bar{p}$ with H and He$^+$ (some of them are given in the Table I). Particularly, we have calculated for the first time the cross sections from the initial states with all possible $(l_i, m_i)$ $\neq 0$ to all possible excitations up to $n_f=10$. The developed quantum time-dependent approach based on our ideas suggested in [5, 10] opens, thanks to its efficiency and flexibility, unique possibilities for treating different cascade processes in antiproton physics.

| $E_\bar{p}$ | 100 keV | 10 keV | 1 keV |
|---------|---------|--------|--------|
| $n_l/\ell$ | 1s | 2s | 2p | 1s | 2s | 2p | 1s | 2s | 2p |
| $n_f = 1$ | 0.920 | 0.920 | 0.667 | 1.07 | 8.66 | 8.66 |
| $n_f = 2$ | 8.03 | 3.99 | 3.99 |
| $n_f = 3$ | 1.59 | 186.0 | 186.0 | 0.927 | 190.0 | 202.0 | 0.927 | 145.0 | 145.0 |
| $n_f = 4$ | 0.580 | 34.3 | 34.3 | 0.370 | 57.8 | 59.9 | 0.370 | 36.8 | 36.8 |
| $n_f = 5$ | 0.279 | 12.8 | 12.8 | 0.188 | 24.0 | 24.1 | 0.188 | 33.2 | 33.2 |
| $n_f = 6$ | 0.156 | 63.6 | 63.6 | 0.108 | 12.6 | 12.5 | 0.108 | 15.8 | 15.8 |
| $n_f = 7$ | 0.096 | 3.67 | 3.67 | 0.067 | 7.53 | 7.42 | 0.067 | 9.74 | 9.74 |
| $n_f = 8$ | 0.064 | 2.35 | 2.35 | 0.045 | 4.90 | 4.82 | 0.045 | 6.57 | 6.57 |
| $n_f = 9$ | 0.044 | 1.58 | 1.58 | 0.031 | 3.34 | 3.28 | 0.031 | 4.65 | 4.65 |
| $n_f = 10$ | 0.032 | 1.12 | 1.12 | 0.023 | 2.40 | 2.35 | 0.023 | 3.45 | 3.45 |
| ionization | 9.76 | 93.0 | 93.0 | 4.73 | 180.0 | 162.0 | 4.73 | 86.6 | 86.6 |

B. Anisotropy effects in control of ultracold atom-atom collisions by laser fields

Possible controlling the atom-atom interaction of quantum gases is an important problem of Bose-Einstein condensation (BEC) at ultralow temperatures. Applying for that near resonant lasers, radio frequency fields, Feschbach resonances induced by a magnetic field, and static electric fields are broadly discussed [14]. We have suggested an alternative possibility: to use a nonresonant laser field [11]. Including into consideration the finiteness of the laser wavelength $\lambda_L$ or the alteration of the laser polarization makes the problem of the atom-atom collisions in the laser field nonseparable over both angular variables $\theta$ and $\phi$ (scattering angles). It leads to essentially anisotropic scattering and has demanded to extend our scheme for a nonseparable three-dimensional stationary scattering problem [11].

With this approach we have found considerable influence of a nonresonant optical laser of intensity $I \geq 10^5 \text{W/cm}^2$ on the Cs-Cs ultracold collisions. In such field the scattering becomes
strongly anisotropic even in the region of ultra-low colliding energies where the s-wave dominates at $I = 0$. I.e. the usual scattering length approach $f(k, \hat{k}_i, \hat{k}_f) = -a_0$ does not work and one has to analyze the stability of BEC for unusual behavior of the amplitude $f(k, \hat{k}_i, \hat{k}_f) = f(\hat{k}_i, \hat{k}_f)$ at $k \to 0$. At that the amplitude may be strongly dependent on the $\lambda_L$, on the relative atom-atom orientation with respect to the field $\hat{k}_i$ and on the scattering angle $\hat{k}_f$ [12].

The developed computational scheme opens new possibilities for study the actual problem of few-dimensional wave-packets collisions in the strong confinement induced by laser or magnetic traps.

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