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Some applications of the Faddeev–Yakubovsky equations to the cold-atom physics

Quelques applications des équations de Faddeev–Yakubovsky à la physique des atomes froids

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ABSTRACT

We present some recent applications of the Faddeev–Yakubovsky equations in describing atomic bound and scattering problems. We consider the scattering of a charged particle X by atomic hydrogen with special interest in $X = p, e^{\pm}$, systems of cold bosonic molecules and the bound and scattering properties of $N = 3$ and $N = 4$ atomic ^{4}He multimers.

RÉSUMÉ

Nous présentons quelques applications récentes des équations de Faddeev–Yakubovsky pour décrire des systèmes atomiques et moléculaires. Nous avons considéré la diffusion d'une particule chargée X par l'atome d'hydrogène avec un intérêt spécial pour les cas $X = p, e^{\pm}$, des systèmes de molécules bosoniques ainsi que les propriétés des états liés et de diffusion des $N = 3$ et $N = 4$ atomes d'^{4}He.

1. Introduction

The Faddeev–Yakubovsky (FY) equations constitute a rigorous mathematical formulation of the quantum mechanical N-body problem in the framework of non-relativistic dynamics. They allow obtaining exact solutions – in the numerical sense – of the Schrödinger equation for bound and scattering states, in principle for an arbitrary number of particles. They were first formulated as integral equations in momentum space by Faddeev in the early sixties [1], in the context of 3-nucleon problem with short range interactions, and were generalized some years latter to an arbitrary number (N) of particles by Yakubovsky [2].

A substantial progress in their numerical solution was made when the boundary conditions in the configuration space were established for $N = 3$ in [3–5] and for $N > 3$ in [6]. A reformulation of the original Faddeev equations, allowing to incorporate long range Coulomb-like interactions was derived in [7,8]. A brief review of the different steps in elaborating the Faddeev–Yakubovsky approach to N-body problem can be found in [9].

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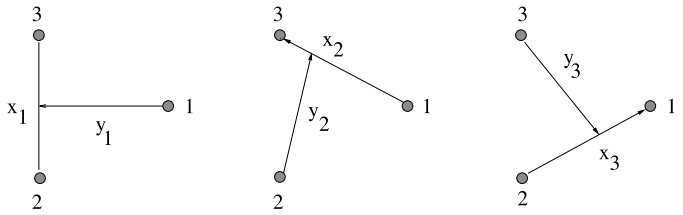

Fig. 1. Sets of three-particle Jacobi coordinates.

Until now only $N = 3$ and $N = 4$ systems have been explored, although there is no any formal nor practical impediment to go beyond. Nowadays very accurate FY solutions have been obtained for the bound state problems on hadronic, nuclear and atomic systems, in configuration as well as in momentum space [10–14], still with a smaller accuracy than the variational methods. The real advantage in using the FY equations, which was also their original motivation, is in describing on the same foot the scattering states. They play there an unavoidable role, especially when many channels are open including the break-up ones (dissociation into more than two clusters). At present, there exist three-body reliable scattering results in nuclear and atomic physics including the break-up process [15–19]. In the four-body case, the progress remains limited to elastic and rearrangement $1+3$ and $2+2$ particle channels in nuclear and atomic problems [20,21,13,22,12,23].

We present in this contribution some recent applications of the Faddeev–Yakubovsky formalism to describe cold atomic structures. A short introduction to the Faddeev equations is given in Section 2. Section 3 is devoted to present some results of a charged particle interacting with atomic hydrogen, with special interest in the p–H (or H_2^+ molecular ion) and $e^{\pm}$–H systems. We study in Section 4 universal properties of the weakly bound $N = 3$ and $N = 4$ cold bosonic molecules. Some results concerning ^{4}He atomic multimers are given in Section 5. The last section is devoted to drawing some conclusion and perspectives.

2. The formalism

We will develop in what follows the main ideas of the Faddeev equations for solving the three-body problem in configuration space. This form is the best adapted to deal with atomic problems. Let us consider three different spinless particles with masses m_i, coordinates $\vec{r}_i$ and denote by $(\vec{x}_i, \vec{y}_i)$ the three different sets of Jacobi coordinates defined by

$$\vec{x}_i = \sqrt{\frac{2m_j m_k}{m_0(m_j+m_k)}}(\vec{r}_j - \vec{r}_k), \quad i = 1,2,3 \tag{1}$$

$$\vec{y}_i = \sqrt{\frac{2m_i(m_j+m_k)}{m_0 M}}\left[\vec{r}_i - \frac{m_j\vec{r}_j + m_k\vec{r}_k}{m_j+m_k}\right] \tag{2}$$

where (ijk) denotes a cyclic permutation of the particle numbers (123), $M = m_1 + m_2 + m_3$ is the total mass of the system and m_0 an arbitrary mass to be fixed at convenience. We will also assume that these particles interact via pairwise short range local potentials $V_i(x_i)$ vanishing at some distance R_i.

The dynamics of the system can be alternatively described by $\{\vec{r}_i\}_{i=1,2,3}$ or by choosing one of the Jacobi coordinate sets $(\vec{x}_i, \vec{y}_i)$, completed by the center of mass coordinate $\vec{R}$

$$M\vec{R} = m_1\vec{r}_1 + m_2\vec{r}_2 + m_3\vec{r}_3$$

The three-body Hamiltonian is assumed to have the form

$$\mathcal{H} = \mathcal{H}_0 + V \tag{3}$$

where $\mathcal{H}_0$ is the kinetic energy which can be written in one of these forms

$$\mathcal{H}_0 = -\frac{\hbar^2}{2}\left(\frac{1}{m_1}\Delta_{\vec{r}_1} + \frac{1}{m_2}\Delta_{\vec{r}_2} + \frac{1}{m_3}\Delta_{\vec{r}_3}\right) = -\frac{\hbar^2}{m_0}\left[\Delta_{\vec{x}_i} + \Delta_{\vec{y}_i} + \frac{m_0}{2M}\Delta_{\vec{R}}\right]$$

and V the total potential

$$V = V_1(x_1) + V_2(x_2) + V_3(x_3) \tag{4}$$

In order to remove the center of mass motion, the choice of a Jacobi set is mandatory. Only in terms of it, the three-body wavefunction Ψ, eigenstate of the total three-body Hamiltonian (3), factorizes into

$$\Psi(\vec{x}_i, \vec{y}_i, \vec{R}) = \Phi(\vec{x}_i, \vec{y}_i)\, e^{i\vec{P}\cdot\vec{R}}$$

where $\Phi(\vec{x}_i, \vec{y}_i)$ is an eigenstate of the intrinsic Hamiltonian

$$H\Phi = E\Phi, \qquad H = -\frac{\hbar^2}{m_0}[\Delta_{\vec{x}_i} + \Delta_{\vec{y}_i}] + V \tag{5}$$

the only one that we are going to consider from now.

As it can be already seen from (4), none of the Jacobi sets is neither privileged nor fully satisfactory. The "non-interacting" region of particles 2 and 3 is simply given by $x_1 > R_1$ but it is difficult to define this region in terms of say $(\vec{x}_2, \vec{y}_2)$.

On the other hand, if we wish to describe for instance the scattering of particle 1 on a bound state of particles 2 and 3 – denoted symbolically by $1(2,3)$ – it will be natural to chose the coordinate set $(\vec{x}_1, \vec{y}_1)$. However, the final state can contain, together with the initial state, a superposition of channels $2(1,3)$ and/or $3(1,2)$ which can be hardly described in terms of the same coordinate set. For the bound states and break-up channels the three ensembles will appear naturally on the same footing.

The Faddeev equations are based on a partition of the total wave function on as many components as two-body asymptotic channels:

$$\Phi = \Phi_1 + \Phi_2 + \Phi_3$$

It is straightforward to see that the three-body Schrödinger equation (5) is equivalent to the set of coupled partial differential equations for the Faddeev components Φ_i

$$\begin{aligned}
\big[E - H_0 - V_1(x_1)\big]\Phi_1(\vec{x}_1, \vec{y}_1) &= V_1(x_1)\big[\Phi_2(\vec{x}_2, \vec{y}_2) + \Phi_3(\vec{x}_3, \vec{y}_3)\big] \\
\big[E - H_0 - V_2(x_2)\big]\Phi_2(\vec{x}_2, \vec{y}_2) &= V_2(x_2)\big[\Phi_3(\vec{x}_3, \vec{y}_3) + \Phi_1(\vec{x}_1, \vec{y}_1)\big] \\
\big[E - H_0 - V_3(x_3)\big]\Phi_3(\vec{x}_3, \vec{y}_3) &= V_3(x_3)\big[\Phi_1(\vec{x}_1, \vec{y}_1) + \Phi_2(\vec{x}_2, \vec{y}_2)\big]
\end{aligned} \tag{6}$$

The coupling is ensured by the right-hand side. It is highly nonlocal due to the linear relations between two different sets of Jacobi coordinates: $\vec{x}_\alpha(\vec{x}_\beta, \vec{y}_\beta)$, $\vec{y}_\alpha(\vec{x}_\beta, \vec{y}_\beta)$. In the non-interacting region, $V_i = 0$, the three Faddeev equations decouple and the boundary conditions for each component take a simple form when expressed in their own Jacobi coordinate set.

These boundary conditions are more easily implemented in terms of the reduced Faddeev components ϕ_i defined by:

$$\phi_i = x_i y_i \Phi_i \tag{7}$$

and take the following Dirichlet form:

- they vanish for $x_i = 0$ and $y_i = 0$:

$$\phi_i(\vec{x}_i = 0, \vec{y}_i) \equiv 0, \qquad \phi_i(\vec{x}_i, \vec{y}_i = 0) \equiv 0 \tag{8}$$

- for a 3-body bound state they decrease exponentially in all the directions. In practice one can force them to vanish at sufficiently large distances

$$\phi_i(x_i \geqslant x_{max}, y_i \geqslant y_{max}) = 0 \tag{9}$$

- for an open $i + (jk)$ elastic or rearrangement scattering, the i-th Faddeev component splits into the product of the two-body bound state wave function $\varphi_i(x_i)$ of the particle pair (jk) and the scattering wave of particle i with respect to the center of mass of this pair $\chi_i(\vec{y}_i)$:

$$\phi_i(\vec{x}_i, \vec{y}_i) = \varphi_i(x_i)\chi_i(\vec{y}_i) \tag{10}$$

- for the break-up reactions at large values of the hyperradius $\rho = \sqrt{x_i^2 + y_i^2}$ one overimposes to (10) the behavior

$$\phi_i(\vec{x}_i, \vec{y}_i) \sim \frac{e^{ik\rho}}{\rho^{1/2}} \tag{11}$$

As mentioned in the Introduction, the original Faddeev equations, above formulated, are not suitable for the Coulomb scattering problems. The reason is that the right-hand sides of Eq. (6) do not decrease fast enough to ensure the decoupling of Faddeev amplitudes in the asymptotic region and to allow unambiguous implementation of the boundary conditions. In order to circumvent this problem, Merkuriev [7,8] proposed to split the Coulomb potential V into two parts, $V = V^s + V^l$, by means of some arbitrary cut-off function η:

$$V^s(x, y) = V(x)\eta(x, y), \qquad V^l(x, y) = V(x)\big[1 - \eta(x, y)\big] \tag{12}$$

One is then left with a system of equivalent equations

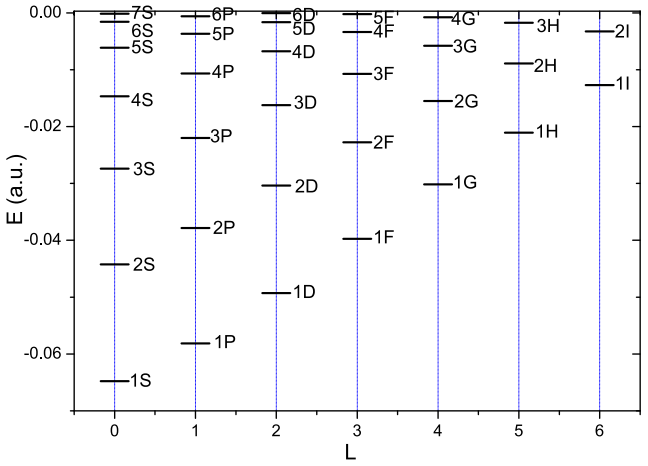

Fig. 2. Bound state spectrum (atomic units) for π–H in a two-body approach with a regularized polarization potential (14).

$$\left[E - H_0 - W_i - V_i^s\right]\Phi_i = V_i^s[\Phi_j + \Phi_k], \qquad W_i = V_i^l + V_j^l + V_k^l \tag{13}$$

with the right-hand side containing only short range contributions (V_s) and with a 3-body potential (W_α) in the left-hand side to account for the long range parts. As it will be demonstrated in the following, this approach was found to be very efficient in calculating the positron–positronium (Ps) and positron–hydrogen (H) cross sections [17,18].

The main advantage of the Faddeev formulation is to allow a proper description of the different asymptotic states, each of them well separated by the corresponding Faddeev component and easily described in terms of their natural Jacobi coordinates. It is clear that the implementation of multichannel boundary conditions listed in (8)–(11) is impossible by means of one single function. Let us just however mention that this is not the only reason for using this approach, after all when working in momentum space there is no any need to implement any kind of boundary conditions. In fact there are also deeper reasons related to the mathematical structure of the underlying Lipmann–Schwinger like integral equations. The reader interested can take benefit in consulting [24,25].

Eqs. (13) allow us to treat any physical non-relativistic quantum three-body problem with the only exception of break-up reaction with at least one attractive Coulomb interaction, despite numerous attempts [26].

Last but least, this formulation is also advantageous in the numerical calculations. Indeed, the Faddeev decomposition takes benefit of the symmetry properties of the system. As a consequence, the Faddeev components have simpler structure than the total wave function itself and are therefore easier to interpolate numerically.

The above described formalism has been extended to account for particles with spin, interacting via three-body and/or nonlocal forces. A few years after their formulation, the Faddeev equations were generalized to an arbitrary number (N) of particles by Yakubovsky [2]. However their numerical solution is still limited to $N = 4$ case and for the energies below the first three-body break-up threshold. In this manuscript we will not present the formalism of Yakubovsky equations and their numerical implementation techniques. The interested reader may refer to [27]. Still, in Sections 4–5, we present some results, which were obtained by solving four-particle Yakubovsky equations.

One should also mention that, although we have described Faddeev approach in coordinate space in terms of coupled differential equations, the equivalent formulation is available in momentum space using coupled integral equations. Both formulations have its own advantages, namely higher energy scattering is easier to treat in momentum space [15,28], while configuration space is more convenient for Coulomb related problems [25,17,19,14].

3. Charged particle interaction with *H*

An interesting atomic physics problem is related to the polarization of neutral atoms. In the vicinity of a charged particle $X^\pm$, the electronic density of a neutral atom A polarizes, giving rise to a central long range $X^\pm$–A interaction which behaves asymptotically like

$$V_P(r) = -\frac{1}{2}\frac{\alpha_d}{r^4} \tag{14}$$

where α_d is the dipole polarizability, characteristic of the atom ($\alpha_d = 9/2$ for H in the $m_p \to \infty$ limit). This interaction is very shallow but if the charged particle is heavy enough to reduce the repulsive kinetic energy, it generates a rich spectrum of bound and resonant states. This can be qualitatively illustrated in a simple two-body approach by assuming an $X^\pm$–A two-body interaction of the form (14) with the replacement [29]:

$$\alpha_d \to \alpha(r) = \alpha_d - \frac{2}{3}e^{-2r}\left(r^5 + \frac{9}{2}r^4 + 9r^3 + \frac{27}{2}r^2 + \frac{27}{2}r + \frac{27}{4}\right)$$

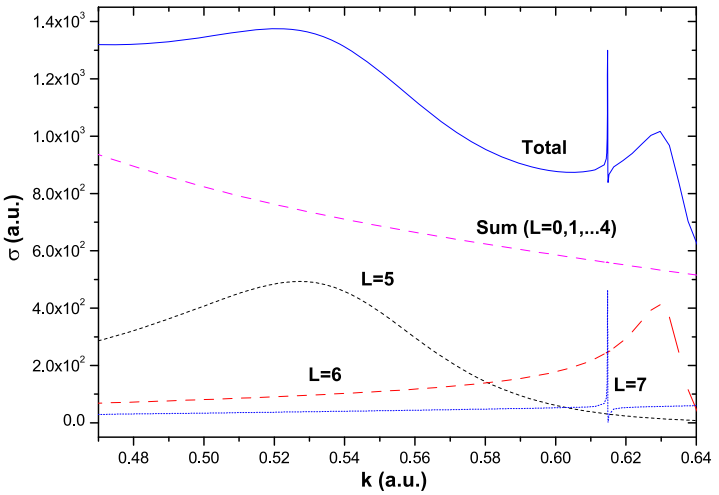

Fig. 3. Resonant μ–H states in the same two-body approximation as in Fig. 2.

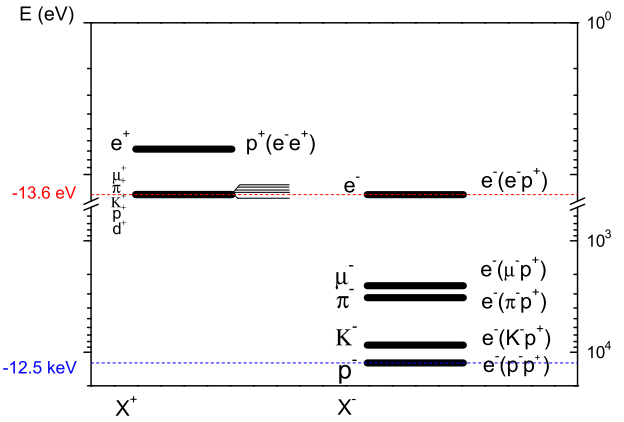

Fig. 4. Different three-body reactions with atomic hydrogen and the existing particles.

This particular choice of $\alpha(r)$, valid for scattering on H atom, regularizes (linearly) the polarization potential (14) at short distances, keeping also the right asymptotic behavior.

We have plotted in Fig. 2 the bound state spectrum of the π–H system thus obtained. It contains a large number of states up to $L = 6$. In the case of a positively charged particle, X^+, these states would lay below the rearrangement threshold $p + (e^- X^+)$. Fig. 3 represents the μ–H elastic cross section obtained in the same approximation, displaying very narrow resonances in high angular momentum states [19].

In view of having reliable quantitative predictions, an exact calculation must, however, be performed, taking into account the internal structure of the atom. In the present Few-Body *state of the art*, this is only possible for the H and He atoms. The simplest case for which the calculations can be performed exactly is the scattering on atomic hydrogen. This constitutes a genuine three-body problem and a challenge for the Few-Body community.

We have first considered the case of positively charged particle X^+ with $m_{X^+} \leqslant m_p$, for they have at zero energy a single open channel corresponding to elastic scattering (see Fig. 4). The first exact three-body solutions of the $X^+(e^- p^+)$ have been obtained in [19]. We display in Fig. 5 the X^+–H scattering length as a function of the mass of the projectile m_X. The values corresponding to physical particles (μ, π) are indicated by arrows. As one can see from this figure, the scattering length is divergent for some values of the incoming particle mass, indicating the appearance of an additional bound state in the (X, p, e) system.

Of special interest is the scattering of protons. Not only for they constitute experimentally the most accessible physical particle but also because it corresponds, by chance, to one of the resonant cases displayed in Fig. 5 for smaller projectile masses.

Indeed, we have computed the p–H scattering length for the S-wave symmetric (pp spin singlet) and antisymmetric (pp spin triplet) states. For the symmetric case we found $a_s = -29.3$ a.u. while the antisymmetric one provided the value of $a_t = 750 \pm 5$ a.u. The analysis of the nodal structure of the corresponding Faddeev amplitude indicated that such a big

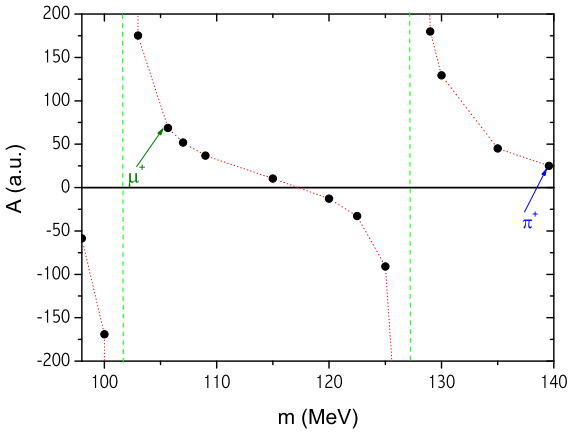

Fig. 5. X^+–H scattering length (in atomic units) as a function of the projectile mass (in MeV). The values corresponding to physical particles are indicated by arrows.

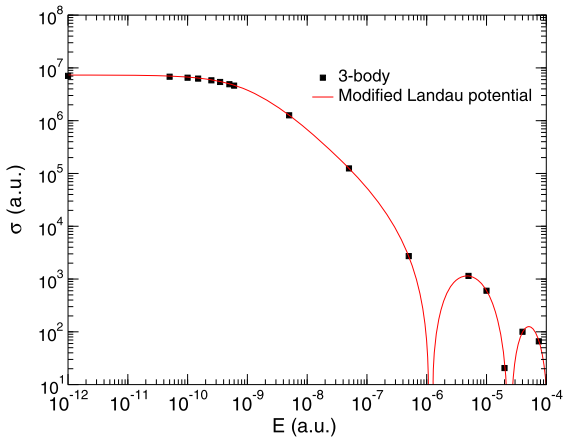

Fig. 6. Cross section for the $L = 0$ pH scattering in pp spin triplet state as a function of the energy (in atomic units). Three body results (filled squares) are compared to those (solid line) given by the two-body Landau potential [34] modified in order to reproduce the binding energy the first excited state.

value is due to the existence of a first excited bound state with extremely small binding energy. By using the effective range expansion, its binding energy was found to be $B = (1.135 \pm 0.035) \times 10^{-9}$ a.u. that is ≈ 30 neV.

This state can be also viewed as the first excited vibrational level $v = 1$ of $2p\sigma_u$ symmetry in the H_2^+ molecular ion. A direct computation of this state using ad-hoc variational techniques [30] confirmed its existence and provided a more accurate value of the binding energy $B = 1.085045 \times 10^{-9}$ [31]. Further work showed that it is stable with respect to the relativistic and leading order QED corrections. Taking them into account, its binding energy is only slightly modified and becomes $B = 1.082247 \times 10^{-9}$ [32].

It is worth mentioning that this H_2^+ first excited antisymmetric state exists also in the so-called Landau p–H potential [34]. The latter consists in adding to the polarization term (14) a repulsive one due to the Pauli principle between protons in the spin triplet state and reads (in atomic units)

$$V_L(x) = \eta \frac{2x}{e^{x+1}} - \frac{\alpha_d}{2x^4} \tag{15}$$

The total potential V_L is regularized to a constant below $x_c = 2.5$. In its original formulation ($\eta = 1$) it entails an excited S-wave state, although with binding energy two order of magnitude smaller than the exact three-body value and a p–H scattering length consequently larger.

To our knowledge the H_2^+ first vibrational $2p\sigma_u$ state above described constitutes the most weakly bound natural molecule ever predicted.[1] A direct computation provides a root mean squared radius $R = 270$ a.u. and its wavefunction has still sizeable values well beyond 1000 a.u. That makes the state extremely unstable against any kind of perturbation.

[1] It is, however, possible to prepare arbitrarily weakly bound systems suitably adjusting external magnetic fields, like for instance in [33].

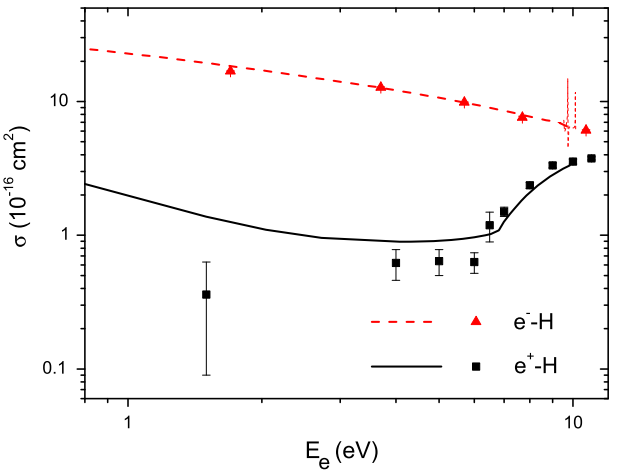

Fig. 7. $e^{\pm}$–H scattering cross section below $H(n=2)$ threshold: calculated values are compared with experimental ones [35].

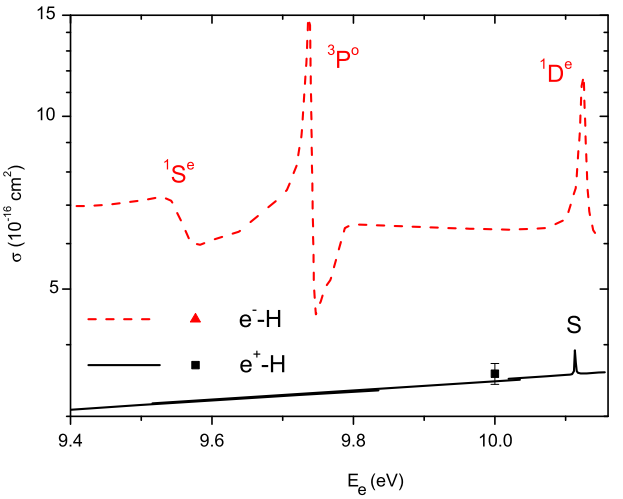

Fig. 8. A zoom in the resonance region of $e^{\pm}$–H scattering close to $H(n=2)$ threshold.

The low energy p–H scattering will be however totally dominated by the existence of this nearthreshold state. Corresponding S-wave elastic p–H cross section is shown in Fig. 6. The Faddeev results (filled squares) are compared to those (solid line) obtained with the Landau potential (15), whose parameter was adjusted to $\eta = 0.9254$ in order to reproduce the exact 3-body binding energy. The huge values of the cross section are a consequence of the large triplet scattering length a_t. Notice that the resonant region is however limited to $E < 10^{-7}$ a.u. Below this energy range, a proton approaching a hydrogen atom will feel an object of nanoscopic size.

Electron and positron scattering on hydrogen atoms in their ground state presents one of the rare three charge structures for which experimental data are available. In Fig. 7 we compare our calculated total scattering cross sections with the measured ones [35], for $e^{\pm}$ energies below $H(n=2)$ threshold ($E_2 \approx 10.2$ eV). One may see an excellent agreement between measured and calculated values. The only exception is in the e^+–H scattering at very low energies ($E \approx 1$ eV), where the experimental result has a big error bar, probably due to the strong positron annihilation probability.

We have displayed in Fig. 8 a zoom of the resonance region, close to the $H(n=2)$ threshold. One may identify three well-known narrow resonances in e^-–H system, which are also confirmed experimentally [36–38]. One S-wave resonance is visible in e^+–H system.

If the incoming particle is heavier than the proton, e.g. $X^+ = d$, the rearrangement process

$$X + \left(e^- p\right) \to p + \left(e^- X^+\right)$$

is kinematically open and even at zero kinetic energy we are left with a two channel problem. By increasing the scattering energy, the number of open $1+2$ channels before the 3-body breakup threshold becomes infinite.

The situation is even more interesting in the case of an incoming negatively charged X^- which presents even at zero incoming energy a large numbers of open channel corresponding to Coulomb (X^-, p) ground and excited states (see Fig. 4).

All of them provide a very rich variety of phenomena, most of them remaining unexplored both from the theoretical as well as from the experimental point of view.

4. Cold molecules

An important simplification of the Faddeev equations may take place if one considers a system of identical particles. In this case, the three Faddeev equations, as well as the corresponding components, become identical and therefore the full solution of the problem is obtained by solving only one of them. Such symmetrized equation may be applied to study a system of identical bosons. This is the simplest few-body problem, nevertheless revealing genuine peculiarities of quantum many-body systems.

Two of the striking phenomena manifested in few-body physics are the Thomas collapse [39] and the so-called Efimov states [40,41].

The first of these two effects, the Thomas collapse, attests that an $N > 2$ boson system will shrink into a state with an infinite binding energy, if the pairwise particle interaction is attractive and of zero-range.

The second phenomenon, i.e. Efimov states, manifests in a series of weakly bound three-body states, which move below the two-body threshold by slightly increasing the two-body attractive interaction. These states can appear in a realistic physical system with finite range interaction, if one of its two-body subsystems is S-wave resonant, i.e. when the two-body scattering length (a_0) turns to be much larger than the interaction range (r_0). The interest in Efimov states has been fueled lately by the important progress of experimental low temperature physics and particularly by the recent discovery of an Efimov state in caesium atoms [42] and the subsequent, even more conclusive, experimental works of Refs. [43–46].

Efimov physics involves systems having largely separated length (or momenta) scales and therefore turns to be a natural laboratory to test Effective field theories (EFT). To analyze Efimov states it is then natural to introduce EFT expansions in terms of two small dimensionless parameters r_0/a_0 and kr_0, k being a characteristic center-of-mass (c.m.) momenta.

It is a common believe that, at the leading order of EFT, all the low-energy properties of a three-boson system are set by two parameters: one two-body parameter – like two-boson (dimer) binding energy or scattering length – and one three-body parameter – like three-boson (trimer) binding energy or particle-dimer scattering length [47,48]. This means that whenever in a three-body system the particle interdistance R satisfies the Efimov condition, $r_0 \ll R \ll |a_0|$, its low-energy properties must be interaction independent and be governed by the only two low energy aforementioned parameters.

More recently, it has even been demonstrated that the properties of the four-boson system (tetramer) are determined by the same two parameters and no additional four-body scale is required to establish universal relations between three- and four-boson observables [49,50]. These universality studies have been also extended to fermionic three- and four-body systems, recovering series of phenomenologically observed correlation rules in multi-particle system [51]. Most of these relations have been derived relying on purely attractive (and often contact) two-particle interactions, while $N > 2$ systems are balanced by introducing repulsive three-particle force to prevent Thomas collapse.

We present in this section a slightly different quantum-mechanical approach, based on a family of short range separable, rank-1 and rank-2, interactions having the same two-boson scattering length.

These potentials have been derived somehow mimicking interaction between ^{4}He atoms, i.e., choosing the boson mass $\hbar^2/m = 12.12$ K Å^2 and fixing the two-boson scattering length to $a_0 = 104.0$ Å. Nevertheless one cannot pretend with these results a realistic description of ^{4}He multimers, since these separable potentials do not retain well-known properties of the effective interaction of two inert neutral atoms, like strong repulsion at the origin and weak Van der Walls attraction in the asymptote.

The family of two-boson separable (and thereby nonlocal) potentials we use have the form:

$$v = \sum_{ij}^{n_r} |g_i\rangle \lambda_{ij} \langle g_j| \tag{16}$$

where n_r is the rank of the considered potential. For simplicity, these potentials are restricted to S-wave only. In close analogy with most of the EFT potentials [49], the form factors $|g_i\rangle$ are chosen as Gaussian. In the configuration-space they are given by

$$\langle r|g_i\rangle = (\Lambda_i/\sqrt{2})^3 e^{-(\Lambda_i r/2)^2} \tag{17}$$

The rank-1 potential is defined by two parameters: λ_{11} and Λ_1. To preserve the two-body scattering length at $a_0 =$ 104.0 Å, these two parameters must satisfy $\lambda_{11} = [\pi m(1/a_0 - \Lambda_1/\sqrt{2\pi})/2]^{-1}$.

The rank-2 potential is obtained by choosing $\Lambda_j = j\Lambda$ with Λ in the range $[0.133, 0.305]$ Å^{-1}, i.e. $13.8 < a_0\Lambda < 31.7$, and determining the remaining three strength parameters λ_{ij} (we assume $\lambda_{12} = \lambda_{21}$) by a fit of the calculated observables (with a typical four digit accuracy): dimer binding energy $B_2 = 1.318$ mK, scattering length $a_0 = 104.0$ Å and two-particle scattering phase-shifts up to about $50B_2$ c.m. energy. The broad scattering energy interval included in the fit, roughly corresponding to the natural energy scale $\hbar^2/mr_0^2$ [49], guarantees that in the effective range expansion not only k^2 but also higher order terms are well retained. Note that the phase-shift set we have used to fix the parameters of the rank-2 potential differs from the one obtained by realistic interaction (for instance our effective range $r_0 = 15.0$ Å is about two times larger).

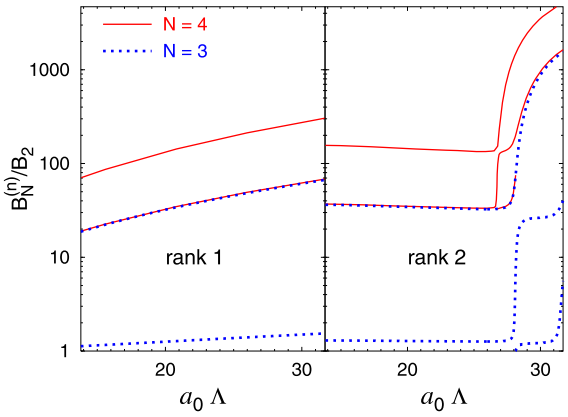

Fig. 9. Evolution of the three- and four-boson binding energies with the Gaussian cutoff Λ.

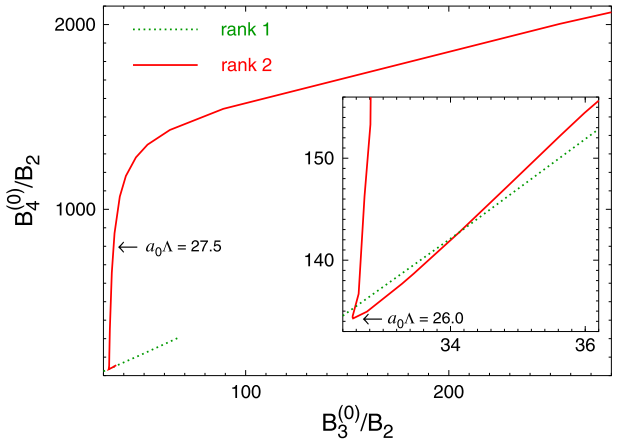

Fig. 10. (Color online.) Correlation between ground state binding energies of trimer and tetramer.

The dependence of the binding energies of $L = 0^+$ three- and four-boson states as a function of the Gaussian cut-off Λ[2] is displayed in Fig. 9 for both rank-1 and rank-2 potentials. By binding energy B_n of a n-particle multimer we denote the difference between the sum of the n free constituent particles masses and the total multimer mass.

The rank-1 results are consistent with the EFT predictions, based on contact 2- and 3-body interactions. There exist two trimers, the ground state which is strongly bound (its binding energy exceeds the dimer one by more than a factor 10), and the first excitation which remains close to the threshold. There are also two tetramers, the ground state being strongly bound relative to trimer one and the excited tetramer which consist in one boson weakly attached to the trimer ground state. The binding energies of these trimers and tetramers reveal almost a linear correlation pattern for rank-1 potential, see Fig. 10, and are in agreement with the EFT results of Ref. [51].

The situation is much more complicated when using the rank-2 potential. The binding energies $B_N^{(n)}/B_2$ are slowly decreasing functions of the cut-off Λ in the range $a_0\Lambda < 26.0$. In this region, all potentials support one ground and one excited state for the trimer as well as for the tetramer, in agreement with the EFT approach. Moreover the trimer and tetramer binding energies follow closely the correlation curves of rank-1 values. However, for larger Λ values, the rank-2 potential results show a nontrivial behavior despite the fact that all the potential parameters λ_{ij} depend smoothly on Λ.

First, at $a_0\Lambda = 26.5$, the binding energy of the excited tetramer $B_4^{(1)}$ detaches from $B_3^{(0)}$. It increases drastically and stabilizes for a moment when it almost attains the tetramer ground state binding energy $B_4^{(0)}$ that, with a tiny delay, also starts to increase rapidly. At the same time, close to $a_0\Lambda = 26.75$, the second excited tetramer state appears with a binding energy $B_4^{(2)}$ only slightly larger than $B_3^{(0)}$. In this region of harsh tetramer variations, the trimer properties remain practically unchanged.

The trimers exhibit qualitatively similar behavior, although at larger Λ values, around $a_0\Lambda = 27.5$. The binding energies of the trimer ground and first excited state, $B_3^{(0)}$ and $B_3^{(1)}$, start to grow very rapidly; the former increases much like

[2] One should notice that the described potentials do not support $L \neq 0^+$ rotational states, neither for trimers nor for tetramers.

$B_4^{(0)}$ did while the latter stabilizes for a while. As $B_3^{(0)}$ increases, the second excited tetramer state disappears below the ground trimer threshold at $a_0\Lambda = 28.14$, whereas the first excited tetramer stalls for a while letting the trimer threshold $B_3^{(0)}$ to approach again. Furthermore, at $a_0\Lambda = 28.12$ the second excited trimer state appears. Unlike the strongly bound trimers, this state behaves like an Efimov one, i.e., it slides under the dimer threshold if the two-boson interaction is made stronger. The second excited trimer loses that property above $a_0\Lambda = 30.7$ where its binding energy $B_3^{(2)}$, much like $B_3^{(1)}$ at $a_0\Lambda = 27.5$, starts a phase of a rapid increase. However, the Efimov property is recovered by the third excited trimer, appearing at $a_0\Lambda = 31.7$. It is interesting to note that the second excited tetramer shows a similar behavior, i.e. it also disappears if the two-boson interaction is made stronger.

While rank-2 potential results seems to be rather confusing, the explanation of such a nontrivial behavior of a few-boson system is rather simple. For this aim one should simply understand the Λ-evolution of the nonlocal interaction. The shape of $n_r = 1$ potential is very simple, and can be represented by a single attractive bell-shape well in (r, r') plane, the width of the bell being constrained by the size of the cutoff Λ. For small Λ values, the $n_r = 2$ potential has also single and rather flat attractive plateau in the (r, r') plane. However for larger Λ values, this plateau splits into a rather complicated saddle-like surface with two asymmetric attractive regions separated by two symmetric repulsive regions. A narrow attractive region is formed at the origin and it deepens when increasing Λ, whereas the second, distant, attractive region is much wider and flatter. Due to the large kinetic energies required to squeeze the particles into the narrow region at the origin, it is energetically preferable for the multi-boson system to stay in the distant attractive plateau. At this moment, the $n_r = 2$ potential presents qualitatively the same features as $n_r = 1$, having a single attractive region. However, for some values close to $a_0\Lambda = 26.0$, the attractive region at the origin becomes deep enough to accommodate the four-boson system, and some kind of a phase transition occurs. The trimer has only three pair interactions compared to six for the tetramer. Therefore the corresponding phase transition in the three-boson system takes place at larger Λ values, when the attractive region near the origin is even more deepened.

One can probably question the reality of such "exotic" nonlocal potentials with several attractive regions. Nevertheless, one must admit that some realistic nucleon–nucleon potentials [52,53] have even more complex structure than the one exhibited in our model. The effective interaction between two complex molecules can, however, reveal an even much more complicated pattern.

The presence of finite range ($r_0 > 0$) interactions does not guarantee that the Thomas-like collapse will not occur in multi-boson system. The interaction can have a short-range or an off-shell structure that may be ignored with the low-energy probe. Such a structure can have no or little effect for low-energy observables of an N particles system, but may be exploited in the $N + 1$ particle one which, having more interacting pairs, can compensate larger kinetic energies and thus regroup itself into a shorter range domain. This fact complicates the possibility to make universal predictions about multi-particle system, in particular about its deeper lying states, based only on the low energy properties of its subsystems, unless one is sure that the eventual size of the few-body system satisfies the Efimov condition $R \gg r_0$. Of course, this condition is never satisfied a priori, although one may expect that it must be valid for higher order excited states [54].

5. ^{4}He multimers

In this section we turn our attention to a realistic description of small structures of ^{4}He atoms. The two electrons of the He atom close the 1s shell, determining its spherical symmetry as well as its inert chemical properties. Two He atoms repel strongly when approaching to each other, but a very weak Van der Vaals attraction is exhibited at large distance, resulting in a shallow attractive pocket with a maximal depth of ≈ 10.9 K, centered at $R_{\text{He–He}} \approx 3$ Å.

This weak attraction is responsible for the fact that at very low temperatures both bosonic ^{4}He but also fermionic ^{3}He become liquid. It is also responsible for the existence of a loosely bound ^{4}He dimer, with binding energies of $B \approx 1$ mK and sizeable ^{4}He–^{4}He scattering length $a_0 \approx 100$ Å, which has been experimentally observed few years ago [55,56].

When trying to study theoretically $N > 2$ ^{4}He clusters, one is faced to a serious theoretical problem. The standard boundary conditions in the Dirichlet form (8), which imposes to the FY components to vanish at the origin, turns to be impractical when considering structures of He atoms. The strong hard-core repulsion describing the inner part of the He–He potential, which dominates the interaction between two He atoms at relative distance $R_{\text{He–He}} \approx 2$ Å, introduce severe numerical complications. The relevant attractive matrix elements which are responsible for the binding fade away in front of these huge repulsive hard-core terms, thus causing numerical instabilities. On the other hand, such strong repulsion close to the origin physically, simply reflects the fact that the two He atoms cannot get close to each other, i.e. closer than some relative distance $r = c$ inside the core.

The wave function of three He atom system, for instance, should vanish in the region of three-particle space $\mathbb{R}^6$, which is the interior of the three multidimensional surfaces $x_i = c$, where x_i is the distance between the particle j and k defined in (1). Therefore one way to attain numerical stability would be to neglect the solution in the strong repulsion region. In practice, as it has been shown by Motovilov and Merkuriev [57], the presence of infinitely repulsive interaction at $x_i < c$, can be formulated in terms of boundary conditions for the Faddeev components, which are implemented by setting:

$$\begin{aligned} &\big[E - H_0 - V(x_i)\big]\Phi_i(\vec{x}_i, \vec{y}_i) = 0 \quad && \text{for } x_i < c \\ &\Phi_i(\vec{x}_i, \vec{y}_i) = 0 && \text{for } x_i = c \end{aligned} \tag{18}$$

Table 1
Predictions for the ^{4}He multimer properties. Binding energies (in mK) and scattering lengths (in Å) obtained using realistic LM2M2 interaction and rank-1 separable model of Section 4.

Pot.	$B_3^{(0)}$	$B_3^{(1)}$	$B_4^{(0)}$	$B_4^{(1)}-B_3^{(0)}$	$a_0^{\{2-1\}}$	$a_0^{\{3-1\}}$
LM2M2	126.39	2.2680	557.7	1.087	115.56	103.7
rank-1	126.39	2.2758	597.9	3.16	114.77	67.38

A similar approach may be applied also to condition Faddeev–Yakubovsky equations for four-body system, see [57].

We compare in Table 1 the calculated properties of three and four ^{4}He atom structures. The binding energies of the ground and excited states (in mK) together with atom–dimer and atom–trimer scattering lengths (in Å) are listed. The realistic model is based on the interaction between two He atoms developed by Aziz and Slaman [58], popularly referred to as LM2M2 potential. These realistic calculations are compared to the values obtained using the rank-1 potential from the previous section, whose parameters (λ, Λ) have been adjusted in order to reproduce the dimer and ground state trimer binding energies obtained with the LM2M2 potential. One may see that the rank-1 approximation reproduces well the excited trimer binding energy $B_3^{(1)}$ and the atom–dimer scattering length $a_0^{\{2-1\}}$. However the description of the four-atom system deteriorates considerably. Probably the main reason is the difference of the off-energy shell properties between these two interaction models: a purely attractive rank-1 potential and the LM2M2 one containing a strong hard-core region. The four-boson system, being a more compact structure, test more strongly the hard-core region than the three-body one, which is also reflected by the fact that the rank-1 potential provides more binding than the LM2M2 one.

It is worth mentioning that a direct calculation of the ^{4}He tetramer excited state still represents a challenging numerical task. This state is very weakly bound and its wave function extend over several hundreds of Å. One is therefore forced to use a very large and dense grid, ensuring at the same time enough accuracy to trace the small binding energy difference with respect to the trimer ground state. Nevertheless the vicinity of the tetramers excited state to the ^{4}He–^{4}He$_3$ continuum makes possible the extraction of its binding energy from the low-energy scattering results as explained in [12].

6. Conclusion

The Faddeev–Yakubovsky equations provide a rigorous quantum mechanical formulation of the non-relativistic few particle problem, taking into account all the possible asymptotic states of the system. First formulated in momentum space and for short range pairwise interactions, they have been generalized to accommodate three-body forces as well as long range Coulomb potentials.

Aside from its well defined mathematical structure, the Faddeev–Yakubovsky formalism turned to be very useful in numerical calculations. A large variety of problems in hadronic, nuclear, atomic and molecular physics have been solved since its appearance. Still limited to $N = 3$ and 4 systems, they can be in principle extended to an arbitrary number of particles. They provide very accurate results for the bound state problems but the genuine feature of this formalism lies on its ability to treat scattering and bound states on the same footing, thus enabling a complete and consistent analysis of the few-body system under consideration.

The configuration space formulation of Faddeev–Yakubovsky equations, made possible once the boundary conditions are well established, is the best adapted to deal with atomic physics problems. Some selected examples of them have been presented in this contribution covering aspects of cold atomic and molecular physics. We have considered the scattering of positively charged particle on atomic hydrogen, systems of cold atomic molecules and bound and scattering states of ^{4}He atoms. In particular, we would like to emphasize the result concerning the p–H scattering: the huge scattering length in the proton–proton spin triplet state $a_t \approx 750$ atomic units.

Even by restricting ourselves to the 3- and 4-body cases, a large variety of unsolved problems remains to be considered. Among them we would like to mention:

- The Coulomb reactions including break-up and/or many open channels, like those presented in Fig. 4.
- The many interesting antiproton physics processes, like $\bar{p} + d$, $\bar{p}H \to e^- + (\bar{p}p)^*$, $\bar{p} + (e^+e^-) \to \bar{H} + e^-$.
- Four-body Coulomb problems, like first principle calculations of positron–positron scattering.
- Four-Body break-up reactions involving $1 + 2 + 1$ and $1 + 1 + 1 + 1$ particle channels.

They constitute altogether a very rich and challenging program for the coming years, both from the theoretical and experimental physics points of view.

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