Physics Letters B 744 (2015) 105–108

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Three-body calculation of the 1*s* level shift in kaonic deuterium

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ARTICLE INFO

Article history:
Received 13 February 2015
Received in revised form 11 March 2015
Accepted 19 March 2015
Available online 24 March 2015
Editor: J.-P. Blaizot

Keywords:
Few-body equations
Mesonic atom
Antikaon–nucleon interaction

ABSTRACT

The first exact calculation of a three-body hadronic atom was performed. Kaonic deuterium 1*s* level shift and width were evaluated using Faddeev-type equations with Coulomb interaction. The obtained exact results were compared with commonly used approximate approaches.

Kaonic deuterium is a very useful exotic atom, which can be accurately studied experimentally and theoretically and after comparing the results give us additional information about antikaon–nucleon interaction.

Interaction of an antikaon with a nucleon is the basis for investigation of strong quasi-bound states in antikaonic–nucleus systems, attracted large interest recently. The most interesting and intensively studied theoretically and experimentally is the lightest K^-pp system, see e.g. [1]. At present, the theoretical predictions for binding energies and widths of the quasibound state differ substantially. The theoretical results, however, agree that the quasibound state really can exist in the K^-pp system. The experimental results also differ from each other; moreover, their binding energies and widths are far from all theoretical predictions. Since the question of the possible existence of the quasibound state in K^-pp system is still actual, new experiments are being planned and performed by HADES and LEPS Collaborations, in J-PARC E15 and E27 experiments.

There are two origins of uncertainty for theoretical results. The first one is different few-body methods, which were used for the calculations. However, it was shown in [1] that even calculations using the same three-body Faddeev-type equations give different results in dependence on the $\bar{K}N$ potential used as the input.

The problem is that available two-body experimental information on the $\bar{K}N$ interaction is insufficient for construction of a unique interaction model. In particular, it was shown e.g. in [2] that phenomenological models of the interaction having one or two poles for the $\Lambda(1405)$ resonance and reproducing all low-energy experimental data on K^-p scattering and kaonic hydrogen equally well can be constructed. The same is true for the recently constructed in [3] chirally-motivated model of the interaction. A way to obtain some additional information about the $\bar{K}N$ interaction is to use it as an input in an accurate few-body calculation and then compare the theoretical predictions with eventual experimental data. Kaonic atoms, in contrast to kaonic nuclear states, can be measured accurately. Kaonic deuterium is the best candidate since energy shift and width of its 1*s* level can be measured directly and calculated accurately. It allows a direct comparison of the theoretical predictions with experimental data on kaonic deuterium, which hopefully will be obtained in the SIDDHARTA-2 experiment [4].

Characteristics of kaonic deuterium, however, are hard to calculate accurately. Due to this only approximate formulas such as Deser [5] or corrected Deser [6], connecting 1*s* level shift and width of an atom with the corresponding scattering length, are used by experimentalists and some theorists. However, it was shown, for example in [7], that even for two-body system, (anti)kaonic hydrogen, the formulas give quite large error in comparison with the exact result. Since no three-body effects can be taken into account by such a formula, the accuracy of the formulas for kaonic deuterium should be less.

To the best of our knowledge, the most accurate evaluation of kaonic deuterium characteristics was done recently in [2] and repeated in [3] with new $\bar{K}N$ potentials. The two-body calculations using effective optical $K^- - d$ potential together with Coulomb interaction were performed. The potential was constructed in such

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http://dx.doi.org/10.1016/j.physletb.2015.03.043

a way that it reproduces elastic amplitudes of K^-d scattering obtained from the Faddeev calculation with strong interactions only.

In this letter we present the results of the first exact calculation of the three-body atom – kaonic deuterium with no reduction to any effective two-body problem. The obtained energy of the $1s$ level of the atom is an exact eigenvalue of the corresponding three-body Hamiltonian with all of its interactions taken into account simultaneously. The dynamically exact results are compared with those of the approximate methods.

At present there are powerful methods to solve three-body problems, especially for the somewhat easier task of finding real or complex eigenvalues: Faddeev equations (in integral or differential form) or variational methods based on wave function expansion in coordinate space. However, just for our case both methods face serious difficulties. In the Faddeev approach we have the everlasting problem of the long range Coulomb force, which is even worse for attractive interaction. As for the coordinate space expansions, the main difficulty lies in the presence of two very different distance scales, both relevant for the calculated level shift.

The usual description of hadronic atoms is based on a two-body picture: a negatively charged hadron in the Coulomb field of the nucleus. The strong interaction with the nuclear few- or many-body system is incorporated into an absorptive nucleus–hadron interaction. Thus the two interaction types, forming the system, are treated not on equal footing: first, the pure strong interaction problem is reduced to an effective two-body one, while the Coulomb force is "added" as a second step.

Some years ago a method for simultaneous treatment of short range plus Coulomb forces in three-body problems was proposed [8]. The method was successfully applied for short range plus repulsive Coulomb forces (nuclear case) [9], and purely Coulomb systems with attraction and repulsion [10]. The present case of three strongly interacting hadrons with Coulomb attraction between certain pairs, which is practically inaccessible by other methods, was not considered.

The basic idea was to transform the Faddeev integral equations into matrix form using a special discrete and complete set of Coulomb Sturmian functions as a basis. Coulomb Sturmian functions in coordinate space have the form

$$\langle \vec{r}|nlm\rangle = \langle \vec{r}|i\rangle = N_{nl} r^l e^{-br} L_n^{2l+1}(2br) Y_{lm}(\hat{\vec{r}}), \tag{1}$$

were b is a range parameter. The functions $\langle \vec{r}|i\rangle$ are orthogonal with the weight function $1/r$, or they form a bi-orthogonal and complete set with their counter-parts $\langle \vec{r}|\tilde{i}\rangle$

$$\left\langle i\left|\frac{1}{r}\right|j\right\rangle = \delta_{ij},\ \langle \vec{r}\,|\tilde{i}\rangle = \frac{1}{r}\langle \vec{r}\,|i\rangle,\ \langle i|\tilde{j}\rangle = \langle \tilde{i}|j\rangle = \delta_{ij}. \tag{2}$$

The most remarkable feature of this particular basis set is, that in this representation the matrix of the $(z-h_c)$ operator, where h_c is the pure two-body Coulomb Hamiltonian, is tridiagonal. Therefore, if we use this property for evaluation the matrix elements of the two-body Coulomb Green's function $\langle \tilde{i}|g_c(z)|\tilde{j}\rangle$, we get an infinite tridiagonal set of equations, which can be solved exactly, see [11] and references therein. The same holds for the matrix elements of the free two-body Green's function $\langle \tilde{i}|g_0(z)|\tilde{j}\rangle$.

The Noble form of the homogeneous Faddeev equations [12] for the K^-pn three-body problem, when the Coulomb interaction appears in Green's functions, reads

$$\begin{aligned}
\Psi_{np} &= \left(z - H_0 - V^s_{np}(x_{np}) + \frac{e^2}{|c_{np}\vec{x}_{np} + \vec{y}_{K^-}|}\right)^{-1} \\
&\quad \times V^s_{np}(x_{np})(\Psi_{nK^-} + \Psi_{pK^-}) \\
\Psi_{nK^-} &= \left(z - H_0 - V^s_{nK^-}(x_{nK^-}) + \frac{e^2}{|c_{nK^-}\vec{x}_{nK^-} + \vec{y}_p|}\right)^{-1} \\
&\quad \times V^s_{nK^-}(x_{nK^-})(\Psi_{np} + \Psi_{pK^-}) \\
\Psi_{pK^-} &= \left(z - H_0 - V^s_{pK^-}(x_{pK^-}) + \frac{e^2}{x_{pK^-}}\right)^{-1} \\
&\quad \times V^s_{pK^-}(x_{pK^-})(\Psi_{np} + \Psi_{nK^-})
\end{aligned} \tag{3}$$

where, as usual for equations of Faddeev type, the total three-body wave function is separated into three components

$$\Psi = \Psi_{np}(\vec{x}_{pn}, \vec{y}_{K^-}) + \Psi_{nK^-}(\vec{x}_{nK^-}, \vec{y}_p) + \Psi_{pK^-}(\vec{x}_{pK^-}, \vec{y}_n). \tag{4}$$

In Eqs. (3) V^s denote the two-body strong potentials, $(\vec{x}_{pn}, \vec{y}_{K^-})$, $(\vec{x}_{pK^-}, \vec{y}_n)$ and $(\vec{x}_{nK^-}, \vec{y}_p)$ are the three sets of Jacobi coordinates, and c are mass coefficients. The Coulomb interaction between the antikaon and the proton $-e^2/x_{pK^-}$ is the same in all three equations, but expressed in different coordinates.

Introducing the shorter notation: $\alpha = (pn, K^-)$, (pK^-, n), (nK^-, p) for the partition channels, $(\vec{x}_\alpha, \vec{y}_\alpha)$ for Jacobi coordinates and inserting (approximate) unit operators into the system of equations

$$\hat{1}_\alpha = \sum_\mu^{N_\alpha} |\mu_\alpha\rangle\langle\tilde{\mu}_\alpha| \sim \hat{1} \tag{5}$$

$$\langle \vec{x}_\alpha, \vec{y}_\alpha|\mu_\alpha\rangle = \langle \vec{x}_\alpha|i\rangle\langle \vec{y}_\alpha|I\rangle = \langle \vec{x}_\alpha|nl\rangle\langle \vec{y}_\alpha|NL\rangle, \tag{6}$$

with three-body μ and two-body iI quantum numbers $\mu = iI = nlNL$, we can write the system of equations for the unknowns $X^\alpha_\mu = \langle\tilde{\mu}_\alpha|\Psi_\alpha\rangle$ to be solved:

$$X^\alpha_\mu = \sum_{(\mu)\gamma\neq\alpha} [G_\alpha(z)]_{\mu\mu''}(V^s_\alpha)_{\mu''\mu'''}(M_{\alpha\gamma})_{\mu'''\mu'}X^\gamma_{\mu'}. \tag{7}$$

The eigenvalue equation is $\mathrm{Det}(\hat{1} - A(z)) = 0$, where matrix $A(z) = G(z)V^sM$.

The matrix elements of the overlap matrix between basis functions from different Jacobi coordinate sets $(M_{\alpha\gamma})_{\mu\mu'} = \langle\tilde{\mu}_\alpha|\mu'_\gamma\rangle$ and of the strong potentials $(V^s_\alpha)_{\mu\mu'} = \langle\mu_\alpha|V^s_\alpha|\mu'_\alpha\rangle$ in Eq. (7) can be calculated numerically. The remaining matrix elements in the kernel – matrix elements of the partition Green's functions:

$$\begin{aligned}
&[G_\alpha(z)]_{\mu\mu'} \\
&= \left\langle \tilde{\mu}_\alpha \left| \left(z - h_0(x_\alpha) - h_0(y_\alpha) - V^s_\alpha(x_\alpha) - \frac{e^2}{x_{pK^-}}\right)^{-1} \right| \tilde{\mu'}_\alpha \right\rangle,
\end{aligned} \tag{8}$$

are the basic quantities of the method, and their calculation depends on α.

For $\alpha = (pK^-, n)$ the $G_\alpha(z)$ is Green's function of two non-interacting subsystems. Therefore, it can be calculated by a convolution integral along a suitable contour in the complex energy plane [13]

$$G_\alpha(z) = \oint g^{sc}_\alpha(\epsilon; x_\alpha) g^0_\alpha(z-\epsilon; y_\alpha) d\epsilon, \tag{9}$$

where

$$g^{sc}_\alpha(z; x_\alpha) = \left(z - h_0(x_\alpha) - V^s_\alpha + \frac{e^2}{x_\alpha}\right)^{-1} \tag{10}$$

$$g^0_\alpha(z; y_\alpha) = (z - h_0(y_\alpha))^{-1} \tag{11}$$

are two-body Green's functions with strong plus Coulomb potential and free Green's function, respectively. While values of $[g^0_\alpha(z;y_\alpha)]_{ll'}$ can be calculated using the properties of the Coulomb Sturmian basis, the matrix elements of $[g^{sc}_\alpha(z;x_\alpha)]_{ii'}$ can be found from the matrix resolvent equation

$$[g^{sc}_\alpha(z;x_\alpha)]_{ii'} = [g^{c}_\alpha(z;x_\alpha)]_{ii'} + \sum_{i'',i'''}[g^{c}_\alpha(z;x_\alpha)]_{ii''}(V^s_\alpha)_{i''i'''}[g^{sc}_\alpha(z;x_\alpha)]_{i'''i'}. \quad (12)$$

For the other two channels $\alpha \neq (pK^-, n)$ an intermediate step is required. In this case the Coulomb potential is given not in its "natural" coordinates, therefore, we first rewrite it in the form

$$-\frac{e^2}{|c_\alpha\vec{x}_\alpha + \vec{y}_\alpha|} = -\frac{e^2}{y_\alpha} + \left(\frac{e^2}{y_\alpha} - \frac{e^2}{|c_\alpha\vec{x}_\alpha + \vec{y}_\alpha|}\right) = V^{c,ch}_\alpha(y_\alpha) + U_\alpha(\vec{x}_\alpha, \vec{y}_\alpha). \quad (13)$$

Here $V^{c,ch}_\alpha(y_\alpha)$ is the channel Coulomb interaction and $U_\alpha(\vec{x}_\alpha, \vec{y}_\alpha)$ is a (short range) polarization potential, entering in the equation

$$G_\alpha(z) = G^{ch}_\alpha(z) + G^{ch}_\alpha(z)U_\alpha G_\alpha(z) \quad (14)$$

for calculation of $G_\alpha(z)$. Its matrix elements $(U_\alpha)_{\mu\mu'} = \langle\mu_\alpha|U_\alpha|\mu'_\alpha\rangle$ can be evaluated by numerical integration. The channel three-body Green's function in Eq. (14) is defined by

$$G^{ch}_\alpha(z) = \left(z - h_0(x_\alpha) - h_0(y_\alpha) - V^s_\alpha(x_\alpha) + \frac{e^2}{y_\alpha}\right)^{-1} \quad (15)$$

and, again, it corresponds to non-interacting subsystems, therefore, can be found by a convolution integral

$$G^{ch}_\alpha(z) = \oint g^s_\alpha(z;x_\alpha)g^{c,ch}_\alpha(z-\epsilon;y_\alpha)d\epsilon \quad (16)$$

with the two-body Green's functions

$$g^s_\alpha(z;x_\alpha) = \left(z - h_0(x_\alpha) - V^s_\alpha\right)^{-1}, \quad (17)$$

$$g^{c,ch}_\alpha(z;y_\alpha) = \left(z - h_0(y_\alpha) + \frac{e^2}{y_\alpha}\right)^{-1}, \quad (18)$$

which can be obtained from resolvent equations similar to Eq. (12).

This schematic description of the formalism does not reflects the fact, that $\bar{K}N$ interaction is isospin dependent and acts in $I=0$ and $I=1$ states. In particle representation it means that the potential is a 2×2 matrix:

$$\begin{pmatrix} V^s_{pK^-,pK^-} & V^s_{pK^-,n\bar{K}^0} \\ V^s_{n\bar{K}^0,pK^-} & V^s_{n\bar{K}^0,n\bar{K}^0} \end{pmatrix}, \quad (19)$$

therefore, our final equations have 4 Faddeev components, including $\Psi_{(n\bar{K}^0,n)}$, instead of three. A more detailed description of the formalism will follow in a subsequent paper.

Our aim was to evaluate $1s$ level shift and width of kaonic deuterium caused by strong interaction between the antikaon and the nucleons. The reference point z_0, from which the energy shift $\Delta z = z - z_0$ is measured, is the lowest eigenvalue of the "dominant" channel Green's function $G^{ch}_{(pn,K^-)}(z)$. It corresponds to a deuteron and a kaon "feeling" a Coulomb force from the center of mass of the deuteron. At $z = z_0$ all matrix elements of $G^{ch}_{(pn,K^-)}(z)$ are singular, the search for $\mathrm{Det}(\hat{1} - A(z)) = 0$ was performed in the vicinity of z_0.

Table 1
Range $\beta_{\bar{K}N}$ (fm^{-1}) and strength $\lambda_{\bar{K}N,I=0}$, $\lambda_{\bar{K}N,I=1}$ (fm^{-2}) parameters of the four complex $\bar{K}N$ potentials V_I, V_{II}, V_{III}, and V_{IV} in isospin representation.

	$\beta_{\bar{K}N}$	$\lambda_{\bar{K}N,I=0}$	$\lambda_{\bar{K}N,I=1}$
V_I	3.0000	$-1.7258 - i\,0.8570$	$-0.7323 - i\,0.4201$
V_{II}	3.6367	$-2.1606 - i\,0.5937$	$-1.0998 - i\,0.4861$
V_{III}	3.6367	$-1.9563 - i\,0.4534$	$-0.9761 - i\,0.3787$
V_{IV}	2.1978	$-0.5669 - i\,0.2744$	$-0.1666 - i\,0.1489$

In fact, even in the absence of the strong interaction of the kaon with the nucleons, the presence of the polarization potential $U_{(pn,K^-)}$ causes a certain real shift of the eigenvalue from z_0 to z_1. It reflects the fact, that Coulomb interaction acts between the antikaon and the proton, not between K^- and d. In principle, the strong shift should be measured from z_1 instead of z_0. However, the effect is small, in our case $z_1 - z_0 \approx 10$ eV.

The calculation itself demands a rather heavy numerical work with a lot of small but important technical details. The convergence of the method depends on the good choice of the range parameters b of the Sturmian functions. The optimal parameters are different in different partition channels and are non-equal for the x and y variables. For a good choice of the b-s 30–40 functions for every variable give an accuracy of $\sim 0.5\%$ ($\sim 1-2$ eV). The dimension of the final matrix is rather large, for 40 functions in each variable it is about 5000.

We used four models of $\bar{K}N$ interaction, all are one-term separable complex potentials with Yamaguchi form factors. The isospin dependent $I=0$ and $I=1$ potentials (their parameters are shown in Table 1) were transformed into particle basis, see Eq. (19). Two potentials reproduce low-energy characteristics of the $\bar{K}N$ system, obtained from a coupled-channel chirally motivated model of the interaction from [3]: either the $I=0$ and $I=1$ $\bar{K}N$ scattering lengths (V_{III}) or the K^-p scattering length and the upper pole forming $\Lambda(1405)$ resonance (V_{II}). The other two models were fitted to the experimental values of $1s$ level shift and width of kaonic hydrogen, measured by SIDDHARTA Collaboration [14] (V_I, V_{IV}), and to the low-energy K^-p cross-sections (V_{IV}). As a result, all four potentials give $1s$ level shift of kaonic hydrogen (presented in Table 2) within or close to the SIDDHARTA data and a reasonable fit to the elastic $K^-p \to K^-p$ and charge exchange $K^-p \to \bar{K}^0n$ cross-sections.

For the NN interaction we took a separable potential, which reproduces NN scattering lengths, low-energy phase shifts and deuteron binding energy in np state.

The results of the calculations are shown in Table 2. The exact (accurate to ≈ 1 eV) results are compared with commonly used approximations, mentioned in the introduction. For the approximate evaluations we used outputs of our Faddeev calculations of low-energy K^-d scattering without Coulomb interaction. In particular, the corrected Deser [6]

$$\Delta E^{cD} - i\frac{\Gamma^{cD}}{2} = -2\alpha^3\mu^2_{K^-d}a_{K^-d} \times [1 - 2\alpha\mu_{K^-d}a_{K^-d}(\ln\alpha - 1)] \quad (20)$$

and the original Deser formula [5], which contains only the first term in the brackets of the Eq. (20), use the K^-d scattering length a_{K^-d}, calculated with the corresponding $\bar{K}N$ potentials. The reduced mass of the K^-d system is denoted by μ_{K^-d} in Eq. (20), while α is the fine structure constant. The effective optical $K^- - d$ potential was fitted to the low-energy K^-d amplitudes from Faddeev calculation and then used in Lippmann–Schwinger equation together with Coulomb potential in the same way as in [2]. Keeping in mind relative values of deuteron and Bohr radius of kaonic deuterium, the approximation seemed well grounded.

Table 2
Kaonic deuterium and hydrogen 1s level shifts ΔE and widths Γ in a form $\Delta(E) - i\,\Gamma/2$ (eV) for the four complex $\bar{K}N$ potentials. The first and last column show two- and three-body exact results, respectively, while the approximate Deser, corrected Deser values and those obtained with optical $K^- - d$ potential are in columns 2, 3 and 4, respectively.

	Kaonic hydrogen shift	Kaonic deuterium shift			
		Deser	Corrected Deser	Complex $V_{K^- - d}$	Exact Faddeev
V_I	$-280 - i\,268$	$-723 - i\,596$	$-675 - i\,351$	$-650 - i\,434$	$-641 - i\,428$
V_{II}	$-217 - i\,292$	$-732 - i\,634$	$-694 - i\,370$	$-658 - i\,460$	$-646 - i\,444$
V_{III}	$-219 - i\,293$	$-837 - i\,744$	$-795 - i\,390$	$-747 - i\,517$	$-732 - i\,490$
V_{IV}	$-280 - i\,266$	$-854 - i\,604$	$-750 - i\,310$	$-740 - i\,422$	$-736 - i\,413$

It is seen from the table that the original Deser formula can be considered only as a rough estimate. The corrected Deser gives somewhat better real part of the 1s level shift, but has quite large error for the width of the level. The most accurate approximation is the exact two-body calculation with the $K^- - d$ effective optical potential supplemented by the Coulomb interaction.

The next step could be a more realistic calculation of the kaonic deuterium atom. In particular, the formalism should be extended to treat energy dependent $\bar{K}N$ interaction models. This is necessary for the inherently energy dependent chirally motivated potentials and for a proper account of the $\pi\Sigma$ channel via an energy dependent exact optical potential.

Acknowledgements

The work was supported by the Czech GACR grant 15-04301S and the Hungarian OTKA grant 109462.

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