# Constraining the $\bar{K}N$ interaction from the 1S level shift of kaonic deuterium

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Motivated by the precise measurement of the 1S level shift of kaonic hydrogen, we perform accurate three-body calculations for the spectrum of kaonic deuterium using a realistic antikaon-nucleon ( $\bar{K}N$ ) interaction. In order to describe both short- and long-range behaviors of the kaonic atomic states, we solve the three-body Schrödinger equation with a superposition of a large number of correlated Gaussian basis functions covering distances up to several hundreds of fm. Transition energies between 1S, 2P, and 2S states are determined with high precision. The complex energy shift of the 1S level of kaonic deuterium is found to be  $\Delta E - i\Gamma/2 = (670 - i\ 508)$  eV. The sensitivity of this level shift with respect to the isospin I = 1 component of the  $\bar{K}N$  interaction is examined. It is pointed out that an experimental determination of the kaonic deuterium level shift within an uncertainty of 25% will provide a constraint for the I = 1 component of the  $\bar{K}N$  interaction significantly stronger than that from kaonic hydrogen.

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#### I. INTRODUCTION

In recent years, systems involving antikaons ( $\bar{K} = K^-, \bar{K}^0$ ) have been widely explored in hadron and strangeness nuclear physics. Studies of the  $\Lambda(1405)$ , as a  $\bar{K}N$  quasibound state coupled to the  $\pi$   $\Sigma$  continuum, suggested early on [1,2] that the low-energy interaction between  $\bar{K}$  and nucleon (N) is strongly attractive. This implies the principal possibility of forming  $\bar{K}$ -nuclear quasibound states, or kaonic nuclei [3–7]. Many experiments and theoretical calculations have been devoted to search for such exotic nuclear systems (see, for example, Refs. [8,9] for recent reviews).

The  $\bar{K}NN$  three-body system, as the lightest prototype of a kaonic nucleus, has been studied actively. A number of theoretical works suggested the existence of this quasibound state [4,5,10–19] and pointed to its possible signatures in production reactions [20–23], but no consensus has been reached so far; the quantitative results depend strongly on the  $\bar{K}N$  interaction employed in the calculations.

Experimentally, the existence of kaonic nuclei is controversial as well. In some reports, a peak structure is observed around 100 MeV below the  $\bar{K}NN$  threshold [24–26]. But, if interpreted as a  $\bar{K}$ -nuclear bound state, such a large binding energy could not be accounted for in any of the theoretical studies [4,5,10–19]. On the other hand, measurements reported in Refs. [27–29] did not find a corresponding prominent signal in their spectra. Recently the J-PARC E15 experiment [30] observed a peak structure near the  $\bar{K}NN$  threshold in the  $^3$ He( $K^-, \Lambda p$ )n reaction, which awaits further analysis and interpretation.

In the theoretical calculations of kaonic nuclei, the  $\bar{K}N$  interaction below the  $\bar{K}N$  threshold energy is an essential ingredient. Since the subthreshold energy region cannot be directly accessed by  $\bar{K}N$  scattering experiments, extrapolations are necessary in order to construct the scattering amplitude below the  $\bar{K}N$  threshold. Such extrapolations are subject to uncertainties in the  $\bar{K}N$  interaction itself.

A kaonic atom in which a  $K^-$  is bound to an ordinary nucleus by the Coulomb force is a useful object for investigating the  $\bar{K}N$  interaction just below threshold. In an ordinary atomic systems, electrons are bound exclusively by the Coulomb interaction. In a kaonic atom, the binding energy is determined by both Coulomb and strong  $\bar{K}N$  interactions. The purely Coulombic energy of the 1S atomic orbit,  $E_{1S}^{C} < 0$ , is shifted to a complex energy  $E_{1S}$  by the  $\bar{K}N$  interaction and the absorptive transitions to lower energy  $\pi \Lambda$  and  $\pi \Sigma$  channels. This 1S level shift and width,  $\Delta E - i\Gamma/2 = E_{1S} - E_{1S}^C$ , reflects the  $\bar{K}N$  interaction at threshold. Actually, this level shift is measured by the x-ray transition energy from 2P to 1S, assuming that the 2P state is not affected by the  $\bar{K}N$ interaction. A prominent example is the 1S level shift of kaonic hydrogen, the  $K^-$ -proton (p) atomic system, determined as  $\Delta E = 283 \pm 36 \pm 6$  eV and  $\Gamma = 541 \pm 89 \pm 22$  eV by the SIDDHARTA experiment [31,32].

The SIDDHARTA data helped reduce significantly the theoretical uncertainties of the scattering amplitude at and below the  $\bar{K}N$  threshold [33,34]. However, these data are not sufficient in order to determine the full isospin dependence of the  $\bar{K}N$  interaction. The isospin I=0 component is well constrained by the properties of the  $\Lambda(1405)$  as a  $\bar{K}N(I=0)$  state coupled to the strongly interacting  $\pi\Sigma$  continuum. Kaonic hydrogen involves both isospin I=0 and I=1 components equally, but a large uncertainty still remains in the I=1 component of the  $\bar{K}N$  interaction [35].

In order to extract further information on this I=1 component, we consider kaonic deuterium, the  $K^-$ -deuteron (d) atomic system. In  $K^-d$ , the ratio of I=0 to I=1 is 1:3; therefore kaonic deuterium is expected to be a more sensitive probe than kaonic hydrogen for the I=1 component of the  $\bar{K}N$  interaction. Its full isospin dependence can thus be determined more precisely by combining data from kaonic hydrogen and deuterium.

In the SIDDHARTA experiment [31], a kaonic deuterium run was performed simultaneously with the hydro-

gen run but the statistics was not sufficient for a reliable separation of signal versus background. New experiments are now being planned to measure kaonic deuterium: J-PARC E57 [36] and SIDDHARTA-2 [37,38]. The tentatively expected precision of these measurements is 60 (30) eV for the shift and 140 (70) eV for the width at J-PARC E57 (SIDDHARTA-2).

In the present work we investigate the level shifts and decay widths of kaonic deuterium by performing a full three-body calculation, aiming at a more stringent constraint for the I=1 component of the  $\bar{K}N$  interaction. We use a modern  $\bar{K}N$  interaction, the Kyoto  $\bar{K}N$  potential [39] that has been constructed based on chiral SU(3) effective field theory. Thanks to systematic improvements with inclusion of higher order terms, this potential reproduces very well all available low-energy  $\bar{K}N$  empirical data ( $K^-p$  total cross sections, branching ratios at  $K^-p$  threshold and the SIDDHARTA data) with an accuracy of  $\chi^2/\text{d.o.f.} \simeq 1$  [33,34].

There are several theoretical studies of kaonic deuterium as an approximate  $K^-d$  two-body problem [40–42]. The relationship between kaonic deuterium observables and  $\bar{K}$  N two-body scattering lengths has been discussed in Refs. [43–45]. Three-body Faddeev calculations of kaonic deuterium also have their own history; see, for example, Ref. [46]. Recently, advanced Faddeev calculations with separable potentials constrained by the SIDDHARTA kaonic hydrogen data have been performed [47,48]. The 1S  $K^-d$  atomic state was evaluated assuming isospin symmetry for the  $\bar{K}$  and nucleon doublets.

Experimentally the 1S level shift is determined from the transition between 2P and 1S states. It is thus important to calculate the precise transition energy between these two states. We perform highly accurate three-body calculations for the 1S, 2P, and 2S energy levels using physical masses of all particles involved, and examine how those levels are affected by the strong  $\bar{K}N$  interaction. Finally, we quantify the accuracy requirement for a measurement of the kaonic deuterium level shift and width aimed at improving constraints on the I=1 components in the  $\bar{K}N$  interaction.

The following section discusses first the properties of the  $\bar{K}N$  interaction by examining the kaonic hydrogen two-body system. Details of the three-body calculation of kaonic deuterium are explained in Sec. III. Section IV presents numerical results of the full three-body calculations. In Sec. IV A, the energy spectrum of kaonic deuterium is presented. The impact of strong-interaction effects on the spectrum is discussed by comparing spectra with and without the  $\bar{K}N$  interaction. In Sec. IV B, the sensitivity with respect to the I=1 component of the  $\bar{K}N$  interaction is tested by changing selectively its strength within presently existing uncertainties. In Sec. IV C, we compare our results to the improved Deser formula, a frequently used approximation to evaluate the 1*S* level shift. A summary is given in Sec. V.

# II. $\bar{K}N$ INTERACTION and Kaonic hydrogen

In the present work, we employ the recently developed, complex, and energy-dependent Kyoto  $\bar{K}N$  potential [39] as the basic antikaon-nucleon interaction. This potential reproduces the scattering amplitudes that were calculated previously

based on chiral SU(3) coupled-channels dynamics [33,34]. The potential in its original form is written in the isospin basis, from which the particle basis potential is constructed as

$$\hat{V}_{ij}^{\bar{K}N} = \frac{1}{2} \left[ \hat{V}_{ij}^{\bar{K}N(I=0)} + \hat{V}_{ij}^{\bar{K}N(I=1)} \right] 
- \frac{1}{2} \left[ \hat{V}_{ij}^{\bar{K}N(I=0)} - \hat{V}_{ij}^{\bar{K}N(I=1)} \right] P_{\tau}^{ij},$$
(1)

where the Heisenberg operator  $P_{\tau}^{ij}=(1+\tau_i\cdot\tau_j)/2$  exchanges the ith and jth particles in the isospin wave function. In the particle basis, which is going to be used in the following, the exchange operator acts as  $P_{\tau}^{ij}|K^-n\rangle=|K^-n\rangle$ ,  $P_{\tau}^{ij}|K^-p\rangle=-|\bar{K}^0n\rangle$ , and  $P_{\tau}^{ij}|\bar{K}^0n\rangle=-|K^-p\rangle$ . The charge exchange channel coupling between  $K^-p$  and  $\bar{K}^0n$  occurs through the isospin dependence of the  $\bar{K}N$  interaction.

Effects of the decay processes into  $\pi \Sigma$  and  $\pi \Lambda$  channels are encoded in the imaginary part of the  $\bar{K}N$  potential. The strength of the interaction depends on the energy  $E_{\bar{K}N}$  being treated self-consistently in the Schrödinger equation in order to reproduce the coupled-channels scattering amplitudes.

Before proceeding to the calculation of kaonic deuterium, it is mandatory to check the applicability of the Kyoto  $\bar{K}N$  potential for the present study. We recall that the fitting to the kaonic hydrogen data in Refs. [33,34] was performed making use of the improved Deser formula [60], whereas in the present work we solve the Schrödinger equation to evaluate the level shift and width. Moreover, the threshold energy difference between the  $K^-p$  and  $\bar{K}^0n$  channels is about 5 MeV and should properly be taken into account in the level shift calculation. While the amplitudes in Refs. [33,34] were calculated using physical hadron masses, the Kyoto  $\bar{K}N$  potential of Ref. [39] has originally been formulated in the isospin basis with isospin-averaged masses, and so this potential is converted to the particle basis with physical masses for the application reported in the present work.

As a first test, the energy of kaonic hydrogen is computed by solving the coupled-channels Schrödinger equation

$$\begin{pmatrix}
\hat{T} + \hat{V}^{\bar{K}N} + \hat{V}^{C} & \hat{V}^{\bar{K}N} \\
\hat{V}^{\bar{K}N} & \hat{T} + \hat{V}^{\bar{K}N} + \Delta m
\end{pmatrix}
\begin{pmatrix}
|K^{-}p\rangle \\
|\bar{K}^{0}n\rangle
\end{pmatrix}$$

$$= E \begin{pmatrix}
|K^{-}p\rangle \\
|\bar{K}^{0}n\rangle
\end{pmatrix} \tag{2}$$

with the kinetic energy  $\hat{T}$ , the Coulomb interaction  $\hat{V}^C$ , and the Kyoto  $\bar{K}N$  potential in the particle basis, using the following physical masses:  $M_p = 938.272$  MeV,  $M_n = 939.565$  MeV,  $M_{K^-} = 493.677$  MeV, and  $M_{\bar{K}^0} = 497.648$  MeV for protons, neutrons, and antikaons, respectively [49].  $\Delta m$  denotes the mass difference of the  $K^-p$  and  $\bar{K}^0n$  channels. The kaonic hydrogen wave function is expressed as a superposition of a large number of square-integrable Gaussian basis functions reaching out to far distances. In the Coulomb-bound state the  $K^-p$  channel is closed and the  $\bar{K}^0n$  channel with its higher physical mass is closed as well, and so the relevant matrix elements are accurately determined.

The results for the  $K^-$ -hydrogen shift and width are listed in Table I. As shown in the first line of this table, the self-consistent solution of the Schrödinger equation using physical masses reproduces the experimental SIDDHARTA

TABLE I. Level shifts and decay widths of the 1*S* atomic state of the kaonic hydrogen with physical masses and with isospin averaged masses. Results by setting  $E_{\bar{K}N}=0$  in the  $\bar{K}N$  interaction are also shown.

Mass	E dependence	$\Delta E \text{ (eV)}$	Γ (eV)
Physical	Self-consistent	283	607
Isospin	Self-consistent	163	574
Physical	$E_{\bar{K}N}=0$	283	607
Expt. [31,32]		$283 \pm 36 \pm 6$	$541 \pm 89 \pm 22$

result [31,32] within its uncertainties. The Kyoto  $\bar{K}N$  potential in the particle basis thus proves to be a valid input even though the original construction of the potential was not optimized for this purpose. On the other hand, when calculating kaonic hydrogen with isospin-averaged masses of the antikaon and nucleon doublets, we obtain the result shown in the second ("Isospin") row of Table I. One observes a quantitative change of the energy shift by more than 100 eV, exceeding by far the uncertainty of the measurement [31,32]. While it is common practice in strong-interaction calculations to assume that isospin breaking effects are not very significant, these effects can be kinematically enhanced in near-threshold observables. To elucidate the difference, we show in Table II the  $\bar{K}N$  scattering lengths calculated with physical masses and with isospin-averaged masses. The isospin averaging implies an upward shift of the  $K^-p$  threshold by 2.6 MeV from its physical location. As a consequence, the real part of the  $K^-p$ scattering length  $a_{K^-p}$  is reduced in magnitude by 0.26 fm (i.e., by about 40%). The more detailed discussion of the resulting kaonic hydrogen energy shift and width follows in Sec. IV C featuring the improved Deser formula. Hence, it is obvious that precise physical masses must be used in the level shift computation.

Next we examine the effect of the energy dependence of the Kyoto  $\bar{K}N$  potential. This energy dependence is essential in determining the binding energies (several tens of MeV) of  $\bar{K}$ -nuclear systems with few to several nucleons [19]. However, the atomic states are located in the near neighborhood of the threshold. Their binding energies are as small as a few keV. To study the effect of the energy dependence, we perform the same calculation as previously described, but setting  $E_{\bar{K}N}=0$  in the potential. As shown in the third row of Table I, the self-consistent and fixed  $E_{\bar{K}N}=0$  results turn out to be numerically identical. Therefore, in the level shift calculation of the atomic states, the energy dependence of the  $\bar{K}N$  potential can be safely neglected, and this is how we shall proceed hereafter, setting  $E_{\bar{K}N}=0$  throughout.

# III. THREE-BODY APPROACH TO KAONIC DEUTERIUM

#### A. Three-body Hamiltonian

We start from the following three-body Hamiltonian for kaonic deuterium:

$$\hat{H} = \sum_{i=1}^{3} \hat{T}_{i} - \hat{T}_{cm} + \hat{V}_{23}^{NN} + \sum_{i=2}^{3} (\hat{V}_{1i}^{\bar{K}N} + \hat{V}_{1i}^{EM}), \quad (3)$$

where  $\hat{T}_i$  denotes the kinetic energy of the *i*th particle (i = 1 for an antikaon and i = 2, 3 for two nucleons), including physical masses of p, n,  $K^-$ , and  $\bar{K}^0$ . The center-of-mass kinetic energy,  $\hat{T}_{cm}$ , is properly subtracted.

We use the Minnesota potential [50] as the NN interaction,  $\hat{V}^{NN}$ . This potential is technically convenient for three-body computations. It operates with a central force only but reproduces the binding energy and radius of the deuteron. In fact, what matters primarily in the kaonic deuterium calculation is a deuteron density distribution,  $\rho_d(r)$ . We checked that  $r^2\rho_d(r)$  deduced from the Minnesota potential agrees perfectly and quantitatively with the radial density profile generated by realistic NN interactions such as the CD-Bonn potential [51].

For the antikaon-nucleon interaction,  $\hat{V}^{\bar{K}N}(\hat{E})$ , we employ the Kyoto  $\bar{K}N$  potential [39]. As just pointed out, the choice of the two-body antikaon-nucleon energy at threshold,  $E \equiv E_{\bar{K}N} = 0$ , is justified for kaonic hydrogen. For kaonic deuterium, this issue requires further discussion. The energy of the  $\bar{K}N$  two-body subsystem within the  $K^-d$  three-body system is not a well-defined concept. Different prescriptions [13,14,17,19] are available to take into account the motion of the bound nucleons while they interact with the antikaon. In the present work, we use the prescription of Refs. [13,14,19], where  $E_{\bar{K}N}$  is proportional to the kaon binding energy. This amounts to setting  $E_{\bar{K}N} = 0$  in the two-body potential  $\hat{V}^{\bar{K}N}$  also for kaonic deuterium, the choice we take as our default input in the following three-body calculations. Leading corrections to this minimal choice are discussed in the appendix and numerically estimated using the resummed Deser formula in Sec. IV C.

The electromagnetic (Coulomb) interaction is denoted by  $\hat{V}^{EM}$ . The effect of higher order QED corrections will be discussed in Sec. IV C. The explicit three-body coupled-channels equation is written as

$$\begin{pmatrix}
\hat{H}_{K^{-}pn} & \hat{V}_{12}^{\bar{K}N} + \hat{V}_{13}^{\bar{K}N} \\
\hat{V}_{12}^{\bar{K}N} + \hat{V}_{13}^{\bar{K}N} & \hat{H}_{\bar{K}^{0}nn}
\end{pmatrix}
\begin{pmatrix}
|K^{-}pn\rangle \\
|\bar{K}^{0}nn\rangle
\end{pmatrix}$$

$$= E \begin{pmatrix}
|K^{-}pn\rangle \\
|\bar{K}^{0}nn\rangle
\end{pmatrix} \tag{4}$$

with

$$\hat{H}_{K^{-}pn} = \sum_{i=1}^{3} \hat{T}_{i} - \hat{T}_{cm} + \hat{V}_{23}^{NN} + \sum_{i=2}^{3} (\hat{V}_{1i}^{\bar{K}N} + \hat{V}_{1i}^{EM}), (5)$$

$$\hat{H}_{\bar{K}^0 nn} = \sum_{i=1}^{3} \hat{T}_i - \hat{T}_{cm} + \hat{V}_{23}^{NN} + \sum_{i=2}^{3} \hat{V}_{1i}^{\bar{K}N} + \Delta M, \quad (6)$$

with  $\Delta M$  denoting the mass difference of the  $K^-pn$  and  $\bar{K}^0nn$  channels. In the following subsection, we describe how the coupled-channels three-body equation is solved in practice.

#### **B.** Basis functions

The three-body Schrödinger equation is solved using a variational method with basis expansion. The generic basis function is expressed as

$$\Phi = \mathcal{A}[\psi^{(\text{space})} \otimes \psi^{(\text{spin})} \otimes \psi^{(\text{isospin})}], \tag{7}$$

Mass	$a_{K^{-}p}$ (fm)	$a_{K^-p^-\bar{K}^0n}$ (fm)	$a_{\bar{K}^0n}$ (fm)	$a_{K^{-}n}$ (fm)
Physical Isospin	-0.66 + i0.89 $-0.40 + i0.81$	-0.85 + i0.26 $-0.99 + i0.04$	-0.40 + i  1.03 $-0.40 + i  0.81$	$0.58 + i0.78 \\ 0.58 + i0.77$

TABLE II.  $\bar{K}N$  scattering lengths with physical masses and with isospin averaged masses.

where A is the antisymmetrizer for two nucleons.

Since the Hamiltonian considered in this paper does not change the total orbital angular momentum, L, and the total spin, S, of the particles, we can introduce an L=0 and S=1 state with isospin-3 component  $M_T=-\frac{1}{2}$  as a basis to describe kaonic deuterium. The spin wave function S=1 is given explicitly as

$$\psi^{(\text{spin})} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \tag{8}$$

where the first (second) arrow indicates the spin of the nucleon with index i=2 (i=3). The isospin part,  $\psi^{(\text{isospin})}$ , of the wave function written in the particle basis includes the following two channels:

$$|K^-pn\rangle = |\downarrow\uparrow\downarrow\rangle, \quad |\bar{K}^0nn\rangle = |\uparrow\downarrow\downarrow\rangle.$$
 (9)

For the radial part of the wave function, we use correlated Gaussian (CG) basis functions [52,53]. This method is sufficiently flexible so that it enables us to describe both short-and long-range behaviors of the wave function accurately, a necessary condition when dealing with systems such as kaonic deuterium in which the very different distance scales characteristic of Coulomb and strong interactions must be treated simultaneously. (See recent reviews, Refs. [54,55], for many applications of the CG method.)

Let x denote a two-dimensional column vector whose ith element is a usual three-dimensional coordinate vector,  $x_i$ . The spatial part of the wave function in Eq. (7) is written in the form [56]

$$F_{LM_L}(u, v, A, \mathbf{x}) = \exp\left(-\frac{1}{2}\tilde{\mathbf{x}}A\mathbf{x}\right) [\mathcal{Y}_{L_1}(\tilde{u}\mathbf{x})\mathcal{Y}_{L_2}(\tilde{v}\mathbf{x})]_{LM_L},$$
(10)

with solid spherical harmonics

$$\mathcal{Y}_{lm}(\mathbf{r}) = r^l Y_{lm}(\hat{\mathbf{r}}). \tag{11}$$

In Eq. (10), A is a  $2 \times 2$  positive-definite symmetric matrix, and a tilde stands for the transposed matrix. The product  $\tilde{x}Ax$  is a short-hand notation for  $A_{11}x_1^2 + A_{22}x_2^2 + 2A_{12}x_1 \cdot x_2$ . The off-diagonal element,  $A_{12}$ , induces correlations between the coordinates  $x_1$  and  $x_2$ . The global vector (GV),  $\tilde{u}x = u_1x_1 + u_2x_2$ , describes rotational motion of the system, with u and v being two-dimensional column vectors which specify the rotation axes.

One of the advantages of the combined CG+GV method is that its functional form does not change under linear coordinate transformations. Suppose that the matrix A and the vectors u and v are defined in the x coordinate set. Defining a transformation matrix T as y = Tx, we can work equivalently with the y coordinate set, simply replacing A, u, and v by  $\tilde{T}AT$ ,  $\tilde{T}u$ , and  $\tilde{T}v$ , respectively.

Consider two sets of Jacobi coordinates:

$$x_1 = r_2 - r_3,$$
  
 $x_2 = \frac{m_2}{m_2 + m_3} r_2 + \frac{m_3}{m_2 + m_3} r_3 - r_1,$  (12)

and

$$y_1 = r_1 - r_2,$$
  
 $y_2 = \frac{m_1}{m_1 + m_2} r_1 + \frac{m_2}{m_1 + m_2} r_2 - r_3,$  (13)

where  $r_i$  stands for the single-particle coordinate of the ith particle. Both of these sets are equally suitable for the three-body calculation. However, when dealing with the channel coupling between systems of different mass, the coordinates  $x_2$  and  $y_2$  are not common to the  $K^-pn$  and  $\bar{K}^0nn$  channels. We therefore use the following integral coordinates which do not depend on any particle masses:

$$z_1 = r_1 - r_2,$$
  
 $z_2 = r_2 - r_3,$  (14)

for evaluating the off-diagonal matrix element between the  $K^-pn$  and  $\bar{K}^0nn$  channels.

# C. Energy convergence

In this work, short-range strong interactions as well as the long-range Coulomb interactions have to be treated simultaneously with high precision. To extract the detailed effects of the  $\bar{K}N$  interaction from the spectrum of kaonic deuterium, we need to calculate the binding energy with an accuracy of a few eV. This is a computational challenge that demands great care. In this subsection, we discuss how to meet this challenge of calculating wave functions with the required precision.

The wave function is expanded in a large set of basis functions, Eq. (7), and the generalized eigenvalue problem

$$\sum_{i=1}^{K} (H_{ij} - EB_{ij})C_j = 0,$$
(15)

is solved to determine the coefficients  $C_i$  and eigenenergy E, with the Hamiltonian matrix  $H_{ij} = \langle \Phi_i | H | \Phi_j \rangle$  and the overlap matrix  $B_{ij} = \langle \Phi_i | \Phi_j \rangle$ . Here K is the number of basis functions. To achieve energy convergence for the kaonic atom, it turns out that we need to include basis functions reaching over distance scales from one tenth to several hundreds of fm. Given the large number of nonorthogonal basis functions, we cannot solve the generalized eigenvalue problem due to round-off errors in the double-precision computation [57]. To avoid this problem, we reconstruct a new orthonormal basis set from the prepared basis functions by diagonalizing the overlap

TABLE III. Cutoff parameter  $\lambda_{\text{cut}}$ , number of basis functions N, and the real part of the energy of the 1S state of kaonic deuterium.

$log_{10} \lambda_{cut}$	N	Re[E] (MeV)
16	1677	-2.211689436
17	2194	-2.211722964
18	2377	-2.211732072
19	2511	-2.211735493
20	2621	-2.211737242
21	2721	-2.211737609
22	2806	-2.211737677
23	2879	-2.211737682

matrix  $B_{ij}$ :

$$\phi_{\mu} = \frac{1}{\sqrt{\mu}} \sum_{i=1}^{K} c_i^{(\mu)} \Phi_i.$$
 (16)

The number of new basis functions  $\{\phi_{\mu}\}$  is again K, and each function is labeled by its eigenvalue  $\mu$ . The Hamiltonian is then diagonalized with this set of basis functions, omitting those which give very small  $\mu$ . If a whole set of basis functions emerges with very small  $\mu$ , we discard this set altogether and try another one. In practice, a cutoff parameter is introduced, defined by the ratio of minimum to maximum eigenvalues  $\mu$  as  $\lambda_{\rm cut} = \mu_{\rm max}/\mu_{\rm min}$ . Basis functions with  $\mu < \mu_{\rm min}$  are discarded. The cutoff parameter is taken as large as possible within significant digits of the double-precision computation.

To generate the elements of the matrix A (the variational parameters), we use a geometric progression [58] for diagonal matrix elements of A with the x coordinates defined in Eq. (12). For the global vectors, we simply take  $\tilde{u}=(1,0)$  and  $\tilde{v}=(0,1)$  to define an angular momentum for each coordinate. Intermediate angular momenta up to  $L_1+L_2\leqslant 4$  are taken into account.

For the diagonal elements of the matrices A, u, and v, the variational procedures can actually be optimized by suitably combining a representation using the coordinates x of Eq. (12) with the equivalent representation in the so-called rearrangement channel, using the coordinates y of Eq. (13). The evaluation of the Hamiltonian matrix elements is then performed in x coordinates applying the transformations  $A \to \tilde{T}AT$ ,  $u \to \tilde{T}u$ , and  $v \to \tilde{T}v$  where appropriate.

With one-by-one inclusion of those channels just mentioned, several sets of variational parameters are prepared covering distance scales from 0.1 fm to 300–1000 fm, in a search for the lowest energy. We need more than 30 Gaussian basis functions for each coordinate to achieve energy convergence within a few eV. After a careful examination of the energy convergence by introducing the cutoff parameter  $\lambda_{\text{cut}}$ , the total number of basis functions K is 4096 and 8192 for the S and P states, respectively.

Table III shows the cutoff dependence of the real part of the energy of the kaonic deuterium 1S state measured from the three-body break-up threshold. N denotes the number of basis functions that actually appear in the diagonalization. The number of primary basis functions, K = 4096, is reduced with decreasing  $\lambda_{\text{cut}}$ . It turns out that we cannot diagonalize

the Hamiltonian for  $\lambda_{cut}\gtrsim 10^{23}$  due to round-off errors in the double-precision calculations. Finally we reach convergence within eV accuracy for  $\lambda_{cut}\gtrsim 10^{20}$ , in which case the number of basis functions becomes approximately half of the number of primary basis functions. For the 2P state, we take  $\lambda_{cut}\gtrsim 10^{28}$ , and  $N\gtrsim 3508$  basis functions are actually needed in the diagonalization.

# IV. RESULTS AND DISCUSSION

#### A. Spectrum and level shifts

Table IV lists binding energies, measured from the  $K^-d$  threshold, and decay widths of kaonic deuterium. The threebody calculation with Coulomb interaction only is shifted slightly from the energy levels produced in the  $K^-d$  two-body calculations with point charge, by 8 and 1 eV for the 1S and 2S states, respectively. The 2P energy remains unchanged in the three-body calculation because the P-wave function around the origin is suppressed by the centrifugal barrier. This behavior is consistent with the  $K^-d$  two-body estimate of the energy shift, assuming a uniform charge distribution as listed in the table.

With inclusion of the  $\bar{K}N$  interaction, the 1S state is shifted by  $\sim$ 670 eV from the  $K^-d$  Coulomb (point charge) 1S level. The level shift and width of the 2S level are an order of magnitude smaller than those of the 1S state because the 2S wave function has a smaller amplitude around the origin than the one of the 1S state. The 2P energy remains unchanged and its decay width is found to be less than 1 eV; the  $\bar{K}N$  interaction has virtually no effect on the 2P state of kaonic deuterium because of the presence of the centrifugal barrier. We can therefore safely extract the 1S level shift from the 2 $P \rightarrow 1S$  transition energy. In summary, the 1S level shift and decay width resulting from the full three-body calculation are predicted as

$$\Delta E - i\frac{\Gamma}{2} = (670 - i\,508)\,\text{eV},$$
 (17)

namely,  $(\Delta E, \Gamma) = (670, 1016)$  eV using the Kyoto  $\bar{K}N$  potential. These values are roughly consistent with those found in a recent Faddeev calculation [48], although the basic interactions used in that approach are different from ours.

For comparison, a full three-body computation of the level shift and width has also been performed using isospin-averaged meson and baryon masses, with the result  $\Delta E - i\Gamma/2 = (672 - i\,509)$  eV. The small deviation, by just a few eV, from the corresponding calculation using physical masses is of some interest here, as this is in unexpected contrast to the relatively large isospin-breaking effects seen in kaonic hydrogen. Some insight into the origin of this difference can be gained by a closer look into the multiple scattering series and the improved Deser formula which relates the level shift and width to the pertinent scattering lengths; see Subsec. IV C.

Up to this point, the determination of the width  $\Gamma$  incorporates the decay channels  $\bar{K}N \to \pi Y$ , where Y stands for  $\Lambda$  and  $\Sigma$  hyperons. The question arises about possible additional contributions to the width from antikaon absorption on two nucleons, with the coupled  $K^-pn$  and  $\bar{K}^0nn$  channels decaying into  $\Lambda n + \Sigma^0 n + \Sigma^- p$ . Early measurements at

TABLE IV. Energy spectrum of kaonic deuterium. Three- and two-body calculations with Coulomb interaction only (omitting the strong  $\bar{K}N$  interaction) are listed in the first three rows. Energy levels resulting from the three-body calculation are measured relative to the calculated  $K^-d$  threshold. For the  $K^-d$  two-body calculations, the deuteron mass  $M_d=1875.613$  MeV has been used [49].

	$E_{1S}(\text{keV})$	$E_{2P}(\text{keV})$	$E_{2S}(\text{keV})$
Coulomb	-10.398	-2.602	-2.600
Uniform charge (2-body)	-10.401	-2.602	-2.601
Point charge (2-body)	-10.406	-2.602	-2.602
Coulomb + $\bar{K}N$	$-9.736 - i\ 0.508$	$-2.602 - i\ 0.000$	$-2.517 - i\ 0.067$

Brookhaven with  $K^-$  stopped on liquid deuterium in the BNL bubble chamber [59] demonstrated that these processes are strongly suppressed as compared to the leading single-nucleon channels,  $\bar{K}N \to \pi Y$ . The ratio of two-nucleon absorption reactions to the single-nucleon processes was found to be as small as  $(1.2 \pm 0.1)\%$  [59]. Taking this value for orientation, the kaonic deuterium 1S width would increase through two-nucleon absorption by only about 10 eV, a correction that can be safely neglected within an uncertainty range of approximately 10 % assigned to the calculated width of about a keV. The smallness of the two-body absorptive width can be understood as follows. Kinematical conditions for the  $\bar{K}NN \to YN$  process require a large momentum transfer of order 1 GeV/c to be provided by the initial deuteron wave function at short distances. The probability for this to take place in a weakly bound, dilute system like the deuteron is small. Similar considerations hold, for example, in the analysis of the  ${}^{3}\text{He}(K^{-}, \Lambda p)n$  reaction [30]. Background simulations performed for this experiment pointed out that two-nucleon absorption is strongly suppressed in the vicinity of the  $K^-pp$ threshold, whereas three-nucleon reactions dominate.

# B. Constraining the I=1 component of $\bar{K}N$ interaction

To quantify the sensitivity of the kaonic deuterium level shift with respect to the I=1 component of the  $\bar{K}N$  interaction, we vary its strength within the uncertainties of the SIDDHARTA kaonic hydrogen measurement [31,32]. This uncertainty range can be simulated by simply multiplying a constant,  $\beta$ , to the real part of the I=1 component of the  $\bar{K}N$  potential. Within the SIDDHARTA constraint [31,32], the control parameter  $\beta$  can range from -0.17 to 1.08. Evidently this constraint is quite weak: Even  $\beta=0$ , i.e., a vanishing real part of the I=1  $\bar{K}N$  potential, would still be acceptable. Theoretical considerations based on chiral SU(3) dynamics would exclude such a possibility, but it cannot be ruled out by just looking at the SIDDHARTA data.

Table V lists the results of the two- and three-body calculations performed with limiting values of  $\beta$  compared to the standard case,  $\beta=1$ . It is interesting to observe that the sensitivity with respect to the I=1  $\bar{K}$  N interaction strength shows different patterns for  $\Delta E$  and  $\Gamma$  in kaonic hydrogen as compared to kaonic deuterium. In the  $K^-p$  system, a variation of  $\beta$  within its upper and lower limits changes  $\Delta E$  by less than 10%, whereas  $\Gamma$  changes by more than 30%. On the other hand, the same variation of  $\beta$  in the  $K^-pn$  system induces a change  $\Delta E$  by 170 eV while  $\Gamma$  remains stable around 1 keV.

One concludes that an accuracy of about 25% in a measurement of the 1S shift in kaonic deuterium would already improve the determination of the I=1  $\bar{K}N$  interaction considerably over the kaonic hydrogen result. The 30–60 eV precision to be expected in the planned experiments [37,38] falls well within that range.

# C. Improved Deser formulas for kaonic deuterium

The improved Deser formula [43,60], derived from nonrelativistic effective field theory (EFT), is frequently used in the investigation of strong-interaction effects in hadronic atoms. The 1*S* level shift  $\Delta E$  and width  $\Gamma$  of a kaonic atom can be estimated by the relation [43,60]

$$\Delta E - \frac{i\Gamma}{2} = -2\mu^2 \alpha^3 a [1 - 2\mu\alpha(\ln\alpha - 1)a], \qquad (18)$$

where  $\mu$  is the kaon-nucleus reduced mass,  $\alpha$  is the fine structure constant, and a is the  $K^-$ -nucleus scattering length. The logarithmically enhanced correction term can be resummed to all orders [61], providing a "double-improved" Deser formula:

$$\Delta E - \frac{i\Gamma}{2} = -\frac{2\mu^2 \alpha^3 a}{1 + 2\mu\alpha(\ln\alpha - 1)a}.$$
 (19)

In this section, we compare our full three-body calculation results with the results obtained from Eqs. (18) and (19). But let us first examine the shift and width of kaonic hydrogen in this context. The  $K^-p$  scattering length obtained by solving the two-body Schrödinger equation with the Kyoto  $\bar{K}N$  potential is shown in Table II. Using Eqs. (18) and (19), one finds the results shown in Table VI. It is evident that the improved Deser formula works reasonably well for kaonic hydrogen and the resummed version indeed improves the accuracy further.

TABLE V. Level shifts and decay widths (in eV) of kaonic hydrogen and deuterium computed with different I=1 strengths of the  $\bar{K}N$  interaction. The experimental level shift data of kaonic hydrogen is  $(\Delta E, \Gamma) = (283 \pm 36 \pm 6, 541 \pm 89 \pm 22)$  eV [31,32].

β	$K^{-}$	- p	$K^-d$	
	$\Delta E$	Γ	$\overline{\Delta E}$	Γ
1.08	287	648	676	1020
1.00	283	607	670	1016
-0.17	310	430	506	980

TABLE VI. Level shift and width of kaonic hydrogen obtained by solving the Schrödinger equation with the Kyoto  $\bar{K}N$  potential and by using the improved Deser formula and its resummed version.

	$\Delta E$ (eV)	Γ (eV)
Full Schrödinger equation	283	607
Improved Deser formula (18)	293	596
Resummed formula (19)	284	605

Estimates of the level shift and width of kaonic deuterium using the Deser formulas require the  $K^-d$  scattering length  $a_{K^-d}$  as input. In the fixed center approximation (FCA) for the nucleons,  $a_{K^-d}$  derived from a multiple scattering series is given as [43,62]

$$a_{K^{-}d} = \frac{\mu_{K^{-}d}}{m_{K^{-}}} \int d^{3}\mathbf{r} \, \rho_{d}(\mathbf{r}) \, \tilde{a}_{K^{-}d}(r), \tag{20}$$

$$\tilde{a}_{K^{-}d}(r) = \frac{\tilde{a}_{p} + \tilde{a}_{n} + (2\tilde{a}_{p}\tilde{a}_{n} - \tilde{a}_{ex}^{2})/r - 2\tilde{a}_{ex}^{2}\tilde{a}_{n}/r^{2}}{1 - \tilde{a}_{p}\tilde{a}_{n}/r^{2} + \tilde{a}_{ex}^{2}\tilde{a}_{n}/r^{3}}, \quad (21)$$

with the  $K^-$ -deuteron reduced mass  $\mu_{K^-d}$ , and  $\rho_d(r)$  is the nucleon density distribution in the deuteron, obtained in the present case using the Minnesota potential. The scattering lengths are defined as  $\tilde{a}_p \equiv \tilde{a}_{K^-p}$ ,  $\tilde{a}_n \equiv \tilde{a}_{K^-n}$  and  $\tilde{a}_{\rm ex}^2 \equiv \tilde{a}_{K^-p,\bar{K}^0n}^2/(1+\tilde{a}_{\bar{K}^0n}/r)$ , and the scattering lengths  $\tilde{a}_{\bar{K}N}$  in the laboratory frame are given as  $\tilde{a}_{\bar{K}N} \equiv \frac{m_K}{\mu_{\bar{K}N}} a_{\bar{K}N}$  with the  $\bar{K}N$  reduced mass  $\mu_{\bar{K}N}$ . Using the Kyoto  $\bar{K}N$  potential, the resulting two-body  $\bar{K}N$  scattering lengths are shown in Table II. These scattering lengths are defined by the scattering amplitudes at the threshold energy for the diagonal channels and at the average of the threshold energies for the off-diagonal  $K^-p-\bar{K}^0n$  channel. Their real and imaginary parts agree well with the original amplitudes [33,34] within their uncertainties. The  $K^-d$  scattering length is then calculated from Eqs. (20) and (21) as

$$a_{K-d} = (-1.42 + i \ 1.60) \,\text{fm}.$$
 (22)

This result remains unchanged when we adopt a realistic deuteron wave function (including the *D*-wave component) generated from the CD-Bonn potential [51].

Next we apply the improved Deser formulas (18) and (19) to kaonic deuterium. The results are summarized in Table VII together with those from the full three-body calculation. The logarithmic correction term is now increased as  $|\mu_{K-d} a_{K-d}/(\mu_{K-p} a_{K-p})| \sim 1.3$ , so the difference between Eqs. (18) and (19) becomes larger than that in kaonic hydrogen.

TABLE VII. Level shift and width of kaonic deuterium obtained by solving the three-body Schrödinger equation with the Kyoto  $\bar{K}N$  potential and by using the improved Deser formula and its resummed version

	$\Delta E \text{ (eV)}$	Γ (eV)
Full Schrödinger equation	670	1016
Improved Deser formula (18)	910	989
Resummed formula (19)	818	1188

In addition, the deviation from the full three-body calculation is of the order of  $\gtrsim 100 \text{ eV}$ .

Note, however, that the  $K^-d$  scattering length in Eq. (22) is estimated in the FCA limit. Hence, it can be different from the exact value. For instance, the importance of recoil corrections, naturally included in the full three-body calculation but neglected in FCA, is discussed in Refs. [61,63]. In addition, the determination of the precise energy of the two-body  $\bar{K}N$  system is subject to some uncertainties.

Another source of small deviations are higher order QED corrections such as electron vacuum polarization. This effect can be included as an effective potential, modifying the Coulomb interaction in the form [64]

$$V(r) = -\frac{\alpha}{r} \left[ 1 + \frac{2\alpha}{3\pi} \int_{1}^{\infty} du e^{-2m_{e}ru} \left( 1 + \frac{1}{2u^{2}} \right) \frac{\sqrt{u^{2} - 1}}{u^{2}} \right],$$

where  $m_e$  is the electron mass. The first term is the ordinary Coulomb potential, and the second term (the Uehling potential) takes into account the vacuum polarization effect, which is found to be small: The 1*S* level shift and width of the kaonic deuterium including this correction is  $\Delta E - i\Gamma/2 = (670 - i519)$  eV. While the level shift is unchanged, the decay width increases slightly by about 10 eV because the Uehling potential is attractive at very short distances.

In summary, the improved Deser formulas work well for kaonic hydrogen but estimates based on these formulas appear to be less accurate for kaonic deuterium, which does require a three-body treatment beyond fixed nucleons if the aim is to reach a precision at the 10-eV level.

At this point, we can add a comment on the previously mentioned surprising fact that isospin-breaking effects, using physical masses of antikaons and nucleons, are large in kaonic hydrogen but turn out to be small in the full three-body calculation of kaonic deuterium. One can trace this phenomenon by examining the improved Deser formulas together with the multiple scattering relation (21). The prime source of the strong effect in kaonic hydrogen is a substantial change of the real part of the  $K^-p$  scattering length when using isospin-averaged instead of physical masses. In kaonic deuterium, on the other hand, the whole set of scattering lengths in Table II enters Eq. (21), including  $a_{K^{-n}}$  with its positive real part, so that the leading effect from  $a_{K^-p}$  is largely compensated. As a consequence, real parts of  $a_{K-d}$  calculated with physical or isospin-averaged masses now differ only by less than 5 %, and this difference is averaged out further in the full three-body approach beyond fixed-scatterer approximation.

Finally we examine possible uncertainties related to the energy dependence of the  $\bar{K}N$  potential,  $\hat{V}^{\bar{K}N}(E_{\bar{K}N})$ . In the present study, we have set  $E_{\bar{K}N}=0$  at threshold, following Refs. [13,14,19]. The binding of the nucleons in the deuteron may cause a shift of  $E_{\bar{K}N}$  toward the subthreshold region. In fact, the prescription in Ref. [17] gives a large negative value for  $E_{\bar{K}N}$ . Our estimate, derived and discussed in the appendix, suggests instead a small average shift,  $E_{\bar{K}N}=-B_d/2\sim-1.1$  MeV, involving the deuteron binding energy  $B_d$ . With this value, we calculate the level shift and width of kaonic deuterium using the resummed Deser formula (19) and find  $(\Delta E, \Gamma)=(869,1310)$  eV, compared to  $(\Delta E, \Gamma)=$ 

(818,1188) eV with  $E_{\bar{K}N}=0$  (see Table VII). Thus the changes induced by correcting the energy dependence in  $\hat{V}^{\bar{K}N}(E_{\bar{K}N})$  for deuteron binding tend to increase the width of kaonic deuterium by about 10%, while the corresponding energy shift changes only marginally.

#### V. CONCLUSIONS

Precise three-body calculations have been performed for the spectrum of kaonic deuterium and the evaluation of the 1S level shift and width. The  $\bar{K}\,NN$  three-body wave function is expressed by a superposition of a large set of correlated Gaussian basis functions. In order to describe both short-range strong interactions and the long-range Coulomb interaction simultaneously, a large model space needs to be considered covering all distance scales ranging from  $0.1\,$  fm to several hundreds of fm.

The  $\bar{K}N$  strong interaction is treated in terms of a complex potential that accurately reproduces previous results of coupled-channels calculations based on chiral SU(3) dynamics. We have calculated the energy levels of 1S, 2S, and 2P kaonic deuterium states and find that the  $\bar{K}N$  strong interaction affects only the S states, inducing energy shifts from the levels characteristic of the pure Coulomb and point charge limit of the  $K^-d$  atomic system. No energy shift is found for the 2P state, so that the 1S level shift can be directly associated with the transition energy from the 2P to the 1Sstate. The calculated 1S level shift of kaonic deuterium is  $\Delta E - i\Gamma/2 = (670 - i508)$  eV, corresponding to a  $2P \rightarrow$ 1S transition energy of 7.134 keV. Following our previous discussions, we assign uncertainties of about 10% to  $\Gamma$  and less than 10% to  $\Delta E$  (not counting the approximately 20% uncertainties in the empirical SIDDHARTA kaonic hydrogen constraints).

In view of upcoming experimental investigations, we have also performed a test of the sensitivity of kaonic deuterium observables with respect to the I=1 component in the  $\bar{K}N$  interaction, by varying selectively the real part of the I=1  $\bar{K}N$  potential strength within the uncertainty limits deduced from the kaonic hydrogen data. One can conclude from this test that the 1S level shift of kaonic deuterium is indeed expected to provide a significantly improved constraint on the I=1 component, as compared to the SIDDHARTA kaonic hydrogen measurement [31,32], if the deuterium level shift can be determined within  $\sim 25\%$  accuracy (corresponding to  $\sim 2\%$  in the  $2P \rightarrow 1S$  transition energy). This sets the physics focus on the yet basically unknown  $K^-$  neutron sector of the  $\bar{K}N$  interaction.

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# APPENDIX: TWO-BODY $\bar{K}N$ ENERGY AND DEUTERON BINDING CORRECTION

Here we consider the average energy  $E_{\bar{K}N}$  of a two-body  $\bar{K}N$  subsystem in kaonic deuterium. In general, the energy of a two-body subsystem within a three-body bound state is not a well-defined notion. An estimate of  $E_{\bar{K}N}$  is nevertheless needed in order to determine the variation of strength of the energy-dependent  $\bar{K}N$  potential close to threshold. Prescriptions for such estimates have been discussed in several previous works. In the present paper, we have argued, following Refs. [13,14,19], that choosing  $E_{\bar{K}N}=0$  is a good approximation. Deuteron binding corrections introducing a subthreshold shift,  $E_{\bar{K}N}=-B_d/2$  with the deuteron binding energy  $B_d\sim 2.2$  MeV, imply uncertainties in the kaonic deuterium width of about 10% and smaller effects on the energy shift. The following considerations are intended to provide a basis for this estimate.

A different prescription is given in Ref. [17], where a considerably larger subthreshold shift,  $E_{\bar{K}N} = -B_d/2 - M_N/(M_N + m_K)\langle T_{N:N}\rangle/2$ , is suggested, involving the pairwise NN kinetic energy  $\langle T_{N:N}\rangle \sim 20$  MeV. In this case, the effective two-body energy turns out to be  $E_{\bar{K}N} \sim -7$  MeV, mostly coming from the kinetic energy term. Such a large subthreshold shift in the  $\bar{K}N$  potential  $V(E_{\bar{K}N})$ , when applied in combination with the resummed Deser formula (19), would produce a massive ( $\sim 60\%$ ) increase of the kaonic deuterium width  $\Gamma$  together with an increase of the energy shift  $\Delta E$  by about 30%.

The expression for  $E_{\bar{K}N}$  in Ref. [17] is deduced from an *ad hoc* ansatz for the average energy of each individual  $\bar{K}N$  subsystem within the  $\bar{K}$ -nuclear many-body system:

$$\sqrt{s_{\text{av}}} = \frac{1}{A} \sum_{i=1}^{A} \sqrt{(E_K + E_i)^2 - (\vec{q} + \vec{p}_i)^2}$$
 (A1)

with the antikaon four-momentum  $(E_K, \vec{q})$  and the *i*th nucleon four-momentum  $(E_i, \vec{p}_i)$ . The number of nucleons is A = 2 in the present case.

We argue instead that the starting point for a discussion of  $E_{\bar{K}N}$  should be a well-defined quantity, namely the total invariant center-of-mass energy of the  $\bar{K}A$  system:

$$\sqrt{s_{\text{tot}}} = \sqrt{(E_K + E_A)^2 - \left(\vec{q} + \sum_{i=1}^A \vec{p}_i\right)^2}.$$
 (A2)

For the kaonic atom case considered here, the Coulomb energy is supposed to be included in  $E_A$ . Equation (A2) is understood in combination with the constraint of conserved total three-momentum,

$$\vec{P} = \vec{q} + \sum_{i=1}^{A} \vec{p}_i = \text{const.}$$
 (A3)

with P=0 in the rest frame of the kaonic atom. A decomposition of  $\sqrt{s_{\text{tot}}}$  into two-body subsystems is then guaranteed

to satisfy all kinematic constraints. Note that there is no such systematic link between Eqs. (A2) and (A1).

For kaonic deuterium, Eq. (A2) becomes

$$\sqrt{s_{\text{tot}}} = \sqrt{(E_K + E_d)^2 - (\vec{q} + \vec{p}_1 + \vec{p}_2)^2},$$
 (A4)

where  $\vec{p}_1$  and  $\vec{p}_2$  now refer to proton and neutron threemomenta within the deuteron. For the purpose of estimating deuteron binding effects, the small Coulomb energy can be dropped. We set, approximately,  $E_K = m_K$  at threshold and  $E_d = M_p + M_n - B_d$ . Three-momentum conservation reads

$$\vec{q} + \vec{p}_1 + \vec{p}_2 = \vec{0} \tag{A5}$$

in the kaonic deuterium rest frame. In this frame, we have

$$\sqrt{s_{\text{tot}}} \approx m_K + M_p + M_n - B_d = \sqrt{s_{\text{th}}} - B_d. \tag{A6}$$

When we identify an average  $\bar{K}N$  energy per nucleon as

$$E_{\bar{K}N} = \frac{1}{2}(\sqrt{s_{\text{tot}}} - \sqrt{s_{\text{th}}}) \tag{A7}$$

with  $E_{\bar{K}N}=0$  at threshold, the subthreshold energy shift per nucleon is simply  $E_{\bar{K}N}=-B_d/2\simeq -1.1$  MeV. The  $\vec{P}=\vec{0}$  constraint implies that there is no additional strong downward shift from a kinetic energy term, as would emerge from applying Eq. (A1).

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