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Molecular Structure Analysis of ppK^-

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Abstract

We have investigated the molecular structure of three-body ppK^- , because the molecular feature is prominent in three-body ppK^- structure calculation. Heitler-london molecular formation model is applied to explain the structure of ppK^- . In this model, K^- is moving around one proton at some time and around another proton at other time to form a molecular-like state. Covalent bonding between K^- and proton plays a significant role in molecular formation mechanism. We calculated the direct kinetic energy, exchange kinetic energy, total kinetic energy and the direct potential energy, exchange potential energy, total potential energy for ppK^- . We also calculated the total energy of ppK^- for symmetric and antisymmetric case. It is obtained as 28 MeV at pp distance 1.9 fm.

Key words: Heitler-london molecular formation model, ppK^-

1. INTRODUCTION

Kaonic atoms and kaonic nuclei carry important informations concerning the K^- -nucleon interaction in nuclear medium. This information is very important to understand the kaon properties at finite density and to determine the constraints on kaon condensation in high density matter. The basic ingredient for this new family of nuclear state is a quasi-bound state of pK^- , which is identified as the $\Lambda(1405)$ with a binding energy 27 MeV and a level width 40 MeV [1]. Light kaonic nuclei are then calculated with this g-matrix. Binding energies of ppK^- , $ppnK^-$ and $ppnnK^-$ are predicted to be 48, 108, 86 MeV respectively with corresponding level widths of 61, 20 and 3 MeV [2, 3, 4]. The distance between the two protons in the ppK^- system is 1.90 fm [5]. However the distance between proton and neutron in deuteron is 3.90 fm. Therefore p-p distance in the ppK^- system is smaller than p-n distance in the ppK^- system is smaller than p-n distance in deuteron due to the strong attraction between K^- and proton.

In the FINUDA experiment, K^- s can be stopped in very thin nuclear targets, and multitracks are detected in the FINUDA spectrometer[6]. It can be interpreted as a bound state composed of a kaon and two protons, hereafter abbreviated as ppK^- . The binding energy $B_{ppK^-} = 115_{-5}^{+5}(\text{stat})_{-4}^{+3}(\text{sys})\text{MeV}$

and the width $\Gamma = 67_{-11}^{+14}(\text{stat})_{-3}^{+2}(\text{sys})\text{MeV}$ are obtained from the fitting in the region of 2.22-2.33 GeV/c².

The theoretical results and experimental results of kaonic nuclear states are very different. Therefore, there remains theoretically and experimentally to confirm that these events are really the deeply bound kaonic molecular state. Existence of the narrow kaonic molecular states is still controversial and we need further studies and more experiments. Also more experiments with better statistics are needed to settle this problem. Therefore, we investigate the molecular structure of kaonic molecular namely ppK^- .

2. Structure Analysis of ppK^- Based on Heitler-london Model

Heitler-london molecular formation model is applied to explain the structure of ppK^- . In this model, K^- is moving around one proton at some time and around another proton at other time to form a molecular-like state. Covalent bonding between K^- and proton plays a significant role in molecular formation mechanism.

Let us first consider $p K^-$ as an atomic state having gaussian density distribution. The second proton is added to form $pp K^-$. Our model based on Heitler-london molecular formation mechanism is to consider that K^- stays in an atomic orbit of either proton half of the time. An extra binding called Covalent bond results from the overlapping between the two orbits. In this model, the molecular orbit is described as

$$\psi_{\pm} = \phi_a \pm \phi_b$$

Where, \pm represents symmetric and antisymmetric states. ϕ 's are atomic orbits of K^- with respect to the fixed protons

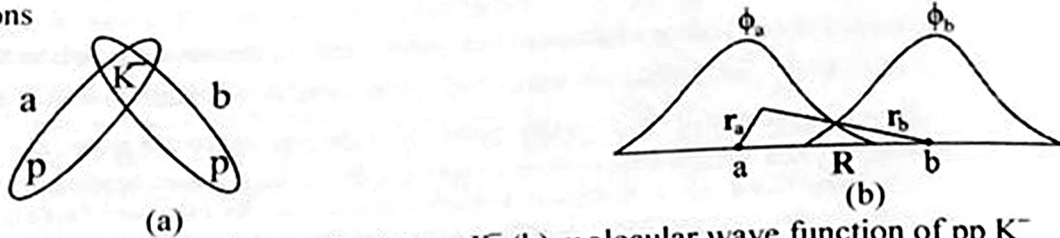


Fig. 2.1 Schematic diagram for (a) $pp K^-$ (b) molecular wave function of $pp K^-$

The total molecular wave functions is $\psi_{\pm} = \phi_a \pm \phi_b$; $\phi = e^{-\frac{1}{2}\alpha r^2}$.

3. CALCULATION OF TOTAL ENERGY OF ppK^-

We will use the Gaussian basis wave function and the standard integral,

$$\int dr e^{-Ar^2+Br} = e^{\frac{1}{4A}B^2} \left(\frac{\pi}{A}\right)^{\frac{3}{2}}$$
 for our consideration system.

By using the Gaussian basis wave function, $\phi = e^{-\alpha r^2/2}$, the normalization of the molecular wave function ppK^- is obtained as follow,

$$\int d\tau \psi_{\pm}^2 = \int d\tau (\phi_a \pm \phi_b)^2 = \int d\tau_a \phi_a^2(r_a) + \int d\tau_b \phi_b^2(r_b) \pm 2 \int d\tau \phi_b(r_b)\phi_a(r_a) \tag{1}$$

$$N = \int d\tau \psi_{\pm}^2 = \left(\frac{\pi}{\alpha}\right)^{3/2} [2 \pm 2e^{-1/4\alpha R^2}] = 2\left(\frac{\pi}{\alpha}\right)^{3/2} [1 \pm e^{-1/4\alpha R^2}] \tag{2}$$

Average kinetic energy of ppK^- molecular system is $\{KE\} = \frac{\langle \psi_{\pm} | -\hbar^2/2m \nabla^2 | \psi_{\pm} \rangle}{\langle \psi_{\pm} | \psi_{\pm} \rangle}$ (3)

$$\begin{aligned} \langle K.E \rangle = & -\frac{\hbar^2}{2m} \times \frac{1}{N} \int d\tau_a e^{-\frac{1}{2}\alpha r_a^2} \nabla_{r_a}^2 e^{-\frac{1}{2}\alpha r_a^2} - \frac{\hbar^2}{2m} \times \frac{1}{N} \int d\tau_b e^{-\frac{1}{2}\alpha r_b^2} \nabla_{r_b}^2 e^{-\frac{1}{2}\alpha r_b^2} \\ & + m \frac{\hbar^2}{2m} \times \frac{2}{N} \int d\tau_b e^{-\frac{1}{2}\alpha (r_b-R)^2} \nabla_{r_b}^2 e^{-\frac{1}{2}\alpha r_b^2} \end{aligned} \tag{4}$$

From above equation, first two terms represent the direct kinetic energy and third term represents the exchange kinetic energy.

We solved the direct kinetic energy terms in equation (4) which become to be

$$\langle K.E \rangle_{dir} = 2 \times \frac{3}{4} \hbar\omega \times \frac{1}{2 \times (1 \pm e^{-\alpha R^2/4})} = \frac{3}{4} \hbar\omega \times \frac{1}{2 \times (1 \pm e^{-\alpha R^2/4})} \tag{5}$$

We solved the exchange kinetic energy term in equation (4) which become to be

$$\langle KE \rangle_{exc} = m\hbar\omega/2(1 \pm e^{-\alpha R^2/4}) \times \{-3/2 + \alpha R^2/4\} e^{-\alpha R^2/4} \tag{6}$$

The molecular kinetic energy of $K^- pp$ system is obtained as

$$T_{mol}^{\pm} = \frac{3}{4} \hbar\omega \frac{\{1 m(-1 + \frac{2}{3}\alpha R^2/4) e^{-\alpha R^2/4}\}}{\{1 \pm e^{-\alpha R^2/4}\}} \tag{7}$$

And then, the molecular kinetic energy of $K^- pp$ system can be divided into two parts as symmetric case (T_{mol}^+) and antisymmetric case (T_{mol}^-).

Now the kinetic energy of K^+p atom is calculated as follow, $T_{at} = 3\hbar\omega/4$ (8)

The difference kinetic energy between K^+pp molecule and K^+p atom in symmetric is obtained as

$$\Delta T^+ = 3\hbar\omega \left\{ 1 - 2 \frac{3 \frac{\alpha R^2/4}{e^{\alpha R^2/4} + 1} - 1 \right\} = -1/2\hbar\omega \frac{\alpha R^2/4}{e^{\alpha R^2/4} + 1} \quad (9)$$

The difference kinetic energy between K^+pp molecule and K^+p atom in antisymmetric is obtained as

$$\Delta T^- = 3\hbar\omega \left\{ 1 + 2 \frac{3 \frac{\alpha R^2/4}{e^{\alpha R^2/4} - 1} - 1 \right\} = \hbar\omega/2 \frac{\alpha R^2/4}{e^{\alpha R^2/4} - 1} \quad (10)$$

To solve the average potential energy of ppK^+ , we used the potential, $V(r) = \bar{V}_0 e^{-\beta r^2}$. And then, the we will use the Gaussian basis wave function for our consideration system.

$$V_{sym} = \bar{V}_0 (\alpha / (\alpha + \beta))^{3/2} \frac{\{1 + e^{-\alpha\beta R^2 / (\alpha + \beta)}\}}{\{1 \pm e^{-\alpha R^2 / 4}\}} \quad (11)$$

$$V_{as} = \bar{V}_0 (\alpha / (\alpha + \beta))^{3/2} \frac{\{\pm 2 \times e^{-\alpha(\alpha + 2\beta)R^2 / 4(\alpha + \beta)}\}}{\{1 \pm e^{-\alpha R^2 / 4}\}} \quad (12)$$

By adding the equations (11) and (12), the average potential energy of K^+pp molecule is obtained as

$$V = V_{sym} = \bar{V}_0 (\alpha / (\alpha + \beta))^{3/2} \frac{\{1 + e^{-\alpha\beta R^2 / (\alpha + \beta)} \pm 2 \times e^{-\alpha(\alpha + 2\beta)R^2 / 4(\alpha + \beta)}\}}{(1 \pm e^{-\alpha R^2 / 4})} \quad (13)$$

The potential energy of ppK^+ system can be divided into two parts as symmetric and antisymmetric use. And then, potential energy of pK^+ atom is

$$V_{at} = \bar{V}_0 (\alpha / (\alpha + \beta))^{3/2} \times \frac{1}{2 \times (\pi/\alpha)^{3/2}} = V_0 \{\alpha / (\alpha + \beta)\}^{3/2} \quad (14)$$

The difference potential energy between molecular ppK^+ and pK^+ atom in symmetric is obtained as

$$\Delta V^+ = \bar{V}_0 \{\alpha / (\alpha + \beta)\}^{3/2} \left\{ \frac{1 + e^{-\alpha\beta R^2 / (\alpha + \beta)} + 2e^{-\alpha(\alpha + 2\beta)R^2 / 4(\alpha + \beta)}}{1 + e^{-\alpha R^2 / 4}} - 1 \right\} \quad (15)$$

The difference potential energy between molecular ppK^+ and pK^+ atom in antisymmetric is obtained as

$$\Delta V^- = \bar{V}_0 \{\alpha / (\alpha + \beta)\}^{3/2} \left\{ \frac{1 + e^{-\alpha\beta R^2 / (\alpha + \beta)} - 2e^{-\alpha(\alpha + 2\beta)R^2 / 4(\alpha + \beta)}}{1 - e^{-\alpha R^2 / 4}} - 1 \right\} \quad (16)$$

The total direct energy is obtained as $\langle E \rangle_{dir} = \langle KE \rangle_{dir} + \langle V \rangle_{dir}$.

$$\langle E \rangle_{dir} = 3\hbar\omega/4 \times \frac{1}{(1 + e^{-\alpha R^2 / 4})} + \bar{V}_0 \{\alpha / (\alpha + \beta)\}^{3/2} \frac{\{1 + e^{-\alpha\beta R^2 / (\alpha + \beta)}\}}{(1 + e^{-\alpha R^2 / 4})} \quad (17)$$

The total exchange energy is

$$E_{ex} = m \frac{\hbar\omega}{2(1 + e^{-\alpha R^2 / 4})} \times \{-3/2 + \alpha R^2 / 4 e^{-\alpha R^2 / 4} + \bar{V}_0 \{\alpha / (\alpha + \beta)\}^{3/2} \frac{\{\pm 2 \times e^{-\alpha(\alpha + 2\beta)R^2 / 4(\alpha + \beta)}\}}{(1 \pm e^{-\alpha R^2 / 4})} \quad (19)$$

The total energy is obtained as

$$E_{tot} = T_{at}^+ + V_{at}^+ = 3\hbar\omega/4 \frac{\{1 + m(-1 + (\alpha R^2 / 6)e^{-\alpha R^2 / 4})\}}{\{1 \pm e^{-\alpha R^2 / 4}\}} + \bar{V}_0 \{\alpha / (\alpha + \beta)\}^{3/2} \frac{\{1 + e^{-\alpha\beta R^2 / (\alpha + \beta)} \pm 2e^{-\alpha(\alpha + 2\beta)R^2 / 4(\alpha + \beta)}\}}{(1 \pm e^{-\alpha R^2 / 4})} \quad (20)$$

We calculate numerically the above equation to obtain the total energy of ppK^+ energy by using FORTRAN CODE.

4. RESULTS AND DISCUSSION

Kinetic energy, potential energy and total energy of K^- in ppK^- system are determined by using equations of section 3. We calculated numerically equation (6) and (13). The total kinetic energy and potential energy of the molecular system (ppK^-) for symmetric and antisymmetric states are shown in Fig. (4.1) and (4.2). The total kinetic energy in symmetric case is smaller than the kinetic energy in antisymmetric case. In both cases, kinetic energy of ppK^- molecule is generally smaller than twice the kinetic energy of (pK^-) atom which is 30 MeV. For very small distances, the potential energy in symmetric case is more attractive than antisymmetric case. The total direct and exchange energy of the molecular system (ppK^-) for symmetric and antisymmetric states are shown in Fig. (4.3) and (4.4). Fig. (4.5) shows that total energies of molecular structure (ppK^-) for symmetric and antisymmetric case gives the binding energies of this molecule. It is seen that the binding energy of ppK^- as 28 MeV at pp distance 1.9 fm. The molecular binding energy in symmetric is more strong than the antisymmetric case. From our study, it is found that exchange terms arising from molecular picture is significant in binding mechanism of this system. This is similar to the covalent bonding in molecule. The ATMS three-body calculation of Yamazaki and Akaishi has predicted that ppK^- system has binding energy 48MeV with 1.9 fm distance between the two protons [7]. From our calculation, it is found that at 1.9fm p-p distance, the binding energy is 28 MeV.

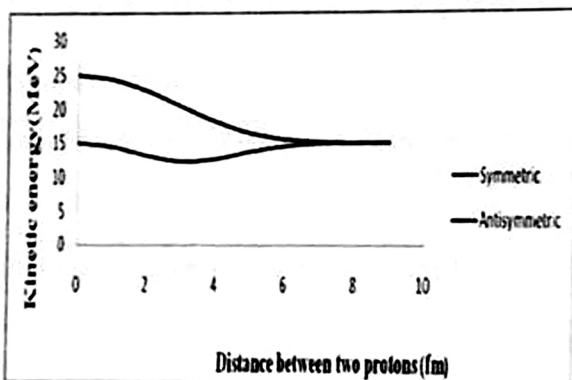


Fig.(4.1) Illustration of total kinetic energy versus the distance between two protons for ppK^-

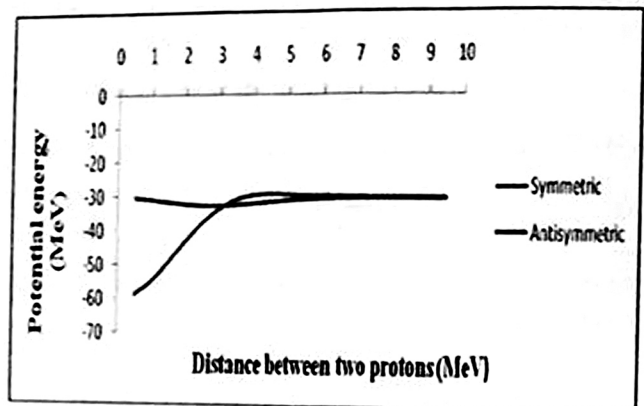


Fig.(4.2) Illustration of total potential energy versus the distance between two protons for ppK^-

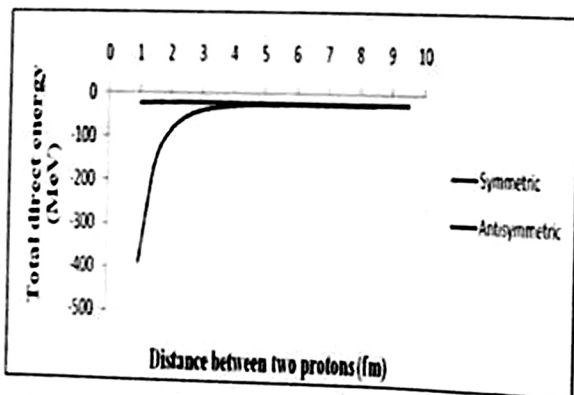


Fig.(4.3) Illustration of total direct energy versus the distance between two protons for ppK^-

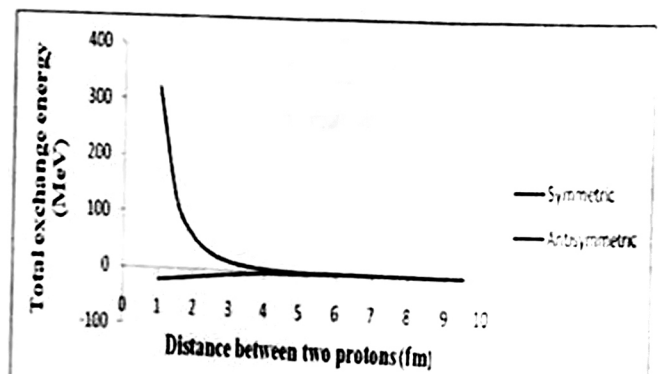


Fig.(4.4) Illustration of total exchange energy versus the distance between two protons For ppK^-

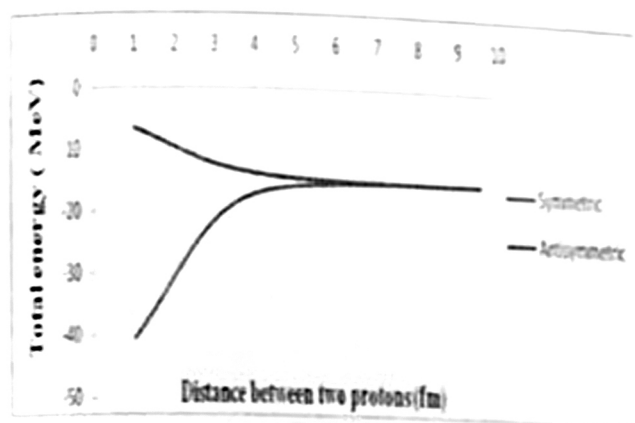


Fig.(4.5) Illustration of total energy versus the distance between two protons for ppK^-

CONCLUSION

We have investigated the molecular structure of three body ppK^- system. In this system, kaon is coherently migrating between two protons. To get a better understanding of the molecular structure, we have calculated the kinetic energies and potential energies for three body ppK^- system. From our calculated results, it is found that the structure of ppK^- system is deeply bound with binding energies of 28 MeV at p-p distance 1.9 fm. Besides, we also observed that the exchange energy arising from molecular picture is significant in binding mechanism of this system.

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