

A SIMPLE VARIATIONAL CALCULATION FOR A THREE-BODY
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Several experiments with high-energy radioactive nuclear beams have attracted a special interest to the case of ^{11}Li in which two neutrons form a loosely bound “halo” surrounding a ^9Li core. Different sophisticated three-body calculations (HH, COSMA, CSF) were employed to explore its ground-state structural properties. Due to the lack of experimental information about $^9\text{Li} - n$ potential and difficulty to incorporate the Pauli principle between the valence and core nucleons, even sophisticated three-body calculations are not completely reliable. We show that a simple variational technique can reproduce the physical structure of ^{11}Li and the results compare well to the other three-body calculations.

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1. Introduction

Recent experiments with high-energy radioactive nuclear beams have opened up new and exciting possibilities in the physics of light radioactive nuclei. Nuclei like ^{11}Li , ^{11}Be , ^{14}Be near the neutron drip line exhibit a “halo” structure for a few outer neutrons. Perhaps the most striking among these is the nucleus ^{11}Li for which experimental results [1] indicate that two neutrons form a loosely bound “halo” surrounding a ^9Li core. Different experimental facts, like large interaction cross section, large matter radius and small two-neutron separation energy [1,2] support the idea of a halo structure. In the dominant reaction channel, ^{11}Li dissociates into ^9Li and two neutrons, and both neutrons and the fragment have sharply forward-peaked angular distributions [3–7] which correspond to a large spatial distribution of valence neutrons. The halo structure is further confirmed in momentum distribution

experiments which show a narrow width for the transverse momentum distribution, which, according to the uncertainty principle, corresponds to a large spatial distribution of valence neutrons. This halo structure causes a low binding energy (BE) of the valence neutrons. Thus ^{11}Li is expected to have a loose three-body structure and no two-body subsystem (dineutron or ^{10}Li) is bound.

Experiments show that the ground state of ^{11}Li is bound by an energy (295 ± 35) keV. Several three-body calculations, using different types of wave-function expansions, have been reported in the literature. Among these are hyperspherical harmonics (HH) method, coordinate-space Faddeev (CSF) approach, cluster-orbital-shell model (COSM) calculation, etc. In the HH expansion method [8,9], one introduces the hyperspherical variables in terms of the relative Jacobi coordinates of the three-body system, and the relative wave function is expanded in the complete set of hyperspherical harmonics spanning the hyper-angular space. The Schrödinger equation reduces to a system of coupled differential equations. For a practical calculation, one has to truncate the expansion basis and then the question of convergence looms large, as the rate of convergence of the HH expansion is notoriously slow. In the CSF approach [10], the three-body wave function ψ is decomposed into three components, corresponding to three partitions:

$$\psi = \psi_{12} + \psi_{c1} + \psi_{c2}, \quad (1)$$

where 1 and 2 refer the two valence neutrons and c represents the core. Expressing each component of the wave function in terms of the Jacobi coordinates, one gets a set of two-dimensional coupled differential equations, which are solved numerically. The cluster-orbital-shell model [11] is an extended version of the conventional shell model for the valence neutrons coupled to a core. Translationally invariant coordinates between the core and the valence neutrons are introduced, which eliminate the spurious centre-of-mass excitations of the valence neutrons. This also allows the potential between the core and valence neutrons to be different from the potential between nucleons within the core. However, the convergence of the binding energy is slow.

In addition to the fact that all these sophisticated three-body calculations are quite difficult, there are two serious problems with all three-body calculations:

(a) $^9\text{Li} - n$ potential is not exactly known - there are no direct experimental informations about this interaction.

(b) The Pauli principle between the valence and the core nucleus is difficult to incorporate [12]. This is either treated approximately or taken indirectly introducing a "Pauli repulsive core" in the core - n potential.

Unless these two points are resolved beyond reasonable doubts, very sophisticated three-body calculations cannot produce the desired credibility, and a simple approach is worth exploring. In this situation, it is desirable to have as much physical insight as possible, without devoting too much effort towards solving the three-body equations precisely. In this communication, we apply a simple variational technique to explore the ground state structure of ^{11}Li using the known $n - n$ potential and a sum of Gaussians for the $^9\text{Li} - n$ potential, whose parameters

are adjusted to reproduce the experimental two-neutron separation energy of ^{11}Li and the fact that ^{10}Li is unbound by about 0.5 MeV. Due to a weaker spin-orbit interaction in neutron rich nuclei [12], we disregard this interaction. Motivation behind the present work is to get a clear and transparent physical picture obtained analytically with very little numerical effort. We find that the results for the ground state compare quite well to those obtained by sophisticated three-body calculations, including elaborate variational calculations using several variational parameters [12]. We have been able to obtain the binding energy, complete internal structure observables, and density and momentum distributions of the ground state of ^{11}Li .

In Sect. 2, we describe the variational calculation for the ground state of ^{11}Li . In Sect. 3, comparison with other theoretical calculation and some remarks are presented.

2. Variational approach for the ground state of ^{11}Li

We consider ^{11}Li as a three-body system consisting of a ^9Li core (labelled 3) and two loosely bound neutrons (labelled 1 and 2) (see Fig. 1). The Hamiltonian of the system is

$$H = -\frac{\hbar^2}{2m_1}\nabla_{r_1}^2 - \frac{\hbar^2}{2m_2}\nabla_{r_2}^2 - \frac{\hbar^2}{2m_3}\nabla_{r_3}^2 + V_{nn}(r_{12}) + V_{cn}(r_{23}) + V_{cn}(r_{31}), \quad (2)$$

where m_i and \vec{r}_i are the mass and position vector of the i^{th} particle ($i = 1, 2, 3$). The n - n and the core - n interaction potentials are denoted by V_{nn} and V_{cn} , re-

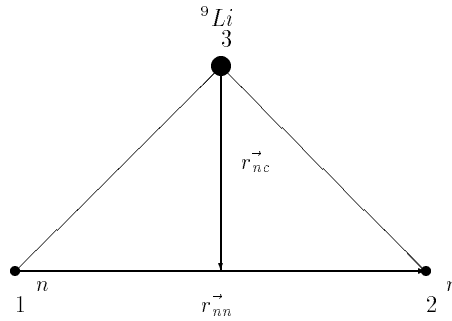


Fig. 1. Choice of the Jacobi coordinates in terms of \vec{r}_{nn} and \vec{r}_{nc} .

spectively. In order to separate the centre-of-mass motion, we define Jacobi ($\vec{\xi}_1, \vec{\xi}_2$) and centre mass (\vec{R}) coordinates through (note that $m_1 = m_2$)

$$\vec{\xi}_1 = \sqrt{\frac{m_1 m_2}{(m_1 + m_2)m}} (\vec{r}_2 - \vec{r}_1) = \sqrt{\frac{m_1}{2m}} (\vec{r}_2 - \vec{r}_1), \quad (3)$$

$$\vec{\xi}_2 = \sqrt{\frac{m_3(m_1 + m_2)}{mM}} \left(\vec{r}_3 - \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2} \right) = \sqrt{\frac{2m_3m_1}{mM}} \left(\vec{r}_3 - \frac{1}{2}(\vec{r}_1 + \vec{r}_2) \right), \quad (4)$$

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2 + m_3\vec{r}_3}{M} \quad (5)$$

where

$$m = \frac{m_1m_2 + m_2m_3 + m_3m_1}{m_1 + m_2 + m_3} = \frac{m_1(m_1 + 2m_3)}{2m_1 + m_3} \quad (6)$$

and

$$M = m_1 + m_2 + m_3 = 2m_1 + m_3. \quad (7)$$

In terms of these variables, the centre-of-mass motion is separated and the Schrödinger equation for the relative motion is

$$-\frac{\hbar^2}{2m} (\nabla_{\xi_1}^2 + \nabla_{\xi_2}^2) \psi + V(\vec{\xi}_1, \vec{\xi}_2) \psi = E \psi, \quad (8)$$

where $V(\vec{\xi}_1, \vec{\xi}_2)$ is the sum of three pairwise interactions, expressed in terms of the relative vectors $\vec{\xi}_1$ and $\vec{\xi}_2$. The n - n interaction, V_{nn} , is chosen as a standard singlet n - n interaction given by

$$V_{nn}(r) = V_{10} e^{-\mu_1 r^2}, \quad (9)$$

with $V_{10} = -31$ MeV and $\mu_1 = 0.3086$ fm⁻², which fits the two-nucleon singlet scattering data to yield, respectively, the effective range and scattering length

$$r_{0s} = 2.76 \text{ fm} \quad \text{and} \quad a_s = 23.72 \text{ fm}. \quad (10)$$

As mentioned in the Introduction, the core - n interaction is not accurately known and we choose a sum of two Gaussians

$$V_{cn}(r) = V_{20} e^{-\mu_2 r^2} + V_{r0} e^{-\mu_r r^2}, \quad (11)$$

with $\mu_2 = 0.153786$ fm⁻², and V_{20} is varied to reproduce the two-neutron separation energy. A short range ($\mu_r = 0.6$ fm) and a strongly repulsive ($V_{r0} = 65$ MeV) term is included in V_{cn} to simulate the Pauli exclusion principle between the valence neutrons at the core nucleons. In choosing the parameters μ_2 and V_{r0} , we make sure that the two-body ⁹Li - n system is unbound by about 0.5 MeV. In order to study the importance of the Pauli principle in V_{cn} , we here repeat our calculation without the repulsive term in Eq. (11) and once again adjust V_{20} to reproduce the two-neutron separation energy, and demanding that the ⁹Li - n system is unbound by 0.5 MeV.

The trial wave function for the ground state is chosen as

$$\psi_0(\vec{\xi}_1, \vec{\xi}_2) = N_0 e^{-\alpha_0(\xi_1^2 + \xi_2^2)}, \quad (12)$$

where α_0 is a variational parameter and N_0 is the normalization constant given by

$$N_0 = \sqrt{\frac{2\alpha_0}{\pi}}. \quad (13)$$

Calculation of the expectation value of the Hamiltonian of Eq. (8) is straightforward and can be done analytically. The result is

$$\begin{aligned} E_0(\alpha_0) = \langle \psi_0 | H | \psi_0 \rangle &= \frac{3\hbar^2\alpha_0}{m} + V_{10} \left[1 + \frac{\mu_1}{\alpha_0} \frac{m_1 + 2m_3}{2m_1 + m_3} \right]^{-1/2} \\ &+ 16V_{20} \left[4 + \frac{2\mu_2}{\alpha_0} \frac{(m_1 + 2m_3)(m_1 + m_3)}{m_3(2m_1 + m_3)} \right]^{-1/2} \\ &+ 16V_{r0} \left[4 + \frac{2\mu_r}{\alpha_0} \frac{(m_1 + 2m_3)(m_1 + m_3)}{m_3(2m_1 + m_3)} \right]^{-1/2}. \end{aligned} \quad (14)$$

Employing the Rayleigh-Ritz variational principle, the variational parameter α_0 is determined by the condition.

$$\frac{\partial E_0}{\partial \alpha_0} = 0. \quad (15)$$

The differentiation with respect to α_0 is done analytically and the resulting equation is solved numerically by the bisection method [13] followed by the Newton-Raphson method [13] to obtain α_0 . This is then used in Eq. (14) to obtain the ground state energy $E_0 = E_0(\alpha_0)$. We next repeat the calculation varying the strength of the *core* - n potential (V_{20}), to get the binding energy (BE) of the ground state of ^{11}Li (as a ^9Li -n-n system) at about 0.3 MeV, in agreement with the currently accepted experimental value of (295 ± 35) keV [14]. Our calculation yields $\alpha_0 = 0.055 \text{ fm}^{-2}$ corresponding to a BE of 0.297 MeV for $V_{20} = -23.75$ MeV, $V_{r0} = 65$ MeV and $\mu_r = 0.6 \text{ fm}^{-2}$. A two-body calculation with these parameters in V_{cn} shows that ^{10}Li is unbound by 0.5 MeV in agreement with the observed result. This fact implies that the interactions between the two valence neutrons in ^{11}Li are responsible for its stability.

We have next calculated the m.s. halo radius defined as

$$(R_{\text{halo}})_{\text{gs}}^2 = \langle \frac{1}{2}(R_{13}^2 + r_{23}^2) \rangle_{\text{gs}} = \langle (b^2\xi_2^2 + \frac{a^2}{4}\xi_1^2) \rangle_{\text{gs}} = \frac{3}{4\alpha_0} (\frac{a^2}{4} + b^2), \quad (16)$$

where $a = \sqrt{2m/m_1}$ and $b = \sqrt{mM/(2m_3m_1)}$. The numerical value of $(R_{\text{halo}})_{\text{gs}}$ turns out to be 5.11 fm. Then the m.s. matter radius of ^{11}Li is given by

$$(R_{\text{rms},^{11}\text{Li}})^2 = \frac{9}{11}(R_{\text{rms},^9\text{Li}})^2 + \frac{2}{11}(R_{\text{halo}})_{\text{gs}}^2. \quad (17)$$

Taking $R_{\text{rms},^9\text{Li}} = 2.5$ fm, we get $R_{\text{rms},^{11}\text{Li}} = 3.14$ fm. We also calculate the average nn separation as

$$\langle r_{\text{nn}}^2 \rangle_{\text{gs}} = \langle 4a^2 \xi_1^2 \rangle_{\text{gs}} = \frac{3a^2}{\alpha_0}. \quad (18)$$

Putting in the values of a^2 and α_0 , we get $\langle r_{\text{nn}}^2 \rangle_{\text{gs}}^{1/2} = 6.86$ fm.

To check the effect of the non-inclusion of the Pauli principle between the valence neutrons and the nucleons in the core, we repeated our calculation by switching off the repulsive part in V_{cn} and readjusting the parameters of the potential. The constraints imposed are the same as before, namely: (1) the two-neutron separation energy of ^{11}Li at about 0.3 MeV (2) ^{10}Li is unbound by about 0.5 MeV. The results together with our previous result including the repulsive part in V_{cn} are shown in Tables 1 and 2. One can immediately notice from Table 2 that without the repulsive part, the three-body system is too compact and all radii turn out to be too small compared to the experimental values, although the two-neutron separation energy is reproduced. This shows that it is indeed the Pauli principle which gives rise to the halo structure with the neutron cloud well outside the core for such neutron-rich nuclei. All calculated quantities, including the repulsive part in V_{cn} agree nicely with the available experimental data and also with other three-body calculations [12].

TABLE 1. Results for the ground state of ^{11}Li with (Model I) and without (Model II) repulsive part in V_{cn} ($V_{10} = -31$ MeV, $\mu_1 = 0.3086$ fm $^{-2}$, $\mu_2 = 0.153786$ fm $^{-2}$).

Calculation	V_{20} MeV	V_r MeV	μ_r fm $^{-2}$	α_0 fm $^{-2}$	E MeV
Model I	-23.75	65.0	0.6	0.055	-0.299
Model II	-10.8	-	-	0.109	-0.298

TABLE 2. Comparison of the structure properties of ^{11}Li ground state in different three-body models including our present calculation (Model I and Model II).

Properties	Model I	Model II	COSMA $_2$	CSF(Q9)	HH	Exptl.
BE (keV)	297	298	-	296	-	-
R_{halo} (fm)	5.11	3.849	61	5.47	5.02	5.1 $^{+0.6}_{-0.9}$
R_{rms} (fm)	3.14	2.794	3.2	3.14	3.11	3.10 \pm 0.17
$\langle r_{\text{nn}} \rangle$ (fm)	6.86	4.87	6.71	6.7	-	-
$\langle r_{\text{nc}} \rangle$ (fm)	3.79	2.69	5.1	4.6	-	-

To get a physical picture of the structure of ^{11}Li , we present in Fig. 2. the halo density distribution $|\psi_0(\xi_1, \xi_2)|^2$ for the ground state as a three-dimensional plot against r_{nn} ($= 2a\xi_1$) and r_{nc} ($= 2b\xi_2$). It is seen that the halo density has

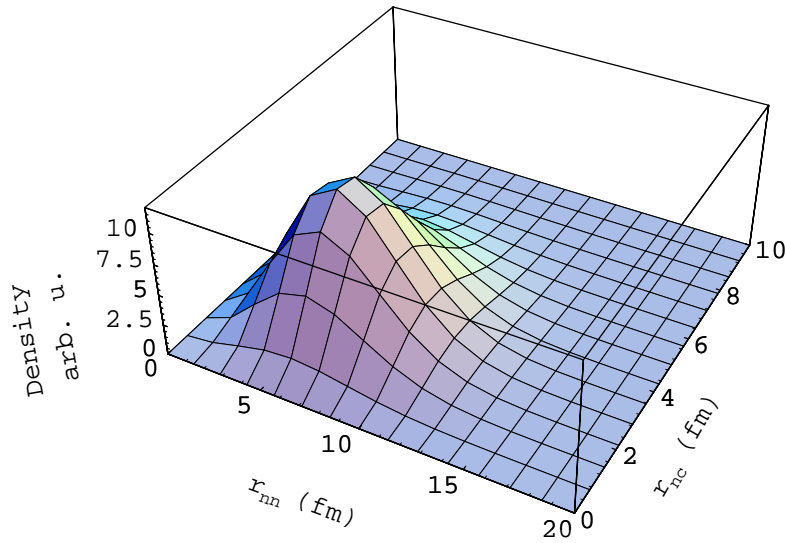


Fig. 2. 3-D plot of the halo density distribution (in arbitrary units) of the ground state of ^{11}Li , $|\psi_0(\xi_1, \xi_2)|^2$ as a function of r_{nn} and r_{nc} .

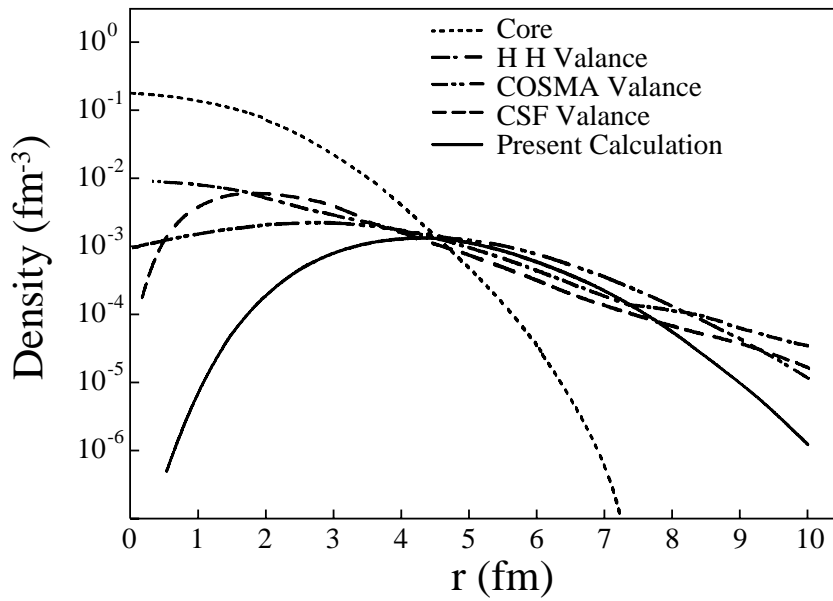


Fig. 3. Single-particle radial densities of ^{11}Li , provided by the core nucleons and valence neutrons. Results of other calculations as read from Fig. 1 of Ref. [15].

a maximum at $r_{\text{nn}} \simeq 5.57$ fm and $r_{\text{nc}} \simeq 3.08$ fm. This corresponds to a cigar-shaped structure with the two valence neutrons on either side of the core. The density decreases rather slowly as either of these two separations increases. The structureless peak is similar to the one obtained for a “shallow potential” case (Z2) by the CSF method [12]. In Fig. 3., we plot the single halo neutron density as a function of r , which is the separation of the halo neutron from the centre-of-mass of the three-body system. This is obtained by integrating the single-neutron probability density over all other variables for a fixed value of r . Our result (the continuous curve) shows a long tail of tenuous neutron matter, extending well beyond the r.m.s. radius of ^{11}Li . In the same figure, we also include the results of other calculations (as read off from Fig. 1 of Ref. [15]) for comparison. We notice that our result agrees fairly well with CSF, HH and COSMA results in the outer region ($3 \text{ fm} \leq r \leq 8 \text{ fm}$). This was expected, as mentioned in Ref. [15], since in a three-body model with a defined core and specified total nuclear r.m.s. radius,

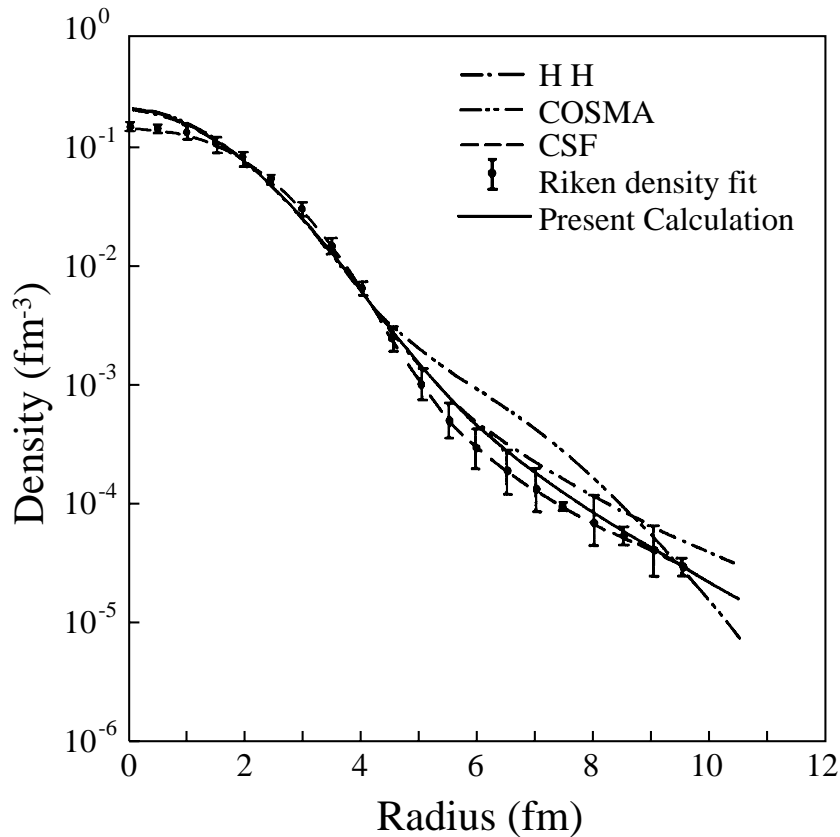


Fig. 4. Total (the core plus valence neutron) one-particle density distribution of ^{11}Li . Results of other calculations have been read off from Fig. 11 of Ref. [12].

the valence neutron density is fairly constrained. However, it is important to notice that the one-particle densities by both HH and COSMA [15] have the *largest value at the origin*, whereas CSF density decreases at small values of r . Our calculation also shows a similar trend, although more pronounced. Since the valence neutron is not expected to penetrate the core due to the Pauli principle, a decrease of single-neutron density within the core is intuitively expected, in agreement with our result. In Fig. 4, we plot the total (the core plus valence neutron) one-particle density as a function of r . In the same figure, we also include the results of other calculations (as read off from Fig. 11 of Ref. [12]) for comparison. Our results are in excellent agreement with the Riken fit and CSF calculation. Considering the simplicity of our calculation, this agreement is remarkable.

The transverse momentum distribution is given by

$$\frac{dN}{dk_{cx}} = \int dp_{cy} dp_{cz} d^3 p_{nn} |\phi(\vec{k}_1, \vec{k}_2)|^2, \quad (19)$$

where $\phi(\vec{k}_1, \vec{k}_2)$ is the Fourier transform of $\psi(\vec{\xi}_1, \vec{\xi}_2)$. The momenta of the two neutrons and the core in the centre-of-mass frame are \vec{k}_1 , \vec{k}_2 and \vec{k}_c , respectively, such that $\vec{k}_1 + \vec{k}_2 + \vec{k}_c = 0$. The relative momentum of the two neutrons (\vec{p}_{nn}) and that of the core relative to the centre-of-mass of the two neutrons (\vec{p}_c) are given by

$$\vec{p}_{nn} = \frac{1}{\sqrt{2}}(\vec{k}_2 - \vec{k}_1), \quad \vec{p}_c = \frac{1}{\sqrt{2}}(\vec{k}_2 - \vec{k}_1). \quad (20)$$

The Fourier transform of $\psi(\vec{\xi}_1, \vec{\xi}_2)$ is

$$\phi(\vec{k}_1, \vec{k}_2) = \frac{1}{(2\pi)^3} \iint \psi_0(\vec{\xi}_1, \vec{\xi}_2) e^{-i\vec{k}_1 \cdot \vec{\xi}_1} e^{-i\vec{k}_2 \cdot \vec{\xi}_2} d^3 \xi_1 d^3 \xi_2 = \frac{1}{\pi^3} e^{-(k_1^2 + k_2^2)/(4\alpha_0)}. \quad (21)$$

Substituting this in Eq. (19), we have

$$\frac{dN}{dk_{cx}} = \frac{1}{\pi} \sqrt{\frac{2\alpha_0}{\pi}} e^{-p_{cx}^2/(2\alpha_0)}, \quad (22)$$

where $p_{cx} = \hbar k_{cx}$. In Fig. 5, we plot dN/dk_{cx} against k_{cx} . In the same figure, experimental values from Ref. [12] are also shown. We see that the agreement is good. As already mentioned, the narrow momentum distribution corresponds to an extended spatial distribution, once again pointing to the halo structure of ^{11}Li .

3. Summary and conclusions

We have investigated the ground state of the two-neutron halo nucleus (^{11}Li treated as a three-body system consisting of ^9Li core and two valence neutrons)

by a simple-minded variational method with a simple analytic trial wave function.

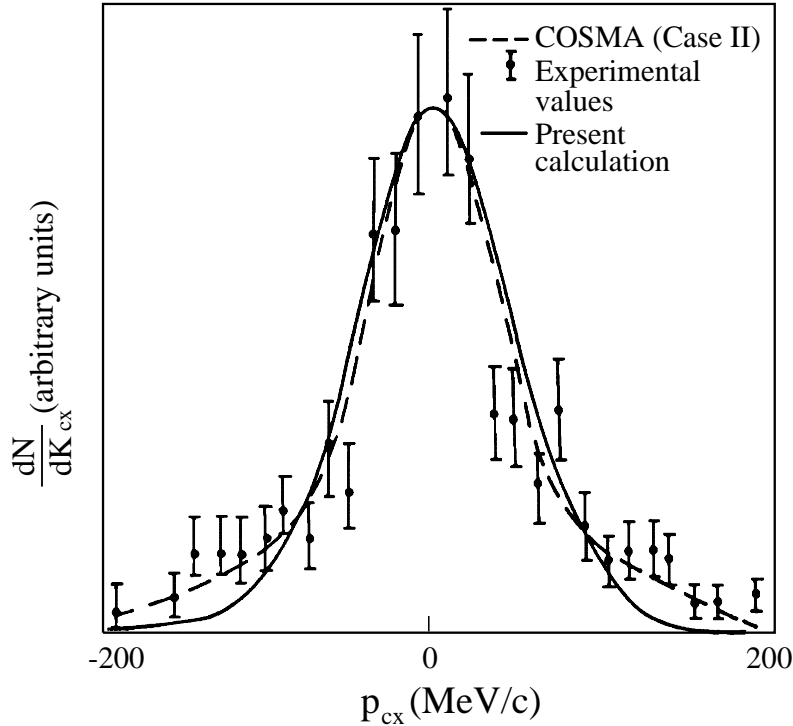


Fig. 5. The ${}^9\text{Li}$ transverse momentum distributions. The experimental data and the COSMA (II) plot are taken from Fig. 8 of Ref. [12].

The $n-n$ interaction has been taken as a standard one-term Gaussian, while the form of the ${}^9\text{Li}-n$ potential was adjusted to reproduce the two-neutron separation energy (S_{2n}) and the r.m.s. matter radius ($R_{\text{rms}}({}^{11}\text{Li})$), making sure that the ${}^9\text{Li}-n$ system is unbound by about 0.5 MeV. It was found that a repulsive core in the ${}^9\text{Li}-n$ potential was necessary; it reflects the effect of the Pauli principle between the valence neutrons and the core nucleons, for which no theoretical provision is made in the strictly three-body model. We find that not only S_{2n} and $R_{\text{rms}}({}^{11}\text{Li})$ are reproduced well, but many other observables like the neutron halo radius (R_{halo}), $\langle r_{\text{nc}} \rangle$, $\langle r_{\text{nn}} \rangle$, halo and single particle density distribution, transverse momentum distribution, etc., agree well with the experimental results and with the results of other sophisticated three-body calculations. On the other hand, appreciable variations of the computed observables by different three-body methods are found (Table 2), reflecting uncertainties inherent in these theoretical methods.

The main interest of the present work is that it uses a single variational parameter. Although the ground-state variational treatment is rather simple, we find that

the quality of agreement of the ground-state results calculated using the simple trial wave function with experimental results is comparable to that by very sophisticated three-body calculations. In spite of the simplicity, our trial wave function gives many fairly precise informations about the ground state. It is worth noting that while other few-body approaches face many problems regarding the convergence of energy, we are able to reproduce the ground state by a simple analytic calculation, within the framework of our model. At the same time, we get a lot of physical information and insight with much less calculational effort and by using only one variational parameter.

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JEDNOSTAVAN VARIJACIJSKI RAČUN TRI TIJELA ZA ^{11}Li

Nedavna mjerenja s visoko-energijskim radioaktivnim nuklearnim snopovima potakla su zanimanje za ^{11}Li u kojemu dva slabo vezana neutrona čine aureolu oko sredice ^9Li . Razne zamršene račune tri tijela (HH, COSMA, CSF) rabi više autora za istraživanje strukture ^{11}Li . Zbog nedostatka eksperimentalnih podataka o potencijalu $^9\text{Li} - n$ i teškoća u primjeni Paulijevog principa među neutronima sredice i valentnih neutrona, čak su i ti računi tri tijela nepouzdana. Ovdje pokazujemo kako jednostavan varijacijski pristup može opisati fizička svojstva ^{11}Li , a ishodi računa posve se dobro uspoređuju s drugim računima tri tijela.