Investigation of $^9$Be with THSR wave function

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Abstract. We extend the THSR wave function into $N\neq Z$ nucleon $^9$Be and perform calculations for its ground state. The negative parity of the ground state is correctly described by the introduction of an extra phase factor. The calculation result of the ground state agrees well with other model. We also calculate the density distribution of the extra neutron. The molecular orbit structure of the extra neutron is found to be reproduced correctly with the THSR wave function without prior assumptions.

1. Introduction
Since the discovery of $\alpha$-cluster in 1930s, the cluster structure has become a fundamental concept in understanding nuclear structures. The light nucleus $^9$Be, which is a typical three body system consists of two alpha clusters and an extra nucleon, has been used widely in testing different
cluster models. This includes nuclear Molecular Orbit (MO) models which considers the extra neutron in $^9$Be to occupy an orbit constructed with two cluster orbits (LCCO) [1, 2, 3]. These models successfully reproduced physical properties of $^9$Be and provided good description of its structure. However, these calculations did not illustrate clearly the motion dynamics of clusters inside nucleus.

The Tohsaki-Horiuchi-Schuck-Ropke (THSR) wave function [4], which was first proposed to study 4-n nuclei $^{12}$C and $^{16}$O, is now considered to provide a new concept of nonlocalized clustering dynamics in nuclei [5, 6]. The nonlocalized motion of clusters inside the nucleus has been tested with both positive and negative bands of nucleus $^{20}$Ne [5, 6, 7]. Considering these successful calculation of these 4-N nuclei, the application of the THSR wave function to non-4N nuclei $^9$Be worth investigation. In this paper, we will apply the THSR wave function into nucleus $^9$Be, and perform calculations for its ground state.

2. The THSR Wave Function of $^9$Be with Intrinsic Negative Parity

The THSR wave function of $^9$Be starts from the integration of Brink wave function $\Phi^B$ over generate coordinates,

$$\Phi = \int G_\alpha(R_1) \int G_\alpha(R_2) \int G_n(R_n) \Phi^B(R_1, R_2, R_n) d^3R_1 d^3R_2 d^3R_n$$  \hspace{1cm} (1)

where $\Phi^B(R_1, R_2, R_n)$ is the Brink wave function with generate coordinates $R_1, R_2$ for the two alpha clusters and generate coordinate $R_n$ for the extra nucleon. The Brink wave function is the total antisymmetrization of nine single nucleon wave functions,

$$\Phi^B(R_1, R_2, R_n) = \hat{A}\{\psi_{R_1}(r_1)\psi_{R_1}(r_2)\psi_{R_1}(r_3)\psi_{R_1}(r_4) \times \psi_{R_2}(r_5)\psi_{R_2}(r_6)\psi_{R_2}(r_7)\psi_{R_2}(r_8)\psi_{R_n}(r_9)\}. \hspace{1cm} (2)$$

Here $\hat{A}$ is the total antisymmetrizer, $\phi_{R_n}$ is the single nucleon wave function. For the eight nucleons inside two alpha clusters, we use the single nucleon wave function of the Gaussian form,

$$\psi_{R}(r) = \left(\frac{1}{\pi b^2}\right)^{3/4} e^{-(r-R)^2/2b^2} \chi_{1,2,3,4} \hspace{1cm} (3)$$

where $b$ is the size parameter of the Gaussian function and $\chi$ is the corresponding spin and isospin of the nucleon. The function $G_\alpha(R)$ in Eq. 1 is also of Gaussian style,

$$G_\alpha(R) = \exp \left( -\frac{R_{i,x}^2}{\beta_{a,xy}^2} - \frac{R_{i,y}^2}{\beta_{a,xy}^2} - \frac{R_{i,z}^2}{\beta_{a,z}^2} \right) \hspace{1cm} (4)$$

where $\beta_{a,xy}$ and $\beta_{a,z}$ are size parameters of the $\alpha$-cluster container. The same parameter $\beta_{a,xy}$ is used for the $x$ and $y$ axis to ensure the rotational symmetry about the $z$-axis. Usually, the THSR wave function is used for systems with intrinsic angular momentum $l = 0$. However this is not suitable for the ground state of $^9$Be which has intrinsic angular momentum $l = 1$ with negative parity. To describe this negative parity of the ground state of $^9$Be, an extra phase factor is introduced in the function $G_n(R_n)$ for the extra neutron as,

$$G_n(R_n) = \exp \left( -\frac{R_{n,x}^2}{\beta_{n,x}^2} - \frac{R_{n,y}^2}{\beta_{n,xy}^2} - \frac{R_{n,z}^2}{\beta_{n,z}^2} \right) e^{im\phi_{R_n}} \hspace{1cm} (5)$$

where $\beta_{n,xy}$ and $\beta_{n,z}$ are size parameters of the extra neutron container. $\phi_{R_n}$ in the extra phase factor $e^{im\phi_{R_n}}$ is the azimuthal angle in spherical coordinates $(R_{R_n}, \theta_{R_n}, \phi_{R_n})$ of vector $R_n$. 


When the spherical coordinates \((R_{n,x}, R_{n,y}, R_{n,z})\) are transformed as,
\[
(R_{n,x}, R_{n,y}, R_{n,z}) \rightarrow (-R_{n,x}, -R_{n,y}, -R_{n,z}),
\]
the sign of phase \(\phi_{R_n}\) and the phase factor \(e^{im\phi_{R_n}}\) will be determined by the choice of parameter \(m\). When choosing \(m = 1\), we will obtain
\[
\phi_{R_n} \rightarrow -\phi_{R_n}, \quad e^{im\phi_{R_n}} \rightarrow -e^{im\phi_{R_n}}.
\]
Thus the negative parity of this intrinsic wave function is proved. With similar argument, we can also obtain the traditional THSR wave function with positive parity for the case of \(m = 0\). The extra phase factor also lead to a changed sign of phase \(\phi\) and the phase factor \(e^{im\phi}\) in the one-body wave function.

For the ground state of \(^9\text{Be}\), we have \(l_z = m = 1\) because of the rotational symmetry of the two-\(\alpha\)-clusters subsystem.

The wave function \(\Phi\) is then transformed in coordinates by
\[
r_i \rightarrow r_i - X_G.
\]
This technique ensures that the center-of-mass (c.o.m.) motion is an 0s state of harmonic oscillator so that the spurious c.o.m. motion can be analytically removed.

The angular-momentum projection technique is applied to \(\Phi\) to obtain correct angular momentum as \(8\),
\[
\left| \Phi^{JM} \right| = \hat{P}_{MK}^J \left| \Phi \right|
\]
\[
= \frac{2I + 1}{8\pi^2} \int d\Omega D^J_{MK}(\Omega) \hat{R}(\Omega) \left| \Phi \right|,
\]
where \(I\) is the orbital angular momentum of the total system.

The Hamiltonian of \(^9\text{Be}\) system is calculated as,
\[
H = \sum_{i=1}^{9} T_i - T_{c.m.} + \sum_{i<j}^{9} V^{N}_{ij} + \sum_{i<j}^{9} V^{C}_{ij} + \sum_{i<j}^{9} V^{ls}_{ij},
\]
where \(T_{c.m.}\) is the kinetic energy of the center-of-mass motion. The Volkov No. 2 interaction is taken as the central force of nucleon-nucleon potential \(9\),
\[
V^{N}_{ij} = \{V_1 e^{-\alpha_1 r^2_{ij}} - V_2 e^{-\alpha_2 r^2_{ij}}\}\{0.6 - 0.4 \hat{P}_y \hat{P}_x + 0.125 \hat{P}_x - 0.125 \hat{P}_y\},
\]
where \(V_1\), \(V_2\), \(\alpha_1\) and \(\alpha_2\) are parameters. The G3RS term is taken as the spin-orbit part of interaction \(10\),
\[
V^{ls}_{ij} = V^{ls}_{0} \{e^{-\alpha_1 r^2_{ij}} - e^{-\alpha_2 r^2_{ij}}\} L \cdot S \hat{P}_{31},
\]
where \(V^{ls}_{0}\), \(\alpha_1\), and \(\alpha_2\) are parameters and \(\hat{P}_{31}\) is an operator which projects two-body systems into triplet odd states.

Parameter \(m\) in the phase factor \(e^{im\phi_{R_n}}\) in Eq. (5) is taken to be \(m = 1\) as discussed above to describe the negative parity of the ground state of \(^9\text{Be}\). \(I = 1\), \(M = 1\) and \(K = 1\) are used in the angular momentum projection operators. The spin of the extra nucleon is taken to be parallel to the orbital angular momentum.

The parameters \(\beta_{n,x, y}, \beta_{n,z}, \beta_{n,x, y}\), and \(\beta_{n,z}\) relates to the size of the containers of clusters. They are determined by variational methods respect to the binding energy. Two different values of parameter \(b\) in single nucleon wave functions are used in our calculations. The first one is to treat \(b\) as a variational parameter with the optimum value as \(b = 1.35\) fm. We also use another value which is the same value \(b = 1.46\) fm as used in Ref. [3],

\[
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3. Results and Discussions
The binding energy of the ground state of $^9$Be is calculated with previous wave function and parameters. The Monte Carlo method is adopted to perform numerical calculations of the integration in the wave function. The calculated binding energies of the ground states $3/2^-$ of $^9$Be with different parameter $b$ are listed in Table 1 and compared with other results. The optimum parameters for the ground state are $\beta_{\alpha,xy} = 0.1$ fm, $\beta_{\alpha,z} = 4.2$ fm, $\beta_{n,xy} = 2.5$ fm and $\beta_{n,z} = 2.8$ fm. When $b = 1.46$ fm as the same value in Ref. [3], the calculated binding energy for the ground state is -54.8 MeV. This value agrees with the result of the Molecular Orbit (MO) Model with model space II in Ref. [3], which shows that our wave function is a good description for the ground state of $^9$Be. The difference between our result and MO+GCM method is relatively larger but still acceptable. We also choose $b$ as the variational optimum value $b = 1.35$ fm, which is the same as used in previous calculations of $^8$Be [11]. This agreement of parameter $b$ after variational optimization is natural because the motion of $\alpha$-clusters in $^9$Be does not change much with the existence of the relatively small neutron. With this $b = 1.35$, the obtained binding energy of the $3/2^-$ ground state is -56.0 MeV which is 1.2 MeV improved than the previous one and closer to the experimental value -58.2 MeV.

Table 1. The binding energy of the ground state of $^9$Be calculated with different methods. $E$ denotes the binding energy of the ground state. THSR, MO, and MO+GCM denotes corresponding models.

| Model          | $b$ (fm) | $E(3/2^-)$ (MeV) |
|----------------|----------|------------------|
| THSR           | 1.35     | -56.0            |
| THSR           | 1.46     | -54.8            |
| MO [3]         | 1.46     | -54.8            |
| MO + GCM [3]   | 1.46     | -56.1            |
| Exp.[12]       | —        | -58.2            |

The agreement of the THSR wave function and the Molecular Orbit model implies that the molecular orbit structure is correctly reproduced by the THSR wave function. To clearly show the molecular orbit structure of the extra neutron, the density distribution of the extra neutron is calculated. Here the density distribution is calculated as the opportunity that a nucleon, which occupies the single nucleon state $\psi_{R_n}$, exist at position $r'$. The corresponding equation is,

$$\rho(r') = \left< \frac{1}{9} \sum_{i=1}^{9} \delta (r_i - X_G - r'_n) \right> / \left< \psi \right| \left< \psi \right> .$$

(13)

In this equation, the states that the $i$th nucleon occupies the single nucleon state $\psi_{R_n}$ is picked out by the operator $\hat{P}_{i,n}$. Then the opportunity that the $i$th nucleon appears at position $r'_n$ is calculated with the $\delta$ function. The calculated density distribution of the extra nucleon is shown in Fig. 1. This figure is a cross section at $y = 0$ of the density distribution in total space. There are two parts on this cross section, each covers one side of the two $\alpha$ clusters. Considering the rotational symmetry about the $z$-axis of the $^9$Be system, this distribution clearly shows a $\pi$-orbit structure and the molecular orbit structure is correctly reproduced. In previous calculations such as in Ref. [2] and Ref. [3], the molecular orbit structure is a presumption of the system. However, this presumption is not used in our calculations where the molecular orbit structure comes naturally from the THSR wave function and the constraint of symmetries.
Figure 1. The calculated density distribution of the extra neutron on the $y = 0$ cross section. The density at each point is denoted by gray scale. The unit of the density at each point is fm$^{-3}$.

4. Conclusion
In this paper, we formulate the THSR wave function for the ground state of $^9$Be. An extra phase factor is introduced into the THSR wave function to obtain intrinsic negative parity. The calculation result of the ground state agrees well with other calculations. By calculating the density distribution of the extra nucleon, we found clearly that the molecular orbit structure of the extra nucleon is reproduced correctly by the THSR wave function. This shows the power of the THSR wave function because no prior assumptions of molecular orbit are made in our calculations. All this calculations show us the possibility to apply THSR wave function into $^9$Be and other $N \neq Z$ nuclei.

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