Structure of Exotic Neutron-Rich Nuclei

Takaharu Otsuka, Nobuhisa Fukunishi, and Hiroyuki Sagawa
Department of Physics, University of Tokyo, Hongo, Bunkyo-ku, Tokyo, 113, Japan
(Received 13 November 1992)

A new framework, the variational shell model, is proposed to describe the structure of neutron-rich unstable nuclei. An application to ^{11}Be is presented. Contrary to the failure of the spherical Hartree-Fock model, the anomalous $\frac{1}{2}^+$ ground state and its neutron halo are reproduced with the Skyrme (SIII) interaction. This state is bound due to dynamical coupling between the core and the loosely bound neutron, which oscillates between the $2s_{1/2}$ and the $1d_{5/2}$ orbits.

PACS numbers: 21.60.Cs, 21.10.Gv, 21.60.Jz, 27.20.+n

The recent developments of radioactive nuclear beams are opening a new rich field of nuclear physics: the structure of neutron-rich unstable nuclei. The observation of the neutron halo [1] is an example. In this Letter, we discuss the single-particle motion of nucleons in exotic circumstances such as extremely neutron-rich nuclei. Neutron-rich unstable nuclei are characterized by $N \gg Z$ with N (Z) being the neutron (proton) number. In such nuclei, neutrons occupy single-particle orbits from the bottom up to weakly bound states in the mean potential for nucleons. In addition, if the number of nucleons is small, the mean potential itself may not be very static. Thus, the shell structure of light neutron-rich unstable nuclei can be different from that of stable nuclei, and provides various intriguing problems. One good example of such problems is the ground state of $^{11}_{4}Be_7$, where the ratio N/Z is nearly 2. The naive picture of this state is that neutrons occupy $1s_{1/2}$ and $1p_{3/2}$ completely, while $1p_{1/2}$ holds just one neutron. The ground state J^π is then expected to be $\frac{1}{2}^-$, whereas experimentally it is known to be $\frac{1}{2}^+$ [2]. Although this has been pointed out by Talmi and Unna more than three decades ago [3], this anomaly has remained a challenge to theories. For instance, the Hartree-Fock (HF) approach, which normally gives a satisfactory description of nuclei around the ground state, has been shown to fail in this case [4]. Recently, a new framework has been proposed to handle many-body systems containing loosely bound particles in general. In this Letter, we present the outline of this framework, called hereafter variation shell model (VSM), and its first result applied to ^{11}Be. This nucleus is known by the anomalous ground state, as stated earlier, and its neutron halo [5]. The result of the VSM with the Skyrme SIII interaction [6,7] nicely reproduces these exotic features, as shown later.

In conventional shell model calculations, the single-particle wave functions are provided by other methods such as the harmonic oscillator potential, HF calculation, etc. In other words, one obtains the single-particle wave functions from a certain mean field potential, assuming stable single-particle motion. The shell model calculation is then carried out, in order to treat the "residual" interaction between nucleons moving on such stable single-particle orbits. The validity of this procedure can be questioned, however, in certain neutron-rich unstable nuclei where the last neutrons (or protons) are forced to occupy loosely bound or even unbound orbits of the mean potential.

We shall now formulate the VSM: One parametrizes the radial part, R, of the single-particle wave function, ϕ, in terms of variational parameters denoted collectively by $\{\alpha\}$:

$$\phi_i(x;\{\alpha\}) \equiv R_i(r;\{\alpha\})[Y^{(l)}\times u]^{(j)}, \tag{1}$$

where i stands for the index of a single-particle orbit, x denotes symbolically all relevant coordinates, and r means the distance from the center of the nucleus. Here Y and u imply the spherical harmonics and spin wave function, respectively, and are coupled to the total angular momentum j. Multinucleon wave functions are constructed from the single-particle bases ϕ_i's:

$$|\Psi_i;\{\alpha\}\rangle \propto \mathcal{A}\{\phi_{k_1}(x_1;\{\alpha\})\phi_{k_2}(x_2;\{\alpha\})\phi_{k_3}(x_3;\{\alpha\})\ldots\}|0\rangle, \tag{2}$$

where $|\Psi_i\rangle$ is the ith Slater determinants, the k's stand for single-particle bases forming Ψ_i, $\mathcal{A}\{\}$ denotes an antisymmetrizer, and $|0\rangle$ means the vacuum. One then calculates matrix elements of the Hamiltonian for these multinucleon wave functions, and diagonalizes the matrix. The lowest eigenvalue with the angular momentum J and parity π can be given as a function of $\{\alpha\}$, $E(J^\pi;\{\alpha\})$, and its wave function is written with amplitude c_i as

$$|J^\pi;\{\alpha\}\rangle = \sum_i c_i(J^\pi;\{\alpha\})|\Psi_i;\{\alpha\}\rangle. \tag{3}$$

One carries out the variation for this $E(J^\pi;\{\alpha\})$ with respect to $\{\alpha\}$, by searching the minimum; $\delta E(J^\pi;\{\alpha\})/\delta\{\alpha\}=0$. The single-particle basis $\phi_i(r;\{\alpha\})$, the configuration mixing amplitude c_i, and the energy of the nucleus $E(J^\pi;\{\alpha\})$ are thus determined simultaneously in the VSM.

In practical VSM calculations, the effective nucleon-nucleon interaction has to be chosen so that the density in the interior region satisfies the saturation. The Skyrme interaction [6] is useful for this purpose, and the SIII interaction [7] is actually adopted in the present work. The SIII interaction contains, in its original form, a three-body repulsive force, which prevents the nucleus from collapsing. We take in this work a simplified but widely used version of SIII, where the three-body term is replaced by a density-dependent two-body repulsive term. This version of SIII still brings about the density saturation despite its practical simplicity. Thus, the Hamiltonian consists of the kinetic energy term and the SIII interaction.

There are two methods for the parametrization of the $R_i(r;\{\alpha\})$'s in Eq. (1). In the first method, a "black box" is used for generating radial wave functions. For instance, solutions of the Woods-Saxon potential can be used by changing the values of radius, depth, diffuseness, etc., of the potential [8]. This method is simple and useful, but appears not to be accurate enough for reproducing halo properties. We therefore use, in this work, the second method, which is the direct variation of $R_i(r;\{\alpha\})$ in Eq. (1). For this method, we start from a variational principle. At a local minimum, any infinitesimal variation of R_i does not change the total energy. This leads us to a set of coupled differential equations with a Lagrange multiplier for keeping orthonormalities of the R_i's. These differential equations of VSM contain terms like kinetic energy and average potential from other nucleons in addition to other terms, for instance, those shifting nucleons from one orbit to another, and hence show certain similarities to HF equations. It is not easy, however, to solve the VSM equation because of partial occupancies and jumping of nucleons from one orbit to another. A numerical procedure for this solution has been developed. In the following we present its first result. Details of the procedure and the results will be published elsewhere at length [9].

Figure 1 shows the lowest $\frac{1}{2}^+$ and $\frac{1}{2}^-$ energy levels of the ^{11}Be, obtained by experiment and from VSM. The $\frac{1}{2}^+$ level is shown relative to $\frac{1}{2}^-$. The VSM calculation is performed with SIII without any adjustment. The configuration space for $\frac{1}{2}^-$ is comprised of four (seven) nucleons in the $1s$ ($1p$) shell, whereas one nucleon is raised from the $1p$ shell to the $2s1d$ shell for $\frac{1}{2}^+$. The isospin is conserved. The same levels of ^{13}C are included for comparison in Fig. 1.

The observed ground state of ^{11}Be is $\frac{1}{2}^+$, and VSM reproduces it correctly. Moreover, the VSM reproduces the change from ^{11}Be to ^{13}C where the ordering of $\frac{1}{2}^+$ and $\frac{1}{2}^-$ becomes normal. It should be remarkable that the SIII interaction, which has been utilized for the description of a wide variety of stable nuclei, remains useful for an unstable nucleus such as ^{11}Be. It is of particular importance that, in going from ^{11}Be to ^{13}C, the energy of the $\frac{1}{2}^+$ level relative to the $\frac{1}{2}^-$ is increased in the VSM to about the right amount. One cannot claim that the agreement between experiment and calculation should be perfect in Fig. 1 because SIII is designed so as to be simple yet useful for a global description of ground-

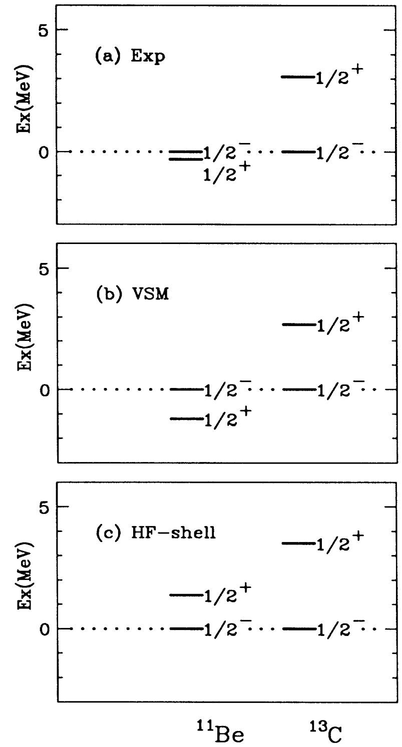

FIG. 1. Energy levels of ^{11}Be and ^{13}C obtained by (a) experiment, (b) VSM, and (c) HF-shell. Levels are shown relative to $\frac{1}{2}^-$.

and near-ground-state properties.

We shall next discuss the physical mechanism responsible for lowering the $\frac{1}{2}^+$ state in ^{11}Be. The major components of the lowest $\frac{1}{2}^+$ state in ^{11}Be can be written as

$$|\tfrac{1}{2}^+\rangle \approx \zeta_1 0_c^+ \times |2s_{1/2}\rangle_\nu + \zeta_2 [2_c^+ \times |1d_{5/2}\rangle_\nu]^{(1/2)}, \qquad (4)$$

where ζ_1 and ζ_2 are amplitudes, 0_c^+ and 2_c^+ stand for the lowest core (i.e., ^{10}Be) state of given J^π, and $|\ \rangle_\nu$ means neutron single-particle orbits. The resulting values are $\zeta_1 \sim 0.74$ and $\zeta_2 \sim 0.63$. Note that the VSM (experimental) value of the 2_1^+ energy level of the core, ^{10}Be, is 3.2 (3.4) MeV, and that its $B(E2;0_1^+ \to 2_1^+)$ is calculated as 54 e^2fm^4 with effective charges $e_p = 1.5e$ and $e_n = 0.5e$ [10] in agreement with the experimental value 52 ± 6 e^2fm^4 [11]. The coupling between the two components on the right-hand side of Eq. (4) plays an indispensable role in ^{11}Be in order to produce the bound $\frac{1}{2}^+$ state [8]. Without this coupling, the system is not bound as discussed below in the context related to the HF calculation. The physical meaning of this coupling is that the motion of the core surface (i.e., ^{10}Be) is coupled dynamically with the motion of the particle (i.e., a neutron in $2s_{1/2}$ or $1d_{5/2}$). It does not matter presently whether the surface motion is vibrational or rotational. The total system then becomes bound, and the above mechanism can be referred to as dynamical mean field. We emphasize that the VSM includes this coupling effect in determining R_i

in Eq. (1), and that this coupling is precisely what was expected when the VSM was proposed [8]. On the other hand, the single-particle explanation is not successful as has been pointed out by Millener and Kurath [12]. As discussed below, if the single-particle motion is restricted on either $2s_{1/2}$ or $1d_{5/2}$ (i.e., no orbital change), the nuclear force does not supply sufficient binding, and thereby the total system is left unbound. In this situation a nucleon cannot complete the circle on either $2s_{1/2}$ or $1d_{5/2}$ in the classical picture.

We note that the structure of the wave function of the anomalous ground state can be examined by g factor or transfer reactions. The calculated value of the g factor of the ground state is $-3.0(\mu_N)$ where the free nucleon g factors are assumed. In the usual single-particle picture, this is $-3.8(\mu_N)$, i.e., free neutron spin g factor. The mixing in Eq. (4) may be too strong due to SIII in the present calculation, and the measurement of the mixing amplitudes provides us with precious information for modifying the effective interaction.

We discuss briefly the relation to the HF approach. Figure 1 also shows the result of the so-called open-shell HF plus shell model (HF-shell) [13]. The HF-shell method is an extension of the usual spherical HF to open-shell nuclei; one starts from a set of single-particle wave functions, and carries out a shell model calculation which produces the occupation number of each single-particle orbit. The spherical HF calculation is then carried out by using these occupation numbers as input, giving rise to a new set of single-particle wave functions. The shell model calculation is repeated with the new single-particle wave functions. One iterates this process until the result is converged.

The HF-shell works well for most stable nuclei, whereas it shows difficulties in nuclei where highest orbits occupied by neutrons turn out to be unbound in the HF-shell calculation. In such cases, the whole scheme breaks down. In order to avoid this obstacle, an infinitely high wall is introduced sometimes [4]. All nucleons are evidently "bound" inside the wall. We carry out such a calculation with the wall at $r=20$ fm. Using SIII, the energies of $2s_{1/2}$ and $1d_{5/2}$ are obtained for ^{11}Be as 0.79 and 1.96 MeV, respectively. These are positive energy solutions bound by the artificial wall, and their wave functions are extremely spread.

Figure 1 includes the lowest $\frac{1}{2}^+$ and $\frac{1}{2}^-$ energy levels of ^{11}Be and ^{13}C calculated by the HF-shell. For ^{11}Be, the HF-shell clearly fails to reproduce the anomalous ground state, while the result is not too bad for ^{13}C. The latter case indicates that the HF-shell is reasonable for stable nuclei.

We shall briefly discuss the origin of this failure, taking the usual HF with two-body interaction for simplicity. The HF equation is written in the form

$$T_{mi}+\sum_{j=1}^{N}\{V_{jm,ji}-V_{mj,ji}\}=\varepsilon_i\delta_{mi}\,, \qquad (5)$$

where T_{mi} is the kinetic term, $V_{ij,kl}$ stands for matrix element of a two-body interaction, ε_i denotes an eigenvalue, and δ_{ij} means Kronecker's symbol. The two-body interaction matrix elements in Eq. (5) are limited to diagonal ones. This limitation remains in the HF-shell calculation. If ε_i is a large negative number, single-particle wave functions are determined well by HF or HF-shell. On the other hand, if $V_{ij,ij}-V_{ij,ji}$ is canceled almost completely by T_{mi} as is the case for loosely bound orbits, Eq. (5) does not produce optimum single-particle wave functions because of other more significant contributions. This is the case for $2s_{1/2}$ and $1d_{5/2}$ of ^{11}Be, where the off-diagonal matrix element shifting a nucleon between $2s_{1/2}$ and $1d_{5/2}$ plays a crucial role as seen in Eq. (4). The deformed HF may be better, but it assumes static deformation. It is of interest to see the result of angular-momentum projected deformed HF. Although a Nilsson calculation with large deformation has not shown the inversion of the $\frac{1}{2}^+$ and $\frac{1}{2}^-$ states [14], the present work and Ref. [14] are qualitatively consistent on the role of deformation.

We now present the density profile obtained by the VSM calculation. Figure 2 shows the matter density profile calculated by the VSM and that measured by Fukuda *et al.* [5]. One sees a reasonable agreement between them. Although the calculation is to be modified by corrections such as center-of-mass and nucleon-size ones, it is unlikely that such corrections change the result

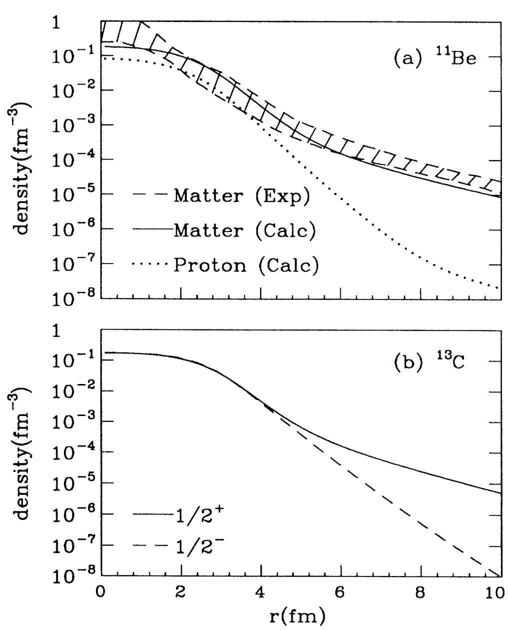

FIG. 2. (a) Density profile of the lowest $\frac{1}{2}^+$ state of ^{11}Be. Experimental matter (hatched area), VSM matter (solid line), and proton (dotted line) densities are shown. (b) Density profile for lowest $\frac{1}{2}^+$ (solid line) and $\frac{1}{2}^-$ (dashed line) of ^{13}C calculated by VSM.

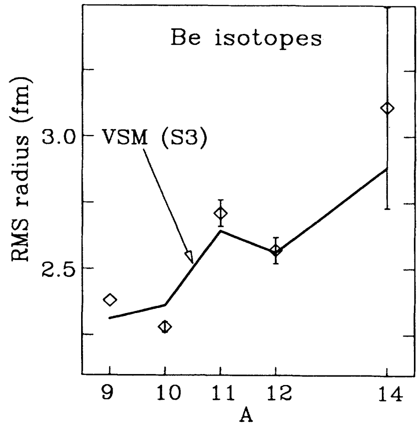

FIG. 3. Experimental (points) and calculated (line) rms matter radius of $^{9-14}$Be.

drastically. We point out that the neutron halo observed for ^{11}Be is clearly seen in the VSM. The calculation is made with SIII without adjustment. This is in contrast to the HF-type calculation by Sagawa [15] where the depth of HF potential for highest orbits is adjusted individually to adjust their separation energies. In fact, the present calculation reproduces the neutron halo ^{11}Be without adjustment for the first time. The halo is primarily due to the slowly damping tail of R_i for $i=2s_{1/2}$ where the radial dependence is very different from that in the harmonic oscillator potential. Wave functions of other orbits, including $1d_{5/2}$, are quite similar to those in the harmonic oscillator potential. The halo information has been pointed out by Hansen and Jonson as a consequence of small separation energy of neutron [16]. If the configuration mixing takes place, however, one cannot relate the single-particle wave function directly to the separation energy of the nucleus. In the VSM, the halo arises as a result of coherence and competition among various effects including configuration mixing.

Figure 2 shows also the density profile of ^{13}C, where one finds again the halo for the first $\frac{1}{2}^+$ state. In other words, the halo structure of the $\frac{1}{2}^+$ state is carried over from ^{11}Be to ^{13}C. This can be viewed as halo universality, if one includes excited states.

The rms matter radius is calculated for some Be isotopes to show the anomalous radius ^{11}Be. Figure 3 shows the result in comparison to experiment [17]. One sees that ^{11}Be has a larger radius, and the VSM result is in good agreement with experiment. The neutron halo in ^{14}Be is seen also in Fig. 3 in both experiment and VSM calculation.

The $E1$ transition between the first $\frac{1}{2}^+$ and $\frac{1}{2}^-$ states is known to be strong in ^{11}Be [18]. The present calculation produces a relatively strong $E1$ matrix element, but does not reach the observed value [18]. The SIII interaction is probably not suitable for the study of this $E1$, because this strong $E1$ transition seems to be sensitive to subtle cancellations of several matrix elements [18]. By the calculation of the center-of-mass kinetic energy, it is confirmed that the mixture of spurious center-of-mass motion is negligible for the states discussed in this work.

In summary, the VSM has been proposed as a scheme to describe the structure of nuclei containing loosely bound nucleons. While the VSM is almost equivalent to HF-shell for stable nuclei, the VSM plays an indispensable role in some neutron-rich unstable nuclei. One of the implications of the VSM is the dynamical determination of the single-particle wave functions, which results in the neutron halo and anomalous ground state for ^{11}Be. We are currently working on calculations on neighboring nuclei, and also on improving the effective interaction suitable for unstable nuclei as well as stable ones.

We are grateful to Professor A. Gelberg for reading the manuscript, and to Dr. D. J. Millener for useful comments. This work is supported in part by Grant-in-Aid for General Scientific Research (No. 01540231 and No. 04804012) by the Ministry of Education, Science and Culture. The VAX 6640 at the Meson Science Laboratory, University of Tokyo has been used for computation.

[1] I. Tanihata, Nucl. Phys. **A552**, 275c (1991).
[2] *Table of Isotopes,* edited by C. Michael Lederer and V. S. Shirley (Wiley, New York, 1978).
[3] I. Talmi and I. Unna, Phys. Rev. Lett. **4**, 469 (1960).
[4] T. Hoshino, H. Sagawa, and A. Arima, Nucl. Phys. **A506**, 271 (1990).
[5] M. Fukuda *et al.*, Phys. Lett. B **268**, 339 (1991).
[6] D. Vautherin and D. M. Brink, Phys. Rev. C **5**, 626 (1972).
[7] M. Beiner *et al.*, Nucl. Phys. **A238**, 29 (1975).
[8] T. Otsuka, N. Fukunishi, and H. Sagawa, in *Structure and Reactions of Unstable Nuclei,* edited by K. Ikeda and Y. Suzuki (World Scientific, Singapore, 1991), p. 100.
[9] N. Fukunishi and T. Otsuka (to be published).
[10] A. Bohr and B. R. Mottelson, *Nuclear Structure* (Benjamin, Reading, 1975), Vol. 2.
[11] S. Raman *et al.*, At. Data Nucl. Data Tables **36**, 1 (1987).
[12] D. J. Millener and D. Kurath, Nucl. Phys. **A255**, 315 (1975).
[13] G. F. Bertsch, B. A. Brown, and H. Sagawa, Phys. Rev. C **39**, 1154 (1989).
[14] I. Ragnarsson *et al.*, Nucl. Phys. **A361**, 1 (1981).
[15] H. Sagawa, Phys. Lett. B **286**, 7 (1992).
[16] P. G. Hansen and B. Jonson, Europhys. Lett. **4**, 409 (1987).
[17] I. Tanihata *et al.*, Phys. Lett. B **206**, 592 (1988).
[18] S. S. Hanna *et al.*, Phys. Rev. C **3**, 2198 (1971); D. J. Millener *et al.*, Phys. Rev. C **28**, 497 (1983).