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Pair correlation in deformed neutron-drip-line nuclei: The eigenphase formalism and asymptotic behavior

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The Hartree-Fock-Bogoliubov (HFB) equation for deformed nuclei in a simplified model is solved in coordinate space with correct asymptotic boundary conditions, in order to study the pair correlation in nuclei close to the neutron drip line. The eigenphase formalism is applied, when the upper components of HFB radial wave functions are continuum wave functions. Calculated occupation probabilities of various Nilsson orbits in the HFB ground state vary smoothly from the region of the upper components being bound wave functions to that of those being continuum wave functions. It is shown that weakly-bound or resonance-like $\Omega^{\pi} = 1/2^{+}$ Nilsson orbits contribute little to the occupation probability of the HFB ground state, while the contribution by the orbits with a large value of Ω, of which the smallest possible orbital-angular-momentum is neither 0 nor 1, may be approximately estimated using the BCS formula.

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The study of nuclei far from the β stability line has been providing a challenge to the conventional theory of nuclear structure. An interesting and important feature unique in the system with some weakly bound nucleons is the importance of the coupling to the nearby continuum of unbound states, as well as the impressive role played by weakly bound nucleons with low orbital angular momenta ℓ, especially in neutron drip line nuclei. Since the Fermi level of drip line nuclei in the mean-field approximation is very close to the continuum, the many-body correlation in the ground state necessarily receives contributions by some of the infinite number of one-particle levels in the continuum.

In the present work we are interested in the many-body pair correlation in deformed neutron-drip-line nuclei. In Ref. [1] we have studied the many-body pair correlation of spherical neutron-drip-line nuclei, while in Ref. [2] one-particle resonant levels in a quadrupole deformed potential are investigated in the absence of pair correlation using eigenphase [3]. One-particle resonant levels defined in a similar way are used also in the study of proton emission in deformed nuclei outside the proton drip line [4]. In the absence of pair correlation in deformed nuclei the eigenphase formalism is needed only when one considers positive-energy one-particle levels [2]. In contrast, in the presence of pair correlation the upper components of the HFB radial wave functions of a bound system can be continuum wave functions. Then, it is absolutely preferable to solve the HFB equation in coordinate space with correct asymptotic boundary conditions instead of restricting the system to a finite box. The solution of this problem was shown in Refs. [5,6] for spherical nuclei, however, to our knowledge it has not been done in deformed nuclei. The eigenphase formalism in deformed potentials is a natural extension of the phase shift used in spherical potentials that is defined for respective (ℓ, j) values. In contrast to the case of Ref. [3] where eigenphase is applied to the study of general positive-energy states in a deformed potential, we are interested in the HFB upper components that are strongly coupled to some weakly-bound Nilsson levels. Extending the simplified HFB model employed in Refs. [1,7,8] to the deformed nuclei, in which continuum wave functions are involved, in the present paper we formulate the model, show numerical solutions, and try to extract the relevant physics.

We consider the time-reversal invariant and axially symmetric quadrupole-deformed system with many-body pair correlation. Single quasiparticle wave functions are written as

$$\Psi^{i}_{\Omega}(\vec{r}) = \sum_{\ell j} R^{i}_{\ell j \Omega}(E_{qp}, r)\mathbf{Y}_{\ell j \Omega}(\hat{r}), \quad i = 1, 2, \tag{1}$$

where Ω expresses the component of one-particle angular momentum $\vec{j}$ along the symmetry axis, which is a good quantum number, and

$$\mathbf{Y}_{\ell j \Omega}(\hat{r}) \equiv \sum_{m_\ell, m_s} C\left(\ell, \frac{1}{2}, j; m_\ell, m_s, \Omega\right) Y_{\ell m_\ell}(\hat{r})\chi_{m_s}. \tag{2}$$

The upper ($i = 1$) and lower ($i = 2$) components of the radial wave functions are introduced as

$$r R^{i}_{\ell j \Omega}(E_{qp}, r) = u_{\ell j \Omega}(E_{qp}, r) \quad \text{and} \quad v_{\ell j \Omega}(E_{qp}, r). \tag{3}$$

Assuming that both the Hartree-Fock (HF) and pair potentials are given by the well-bound core nucleus, our HFB equation is reduced to the coupled equations for $u_{\ell j \Omega}$ and $v_{\ell j \Omega}$, which are written as

$$\left.\begin{aligned}&\left(\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}+\frac{2m}{\hbar^2}(\lambda+E_{qp}^{\Omega}-V(r)-V_{so}(r))\right)u_{\ell j\Omega}(r)-\frac{2m}{\hbar^2}\Delta_0(r)v_{\ell j\Omega}(r)\\&\quad=\frac{2m}{\hbar^2}\sum_{\ell' j'}\langle\mathbf{Y}_{\ell j\Omega}|V_{\text{coupl}}|\mathbf{Y}_{\ell' j'\Omega}\rangle u_{\ell' j'\Omega}(r)+\frac{2m}{\hbar^2}\sum_{\ell' j'}\langle\mathbf{Y}_{\ell j\Omega}|\Delta_{20}|\mathbf{Y}_{\ell' j'\Omega}\rangle v_{\ell' j'\Omega}(r),\\&\left(\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}+\frac{2m}{\hbar^2}(\lambda-E_{qp}^{\Omega}-V(r)-V_{so}(r))\right)v_{\ell j\Omega}(r)+\frac{2m}{\hbar^2}\Delta_0(r)u_{\ell j\Omega}(r)\\&\quad=\frac{2m}{\hbar^2}\sum_{\ell' j'}\langle\mathbf{Y}_{\ell j\Omega}|V_{\text{coupl}}|\mathbf{Y}_{\ell' j'\Omega}\rangle v_{\ell' j'\Omega}(r)-\frac{2m}{\hbar^2}\sum_{\ell' j'}\langle\mathbf{Y}_{\ell j\Omega}|\Delta_{20}|\mathbf{Y}_{\ell' j'\Omega}\rangle u_{\ell' j'\Omega}(r)\end{aligned}\right\}. \tag{4}$$

Since the model Hamiltonian and Eq. (4) are the same as those used in Ref. [8], where Eq. (4) was solved in the case that continuum wave functions are not involved, here we do not repeat the detailed description of all terms. We use the Woods-Saxon potential as a replacement of the HF potential, and some quantities appearing in Eq. (4) are

$$\begin{aligned}V(r)&=V_{WS}f(r),\\V_{\text{coupl}}(\vec{r})&=-\beta k(r)Y_{20}(\hat{r}),\\f(r)&=\frac{1}{1+\exp\left(\frac{r-R}{a}\right)},\\k(r)&=rV_{WS}\frac{df(r)}{dr}.\end{aligned}\tag{5}$$

We fix the parameters to be $a=0.67$ fm and $V_{WS}=-51$ MeV, which are the standard parameters used in β stable nuclei [9]. The strength of the one-body potential is varied by changing the radius of the potential R in units of $r_0=1.27$ fm. We present the numerical results obtained by using the functional form of the volume-type pairing, $\Delta_0(r)\propto f(r)$, and $\Delta_{20}\propto d\Delta_0(r)/dr$. The averaged strength of the pair field defined by

$$\bar{\Delta}\equiv\frac{\int_0^\infty r^2dr\,\Delta_0(r)f(r)}{\int_0^\infty r^2drf(r)}\tag{6}$$

is an input of numerical calculations expressing the strength of the pair field. The way of solving the coupled equations (4) is taken from Ref. [10].

For $(\lambda+E_{qp}^{\Omega})<0$ Eq. (4) is an eigenvalue problem and the asymptotic behavior of HFB wave functions for $r\to\infty$ is

$$\left.\begin{aligned}u_{\ell j\Omega}\big(E_{qp}^{\Omega},r\big)&\propto rh_\ell(\alpha_u r)\\v_{\ell j\Omega}\big(E_{qp}^{\Omega},r\big)&\propto rh_\ell(\alpha_v r)\end{aligned}\right\},\tag{7}$$

where $h_\ell(-iz)\equiv j_\ell(z)+in_\ell(z)$, in which j_ℓ and n_ℓ are spherical Bessel and Neumann functions, respectively, and

$$\left.\begin{aligned}\alpha_u^2&\equiv-\frac{2m}{\hbar^2}\big(\lambda+E_{qp}^{\Omega}\big)\\\alpha_v^2&\equiv-\frac{2m}{\hbar^2}\big(\lambda-E_{qp}^{\Omega}\big)\end{aligned}\right\}.\tag{8}$$

The normalization of the wave functions is written as

$$\sum_{\ell j}\int_0^\infty\left(\left|u_{\ell j\Omega}\big(E_{qp}^{\Omega},r\big)\right|^2+\left|v_{\ell j\Omega}\big(E_{qp}^{\Omega},r\big)\right|^2\right)dr=1\tag{9}$$

and the quantity

$$\sum_{\ell j}\int_0^\infty\left|v_{\ell j\Omega}\big(E_{qp}^{\Omega},r\big)\right|^2dr\quad\text{for}\quad\big(\lambda+E_{qp}^{\Omega}\big)<0\tag{10}$$

describes the occupation probability of the discrete one-particle level in the deformed HF potential, for which E_{qp}^{Ω} is the eigenvalue of the HFB equation (4).

For $(\lambda+E_{qp}^{\Omega})>0$ the solution of Eq. (4) exists for any values of E_{qp} and is looked for, of which the wave functions for $r\to\infty$ are written as

$$\left.\begin{aligned}u_{\ell j\Omega}(E_{qp}^{\Omega},r)&\propto(\cos(\delta_\Omega)rj_\ell(\alpha_c r)-\sin(\delta_\Omega)rn_\ell(\alpha_c r))\\v_{\ell j\Omega}(E_{qp}^{\Omega},r)&\propto rh_\ell(\alpha_v r)\end{aligned}\right\},\tag{11}$$

where

$$\alpha_c^2\equiv\frac{2m}{\hbar^2}\big(\lambda+E_{qp}^{\Omega}\big).\tag{12}$$

For a given set of potential parameters and E_{qp}^{Ω} the coupled equations (4) are integrated both outward from $r=0$ and inward from a large r value. Then, we look for the eigenphase δ_Ω, which is common to all channels (ℓ,j), so that at $r=R_m$ we can match inward-integrated $u_{\ell j\Omega}(E_{qp}^{\Omega},r)$ and $v_{\ell j\Omega}(E_{qp}^{\Omega},r)$ and those of their derivatives with the outward-integrated $u_{\ell j\Omega}(E_{qp}^{\Omega},r)$ and $v_{\ell j\Omega}(E_{qp}^{\Omega},r)$ and those of their derivatives, respectively. We obtain several solutions of δ_Ω, the number of which is equal to that of wave function components with different (ℓ,j) values. The value of δ_Ω determines the relative amplitudes of different (ℓ,j) components. It is found that the only upper components $u_{\ell j\Omega}(E_{qp}^{\Omega},r)$ which can appreciably couple to $v_{\ell j\Omega}(E_{qp}^{\Omega},r)$ of a given Nilsson level are those with a particular one of δ_Ω. The continuum wave function $u_{\ell j\Omega}(E_{qp}^{\Omega},r)$ in Eq. (11) is normalized to the Dirac δ function of energy,

$$\int_0^\infty dr\sum_{\ell j}u_{\ell j\Omega}(E_{qp},r)u_{\ell j\Omega}(E'_{qp},r)=\delta(E_{qp}-E'_{qp}).\tag{13}$$

Then, the quantity

$$\sum_{\ell j}\int_0^\infty\left|v_{\ell j\Omega}\big(E_{qp}^{\Omega},r\big)\right|^2dr\quad\text{for}\quad\big(\lambda+E_{qp}^{\Omega}\big)>0\tag{14}$$

represents the occupation number probability density per unit energy interval, while the quantity

$$\sum_{\ell j} \int_{-\lambda}^{E_{qp}^{\max}} dE_{qp}^{\Omega} \int_0^\infty \left|v_{\ell j \Omega}\left(E_{qp}^{\Omega}, r\right)\right|^2 dr, \tag{15}$$

can be interpreted as the occupation probability of a given Nilsson level.

For convenience, we choose to show numerical results of the Nilsson orbits, of which both the bound and resonant levels in the absence of the many-body pair correlation are already presented in detail in Ref. [2]. Taking $\lambda = -1.0$ MeV, $\bar{\Delta} = -1.0$ MeV and $\beta = 0.5$, in Fig. 1(a) the

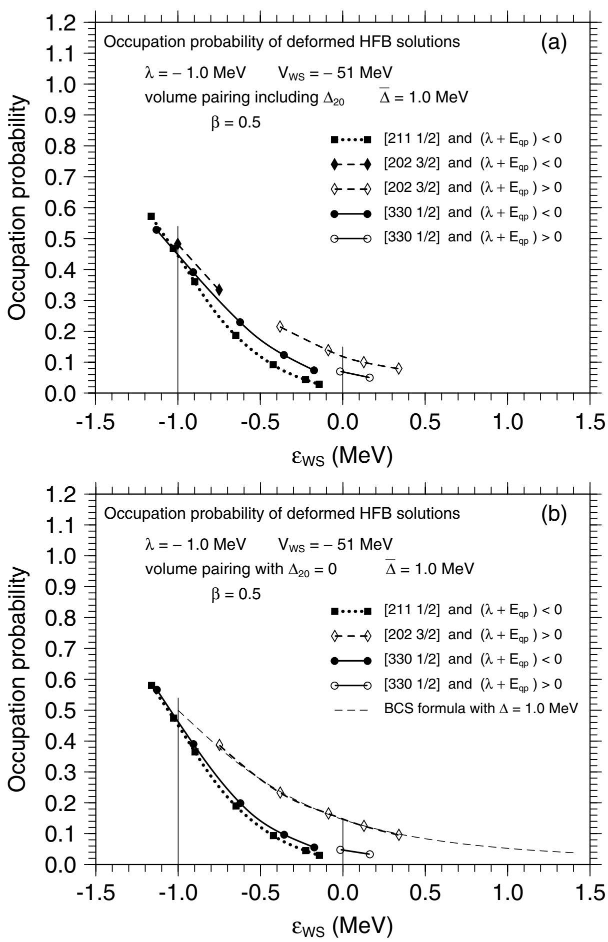

FIG. 1. (a) Calculated occupation probability of the [211 1/2], [202 3/2] and [330 1/2] Nilsson orbits in the HFB ground state as a function of one-particle bound ($\varepsilon_{WS} < 0$) or resonant energy ($\varepsilon_{WS} > 0$) of the Woods-Saxon potentials. The radius of the Woods-Saxon potential is varied for respective orbits, in order to vary respective values of ε_{WS}. The occupation probabilities obtained from the solution with $(\lambda + E_{qp}) > 0$ are denoted by open symbols, while those with $(\lambda + E_{qp}) < 0$ by filled symbols. (b) Calculated occupation probability for the same parameters as those in (a), except setting $\Delta_{20} = 0$. For the [202 3/2] orbit in the case of $\Delta_{20} = 0$ with the present parameters no solution with $(\lambda + E_{qp}) < 0$ exists for any value of ε_{WS}, due to the effectively larger pair gap. The thin dashed curve shows the occupation probability in the BCS approximation with $\Delta = 1$ MeV.

calculated occupation probabilities of three representative Nilsson orbits, which are defined by Eq. (10) for $(\lambda + E_{qp}) < 0$ and Eq. (15) for $(\lambda + E_{qp}) > 0$, respectively, are plotted as a function of one-particle bound ($\varepsilon_{WS} < 0$) and resonant ($\varepsilon_{WS} > 0$) energies of respective Woods-Saxon potentials. Though ε_{WS} does not appear in the HFB equation (4), we have separately calculated it for respective Woods-Saxon potentials. The value of $E_{qp}^{\max}$ in Eq. (15) is set equal to 5 MeV, at which the contribution to the integral is already negligible in the present numerical examples. The distance between the one-particle levels with a given Ω^π in a deformed potential is shorter than that with a given (ℓ, j) in a spherical potential, especially for small Ω values. Thus, if we take a larger value such as $E_{qp}^{\max} = 10$ MeV, there is a risk to include the occupation probability of other Nilsson levels with the same Ω^π than the specified level. In the absence of pair correlation it is shown [2] that no one-particle resonant states are found as a continuation of the bound [211 1/2] level, while the [330 1/2] level has a short continuation for $\varepsilon_{WS} > 0$ and the [211 3/2] level continues up to several MeV as a one-particle resonant level.

For reference, in Fig. 1(b) we show the calculated occupation probabilities of the same Nilsson orbits as those in Fig. 1(a), which are obtained by setting $\Delta_{20} = 0$ in Eq. (4). The inclusion of the Δ_{20} term increases (decreases) the effective pair gap of the [330 1/2] ([202 3/2]) orbit since the quadrupole deformation with $\beta > 0$ is favored (disfavored) by the [330 1/2] ([202 3/2]) orbit, while it hardly affects that of the [211 1/2] orbit. Correspondingly, the occupation probability of the [330 1/2] ([202 3/2]) orbit in Fig. 1(a) decreases less (more) rapidly than in Fig. 1(b), as ε_{WS} increases from -1.0 MeV. Due to the effectively larger pair gap in the [202 3/2] orbit in the absence of the Δ_{20} term, no HFB discrete solution exists for any value of ε_{WS} in contrast to the case shown in Fig. 1(a). In Fig. 1(b) the occupation probability in the BCS approximation is plotted by a thin dashed curve, where $\Delta = 1$ MeV and $\lambda = -1$ MeV are used. It is seen that the occupation probability of the [202 3/2] level obtained by using the present formalism follows closely the BCS value.

It is seen that both [211 1/2] and [330 1/2] levels lose drastically the occupation probability in the HFB ground state or the contribution to the many-body pair correlation, already when $\varepsilon_{WS}(< 0)$ approaches zero. For a given Ω^π value it depends somewhat on the structure of each orbits how quickly their occupation probabilities decrease. When the calculated occupation probability becomes very small for $(\lambda + E_{qp}) > 0$, there is some small numerical ambiguity in the calculated occupation probabilities due to the $E_{qp}^{\max}$ values chosen in Eq. (15). Furthermore, when the eigenvalue E_{qp} approaches $-\lambda$ for $(\lambda + E_{qp}) < 0$, there is a very small contribution to the occupation probability also from the region of $E_{qp} > -\lambda$, as shown in Ref. [1]. This contribution is not included in the filled symbols of Fig. 1.

In Fig. 2 we plot the occupation number probability densities per unit energy of various (ℓ, j) components

$$\int_0^\infty \left|v_{\ell j \Omega}\left(E_{qp}^{\Omega}, r\right)\right|^2 dr \tag{16}$$

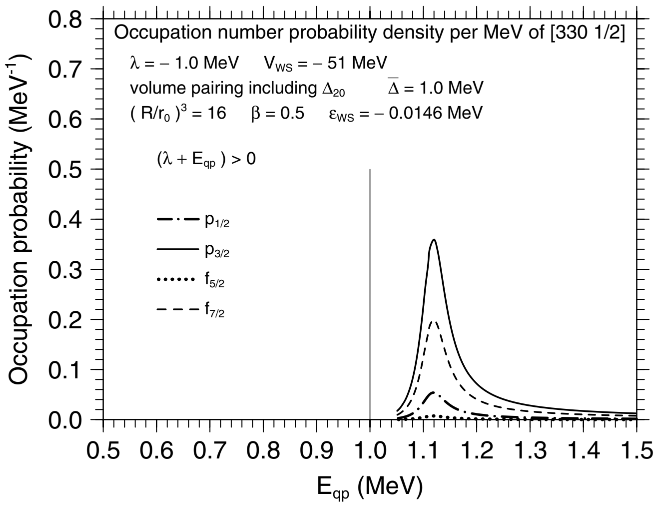

FIG. 2. Occupation number probability density per unit energy of various (ℓ, j) components of the [330 1/2] level, Eq. (16), as a function of quasiparticle energy E_{qp}. No discrete HFB solution exists for the present potential parameters, which produce $\varepsilon_{WS} = -0.0146$ MeV.

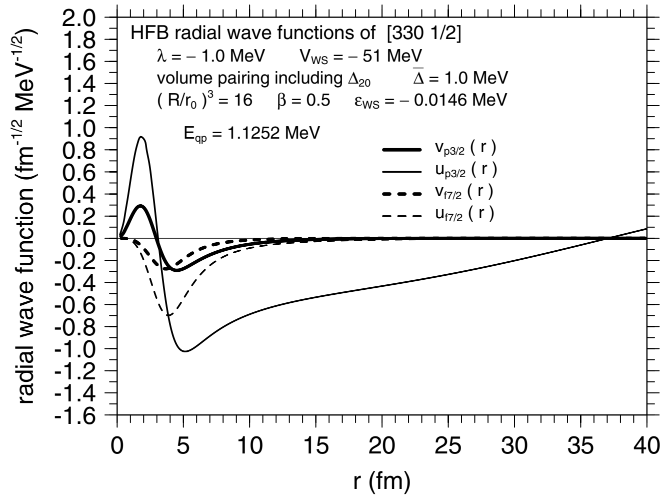

FIG. 3. HFB radial wave functions of the [330 1/2] level as a function of radial variable. At the chosen value of $E_{qp} = 1.1252$ MeV the eigenphase δ_Ω of the upper component of HFB radial wave functions, $u_{\ell j\Omega}(E_{qp}, r)$, increases through $\frac{1}{2}\pi$.

as a function of E_{qp}, taking the [330 1/2] level with the potential which gives $\varepsilon_{WS} = -0.0146$ MeV. Though for a well-bound [330 1/2] level the $f_{7/2}$ component is predominant [11], in Fig. 2 it is seen that $p_{3/2}$ is the major component. See also Fig. 4 of Ref. [7]. The peak of the occupation number probability densities occurs at $E_{qp} = 1.119$ MeV, which is only slightly different from $E_{qp} = 1.1252$ MeV where $\delta_\Omega = \frac{1}{2}\pi$ for $u_{\ell j\Omega}(E^{\Omega}_{qp}, r)$ is obtained.

Taking the value of $E_{qp} = 1.1252$ MeV, in Fig. 3 the HFB radial wave functions of the [330 1/2] level are exhibited for the two major components, $p_{3/2}$ and $f_{7/2}$. For this small positive value of $(\lambda + E_{qp})$= +0.1252 MeV, the continuum wave function $u_{f7/2}(r)$ does not show any violent behavior in the plotted range of r, while $u_{p3/2}(r)$ clearly exhibits the structure of a continuum wave function.

In conclusion, applying the eigenphase formalism to the asymptotic boundary conditions of the upper components of radial wave functions for $(\lambda + E_{qp}) > 0$, the HFB equation for deformed nuclei in a simplified model is solved in coordinate space. Though there are several solutions of eigenphase for a given set of potential parameters and E^{Ω}_{qp}, it is found that the lower components of radial wave functions, $v_{\ell j\Omega}(r)$, of a given Nilsson level couple appreciably only to the upper components with a particular solution of eigenphase. Those $u_{\ell j\Omega}(r)$ with other values of eigenphase may strongly couple to $v_{\ell j\Omega}(r)$ of other Nilsson levels than the present one and, thus, may become important, for example, when excitation modes are considered. It is shown that weakly-bound or resonance-like $\Omega^\pi = 1/2^+$ and $1/2^-$ Nilsson orbits contribute little to the occupation probability of the HFB ground state. Combining this finding together with their considerably small effective pair gaps exhibited in Ref. [8], those orbits may contribute little to the many-body pair correlation of the HFB ground state. On the other hand, the contribution by the orbits with a large value of Ω, of which the smallest possible orbital-angular momentum is larger than 1, may be approximately estimated using the BCS approximation. It remains to see how quantitatively the fully self-consistent HFB calculations solved in coordinate space with correct asymptotic boundary conditions support the results of the present work.

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[1] I. Hamamoto and B. R. Mottelson, Phys. Rev. C **68**, 034312 (2003); **69**, 064302 (2004).
[2] I. Hamamoto, Phys. Rev. C **72**, 024301 (2005).
[3] K. Hagino and N. V. Giai, Nucl. Phys. **A735**, 55 (2004), and references quoted therein.
[4] L. S. Ferreira and E. Maglione, Int. J. Theor. Phys. **42**, 2117 (2003), and references quoted therein.
[5] A. Bulgac, preprint No. FT-194-1980, Institute of Atomic Physics, Bucharest, 1980, nucl-th/9907088.
[6] M. Grasso, N. Sandulescu, N. V. Giai, and R. J. Liotta, Phys. Rev. C **64**, 064321 (2001).
[7] I. Hamamoto, Phys. Rev. C **69**, 041306(R) (2004).
[8] I. Hamamoto, Phys. Rev. C **71**, 037302 (2005).
[9] A. Bohr and B. R. Mottelson, *Nuclear Structure* (Benjamin, Reading, MA, 1969), Vol. I.
[10] T. Tamura, Oak Ridge National Laboratory, Report ORNL-4152, 1967 (unpublished).
[11] A. Bohr and B. R. Mottelson, *Nuclear Structure* (Benjamin, Reading, MA, 1975), Vol. II.