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Reflection Asymmetric Shell Model on the Projected Woods–Saxon+BCS Basis *

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The projected Woods–Saxon (WS) quasi-particle states have been used as the bases in the calculation of the reflection asymmetric shell model (RASM). The WS potential has been modified but constrained to give the similar single-particle levels of the standard WS potential. Correspondingly, the multipole interactions in the total RASM Hamiltonian are constructed according to the modified WS potential. The calculated octupole band of ^{228}Th from this approach is in good agreement with experimental data.

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The shell model has been quite successful in the description of the nuclear structure, especially for spherical nuclei. However, it is almost impossible to describe medium and heavy deformed nuclei in terms of the standard (spherical) shell model. The introduction of the Nilsson model[1] is a major development in the studies of deformed nuclei. In this model, the deformed state is defined in the intrinsic frame of reference, in which the rotational symmetry is broken. If one is just interested in the average behaviour of the rotation, the Coriolis term $-\omega j_x$ can be added to the intrinsic Hamiltonian, which leads to the cranking shell model (CSM) introduced by Inglis[2] and widely used in the high-spin state studies. Despite its great success, the angular momentum in the CSM cannot be treated in a quantum mechanics way. In order to have good angular momentum numbers, it is necessary to restore the broken rotational symmetry in the laboratory frame of reference by using the standard angular momentum projection techniques.[3] Along this line, the projected shell model (PSM) has been developed to project the good angular momentum states in the laboratory frame of reference from the Nilsson+BCS intrinsic states.[4] In the PSM, the angular momentum projection is carried out on a chosen set of Nilsson+BCS states near the Fermi surface, and the projected states are then used to diagonalize a shell model Hamiltonian. The deformed bases are used instead of the spherical ones, which makes the truncation of the many-body bases so efficient that the shell model calculations even for heavier systems become possible. The PSM approach has been successfully used to describe a broad range of nuclear phenomena such as backbending,[5] signature dependence,[6,7] superdeformation[8,9] and identical bands.[10] With those successes, the PSM has been extended to study the triaxial deformed nuclei—triaxial projected shell model (TPSM)[11] and the octupole deformed nuclei—reflection asymmetric shell model (RASM).[12,13]

So far, the projected states used in the PSM and its extensions are the Nilsson+BCS intrinsic states. As the deformed Nilsson potential is expressed in terms of spherical harmonics, it is very easy to construct the self-consistent multipole interactions in the total PSM Hamiltonian. However, in the Nilsson potential, it is a pity that the parameters κ and μ are different for different shells, and this potential cannot supply a geometric picture with a flat bottom and diffused surface. While for the Woods–Saxon (WS) potential, its parameters are more acceptable, and its flat bottom and diffused surface are intuitive. Moreover, the single-particle states from the WS potential are more realistic. For instance, in the actinide region, it has been found that the coupling to octupole deformation is stronger in a potential with a more realistic flat-bottomed shape.[14] The WS potential used by Nazarewicz *et al.*[15] leads to an octupole coupling which is much stronger than that obtained with the modified harmonic oscillator (MHO) potential, in agreement with the observation. Therefore, it is expected that the projected states based on the WS potential may provide a better description for the octupole deformed bands.

As the deformed WS potential is in compact form rather than in the spherical harmonic expansion, it is difficult to construct a multipole interaction corresponding to the deformed WS potential. It will be shown that the WS potential can be expanded in terms of a limited spherical harmonics. Then the multipole interactions can be as easily constructed as those in the RASM.[12] In this letter, the RASM based on the WS potential will be developed and applied to the octupole band in ^{228}Th.

The detailed formalism of the RASM can be found in Ref. [12]. Considering a set of intrinsic states with

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quantum number κ, $\{|\Phi_\kappa\rangle\}$, one may construct another class of states in the laboratory frame of reference as a trial wavefunction

$$|\Psi^p_{IM}\rangle = \sum_{K\kappa} F^{Ip}_{K\kappa} P^p P^I_{MK} |\Phi_\kappa\rangle, \tag{1}$$

where

$$P^p = \frac{1}{2}(1 + p\hat{P}), \quad p = \pm 1,$$
$$P^I_{MK} = \frac{2I+1}{8\pi^2} \int \mathrm{d}\Omega D^I_{MK}(\Omega)\hat{R}(\Omega).$$

The coefficient $F^{Ip}_{K\kappa}$ is determined by the RASM eigenvalue equation

$$\sum_{K\kappa} \{\langle\Phi_{\kappa'}|HP^pP^I_{K'K}|\Phi_\kappa\rangle - E^p_I\langle\Phi_{\kappa'}|P^pP^I_{K'K}|\Phi_\kappa\rangle\} F^{Ip}_{K\kappa} = 0, \tag{2}$$

where E^p_I is the rotational energy with angular momentum I and parity p. The normalization condition for $F^{Ip}_{K\kappa}$ is

$$\sum_{K'\kappa'K\kappa} F^{Ip*}_{K'\kappa'} \langle\Phi_{\kappa'}|P^pP^I_{K'K}|\Phi_\kappa\rangle F^{Ip}_{K\kappa} = 1. \tag{3}$$

It is seen that Eq.(1) is valid for any nuclear shape, although in the present study we only consider the case of axial symmetry.

The intrinsic states $|\Phi_\kappa\rangle$ can be generated from the deformed BCS quasi-particle states. Here the single-particle states were obtained from a modified WS potential.

The standard WS potential is defined as[16]

$$V(\boldsymbol{r}, \hat{\beta}) = \frac{V_0}{1 + \exp[\mathrm{dist}_\Sigma(\boldsymbol{r}, \hat{\beta})/a]}, \tag{4}$$

where $\hat{\beta}$ denotes the deformation parameter sets $\{\beta_\lambda, \lambda \geq 2\}$, $\mathrm{dist}_\Sigma(\boldsymbol{r}, \hat{\beta})$ is the distance (taken with the minus sign inside the surface) between the point $\boldsymbol{r}$ and the nuclear surface Σ represented by (here the axially symmetric case only)

$$R(\theta, \hat{\beta}) = R_0(\hat{\beta}) \left[1 + \sum_{\lambda\geq 2} \beta_\lambda Y_{\lambda 0}(\theta)\right], \tag{5}$$

and the diffuseness parameter is denoted by a. As $V(\boldsymbol{r}, \hat{\beta})$ is one term, it is difficult to construct an exact effective interaction consistent with $V(\boldsymbol{r}, \hat{\beta})$. Similar to the case of the Nilsson potential, Eq. (4) can be expanded in terms of spherical harmonics

$$V(\boldsymbol{r}, \hat{\beta}) = w_0(r) + \sum_{\lambda=1}^{\infty} w_\lambda(r) Y_{\lambda 0}(\theta) \tag{6}$$

where

$$w_0(r) = \frac{1}{2}\int_0^\pi V(\boldsymbol{r}, \hat{\beta}) \sin(\theta)\mathrm{d}\theta,$$
$$w_\lambda(r) = 2\pi \int_0^\pi V(\boldsymbol{r}, \hat{\beta}) Y_{\lambda 0}(\theta) \sin(\theta)\mathrm{d}\theta. \tag{7}$$

It is of course impossible to include all terms on the right-hand side of the above equation, and one can hope that this expansion converges fast enough for the real nuclear surface. As an example, various $w_\lambda(r)$ as a function of r for a normal deformed WS potential corresponding to that of ^{228}Th are shown in Fig. 1. It is seen that $w_0(r)$ is very similar to the spherical WS potential. For spherical nuclei, $w_0(r)$ equals the corresponding WS potential with the same diffuseness, while the other $w_{\lambda\neq 0}(r)$ vanishes. The diffuseness of $w_0(r)$ depends on the deformation as well as the surface diffuseness. With the increase of the deformation, and thus of the diffuseness of $w_0(r)$, simultaneously those terms $w_{\lambda\neq 0}(r)$ will appear and become more and more remarkable. As can be seen from Fig. 1, the most important terms are those with $\lambda \leq 6$, i.e.

$$V(\boldsymbol{r}, \hat{\beta}) \approx w_0(r) + \sum_{\lambda=1}^{6} w_\lambda(r) Y_{\lambda 0}(\theta). \tag{8}$$

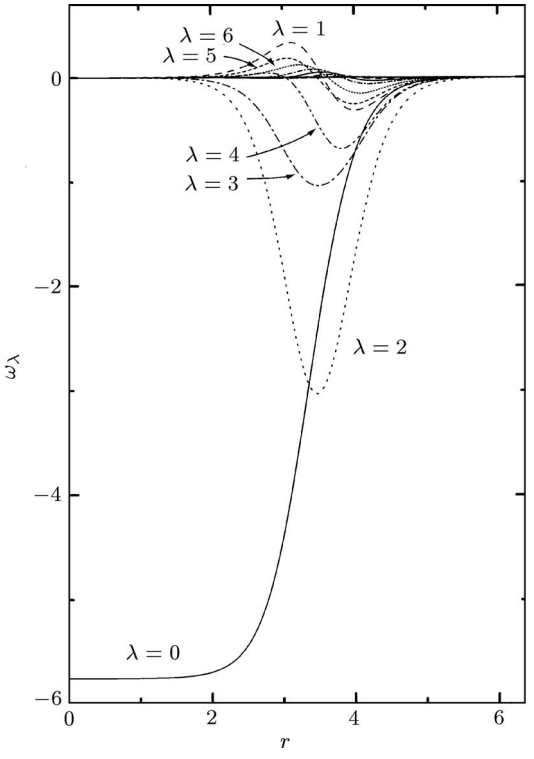


Fig. 1. Expansion coefficients $w_\lambda(r)$ of the WS potential with the deformation $\beta_2 = 0.2$, $\beta_3 = 0.077$, $\beta_4 = 0.034$, $\beta_5 = 0.00418$ and $\beta_6 = 0.00166$.

To check this approximation further, the contour plots corresponding to that in Fig. 1 for both sides of Eq. (8) are shown in Fig. 2. Figure 2(a) represents the

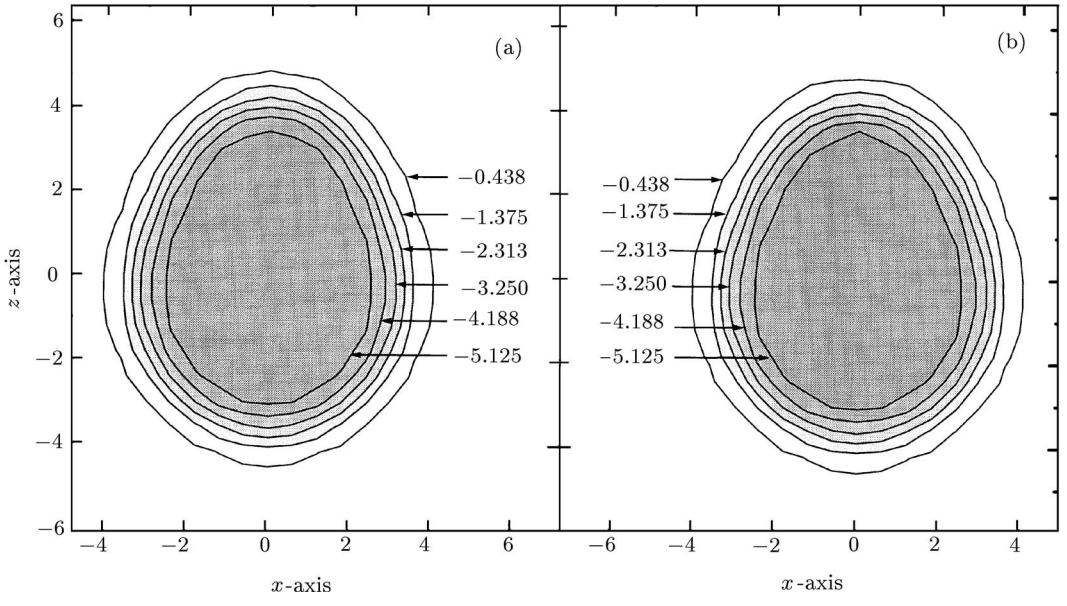


Fig. 2. Contour plots on the plane determined by the x-axis and the axially symmetric z-axis for the WS potential (a) and the corresponding expansion with $\lambda \leq 6$ (b). The deformation for the WS potential is the same as Fig. 1.

WS potential and Fig. 2(b) represents the corresponding expansion up to $\lambda = 6$. It is seen that Fig. 2(b) reproduces Fig. 2(a) well. This gives us confidence to replace the deformed WS potential with Eq. (8)

The spin-orbit term is defined as $[\nabla V \times P] \cdot \sigma$, and it does not have the rotational invariance if V is not spherical. This will lead to difficulty in the present method as the total Hamiltonian in RASM should have the rotational invariance. Therefore, we replace V with $w_0(r)$, i.e.

$$V_{so} = \lambda_{so} \left(\frac{\hbar}{2mc}\right)^2 \frac{2}{r} \frac{\mathrm{d}w_0(r)}{\mathrm{d}r} l \cdot s. \tag{9}$$

As noted above, since $w_0(r)$ depends on the deformation, V_{so} will depend on the deformation despite its spherical form. This modified V_{so} term Eq. (9) will lead to some difference on the single-particle levels compared with the standard spin-orbit term. However, this difference can be compensated for to a great extent by reasonably changing the deformation of $V(\boldsymbol{r}, \hat{\beta})$, and a set of similar single-particle levels (at least in the vicinity of the Fermi level) from Eq. (9) can be obtained.

Generally, the single-particle Hamiltonian in the body-fixed system can be written as

$$\begin{aligned} H_{\mathrm{s.p.}} &= H_0 + \sum_{\lambda=1}^{6} w_\lambda(r) Y_{\lambda 0}(\theta) \\ &= T + w_0(r) + V_{so} + \sum_{\lambda=1}^{6} w_\lambda(r) Y_{\lambda 0}(\theta), \end{aligned} \tag{10}$$

where T is the kinetic energy. The RASM Hamiltonian, consistent with the above single-particle potential, can be written as

$$\begin{aligned} H = H_0 &+ \frac{1}{2} \sum_{\lambda=1}^{6} \chi_\lambda \sum_{\mu=-\lambda}^{\lambda} Q^\dagger_{\lambda\mu} Q_{\lambda\mu} - G_0 P^\dagger_{00} P_{00} \\ &- G_2 \sum_{\mu=-2}^{2} P^\dagger_{2\mu} P_{2\mu}, \end{aligned} \tag{11}$$

where

$$\begin{aligned} Q_{\lambda\mu} &= \sum_{\alpha,\beta} \langle \alpha | w_\lambda(r) Y_{\lambda\mu} | \beta \rangle c^\dagger_\alpha c_\beta, \\ P^\dagger_{00} &= \frac{1}{2} \sum_{\alpha} c^\dagger_\alpha c^\dagger_{\bar{\alpha}}, \\ P^\dagger_{2\mu} &= \frac{1}{2} \sum_{\alpha,\beta} \langle \alpha | w_2(r) Y_{2\mu} | \beta \rangle c^\dagger_\alpha c^\dagger_{\bar{\beta}}. \end{aligned} \tag{12}$$

This Hamiltonian includes multipole–multipole interactions with the rank from 1 to 6, which correspond to the $\lambda \neq 0$ terms in Eq. (8). The radial function of the multipole moments now varies with $w_\lambda(r)$ rather than the previous r^2. As can be seen in Fig. 1, $w_{\lambda \neq 0}(r)$ have a non-zero value only in the vicinity of the surface. These interactions are actually surface effects, and very different from the previous definition.[12]

The coupling constants of the $Q^\dagger_\lambda \cdot Q_\lambda$ forces, χ_λ, in Eq. (11) can be determined by the expression (similar to Ref. [4,12])

$$\chi_{\lambda,\tau\tau'} = \frac{\hbar\omega_\tau \hbar\omega_{\tau'}}{\hbar\omega_n \langle Q_{\lambda 0} \rangle_n + \hbar\omega_p \langle Q_{\lambda 0} \rangle_p}, \qquad (\lambda = 1 \text{ to } 6) \tag{13}$$

where $\langle \cdots \rangle$ means the expectation value with respect to the BCS vacuum state, and $\tau(\tau')$ refers to neutron or proton.

Table 1. Woods–Saxon potential parameters taken from Ref. [18]. The values of r_0 and a are in units of fm, V_0 in MeV, while κ and λ are dimensionless.

$\lambda(P)$	$\lambda(N)$	$r_{0-so}(P)$	$r_{0-so}(N)$	$r_0(P)$	$r_0(N)$	κ	V_0	a
17.8	31.5	0.932	1.28	1.275	1.347	0.86	49.6	0.70

As an example, the octupole bands in ^{228}Th are studied with this method. The WS single-particle states were calculated in the major shells from $N = 4$ to 9 for neutrons and $N = 3$ to 8 for protons. The WS parameters adopted in the present calculation are taken from Refs. [17,18], as shown in Table 1. The BCS procedure involves all the single-particle levels considered and then the pairing strength is chosen as $G_0 = [15.08 \mp 13.49(N - Z)/A]/A$ (minus for neutron and plus for proton) for the actinide region. The strength of the quadrupole pairing is not considered here, as we take $G_2 = 0$. The deformation of ^{228}Th is ($\beta_2 = 0.2, \beta_3 = 0.077, \beta_4 = 0.034, \beta_5 = 0.00418, \beta_6 = 0.00166$), where β_5, and β_6 are determined by the formula mentioned in Ref. [19], as shown in Fig. 2.

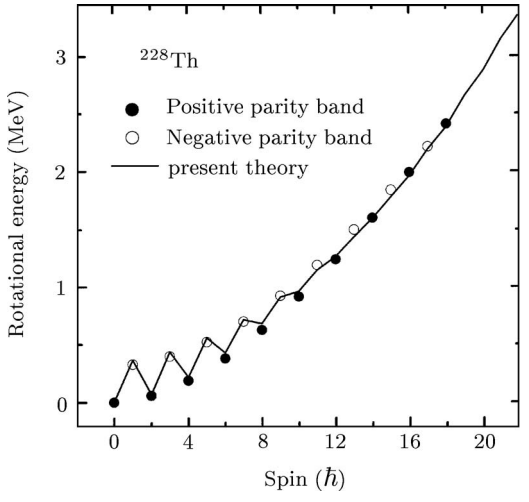


Fig. 3. Yrast octupole bands in ^{228}Th calculated by the RASM with the modified WS potential are compared with the data.[20]

In Fig. 3, the octupole yrast bands calculated by the RASM with the modified WS potential are shown together with the experimental observation.[20] It should be noted that apart from the modification of the WS potential with a harmonic expansion, all the parameters used here are standard. It is seen that the theoretical result is in good agreement with the experimental data. The main characteristics of the octupole rotational band are well reproduced by the present model. As shown in the former paper,[12] the big parity splitting at low spin appears naturally for the RASM no matter whether the WS or Nilsson model is used for the single-particle states. It is well demonstrated that the negative parity band can be explained well in a rotational picture rather than an octupole vibrational one.

In summary, the projected WS quasi-particle states have been used as the bases in the calculation of the reflection asymmetric shell model. The WS potential has been properly modified as an expansion of spherical harmonics and the spin-orbit term has been approximated as a rotational invariant one, but constrained to give the similar single-particle levels of the standard WS potential. Correspondingly, the multipole interactions in the total RASM Hamiltonian is constructed according to the modified WS potential. The calculated octupole band of ^{228}Th from this approach is in good agreement with experimental data.

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