Triaxiality-Driving Effect Extracted by Spin Projection

Ken-Ichi Enami, Kosai Tanabe,* Naotaka Yoshinaga** and Koji Higashiyama

Department of Physics, Saitama University, Urawa 338-8570, Japan

(Received May 19, 2000)

The effect of triaxial spin projection on the potential energy surface in the deformation parameter space $(\varepsilon, \gamma)$ is investigated for three nuclei, $^{142}$Nd, $^{168}$Er and $^{188}$Os. The calculation is performed for two sets of the spherical single-particle space and an effective monopole-pairing plus quadrupole-quadrupole interaction. The correlations taken into account by the spin projection have an effect of driving the system toward a triaxial deformation, irrespective of the shell fillings of the nuclei.

§1. Introduction

In the past several decades, studies of the potential energy surface (PES) have given an insight into nuclear deformation, not only for the ground state but also for high spin states.1, 2 Many microscopic studies of the PES have been based on the symmetry breaking mean-field theories, such as Nilsson BCS and Hartree-Fock-Bogoliubov theories.3 For the quantum mechanical description of a finite system such as a nucleus, it is quite desirable to restore the symmetries broken by the mean-field approximation. Such an investigation in connection with the ground state PES was performed by Hayashi, Hara and Ring.4 They applied the triaxial spin projection to the transitional nucleus $^{188}$Os and the well-deformed $^{168}$Er. Their result for $^{188}$Os shows that the behavior of the $\gamma$-soft PES is modified and that an explicit energy minimum appears at $\gamma \simeq 30^\circ$ due to the energy gain from the spin projection. This result supports the basic assumption of the triaxial rigid rotor model5 of the microscopic point of view. Similar work has been done using the macroscopic interacting boson model in connection with $\gamma$-unstable nucleus in the $O(6)$ limit.7

The purpose of the present paper is to reconsider this problem from a different point of view. Our interest is focused on the problem of determining whether the triaxiality-driving tendency of the spin projection is caused by specific shell filling or not. For this purpose, we apply the triaxial spin projection to three typical cases, the spherical nucleus $^{142}$Nd and the well-deformed nucleus $^{168}$Er, as well as the $\gamma$-unstable nucleus $^{188}$Os. For the basic microscopic interaction, we employ the empirical pairing-plus-quadrupole model.8, 9 In order to avoid the ambiguity concerning the total potential energy, we exclusively investigate the energy gain arising from the triaxial spin projection. The numerical analysis was carried out for two types of the single-particle spaces, each of which is spanned by two or three

* E-mail: tanabe@rihon.ged.saitama-u.ac.jp
** E-mail: yosinaga@rihon.ged.saitama-u.ac.jp
major shells for both kinds of nucleons. Moreover, we perform a similar investigation for the single $j$-shell model with pure quadrupole-quadrupole interaction. In this way, we study the effect of the two-body correlations taken into account through the spin projection on the PES, and find a common feature that does not depend on the adopted single-particle space and the shell fillings.

In §2, we review the theory employed in the present paper. In §3, the results of the numerical analysis are given. In §4, we consider the origin of the results reported in §3 and summarize our results.

§2. Resume of the theory

We determine the deformed mean-field solutions for the pairing-plus-quadrupole model of Kumar and Baranger with some modifications presented below. The intrinsic states determined from this scheme are essentially the same as those obtained from the Nilsson BCS model, so that the input deformation parameters $\varepsilon$ and $\gamma$ can be conveniently used for PES studies.

The Hamiltonian of the pairing-plus-quadrupole model is composed of a spherical single-particle Hamiltonian, quadrupole-quadrupole interaction (QQI) and monopole-pairing interaction (MPI):

$$\hat{H} = \hat{H}_0 - \frac{1}{2} \sum_{\tau, \tau', \mu} \chi_{\tau\tau'} \hat{Q}_{\tau\mu}^\dagger \hat{Q}_{\tau'\mu} - \sum_{\tau} G^{(0)}_{\tau} \hat{P}_{\tau}^\dagger \hat{P}_{\tau}. \quad (2.1)$$

Here, $\hat{Q}_{\tau\mu}$ ($\mu = 0, \pm 1, \pm 2$) is the dimensionless mass quadrupole operator and $\hat{P}_{\tau}$ the monopole pair operator with $\tau$ designating a proton or neutron. The single-particle Hamiltonian $\hat{H}_0$ is given by the spherical modified oscillator (MO) potential. The MO parameters $\kappa$ and $\mu$ of the $\vec{l} \cdot \vec{s}$ and $\{\vec{l}^2 - \langle \vec{l}^2 \rangle_N\}$ terms are the same as those given in Refs. 1) and 10). We carried out the numerical analysis with respect to two types of the single-particle space, I and II. The single-particle space I consists of two major shells of $N = 4, 5$ ($5, 6$) for protons (neutrons) and the space II consists of three major shells of $N = 3, 4, 5$ ($4, 5, 6$) for protons (neutrons). The shell model basis I corresponds to that employed by Kumar and Baranger, and the basis II is utilized in the Projected Shell Model (PSM). In the case of the single-particle space II, the mixing of the states whose principal quantum numbers differ by 2 is partially taken into account by the matrix elements of the quadrupole moment. The oscillator energy $\hbar \omega$ is independent of the deformation, but it depends on the isospin

$$\hbar \omega_{p/n} = \hbar \omega_0 \left(1 \mp \frac{N - Z}{3A}\right), \quad (2.2)$$

where we use the standard value $\hbar \omega_0 = 41.2A^{-1/3}$ MeV. In connection with the volume conservation condition, we modify the oscillator length $b_\tau$ for both protons and neutrons, according to the ansatz in Ref. 9).

We consider an MPI force strength of the form

$$G^{(0)}_{p/n} = \left( g_1 \pm g_2 \frac{N - Z}{A} \right) \frac{1}{A} \text{ MeV.} \quad (2.3)$$
We adopt standard values of the MPI parameters $g_1$ and $g_2$ for both single-particle space I and II, as given in Table I. In contrast to the MPI, for which the same value of $G^{(0)}$ can be used in both the Nilsson BCS and projection stages, there is an ambiguity in determining the force strength of the QQI. We determine the force parameter of the QQI in a manner similar to that of the PSM, as

\begin{equation}
\chi_{\tau\tau'} = \frac{2}{3} \sqrt{\frac{4\pi}{5}} \frac{\hbar \omega_\tau \hbar \omega_{\tau'} \varepsilon \cos \gamma}{\hbar \omega_p \langle \hat{Q}_{\tau 0} \rangle + \hbar \omega_n \langle \hat{Q}_{\tau' 0} \rangle} \, \text{MeV},
\end{equation}

where $\langle \rangle$ denotes the Nilsson BCS quasi-vacuum specified by the deformation parameters $\varepsilon$ and $\gamma$. The force parameter $\chi_{\tau\tau'}$ given by Eq. (2.4) and that of the axially symmetric PSM differ by the factor $\cos \gamma$ due to the triaxiality. We determine $\chi_{\tau\tau'}$ by using $\varepsilon, \gamma$ and $\langle \hat{Q}_{\tau 0} \rangle$ for the equilibrium deformation in the unprojected PES. Then, we calculate the unprojected PES using the Nilsson-Strutinsky method. Since the factor $\varepsilon \cos \gamma$ is effectively canceled by a similar dependence appearing in the denominator of Eq. (2.4), the variation of $\chi_{\tau\tau'}$ in the ($\varepsilon, \gamma$) plane is slight. Therefore, we pick up a reasonable value for a common force parameter $\chi_{\tau\tau'}$ for the microscopic interaction. In practice, we adopt the force strength $\chi_{\tau\tau'}$ for the axially symmetric shape. For the spherical nucleus $^{142}$Nd, for which the minimum of the PES is at $\varepsilon = 0$, where $\langle \hat{Q}_{\tau 0} \rangle = 0$, we use the value of $\chi_{\tau\tau'}$ at $\varepsilon = 0.2 (\gamma = 0^\circ)$. This choice comes from the fact that neutron gap $\Delta_n$, which vanishes in the vicinity of $\varepsilon = 0$, becomes stable around $\varepsilon \sim 0.2$ for both single-particle spaces I and II. At any rate, we confirm that the behavior of the projected PES is not strongly affected by these choices. In Table II, the force parameters of the QQI are summarized.

The spin projected energy for any spin $I$ is determined from the generalized eigenvalue equation

\begin{equation}
\sum_{K'=-I}^{I} \left\{ \langle \hat{H} \hat{P}_{KK'}^I \rangle - E_I \langle \hat{P}_{KK'}^I \rangle \right\} F_{K'}^I = 0 .
\end{equation}

Table II. The force parameter of the QQI, where $\chi' = \chi A^{1.4} \, \text{MeV}$ and $\chi_{pn} = \chi_{np}$.

<table>
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<tr>
<th>s-p space</th>
<th>$\chi'_{pn}$</th>
<th>$\chi'_{pp}$</th>
<th>$\chi'_{nn}$</th>
<th>$\varepsilon (\gamma = 0^\circ)$</th>
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<td>78.3</td>
<td>70.6</td>
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<td>$^{168}$Er</td>
<td>55.2</td>
<td>48.6</td>
<td>62.6</td>
<td>0.26</td>
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<td>$^{188}$Os</td>
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<td>49.4</td>
<td>63.8</td>
<td>0.14</td>
</tr>
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<td>40.3</td>
<td>49.5</td>
<td>0.20</td>
</tr>
<tr>
<td>$^{168}$Er</td>
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<td>38.7</td>
<td>49.9</td>
<td>0.26</td>
</tr>
<tr>
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<td>46.2</td>
<td>40.7</td>
<td>52.5</td>
<td>0.15</td>
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</tbody>
</table>

$^*$) The factor $\frac{2}{3} \sqrt{\frac{4\pi}{5}}$ comes from the different convention for the definition of the quadrupole matrix element, i.e. $\langle k|Q_{\tau \mu}^{(2)}|k' \rangle \equiv \langle k|\hat{r}^2 \hat{Y}_{\mu}^{(2)}|k' \rangle$, with $|k\rangle=|k(\tau nl jm)\rangle$. 

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Table I. The force parameter of the MPI.

<table>
<thead>
<tr>
<th>s-p space</th>
<th>$g_1$</th>
<th>$g_2$</th>
</tr>
</thead>
<tbody>
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<td>24.5</td>
<td>13.0</td>
</tr>
<tr>
<td>II</td>
<td>22.2</td>
<td>11.5</td>
</tr>
</tbody>
</table>

We adopt standard values of the MPI parameters $g_1$ and $g_2$ for both single-particle space I and II, as given in Table I.
In this expression, the spin projection operator is given by
\[ \hat{P}^{I}_{MK} = \frac{2I + 1}{8\pi^2} \int d\Omega D^{I}_{MK}(\Omega) \hat{R}(\Omega), \] (2.6)
where \( \hat{R}(\Omega) \) and \( D^{I}_{MK}(\Omega) \) denote the rotation operator and Wigner’s \( D \)-function, respectively, and \( \Omega \) expresses three Euler angles. For the purpose of calculating the projected ground state PES with \( I = K = K' = 0 \), it is not necessary to solve the eigenvalue equation (2.5). The coefficient \( F^{I=0}_{K=0} \) is simply given by \( \langle \hat{P}^{I=0}_{00} \rangle^{-1/2} \) in this case. Then, the energy gain due to the spin projection is defined by
\[ E_{\text{proj}}(\varepsilon, \gamma) \equiv \frac{\langle \hat{H} \hat{P}^{I=0}_{00} \rangle}{\langle \hat{P}^{I=0}_{00} \rangle} - \langle \hat{H} \rangle. \] (2.7)

The calculation of \( E_{\text{proj}} \) is repeated at various points in the \((\varepsilon, \gamma)\) plane to complete the contour plot.

The simple expectation value \( \langle \hat{H} \rangle \) with the Nilsson BCS state and the empirical Hamiltonian employed in the present paper is often inadequate for describing the unprojected PES. Also, the resultant PES is strongly dependent on the employed single-particle space. Therefore, the first term on the rhs of Eq. (2.7), including \( \langle \hat{H} \rangle \) as a part, does not always reproduce a reasonable total potential energy. There exist some prescriptions to extract the suitable behavior of the unprojected PES, e.g. the shell correction method. The equilibrium deformation predicted by the minimum of the unprojected PES is not strongly dependent on the methods, although the magnitude of the potential energy does depend on the method employed, especially when the single-particle space is restricted. For instance, when the shell correction method is applied to the case of a restricted single-particle space, a qualitatively reasonable PES and Nilsson diagram can be obtained, but the depth of the PES at the equilibrium deformation is often underestimated in comparison with the results that take account of a sufficiently large part of the single-particle space, e.g. \( N = 0 \sim 8 \) major shells for both protons and neutrons. The differences in energy among these alternative estimates often amount to a few MeV at the equilibrium deformation for a well-deformed nucleus with a deep minimum in the PES. On the other hand, the validity of the prescription of Kumar and Baranger\(^9\) is guaranteed only for the single-particle space \( I \). In order to obtain a result which is reasonably free from these ambiguities, we consider the energy gain defined by Eq. (2.7). The characteristic effect of the spin projection is described by contour plots of the energy gain in the next section.

\[\text{§3. Numerical results}\]

For the spherical shape \((\varepsilon = \gamma = 0)\), the energy gain from the spin projection is automatically zero, i.e. \( E_{\text{proj}}(0, 0) = 0 \), since no fluctuation of the angular momentum exists (noting that \( \langle \hat{P}^{I=0}_{00} \rangle = |\rangle \) at \( \varepsilon = 0 \)). Moreover, the pairing-plus-quadrupole model includes only attractive interactions, and the energy gain becomes negative for \( \varepsilon \neq 0 \) with respect to the nuclei investigated in the present paper. Accordingly, all the contour lines in the energy gain plots represent only negative values.
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Fig. 1. The contour plot of the energy gain calculated for $^{142}$Nd with (a) the single-particle space I, and (b) the single-particle space II. The contour line separation is 200 keV. The point where the energy gain takes its minimum is indicated by the symbol “×”.

The numerical results for $^{142}$Nd, $^{168}$Er and $^{188}$Os are displayed in Figs. 1, 2 and 3, respectively.

We recognize some common features for three nuclei. In the region of small deformation, which is typically less than $\varepsilon \sim 0.1$, the energy gain increases rapidly with increasing $\varepsilon$, but it is almost independent of $\gamma$. A more noteworthy effect of the spin projection can be seen in the deformation region for value of $\varepsilon$ beyond $\sim 0.1$.

Fig. 2. The contour plot of the energy gain calculated for $^{168}$Er with (a) the single-particle space I, and (b) the single-particle space II. Other illustrations are the same as those in Fig. 1.
First, in the region of small triaxiality ($\gamma = 0^\circ - 10^\circ$ or $\gamma = 50^\circ - 60^\circ$), the contour lines of the energy gain are almost parallel to the straight line corresponding to $\gamma = 0^\circ$ or $\gamma = 60^\circ$, i.e. the energy gain varies with $\gamma$, but it is not strongly dependent on $\varepsilon$. This implies that the qualitative properties of the unprojected PES are not greatly affected by the spin projection, as long as the projected PES is analyzed along the line of the prolate (oblate) deformation with $\gamma = 0^\circ$ ($\gamma = 60^\circ$). Second, it can be seen that the maximum energy gain is always realized at an explicit triaxial shape for any nucleus. If the energy gain is analyzed for a fixed $\varepsilon$, the shape favored by the spin projection is not axially symmetric but triaxial. In short, the spin projection tends to stabilize the triaxial shape. Such a feature is more pronounced for the single-particle space II. It is quite noticeable that such a triaxiality-driving effect is not restricted to the $\gamma$-unstable nuclei, for which it is simply amplified in the total PES. Regarding $^{168}$Er and $^{188}$Os with the single-particle space I, we can see the similarity between our energy gain plot and the unprojected and projected PESs obtained by Hayashi et al.\textsuperscript{4)} While their emphasis was put on the outstanding energy minimum in the region of large triaxiality with respect to $^{188}$Os, the net effect of the spin projection on the PES turns out to be common to these nuclei in our study.

The maximum difference between the energy gains for the axially symmetric and the triaxial shape for a fixed value of $\varepsilon (> 0.1)$ amounts to about 1.5–2 MeV. Such a large energy difference is comparable with the corresponding energy difference which arises from the shell correction energy. For instance, according to a calculation based on the standard Nilsson-Strutinsky method for $^{168}$Er, the potential energy difference between the maximum in energy located at $\gamma = 60^\circ$, and the minimum located at $\gamma = 0^\circ$ for a fixed $\varepsilon (= 0.26)$ is about 5 MeV. We also carried out numerical analysis...
Fig. 4. The energy gain as a function of the deformation parameter $\gamma$, calculated for the single $j$-shell model with the QQI. Shells are assumed to be half-filled, i.e. $N = \Omega$ ($2\Omega = 2j + 1$), and the force strength of the QQI is assumed to be $\chi = 1.0$. Furthermore, the orbital angular momentum is assumed to be $l = j - 1/2$ and the radial quantum number to be $n = 0$.

using a single-particle space which covers almost 4 major shells, but the trends mentioned above are not changed qualitatively.

In order to obtain additional supporting evidence of this prominent feature, we carried out a similar investigation based on the single $j$-shell model. It is known that an axially symmetric equilibrium deformation is always realized within the mean-field approximation when the pairing-plus-quadrupole model is applied to the single $j$-shell model. For this reason, it is interesting to investigate whether the minimum of the PES remains in the axially symmetric shape under the spin projection. For the sake of simplicity, we consider the $Q \cdot Q$ limit, where the pairing correlation is absent. Under this restriction, the system realizes the maximum deformation, so that the intrinsic state is dependent only on the parameter $\gamma$. Furthermore, we consider the case in which the shells are half-filled (i.e. the particle number is given by $N = \Omega \equiv j + 1/2$). This situation is suitable for the present investigation for the following two reasons. First, two minima of the unprojected potential energy necessarily appear at $\gamma = 0^\circ, 60^\circ$, and the maximum is always realized at $\gamma = 30^\circ$. Second, the self-consistency condition $\tan \gamma = \sqrt{2} \langle \hat{Q}_2 \rangle / \langle \hat{Q}_0 \rangle$ is exactly satisfied at $\gamma = 30^\circ$, as well as at $\gamma = 0^\circ, 60^\circ$.

In Fig. 4, the energy gain from the spin projection is plotted for each value of $j$ from $j = 11/2$ to $31/2$. It is noted that the largest energy gain necessarily appears

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*) This single-particle space is spanned by $N = 2, 3, 4, 5$ major shells plus $1i_{13/2}$ orbitals ($N = 4, 5, 6$ major shells plus $2p_{1/2}$, $2p_{3/2}$, $1f_{5/2}$ and $1j_{15/2}$ orbitals) for protons (neutrons). These shells correspond to 59 (78) Nilsson levels above the $Z = 8$ ($N = 28$) core for protons (neutrons).

**) In the case that $N \neq \Omega$ for the single $j$-shell model, the self-consistency condition is strongly violated, except in the regions of $\gamma \sim 0^\circ$ and $\gamma \sim 60^\circ$. 
Fig. 5. Total PES as a function of the deformation parameter $\gamma$, calculated for the single $j$-shell model. The figure corresponds to the case $j = 23/2$. The parameters adopted in the numerical analysis are the same as in Fig. 4. The projected PES is indicated by solid curve, and the unprojected PES given by the expectation value of the QQI without (with) exchange term is indicated by dotted (dashed) curve.

in the region of large triaxiality, although the minimum at $\gamma = 30^\circ$ is bifurcated, and two minima appear symmetrically with respect to $\gamma = 30^\circ$ for $j \geq 23/2$. Also, the energy gain is always smallest for axially symmetric shapes. It is interesting that the result derived from the single $j$-shell model is quite similar to that for realistic nuclei for which the spin projection acts to increase the binding energy in the triaxial region. The PES calculated in three alternative ways for the case $j = 23/2$ is plotted in Fig. 5. In this figure, the unprojected PES calculated from the expectation value of the QQI without (with) the exchange term is indicated by the dotted (dashed) curve, and the projected PES including the energy gain shown in Fig. 4 by the solid curve. The resultant projected PES of the $j = 23/2$ shell excludes the physical picture of small $\gamma$ oscillation around the axially symmetric shape, since the effect of the spin projection is large enough to shift the gradient of the PES at $\gamma = 0^\circ$ from a positive to a negative value. As for the other systems with different values of $j$, the equilibrium shapes are also realized for large triaxial deformation.

§4. Discussion and conclusion

The triaxiality-driving tendency of the spin projection can be quantitatively understood by considering the intrinsic states given by the Nilsson BCS scheme. The quantity $\langle \hat{P}_{I=0} \rangle$ appearing in Eq. (2.7) is nothing but the probability distribution of the spin $I = 0$ ($K = 0$) component included in the Nilsson BCS state for each deformation. The probability distribution of the $I = 0$ component calculated with the single-particle space I for $^{168}$Er is displayed in Table III. The probability of the
$I = 0$ component is unity for the spherical shape $\varepsilon = 0$, and it decreases with deformation. At the large deformation value $\varepsilon = 0.4$, for instance, this quantity becomes of order 0.01 for all nuclei. In other words, only 1% of the intrinsic state contributes to the projected ground state PES, but the remaining components of 99% corresponding to high-spin states are removed by the spin projection. This feature is not strongly dependent on the nuclides and the choice of the single-particle space. This is a well-known result for the solutions of the mean-field theory. 18)

Furthermore, we can recognize another characteristic common feature in Table III as follows. For fixed $\varepsilon$, which is typically larger than $\varepsilon \sim 0.1$, the value of $\langle \hat{P}_{i=0} \rangle$ near $\gamma = 30^\circ$ is generally small in comparison with that near $\gamma = 0^\circ$ or $\gamma = 60^\circ$, giving an axially symmetric shape. The decrease of the probability toward the triaxial deformation is always quite rapid. In case $\varepsilon = 0.32$, for instance, the value of the probability at $\gamma = 0^\circ$ is about three times as large as that at $\gamma = 30^\circ$. This trend becomes more pronounced as the deformation increases. On the other hand, the kernel of the energy gain $\langle (\hat{H} - \langle \hat{H} \rangle)\hat{P}_{I=0} \rangle$ increases toward the triaxial shape. This quantity is always negative, so that its absolute value for $\varepsilon \neq 0$ decreases as the value of $\gamma$ deviates from the prolate or oblate shape. Since the extent of this increase is not sufficient to cancel the excessive decrease of $\langle \hat{P}_{I=0} \rangle$ that appears in the denominator in Eq. (2.7), the spin projection always lowers the energy in the triaxial deformation region. This consequence appears to be a contradiction at first sight, since the spin projection favors a triaxial shape in spite of the smaller probability for the nucleus to take such a shape. An application of the spin projection method leads to a striking result, as we have seen in the previous section. This is due to another role played by the spin projection, taking account of further residual two-body correlations.

In addition to the spin projection, the number projection should be investigated, since it contributes also to the PES. We have carried out the number projection using a method similar to those used in Refs. 18 and 19. However, we have found that the number projection does not affect the main properties of the unprojected PES, as

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</table>
long as it is performed separately and its contribution is added on top of the energy gain due to the spin projection. It is probable that the “simultaneous” number and spin projection affects the properties of the PES, since the probability distribution of the $I = 0$ component is affected in this case.

In order to clarify the physical meaning of the resultant projected PES, it is desirable to carry out a computation that combines the triaxial spin projection with the generator coordinate method (GCM), taking account of $\varepsilon$ and $\gamma$ as the collective parameters. Recently, we applied the GCM to the single $j$-shell model with pure QQI, and compared its results with the exact solutions of the shell model. In this calculation, we took account of 4 coordinates, three Euler angles concerning the triaxial spin projection and the deformation parameter $\gamma$ ($0^\circ \leq \gamma \leq 60^\circ$). As for the half-filled single $j$-shell, the GCM reproduces the shell model levels belonging to the low-lying collective bands with extremely good accuracy. Moreover, the triaxiality-favored tendency of the ground state PES seen in the previous section is extended to the excited states as well, and clearly reflects the band structure of the shell model levels. Such a characteristic feature has never been anticipated from a mean-field approximation. This consequence also demonstrates the important role played by the triaxial spin projection. Thus, it seems that the assumption of the axially symmetric deformation is not necessarily appropriate, even if a prominent minimum in the unprojected PES is realized for an axially symmetric shape.

In summary, we have analyzed the effect of spin projection on the PES by applying the triaxial spin projection to the mean-field solution of the pairing-plus-quadrupole model for $^{142}$Nd, $^{168}$Er and $^{188}$Os. It turns out that the correct accounting of the correlations provided by the spin projection contributes to lower the potential energy in the triaxial deformation region. Such a tendency is common to all kinds of nuclei and not limited to the $\gamma$-unstable nuclei. This kind of effect should not be overlooked, since many microscopic analyses of the PES have been carried out using the Nilsson BCS theory.

References