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Coupling Parameter in the Single-j Shell Model *

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We propose a modified formula which is used to determine the coupling parameter C in the Hamiltonian of the single-j shell. In comparison with the previously known formula, the new formula improves the agreement between the intruder single-j levels and the Nilsson ones. For studies of chiral bands within the particle rotor model, the new coupling parameter will considerably influence the energy splitting between the doublet bands.

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The single-j shell model has turned out to be quite successful in extensive nuclear structural applications, due to its simplicity and effectiveness. In particular the single-j particle coupled with the triaxial rotor model has led to the understanding of the magnetic rotational bands,[1] and the prediction of the chiral doublet bands.[2] The particle-rotor model, unlike the cranking model, is a full quantum theory where the total angular momentum is a good quantum number and directly yields energy splitting and tunneling between doublet bands. Thus far, this model has been extensively used in the investigation of chiral rotation.[3−8]

For a single-j shell, the quadrupole deformed potential with deformation parameters (β_2,γ) is given by[5,9]

$$V=\frac{206\beta_2}{A^{1/3}}\Big[\cos\gamma Y_{20}(\theta,\phi)+\frac{\sin\gamma}{\sqrt{2}}[Y_{22}(\theta,\phi)+Y_{2-2}(\theta,\phi)]\Big]. \quad (1)$$

The deformed potential results in the single particle energy of the j-shell,

$$h=\pm\frac{1}{2}C\Big[\cos\gamma\Big(\hat{j}_3^2-\frac{j(j+1)}{3}\Big)+\frac{\sin\gamma}{2\sqrt{3}}\Big(\hat{j}_+^2+\hat{j}_-^2\Big)\Big], \quad (2)$$

with the coupling parameter C expressed as

$$C=\frac{195}{j(j+1)}A^{-\frac{1}{3}}\beta_2. \quad (3)$$

This coupling parameter C is responsible for the level splitting in the deformed field and directly proportional to the quadrupole deformation β_2. The formula (3) was extensively used in previous calculations of the particle rotor model with the single-j shell.[3−6] Nevertheless, one should bear in mind that Ref. [9] pointed out that the formula (3) was consistent with the splitting of the $h_{11/2}$ shell in the Nilsson level scheme, and would be most suitable for the single particle (hole) sitting in the $h_{11/2}$ shell. Therefore it is interesting and important to deduce a general formula, which is not only suitable for the $h_{11/2}$ shell but also other single-j shells, such as the $g_{9/2}$ or $i_{13/2}$ shell.

In this Letter, an universal formula for the coupling parameter C will be deduced from the Nilsson Hamiltonian. The differences between the single-j levels by the formula (3) and by the new one will be studied in comparison with the Nilsson levels. The influence of the new formula on the energy splitting of chiral bands will be also studied using the triaxial PRM coupled with one particle and one hole sitting in the high-j shells.

We start from the Nilsson Hamiltonian[10]

$$\hat{h}_{\rm Nilsson}=\Big(\frac{p^2}{2m}+\frac{1}{2}m\omega_0^2\rho^2\Big)-\beta_2\hbar\omega_0\rho^2\Big[\cos\gamma Y_{20}+\frac{1}{\sqrt{2}}\sin\gamma(Y_{22}+Y_{2-2})\Big]-\kappa\hbar\omega_0\{2\boldsymbol{l}\cdot\boldsymbol{s}+\mu(l^2-\langle l_N\rangle^2)\}, \quad (4)$$

where κ and μ are the Nilsson parameters, Y_{2q} is the rank-2 spherical harmonic function. The single particle Hamiltonian matrix element in the spherical harmonic oscillator basis is

$$\langle N'l'j'\Omega'|\hat{h}_{\rm Nilsson}|Nlj\Omega\rangle=\mathrm{Term1}+\mathrm{Term2}+\mathrm{Term3}, \quad (5)$$

where

$$\mathrm{Term1}=\langle N'l'j'\Omega'|\Big(\frac{p^2}{2m}+\frac{1}{2}m\omega_0^2\rho^2\Big)|Nlj\Omega\rangle,$$
$$\mathrm{Term2}=\langle N'l'j'\Omega'|-\kappa\hbar\omega_0\big[2\boldsymbol{l}\cdot\boldsymbol{s}+\mu(l^2-\langle l_N\rangle^2)\big]|Nlj\Omega\rangle,$$
$$\mathrm{Term3}=\langle N'l'j'\Omega'|-\beta_2\hbar\omega_0\rho^2\Big[\cos\gamma Y_{20}$$

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$$+\frac{1}{\sqrt{2}}\sin\gamma(Y_{22}+Y_{2-2})\Big]|Nlj\Omega\rangle. \tag{6}$$

For the case of a single-j shell, Term1 and Term2 simply add an overall constant energy to the single-j energy spectrum, thus can be neglected. Then Eq. (5) becomes

$$\begin{aligned}&\langle Nlj\Omega'|\hat{h}_{\rm single-j}|Nlj\Omega\rangle\\ &=\langle Nlj\Omega'|-\beta_2\hbar\omega_0\rho^2\Big[\cos\gamma Y_{20}\\ &+\frac{1}{\sqrt{2}}\sin\gamma(Y_{22}+Y_{2-2})\Big]|Nlj\Omega\rangle.\end{aligned} \tag{7}$$

Using the relations $\langle Nl|\rho^2|Nl\rangle=(N+3/2)$, and

$$\begin{aligned}&\langle lj\Omega'|\cos\gamma Y_{20}+\frac{1}{\sqrt{2}}\sin\gamma(Y_{22}+Y_{2-2})|lj\Omega\rangle\\ &=-\sqrt{\frac{5}{4\pi}}\frac{3}{4j(j+1)}\langle lj\Omega'|\cos\gamma\Big(\hat{j}_3^2-\frac{j(j+1)}{3}\Big)\\ &+\frac{\sin\gamma}{2\sqrt{3}}\Big(\hat{j}_+^2+\hat{j}_-^2\Big)|lj\Omega\rangle,\end{aligned} \tag{8}$$

we find

$$\begin{aligned}&\langle Nlj\Omega'|\hat{h}_{\rm single-j}|Nlj\Omega\rangle\\ &=\langle Nlj\Omega'|\sqrt{\frac{5}{4\pi}}\Big(N+\frac{3}{2}\Big)\frac{3\hbar\omega_0\beta_2}{4j(j+1)}\Big[\cos\gamma\Big(\hat{j}_3^2\\ &-\frac{j(j+1)}{3}\Big)+\frac{\sin\gamma}{2\sqrt{3}}(\hat{j}_+^2+\hat{j}_-^2)\Big]|Nlj\Omega\rangle.\end{aligned} \tag{9}$$

Then the single-j Hamiltonian reads

$$\begin{aligned}h_{\rm single-j}&=\sqrt{\frac{5}{4\pi}}\Big(N+\frac{3}{2}\Big)\frac{3\hbar\omega_0\beta_2}{4j(j+1)}\Big[\cos\gamma\Big(\hat{j}_3^2\\ &-\frac{j(j+1)}{3}\Big)+\frac{\sin\gamma}{2\sqrt{3}}(\hat{j}_+^2+\hat{j}_-^2)\Big],\end{aligned} \tag{10}$$

where $\hbar\omega_0=41A^{-\frac{1}{3}}$ MeV is the harmonic oscillator frequency of the deformed potential and N is the quantum number of the major shell. The corresponding relation for the coupling parameter C in Eq. (2) is

$$C=\Big(\frac{123}{8}\sqrt{\frac{5}{\pi}}\Big)\frac{(2N+3)}{j(j+1)}A^{-\frac{1}{3}}\beta_2. \tag{11}$$

The new coupling parameter C depends not only on the deformation parameter β_2, the single-j angular momentum j and the mass number A, as shown in Eq. (3), but also the quantum number of the major shell N.

Now the coupling parameter C may be determined in two ways. We label the parameter evaluated from the new formula (11) by C'. The parameters C and C' extracted from formula (3) and new formula (11) are obviously different for the same single-j particle (hole) orbital. For example, for the $g_{9/2}$ shell in the $A\sim100$ mass region, the quadrupole deformation parameter $\beta_2=0.2$ corresponds to $C\sim0.34$ MeV and $C'\sim0.37$ MeV, and for the $i_{13/2}$ shell in the $A\sim190$ mass region, $\beta_2=0.2$ corresponds to $C\sim0.14$ MeV and $C'\sim0.21$ MeV. Detailed values of C and C' with $\beta_2=0.2$ for four representative configurations are listed in Table 1.

In order to check the new Eq. (11), the single particle energy levels obtained from the coupling parameter C and C' have been compared with the corresponding Nilsson levels. Taking $1h_{11/2}$ sub-shell as an example, the calculated single particle energy levels using the new coupling parameter $C=0.28$ MeV according to Eq. (11) and 0.22 MeV according to Eq. (3) are shown in Fig. 1. The Nilsson levels for $1h_{11/2}$ sub-shell are also included, with the Nilsson parameters taking the values of $\kappa=0.06$ and $\mu=0.65$ [11] for the main oscillator quantum number $N=5$ in Eq. (4). It can be clearly seen that, even for the $1h_{11/2}$ sub-shell, the single particle levels obtained from the new coupling parameter formula are much closer to the corresponding Nilsson levels than those from the old one. The difference between the Nilsson levels and the results with $C=0.28$ MeV decreases with the increase of the triaxial deformation, and they become very close at $\gamma=30°$. This difference mainly arises from the mixing of the $1f_{7/2}$ component to the $1h_{11/2}$ sub-shell in the Nilsson levels. A similar trend is found in other intruder orbitals.

As mentioned above, the particle rotor model with single-j single particle Hamiltonian has been extensively used in the investigation of chiral rotation. It is interesting to investigate the influence of the coupling parameter C on the chiral bands. Energy splitting is one critical observable for the chiral bands that carries important information on the tunneling between the left-handed and right-handed states.

Table 1. Comparison of the coupling parameters C and C' obtained respectively from Eq. (3) and (11) for four representative configurations in different mass regions with deformation parameter $\beta=0.2$.

Parameters	$A\sim100$ $\pi g_{g/2}^{-1}\otimes\nu h_{11/2}$	$A\sim130$ $\pi h_{11/2}\otimes\nu h_{11/2}^{-1}$	$A\sim160$ $\pi h_{11/2}^{-1}\otimes\nu i_{13/2}$	$A\sim190$ $\pi i_{13/2}\otimes\nu i_{13/2}^{-1}$
C_p (MeV)	−0.34	0.22	−0.20	0.14
C_n (MeV)	0.24	−0.22	0.15	−0.14
C'_p (MeV)	−0.37	0.28	−0.26	0.21
C'_n (MeV)	0.30	−0.28	0.22	−0.21

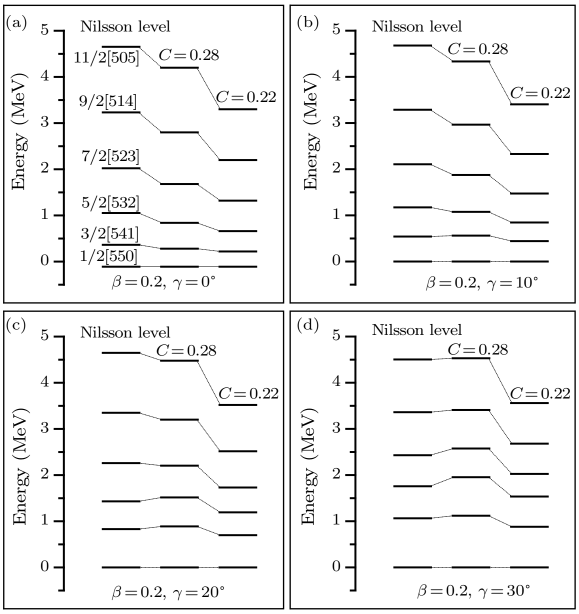

Fig. 1. Calculated single particle energy levels in the $1h_{11/2}$ sub-shell adopting the different coupling parameters C in comparison with the Nilsson level at the deformation parameters ($\beta_2 = 0.2$, $\gamma = 0°$), ($\beta_2 = 0.2$, $\gamma = 10°$), ($\beta_2 = 0.2$, $\gamma = 20°$), and ($\beta_2 = 0.2$, $\gamma = 30°$), respectively. The 1st column in each panel corresponds to the Nilsson levels, while 2nd and 3rd columns correspond to the single-j Hamiltonian with C from Eq. (3) and Eq. (11).

First we investigate the energy splitting of chiral bands for a nucleus with the maximum triaxiality $\gamma = 30°$. The energy splitting ($E_{\rm side}(I) - E_{\rm main}(I)$) between the chiral bands is calculated using the particle-hole-triaxial rotor model for the configurations $\pi g_{g/2}^{-1} \otimes \nu h_{11/2}$, $\pi h_{11/2} \otimes \nu h_{11/2}^{-1}$, $\pi h_{11/2}^{-1} \otimes \nu i_{13/2}$, and $\pi i_{13/2} \otimes \nu i_{13/2}^{-1}$, respectively. A summary of the values of the coupling parameter used in the present work is given in Table 1.

As shown in Fig. 2, the calculated results with C and C' are very close at the spin interval $8 \le I \le 15$ and an evidently increasing energy separation at the spin $I > 16$ for four representative configurations is seen. Moreover, the difference between the cases C and C' increases from the configurations $\pi g_{g/2}^{-1} \otimes \nu h_{11/2}$ to $\pi i_{13/2} \otimes \nu i_{13/2}^{-1}$. For $\pi i_{13/2} \otimes \nu i_{13/2}^{-1}$, the energy separation is around 50 keV at spin $I > 16$. It is known that the energy splitting of chiral bands for a nucleus at the deformation $\gamma = 30°$ is smaller than 50 keV at the chiral region.[12] Even if the triaxiality parameter deviates from $\gamma = 30°$, the average energy splitting between chiral bands is still rather small, about 200 keV.[7,13] Thus the discrepancy of 50 keV cannot be simply neglected.

A similar trend is seen in the case of $\gamma = 20°$, as shown in Fig. 3. The energy difference between the cases C and C' also increases from the configurations $\pi g_{g/2}^{-1} \otimes \nu h_{11/2}$ to $\pi i_{13/2} \otimes \nu i_{13/2}^{-1}$, and a small energy difference occurs in low spins. The calculated result with C is lower than that with C' in a low spin region $I < 14$, whereas the opposite situation occurs at $I > 15$ for four representative cases. At spin $I > 15$, the energy separation is around 40 keV corresponding to the $\pi g_{g/2}^{-1} \otimes \nu h_{11/2}$ and $\pi h_{11/2} \otimes \nu h_{11/2}^{-1}$ configurations, and around 70 keV corresponding to the $\pi h_{11/2}^{-1} \otimes \nu i_{13/2}$ and $\pi i_{13/2} \otimes \nu i_{13/2}^{-1}$ configurations. One can see that the deviation between the results calculated with C and C' for $\gamma = 20°$ is larger than that for $\gamma = 30°$ at the whole spin region. In short, the present calculated results show explicitly the influence of the different coupling parameters C on the energy splitting of chiral doublet bands. In addition, the newly obtained coupling parameter (11) has been applied to describe chiral bands with $\pi g_{g/2}^{-1} \otimes \nu h_{11/2}$ configuration in ^{106}Rh[8] and with $\pi h_{11/2}^2 \otimes \nu h_{11/2}^{-1}$ configuration in ^{135}Nd[14], and both reproduce the experimental energy difference perfectly.

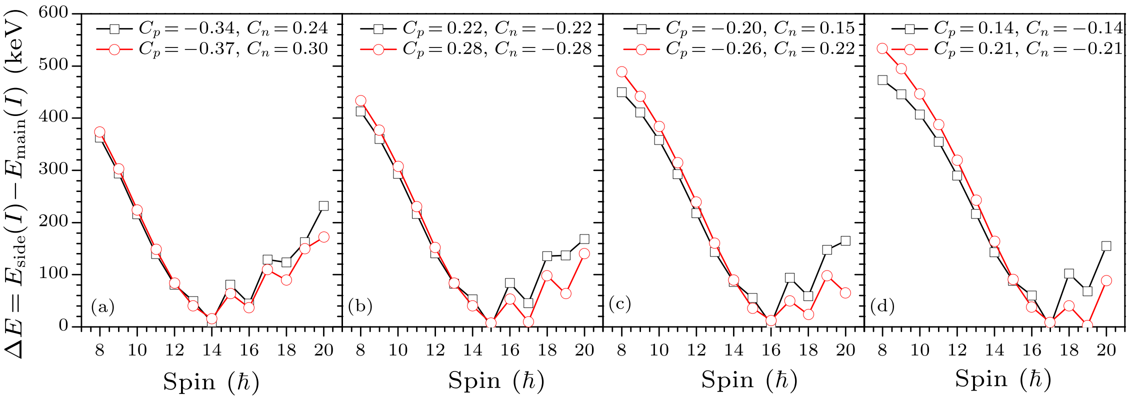

Fig. 2. Calculated energy difference between main and side bands as a function of spin for $\beta_2 = 0.2$ and $\gamma = 30°$: (a) $\pi g_{g/2}^{-1} \otimes \nu h_{11/2}$ in the $A \sim 100$ mass region, (b) $\pi h_{11/2} \otimes \nu h_{11/2}^{-1}$ in the $A \sim 130$ mass region, (c) $\pi h_{11/2}^{-1} \otimes \nu i_{13/2}$ in the $A \sim 160$ mass region, (d) $\pi i_{13/2} \otimes \nu i_{13/2}^{-1}$ in the $A \sim 190$ mass region.

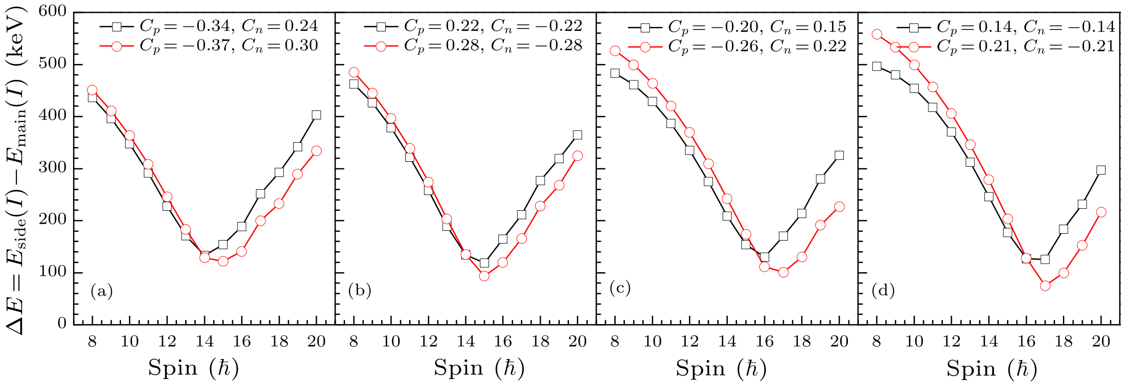

Fig. 3. The same as Fig. 2 but $\gamma = 20°$.

In summary, a modified formula for the coupling parameter C in the Hamiltonian of the single-j shell is deduced from the Nilsson Hamiltonian. The new formula greatly improves the agreement of the intruder single-j levels with the Nilsson ones. The influence on the chiral bands of the new formula related to the previous one has been studied using one particle and one hole coupled to a triaxial rotor model. Although the new coupling parameter does not change the overall energy spectra significantly, it influences the energy splitting between the chiral bands considerably.

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