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Study of Superdeformation with Skyrme-Hartree-Fock Method

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In the last decade superdeformed (SD) bands have been studied extensively both experimentally and theoretically. Since the first observation in ^{152}Dy in 1986[1], SD bands have been found in four mass regions, i.e., $A \sim 80$[2], 130[3,4], 150 and 190[5]. Although these SD bands have been observed only at high spins so far, they may be present at zero spin, too, like fission isomers in actinide nuclei: The familiar generic argument on the strong shell effect at axis ratio 2:1[6] does not assume rotations.

If non-fissile SD isomers exist at zero spin, they may be utilized to develop new experimental methods to study exotic states, in a similar manner as short-lived high-spin isomers are planned to be utilized as projectiles of fusion reactions in order to populate very high-spin near-yrast states[7]. They will also be useful to test theoretical models whether the models can describe correctly the large deformations of rare-earth nuclei without further complications due to rotation.

In this paper, we employ the Skyrme-Hartree-Fock method to study the SD states at zero spin. First, we compare various Skyrme force parameter sets to see whether they can reproduce the extrapolated excitation energy of the SD band head of ^{194}Hg. Second, we study fission isomers in ^{236,238}U. Third, we systematically search large-deformation solutions with the SkM* force.

The feature of our calculations is that the single-particle wavefunctions are expressed in a three-dimensional Cartesian-mesh representation[8]. This representation enables one to obtain solutions of various shapes (including SD) without preparing a basis specific to each shape. Solving the mean-field equations in this representation requires, however, a large amount of computation which can be accomplished only with present supercomputers.

1. ^{194}Hg

Recently, Khoo *et al.*[9] determined the excitation energies and the spins of a SD band in ^{194}Hg down to $I^\pi = 8^+$. By extrapolating the spectrum to $I = 0$, they could predict reliably the excitation energy of the band head to be 6.017 MeV

In table 1, we show the excitation energy E^* of the SD band-head state calculated with various Skyrme force parameter sets. From macroscopic point of view, the softness to deformation is determined by the smallness of the surface energy coefficient a_s specific to each force. The SkM* is a force adjusted so as to reproduce the fission barrier height of ^{240}Pu and thus expected to have the correct surface energy coefficient. Indeed, the SkM* as well as the SkP forces are the best ones to reproduce the experimental value of E^*. On the other hand, the SIII and the SkSC4 forces seems to be too stiff against deformation, while the SGII is too soft.

Table 1. Excitation energy of the SD band head of ^{194}Hg.

	E^* (MeV)
experiment	6.017
SGII	3.925
SkP	6.012
SkM*	6.275
SkSC4	7.350
SIII	8.223

A different strength of the pairing force was used by Krieger *et al.*[10] to calculate the SD band head in ^{194}Hg. Their strength G was given by an empirical formula of their own,

$$G_N = \frac{16.5}{11+N}, \quad G_Z = \frac{17.5}{11+Z}\ [\mathrm{MeV}]. \tag{1}$$

On the other hand, our strength G is determined (for each deformation) such that the so-called classical empirical formula of the average pairing gap,

$$\bar{\Delta} = \frac{12}{\sqrt{A}}\ [\mathrm{MeV}], \tag{2}$$

is reproduced for shell-effect-averaged level density obtained by the Thomas-Fermi approximation. The pairing-active space is the same between their treatment and ours: Single-particle levels below "the Fermi level plus 5 MeV" are taken into account in the BCS calculations.

Krieger's strength G gives a rather large pairing gap ($\Delta_n < 1.8$ MeV), while our strength produces a reasonable size of gap ($\Delta_n < 1.2$ MeV) for deformations less than 0.6.

As a consequence, they obtained E^*=5.0 MeV, which is lower than our value (given in Table 1) by 1.3 MeV. The height of the barrier preventing the decay into the normal-deformation (ND) well is also different: They found it to be 1.8 MeV, while we obtained a larger value 3.5 MeV. Note that the partial halflife of the SD band head for the decay into the ND well is longer

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for higher barriers. We have estimated the halflife in a simple WKB approximation as explained in the next section with $f_{\rm B} = 10$. The resulting halflife is 6×10^{-17} sec for Krieger's pairing force strength while it is 1×10^{-13} sec for our strength. The difference amounts to a factor of order 10^3.

2. ^{236,238}U

We have also applied our HF+BCS scheme to fission isomers. Among several tens of actinide nuclei having fission isomers, ^{236}U and ^{238}U are the only ones whose fission isomers were observed to decay electromagnetically into ND states. The energy of the gamma-ray tells us the excitation energy of the fission isomer, while the measured halflife gives information on the barrier between the SD and the ND wells.

In tables 2 and 3, we compare the results of various calculations with the experimental values.

We employ the SkM* force and the same pairing scheme as we used for ^{194}Hg. We estimate the halflives in the following way.

$$\tau_{1/2} = \frac{\ln 2}{nP}, \tag{3}$$

where halflife $\tau_{1/2}$ is inversely proportional to two quantities. One is the number of assaults in the SD well, n, which may be estimated as

$$n = \frac{2\pi}{\omega_{\beta\text{-vib}}}, \tag{4}$$

where $\omega_{\beta\text{-vib}}$ is the frequency of the β-vibration in the SD well. We assume that $\omega_{\beta\text{-vib}}$ scales as $A^{-1/6}$ and that $\hbar\omega_{\beta\text{-vib}} = 1$ MeV for A=150. The other is the penetration probability through the barrier into the ND well, P, which is related to the action S in the WKB approximation as

$$P = \exp(-S), \tag{5}$$

$$S = \frac{2}{\hbar}\int_{\beta_1}^{\beta_2} \sqrt{2B(\beta)(V(\beta)-E)}\,d\beta. \tag{6}$$

In the r.h.s. of Eq. (6), β_2 is the deformation of the SD isomer while β_1 is the deformation in the ND well where the total energy is the same as that of the SD isomer, i.e., $E(\beta_1) = E(\beta_2) \equiv E$. The action S takes on large values when the barrier is high and broad and/or when the collective mass $B(\beta)$ is large.

The collective mass for small-amplitude irrotational hydrodynamical motions is expressed as

$$B_\lambda = \frac{\rho R_0^5}{\lambda} = \frac{3Am_{\rm N}R_0^2}{4\lambda\pi}, \tag{7}$$

where λ (=2) is the multipolarity of the motion, ρ the nucleon density inside the nucleus ($= 3Am_{\rm N}/4\pi R_0^3$), R_0 the nuclear radius ($= 1.2A^{1/3}$ fm), A the mass number, and $m_{\rm N}$ the bare nucleon mass.

We express the collective mass in unit of B_2, neglecting the dependence on deformation:

$$B(\beta) = B_2 f_{\rm B}. \tag{8}$$

The empirical enhancement factor $f_{\rm B}$ changes between 10 and 40 if it is determined to reproduce the quadrupole vibrational levels of spherical nuclei[11].

The tables 2 and 3 also show the results of calculations by other groups. Chinn *et al.*[12] employed the Hartree-Fock-Bogoliubov (HFB) method with the Gogny D1 force. They calculated the halflives by reducing the Hill-Wheeler equation for the Generator Coordinate Method (GCM) to a Schrödinger equation with the Gaussian Overlap Approximation. Krieger *et al.*[13] applied the HF+BCS method with the SkM* force and the same pairing force as they used for ^{194}Hg. They estimated the halflives with the GCM without further approximations.

Table 2. Excitation energies of fission isomers.

	E^* [MeV]	
	^{236}U	^{238}U
experiment[14]	2.750	2.557
Chinn *et al.*[12]	–	2.828
Krieger *et al.*[13]	–	2.28
HF+BCS with SkM*	1.250	2.273

Excitation energy of ^{238}U is reproduced very well (within $\pm$11%) in all the three calculations. On the other hand, as for ^{236}U, the only available calculation predicts 45 % of the experimental value.

Table 3. Partial halflives of fission isomers for decay into the ground state.

	$t_{1/2}$ [sec]	
	^{236}U	^{238}U
experiment[14]	1.20×10^{-7}	2.98×10^{-7}
Chinn *et al.*[12]	–	8.5×10^{-5}
Krieger *et al.*[13]	–	(0.05 - 20) $\times10^{-9}$
HF+BCS with SkM*		
$f_{\rm B} = 10$	4.4×10^{-13}	4.3×10^{-14}
$f_{\rm B} = 20$	1.0×10^{-9}	4.5×10^{-11}
$f_{\rm B} = 30$	4.0×10^{-7}	8.6×10^{-9}
$f_{\rm B} = 40$	6.1×10^{-5}	7.3×10^{-7}

The partial halflives are not reproduced very accurately by the first two calculations. As for our calculations, we have to determine the enhancement factor $f_{\rm B}$ before estimating the halflives. Conversely, when it is adjusted to reproduce the experimental halflives, the resulting values are $f_{\rm B}$=28 for ^{236}U and $f_{\rm B}$=38 for ^{238}U.

It should be admitted that our estimation of the halflives is very crude. There are many factors which can strongly influence on the halflives, e.g., the landscape of the potential energy curve, the collective mass, the triaxial deformation, the level density in the ND well, and the angular momentum projection effect. Our estimation takes into account only the first two factors.

3. Systematics of the zero-spin SD

With the Skyrme SkM* force, we have explored a wide area of the nuclear chart ranging from $_{40}$Ca to $_{82}$Pb in order to study systematically the SD states at zero spin.

To specify that the spin is zero, we do not perform the angular momentum projection but simply do *not* rotate or crank the mean field.

An early microscopic attempt to explore SD at zero spin was made by Bonche *et al.*[15] for Os-Pt-Hg region using the HF+BCS with the SIII force. Later, Krieger *et al.*[10] changed the force to SkM* and performed an extensive calculation covering from $_{62}$Sm$_{126}$ to $_{92}$U$_{146}$ to obtain SD minima for 148 nuclei.

We employ the same Skyrme force as Krieger et al. used. However, the results of calculations are significantly different because their pairing strength is too strong as demonstrated clearly for ^{194}Hg.

Our calculation does not cover very neutron-rich nuclei, unlike the calculation by Krieger et al. It is because the pairing correlation of neutrons cannot be correctly described within the HF+BCS scheme for these nuclei: When the Fermi level approaches to zero from below, the continuum single-particle states are coupled strongly to the ground state in the pairing channel. This coupling cannot be treated in the HF+BCS scheme, which relies on an assumption that the pair-scattering matrix elements are constant, i.e., independent of the orbitals. For the correct description of the coupling, one has to switch from the HF+BCS to the HFB scheme, of which computer program we are developing presently.

In order to explain how we search the SD solutions, let us define the quadrupole deformation parameter δ,

$$\delta \equiv \frac{3\langle \hat{Q}_z \rangle}{4\langle \hat{r}^2 \rangle}, \tag{9}$$

where $\hat{Q}_z$ is the axially symmetric mass quadrupole moment,

$$\hat{Q}_z \equiv 2\hat{z}^2 - \hat{x}^2 - \hat{y}^2, \tag{10}$$

and $\hat{r}^2$ is the squared mass radius,

$$\hat{r}^2 \equiv \hat{x}^2 + \hat{y}^2 + \hat{z}^2. \tag{11}$$

We take the following procedures:

1) We prepare an initial wavefunction by either using the solution for a neighboring nucleus or taking the wavefunction of the eigenstate of the Nilsson potential of appropriate deformation.

2) If the quadrupole deformation parameter δ of the initial wavefunction is smaller than 0.6, we exert an external potential proportional to $\hat{Q}_z$ on the initial wavefunction until δ exceeds 0.6. Then, we switch off the external potential.

3) We let the wavefunction evolve by itself. If it converges to a local minimum with $\delta > 0.35$, we regard that the nucleus have a SD isomeric state. If the deformation parameter becomes less than 0.35 in the course of the self evolution, we conclude that the nucleus does not have a SD state.

4) If the nucleus has a SD minimum, we calculate the potential energy curve for $0 \leq \delta \leq 0.6$ by imposing a constraint on $\hat{Q}_z$. This step requires more than ten times as long computation time as the previous three steps. It is necessary, however, to estimate the halflife of the isomer.

Following the above prescription, we have explored 642 nuclei and found SD minima in 155 nuclei. We are now analyzing the results[16].

4. Comparison with the results of the Nilsson-Strutinsky method

We have also tried the Nilsson-Strutinsky method to do a similar systematic survey of SD isomers.

With this model, we can calculate the entire region of the nuclear chart, i.e., from the proton drip line to the neutron drip line. It is because the model does not suffer from the problem of neutron pairing in neutron-rich nuclei: There is no other way than to simply neglect the enhancement of the pairing due to the coupling with the continuum states because the Nilsson potential does not have a continuum spectrum. The calculations with this model can be completed in a few hours with a high-grade personal computer.

The Nilsson-Strutinsky code has been offered by Dr. Y.R. Shimizu of Kyushu University. Standard values[17] are used for the parameters κ_N and μ_N of the Nilsson potential. We consider only axially symmetric deformations. For each value of the quadrupole deformation ϵ_2, the hexadecapole deformation ϵ_4 is optimized such that the total energy is minimized.

We are now analyzing the difference of the results between the Nilsson-Strutinsky method and the HF+BCS with the Skyrme SkM* force[16].

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