Deformation around Neutron-Rich Cr Isotopes in Axially Symmetric Skyrme-Hatree-Fock-Bogoliubov Method

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We analyse the deformation mechanism in neutron-rich Cr, Fe and Ti isotopes with $N = 32 - 44$ using a Skyrme-Hartree-Fock-Bogoliubov mean-field code employing a two-dimensional mesh representation in the cylindrical coordinate system. Evaluating the quadrupole deformation energy systematically, we show that the Skyrme parameter set SkM* gives a quadrupole instability around the neutron numbers $N \sim 38 - 42$ in Cr isotopes, where the deformation energy curve suggests a transitional behavior with a shallow minimum extending to a large prolate deformation. The roles of a deformed $N = 38$ gap and the position of the neutron $g_{9/2}$ orbit are analysed in detail.

§1. Introduction

The deformation of the nuclear shape is one of the fundamental features of the nuclear structure. The mechanism of the deformation reflects quantal effects such as the shell effect, the pairing correlation, and the long range proton-neutron correlation. Thus, analyses of a new deformation region often provide us with new insights into the nuclear structure. A recent example is the quadrupole deformation in neutron-rich $Z \sim 12$ isotopes, which have been a crucial probe for disclosing the weakening of the $N = 20$ shell gap in neutron-rich nuclei.\textsuperscript{1)} More recently, another possibility of a new deformation region has been suggested in neutron-rich Cr isotopes.\textsuperscript{2)–7)}

The self-consistent mean-field theory is a powerful scheme for analysing the deformation mechanism when we deal with nuclei far from the stability line in medium- and heavy-mass regions.\textsuperscript{8)} There are three important features that should be taken into account in this case: pairing correlation, continuum states and deformation. The pairing correlation can be described using Bogoliubov’s generalised quasi-particle scheme; the conventional BCS approximation is not suitable for nuclei far from the stability line. The continuum states become important in nuclei near drip lines where the Fermi energy approaches zero. In this case, one has to treat continuum quasi-particle states that have spatially extended wave functions. These two requirements are fulfilled in the Hartree-Fock-Bogoliubov (HFB) formalism once it is represented in the coordinate space.\textsuperscript{9), 10)} To describe the deformation, the HFB method has to be extended to a two- or three-dimensional problem, for which several techniques using the truncated Hartree-Fock basis,\textsuperscript{11)–13)} the transformed harmonic oscillator basis,\textsuperscript{14), 15)} and the B-Spline basis\textsuperscript{16), 17)} have been developed recently.
In the present paper, we develop our own 2D coordinate-space Skyrme-HFB code, which enables us to describe axially deformed unstable nuclei. The formalism is similar to that in Ref. 16), which utilizes the B-Spline and Galerkin methods on top of the cylindrical coordinate system. In the present approach, we adopt a two-dimensional mesh representation using the cylindrical coordinate system and a multi-point formula for differential operators. Since the 2D mesh approach using the cylindrical coordinate has not been explored except for a few Hartree-Fock\textsuperscript{18}) and Hartree-Fock-Bogoliubov calculations,\textsuperscript{19), 20}) we shall test the numerical accuracy of our code. As will be shown later, the energy accuracy of our code employing the simple mesh representation is not better than those of the basis approaches,\textsuperscript{14)–17}) but is sufficient to analyse deformation mechanisms unless an accuracy better than a few hundreds of keV is needed. Then, as an application of this code, we investigate the possible deformation region around neutron-rich Cr isotopes. Global calculations of the ground-state deformation including the neutron-rich Cr isotopes are performed using the Skyrme-HFB\textsuperscript{15), 21), 22}) or relativistic mean-field models.\textsuperscript{23}) Here, we perform detailed analysis of the deformation mechanism by looking into the deformation energy curve and the shell structure of single-particle orbits, and by studying the dependence on Skyrme interactions.

\section{HFB formalism}

\subsection{HFB equation in the cylindrical coordinate system}

The HFB equation in the coordinate space representation is written as

\[
\begin{pmatrix}
 h^q_{\sigma\sigma'}(r) - \lambda & \tilde{h}^q_{\sigma\sigma'}(r) \\
 \tilde{h}^q_{\sigma\sigma'}(r) & -h^q_{\sigma\sigma'}(r) - \lambda
\end{pmatrix}
\begin{pmatrix}
 \phi^{(1)}_{\alpha q}(r) \\
 \phi^{(2)}_{\alpha q}(r)
\end{pmatrix}
= E_{\alpha q}
\begin{pmatrix}
 \phi^{(1)}_{\alpha q}(r\sigma) \\
 \phi^{(2)}_{\alpha q}(r\sigma)
\end{pmatrix}
\] \tag{2.1}

assuming the local HF potential $h^q_{\sigma\sigma'}(r)$ and the local pairing potential $\tilde{h}^q_{\sigma\sigma'}(r)$ for neutrons and protons ($q = n$ or $p$) with $\sigma$ and $\sigma'$ being spin indexes ($\sigma, \sigma' = \uparrow, \downarrow$). In the present paper, we assume the axial symmetry of nuclear deformation and the $z$-axis is chosen as the symmetry axis. The quasi-particle wave function has a quantum number $\Omega$ for the $z$-component of the total angular momentum. Using the cylindrical coordinate $(r, z, \varphi)$, the quasi-particle wave function of the $n$-th eigenstate is written as

\[
\begin{pmatrix}
 \phi^{(1)}_{n\Omega q}(r\sigma) \\
 \phi^{(2)}_{n\Omega q}(r\sigma)
\end{pmatrix}
= \frac{1}{\sqrt{2\pi}}
\begin{pmatrix}
 e^{i(\Omega - \frac{1}{2})\varphi} \phi^{(1)\dagger}_{n\Omega q}(r, z) \\
 e^{i(\Omega + \frac{1}{2})\varphi} \phi^{(2)\dagger}_{n\Omega q}(r, z)
\end{pmatrix}
\begin{pmatrix}
 e^{i(\Omega - \frac{1}{2})\varphi}\phi^{(1)\dagger}_{n\Omega q}(r, z) \\
 e^{i(\Omega + \frac{1}{2})\varphi}\phi^{(2)\dagger}_{n\Omega q}(r, z)
\end{pmatrix}
\]. \tag{2.2}

Expressing the Hartree-Fock Hamiltonian $h(r, z, \varphi)$ and the pairing Hamiltonian $\tilde{h}(r, z, \varphi)$ as

\[
h^q(r, z, \varphi) = \begin{pmatrix}
 h^q_{\uparrow\uparrow}(r, z) & e^{-i\varphi}h^q_{\downarrow\downarrow}(r, z) \\
 e^{i\varphi}h^q_{\downarrow\downarrow}(r, z) & h^q_{\uparrow\uparrow}(r, z)
\end{pmatrix}, \tag{2.3}
\]
\[\tilde{h}^q(r, z, \varphi) = \begin{pmatrix} \tilde{h}^q_{\uparrow\uparrow}(r, z) & e^{-i\varphi}\tilde{h}^q_{\downarrow\uparrow}(r, z) \\ e^{i\varphi}\tilde{h}^q_{\uparrow\downarrow}(r, z) & \tilde{h}^q_{\downarrow\downarrow}(r, z) \end{pmatrix}, \]  

(2.4)

the HFB equation in the cylindrical coordinate representation is written as

\[H_q\Phi_n\Omega_q = E_n\Omega_q\Phi_n\Omega_q,\]  

(2.5)

where

\[H_q = \begin{pmatrix} h^q_{\uparrow\uparrow}(r, z) - \lambda & h^q_{\uparrow\downarrow}(r, z) & \tilde{h}^q_{\uparrow\uparrow}(r, z) & \tilde{h}^q_{\downarrow\downarrow}(r, z) \\ h^q_{\downarrow\uparrow}(r, z) & h^q_{\downarrow\downarrow}(r, z) - \lambda & -h^q_{\downarrow\uparrow}(r, z) + \lambda & -h^q_{\downarrow\downarrow}(r, z) \\ h^q_{\uparrow\downarrow}(r, z) & -h^q_{\downarrow\uparrow}(r, z) & h^q_{\uparrow\uparrow}(r, z) & h^q_{\downarrow\downarrow}(r, z) \\ h^q_{\downarrow\downarrow}(r, z) & h^q_{\downarrow\uparrow}(r, z) & -h^q_{\uparrow\downarrow}(r, z) & h^q_{\uparrow\uparrow}(r, z) \end{pmatrix},\]  

(2.6)

and

\[\Phi_n\Omega_q = \begin{pmatrix} \phi^{(1)\uparrow}_{n\Omega q}(r, z) \\ \phi^{(1)\downarrow}_{n\Omega q}(r, z) \\ \phi^{(2)\uparrow}_{n\Omega q}(r, z) \\ \phi^{(2)\downarrow}_{n\Omega q}(r, z) \end{pmatrix}.\]  

(2.7)

We adopt the Skyrme force, and \(h^q_{\sigma\sigma'}(r, z)\) is expressed\(^{16}\) in terms of the force parameters, the normal density \(\rho_{n,p}(r, z)\), the kinetic density \(\tau_{n,p}(r, z)\) and the spin-orbit density \(J_{n,p}(r, z)\). We adopt the density-dependent delta interaction (DDDI)

\[v_{\text{pair}} = \frac{1}{2} V_0 (1 - P_\sigma) \left(1 - \eta \left(\frac{\rho(r)}{\rho_0}\right)\right) \delta(r - r'),\]

for the effective interaction producing the pairing potential \(\tilde{h}^q_{\sigma\sigma'}\), where \(h^q_{\sigma\sigma'}\) is expressed in terms of the total nucleon density \(\rho(r, z)\) and the pair density \(\tilde{\rho}_q(r, z)\).

The eigenstates and eigenenergies of the quasi-particles are obtained by solving the HFB equation (2.5) for each \(\Omega\). Since we assume time reversal symmetry, we need to solve for only \(\Omega > 0\).

We consider a rectangular area with \(0 \leq r \leq r_{\text{max}}\) and \(-z_{\text{max}} \leq z \leq z_{\text{max}}\) in the \((r, z)\) plane. The \(r\)-axis is discretized at \(r = h/2, 3h/2, \ldots, r_{\text{max}}\) with \(N_r\) mesh points, while the \(z\)-axis is discretized from \(-z_{\text{max}} = -N_z h\) to \(z_{\text{max}} = N_z h\) with the same equidistant interval \(h\). The quasi-particle wave functions \(\phi(r, z)\) (the indices are omitted here for simplicity) and the HFB Hamiltonian \(H_q\) are represented on this two-dimensional mesh. At the outer boundaries \(z = \pm z_{\text{max}}\) and \(r = r_{\text{max}}\), we impose \(\phi(r, \pm z_{\text{max}}) = 0\) and \(\phi(r_{\text{max}}, z) = 0\), respectively. Using the 11-point formula to represent differential operators, we obtain a matrix representation of the HFB Hamiltonian. We adopted the following treatments in applying the 11-point formula to the points near the boundaries. At the origin \(r = 0\), we impose \(\phi(-r, z) = (-)^l z \phi(r, z)\) determined by the parity \((-)^l z\) where \(l_z\) is the \(z\)-component of the orbital angular momentum, and we assumed that the wave function values outside the outer boundaries are zero. Note that we utilize shifted mesh points \(r = (n + \frac{1}{2})h\) so that we do not need to evaluate \(\phi\) at \(r = 0\). We made a comparison
with calculations where the \( r \)-axis is discretized on a slightly different mesh points \( r = 0, h, 2h, \ldots, r_{\text{max}} \) and we found that the adopted discretization with \( r = (n + \frac{1}{2})h \) has better accuracy. Consequently, a quasi-particle wave function is expressed as a vector with an \( N = 4N_zN_r \) dimension and the HFB Hamiltonian is a matrix with a size of \( N^2 \). We obtain eigenvalues and eigenfunctions by diagonalising this Hamiltonian matrix. The Hamiltonian is nonsymmetric because of the finite-point representation of the differential operators near \( r = 0 \). We diagonalise the Hamiltonian using the QR method\(^{25}\) to solve the nonsymmetric eigenvalue problem. Concerning the integrals, we adopt a trapezoidal formula since the high-order formula does not always guarantee better accuracy.\(^{24}\) When we evaluate a derivative of a function such as the density or wave functions, we also use an 11-point formula, however, functional values around the outer boundary \( r \sim N_r h \) and \( z \sim \pm N_z h \) are evaluated using fewer-point formulas.\(^{26}\) At mesh points on the outer boundaries, we adopted the same derivative values as those at points on a neighboring inner layer.

Since we use the delta-type pairing force, we introduce a cutoff with respect to quasi-particle energy. The adopted cutoff energy is 60 MeV. We also need a cutoff with respect to the azimuthal quantum number \( \Omega \), and we adopted a cutoff value of \( \Omega = \frac{15}{2} \). To obtain a self-consistent solution, we utilize an iteration scheme. As an initial condition, we start with single-particle orbits in a deformed Woods-Saxon potential. As an initial pairing potential, we chose one with a Woods-Saxon shape. We revise only a fraction of the densities in each step of iteration. In practice, this fraction is chosen within an interval of 0.2–0.4. When about 200 iterations pass, the energy difference between two consecutive steps becomes smaller than \( 1 \times 10^{-5} \) MeV, at which we stop the iteration. To obtain deformation energy, we also perform a constrained HFB calculation. As a constraint operator, we use the mass quadrupole operator \( \hat{Q}_2 \), which is defined as

\[
\hat{Q}_2 = \sqrt{\frac{16\pi}{5}} R^2 Y_{20}(\hat{r}) = 2z^2 - r^2,
\]

where \( R = \sqrt{r^2 + z^2} \). We use the quadratic constraint method.\(^{27}\)

2.2. Test on numerical code

To check the accuracy of the code, we compare our result with those of the two previous Skyrme-HFB calculation methods. One is the THO basis method developed by Stoitsov et al.\(^{14}\) and the other is the B-Spline basis method developed by Terán et al.\(^{16}\) We choose neutron-rich Zr isotopes. In accordance with Refs. 14) and 16), we adopt the Skyrme parameter SLy4 and the volume-type pairing force, i.e., \( \eta = 0 \). The box size is 12 fm for both \( r_{\text{max}} \) and \( z_{\text{max}} \), and the mesh interval \( h \) is 0.6 fm. The pairing strength \( V_0 \) is the same in Refs. 16) and 17). The obtained ground-state properties of neutron-rich Zr isotopes are shown in Table I and Fig. 1. The density and pair density for neutrons are shown in Fig. 1. The neutron density shows a large quadrupole deformation and the neutron pair density also shows deformation. Note that the pair density exhibits a complex structure in the inner region.

In Table I, we compare our result for \(^{102}\)Zr with the results of the B-Spline and THO methods in Ref. 16). It is seen that our code reproduces the results of the two
Table I. Total binding energy BE, Fermi energy $\lambda_n$, average pairing gap $\Delta_n$ and RMS radius $\sqrt{\langle r^2 \rangle}$ in $^{102}\text{Zr}$ obtained in present work. The values\textsuperscript{16} of the B-Spline and THO methods are compared.

|                  | present work | B-Spline   | THO        |
|------------------|--------------|------------|------------|
| BE [MeV]         | $-856.92$    | $-859.61$  | $-859.40$  |
| $\lambda_n$ [MeV] | $-5.42$      | $-5.46$    | $-5.42$    |
| $\lambda_p$ [MeV] | $-12.07$     | $-12.08$   | $-12.10$   |
| $\Delta_n$ [MeV] | $0.23$       | $0.31$     | $0.56$     |
| $\Delta_p$ [MeV] | $0.35$       | $0.34$     | $0.62$     |
| $\sqrt{\langle r^2 \rangle}$ [fm] | $4.58$       | $4.58$     | $4.58$     |

methods reasonably well. In particular, the root mean square (RMS) radius $\sqrt{\langle r^2 \rangle}$ and the Fermi energies $\lambda_{n,p}$ are in a good agreement. Note however that there is a deficiency in the total binding energy by about 2–3 MeV. This is due to the use of a moderate mesh size, ($h = 0.6$ fm) and the finite-point formula for differential operators as a deficiency due to the finite mesh size has been known in previous HF+BCS calculations.\textsuperscript{28, 29} There is some deviation in the average neutron pairing gap $\Delta_n$. It should be noted that the pairing gap is rather small $\sim 300$ keV. Generally, the pairing gap is sensitive to minor differences, particularly when the pairing gap is small. A small difference in defining the cutoff energy may be suspected because we adopt the quasi-particle energy cutoff, while the THO and B-Spline methods use the so-called equivalent single-particle energy cutoff. The finite mesh size effect could be another origin of these differences.

To make a systematic comparison, we calculated an isotopic chain of zirconium for $N = 102$–122. The mass quadrupole moment $Q_2$, the RMS radius, the neutron and proton pairing gaps, and the two-neutron separation energy are compared with those in Ref. 17) in Figs. 2(a)-(d). In this calculation, we use the pairing strength $V_0 = -187.1305$ MeV fm$^{-3}$ taken from Ref. 17). The quadrupole moment (Fig. 2(a)) and RMS radius (Fig. 2(b)) agree very well with those in the B-Spline and THO
methods in the whole region ($A = 102 – 122$) shown in the figure. In particular, the deformation is described well. The difference in two-neutron separation energy is much better than the 2–3 MeV difference in the absolute value of total binding energy, except at $A = 114$ where a larger deviation is caused by a large jump in the ground-state deformation. The better accuracy in the relative quantities is consistent with the same feature found in the previous Skyrme-HF + BCS calculations using the 3D Cartesian mesh representation. The average pairing gap is also reproduced reasonably well as shown in Fig. 2(c) although a small but non-negligible difference is noted.

In Fig. 3, we display the deformation energy curve as a function of the quadrupole deformation parameter $\beta$ defined by $\beta = \sqrt{\frac{\langle Q_2 \rangle}{\langle r^2 \rangle A}}$. The dependence of quadrupole deformation energy on mesh size is seen from the comparison of the results obtained with mesh sizes 0.6 and 0.8 fm. If we shift the total energy by about 1.8 MeV, we see that the difference between the two curves becomes within about 200 keV. We thus conclude that deformation energy can be evaluated to the accuracy of this order. Since the calculation using $h = 0.6$ fm is very numerically demanding, we adopt $h = 0.8$ fm in the following systematic analyses.

Concluding this section, we have shown that our code employing the direct 2D mesh representation in the cylindrical coordinate system and a finite-point differential formula provides us with reasonable results although the numerical accuracy is not better than those in Refs. 14)–17). As the origins of numerical error, we consider...
the finite mesh size, the use of a finite-point formula and our treatment around box boundaries. Improvements could be achieved, for example, if we use better boundary treatments or use another representation based on the 3D cartesian mesh representation.\textsuperscript{30} We leave such improvements for future work, and in the following we turn to the analysis of the deformation mechanism in neutron-rich nuclei around Cr isotopes to the accuracy obtained in the present code.

§3. Quadrupole deformation around neutron-rich Cr isotopes with \( N \sim 38 \)

3.1. Neutron-rich Cr isotopes and neutron single-particle gaps

The observed \( 2^+_1 \) energy of the neutron-rich Cr isotopes decreases monotonically with increasing neutron number from \( E_2 = 1007 \text{ keV} \) in \( {}^{56}\text{Cr} \) down to 446 keV in \( {}^{62}\text{Cr} \),\textsuperscript{2} suggesting a new region of deformation. The energy ratio \( E_4/E_2 \) between the \( 2^+_1 \) and \( 4^+_1 \) excited states increases to \( E_4/E_2 \sim 2.65 \) in \( {}^{62}\text{Cr} \),\textsuperscript{7} while the ratio is small \( E_4/E_2 \sim 2.2 \) for lighter isotopes.\textsuperscript{6} The proton inelastic scattering experiment\textsuperscript{7} indicates that the \( 2^+_1 \) state accompanies a large quadrupole deformation \( \beta \sim 0.25 \). Shell model analyses\textsuperscript{2,31} suggest a possible deformation for \( N \geq 38 \) as an extended model space including at least the neutron \( 1g_{\frac{7}{2}} \), and \( 2d_{\frac{5}{2}} \) orbits in the higher shell is necessary to describe the decrease in \( E_2 \) with increasing neutron number. There are several self-consistent mean-field calculations\textsuperscript{21-23} for the systematics of the ground-state deformation, including neutron-rich Cr isotopes. The calculation using the Skyrme parameter set SkM*\textsuperscript{21} produces a large prolate deformation around \( {}^{62}\text{Cr} \), but the other Skyrme models using SLy4,\textsuperscript{21} SkP,\textsuperscript{21} BS\textsuperscript{22} and the relativistic mean-field model using NL-SH\textsuperscript{23} do not. Here, we analyse the microscopic deformation mechanism, focusing on the parameter set SkM*.

First, we discuss the deformation energy curve in \( {}^{56-68}\text{Cr} \). We adopt SkM* and the volume-type pairing force \( (\eta = 0) \) with the pairing strength \( V_0 = -200 \text{ MeV} \)
The energy is arbitrarily shifted for the sake of comparison.

$V_0$ is adjusted to reproduce the odd-even mass difference in $^{56-66}$Cr, which are between 1.5 and 2.0 MeV. The ground-state values of $\beta$, $\Delta_n$, and $\Delta_p$ are shown in Table II. The calculated deformation energy curves of neutron-rich Cr isotopes are plotted in Fig. 4. It is seen that the deformation energy curve becomes soft toward the prolate direction with increasing neutron number from $N = 32$. In $^{60}$Cr, the deformation energy is almost flat between $\beta = -0.1$ and 0.3. In $^{62,64,66}$Cr($N = 38-42$), the energy minimum with a large quadrupole deformation appears at around $\beta = 0.25 - 0.3$, but then the deformation of the energy minimum decreases for $N \geq 42$. The calculated isotopic tendency is consistent with the observed trend of $E_2$ from $N = 32$ to $N = 38$. Note, however, that the energy difference between the spherical configuration ($\beta = 0$) and the quadrupole deformed minimum is small. In the case of $^{62}$Cr, the difference is about 290 keV. If we estimate the zero-point energy in terms of the experimental $E_2 = 446$ keV, the deformation and the zero-point energies have comparable magnitudes. Thus, it is suggested, within the SkM* model, that even in $^{62-64}$Cr exhibiting largely deformed minima no well-developed static deformation is realized, and that a large-amplitude quadrupole motion of a transitional character is expected. The transitional nature seems to be consistent with the observed $E_4/E_2$ ratio$^7$ of 2.65 in $^{62}$Cr which lies between the vibrator and the rotor limits 2 and 3.33.

Next, we analyse the mechanism of deformation. For this purpose, we plot Hartree-Fock single-particle energy as a function of $\beta$. Single-particle orbits are obtained by rediagonalising the HF Hamiltonian associated with the constrained Skyrme-HFB solution. The result is shown in Figs. 5(a) and (b). By observing the Fermi energy of $N = 38$ (the thick solid line in Fig. 5(a)), the neutron subshell gap $N = 40$ between the $f_{7/2}$ and $g_{9/2}$ orbits in the spherical region and an energy gap $N = 38$ in the prolate region at $\beta \sim 0.25 - 0.5$ are notable. Because the magnitude of the deformed $N = 38$ gap is comparable to that of the spherical $N = 40$ subshell gap, it is easy to deduce that the deformed $N = 38$ gap may drive the nucleus toward
Fig. 5. Single-particle energies obtained with SkM* (top panels (a)(b)) and SLy4 (bottom panels (c)(d)) for $^{62}$Cr. The left panels (a)(c) are for neutrons, and the right panels (b)(d) are for protons. The thick solid line denotes the Fermi energy. The horizontal axis is the quadrupole deformation parameter $\beta$.

prolate deformation with $\beta \sim 0.3$. We also note that the neutron $g_{\frac{9}{2}}$ orbit plays an important role in forming the deformed states. In particular, the $\Omega = \frac{1}{2}$ and $\frac{3}{2}$ orbits that stem from the deformation splitting of $\nu g_{\frac{9}{2}}$ are relevant as they exhibit the steepest downsloping at $\beta \geq 0$. If neutrons occupy these $\nu g_{\frac{9}{2}}$ orbits, they cause a strong driving force toward prolate deformation. This situation can be realized for $\beta \gtrsim 0.20$. We show in Table II the occupation number for all the $\nu g_{\frac{9}{2}}$ orbits. Here, we evaluate the occupation number at the minimum solution for each quasi-particle state by integrating the square of the lower component of the quasi-particle wave function. We list, in Table II, numbers summed over the quasi-particle states arising from the deformation splitting of the spherical $\nu g_{\frac{9}{2}}$ state. The occupation numbers $\sim 3.0$–$3.8$ in $^{62}$Cr and $^{64}$Cr, where the largest ground state deformation is realized, are consistent with the interpretation that the $\nu g_{\frac{9}{2}}$ $\Omega = \frac{1}{2}$ and $\frac{3}{2}$ orbitals are largely occupied. As neutron number exceeds $N = 38$, the occupation number of $\nu g_{\frac{9}{2}}$ still increases slightly ($3.8$ in $^{64}$Cr with $N = 40$ and $4.4$ in $^{66}$Cr with $N = 42$). However, the extent of quadrupole deformation then decreases at $N = 42$ since the upsloping orbits $[303 \frac{5}{2}]$ and $[301 \frac{1}{2}]$ stemming from $\nu f_{\frac{5}{2}}$ and $\nu p_{\frac{3}{2}}$ are occupied. This explains the reason for the largest quadrupole deformation in $^{52,64}$Cr with $N = 38$–$40$. The
important role of the occupation of $\nu g_{9/2}$ is consistent with the conclusions of the shell model analyses.\textsuperscript{2,3,6,31)}

### 3.2. Neutron-rich Ti and Fe isotopes

It is interesting to investigate neutron-rich Fe and Ti isotopes around $^{62,64}$Cr with $N = 38, 40$ with which the largest deformation is realized in the Cr isotopes. Figure 6 shows the deformation energy curve calculated with SkM* for the $N = 38$ isotones $^{60}$Ti, $^{62}$Cr, $^{64}$Fe and for the $N = 40$ isotones $^{62}$Ti, $^{64}$Cr, $^{66}$Fe. It is seen that the Cr and Fe isotopes have deformed minima at prolate deformation while the Ti isotopes do not exhibit this feature. Since the importance of proton configurations is easily inferred, we look into the proton Nilsson diagram in Fig. 5(b), which is for $^{62}$Cr but essentially the same for the nuclei under discussion. We also show the occupation number in the proton $f_{7/2}$ orbits in Table II. The occupation numbers are $\sim 2$, 4, and 6 in Ti, Cr and Fe, respectively, as naturally expected from Fig. 5(b). Since the $\Omega = \frac{1}{2}$ and $\Omega = \frac{3}{2}$ orbits stemming from $\pi f_{7/2}$ have steep slopes in the prolate direction, the simultaneous occupation of these orbits in Cr gives a large driving force toward the prolate deformation. We can expect that the deformation

Table II. Occupation numbers of neutron $g_{9/2}$ and proton $f_{7/2}$ orbits, average neutron and proton pairing gaps $\Delta_n$, $\Delta_p$ and quadrupole deformation parameter $\beta$ associated with HFB solutions obtained with SkM*.

|        | neutron $g_{9/2}$ | proton $f_{7/2}$ | $\Delta_n$ [MeV] | $\Delta_p$ [MeV] | $\beta$ |
|--------|------------------|------------------|------------------|------------------|--------|
| $^{60}$Ti | 1.28             | 2.02             | 2.042            | 1.198            | 0.0    |
| $^{62}$Ti | 1.28             | 2.02             | 2.096            | 1.157            | 0.0    |
| $^{58}$Cr | 0.355            | 3.98             | 1.619            | 1.427            | 0.0    |
| $^{60}$Cr | 0.794            | 3.98             | 1.970            | 1.388            | 0.0    |
| $^{62}$Cr | 2.98             | 4.00             | 1.908            | 0.405            | 0.257  |
| $^{64}$Cr | 3.85             | 4.02             | 1.904            | 0.212            | 0.262  |
| $^{66}$Cr | 4.39             | 4.00             | 1.833            | 0.280            | 0.247  |
| $^{58}$Cr | 5.40             | 4.00             | 1.756            | 0.456            | 0.222  |
| $^{60}$Fe | 2.58             | 5.99             | 1.999            | 0.280            | 0.212  |
| $^{62}$Fe | 3.76             | 6.00             | 1.951            | 0.008            | 0.231  |
is less favored in Fe than in Cr because protons in Fe occupy $\Omega = \frac{5}{2}$ orbits which are slightly upsloping. Indeed the $\beta$ at the minima in $^{64,66}\text{Fe}$ is slightly smaller than those in $^{62,64}\text{Cr}$ (cf. Table II, Fig. 6). On the other hand the spherical minima in Ti isotopes indicate that the occupation of the $\Omega = \frac{1}{2}$ orbit alone is not sufficient to cause deformation.

The observed $2^+_1$ energies$^{32}$ in $^{64,66}\text{Fe}$ are lower than those in $^{62}\text{Fe}$, and the observed ratio$^{33}$ $E_4/E_2 = 2.36$ in $^{64}\text{Fe}$ is smaller than that ($= 2.65$) in $^{62}\text{Cr}$. The deformation energy curves indicating smaller quadrupole deformation in $^{64,66}\text{Fe}$ than in $^{62,64}\text{Cr}$ are consistent with these experimental trends. In addition, the calculation predicts much less collectivity in Ti isotopes than in Cr and Fe isotopes. This is also consistent with higher $E_2$ in $^{58}\text{Ti}$ than in $^{60}\text{Cr}$.7

3.3. Relation to $N \sim Z = 38–40$ deformed region

The role of the $N = 38$ deformed shell gap brings to mind the mechanism of the prolate deformation in proton-rich Sr and Zr isotopes with $N \sim Z = 38–40$ as the large deformation in the proton-rich $N = Z$ region originates from the presence of a deformed shell gap at $N, Z = 38$ and $40$ at around $\beta \sim 0.4$.28), 34), 35) It is therefore interesting to investigate how the deformation of neutron-rich Cr and Fe nuclei is related to the $N \sim Z = 38–40$ cases. Figure 7 shows a comparison of the deformation energy curve in $^{62}\text{Cr}$ with those in $^{68}\text{Zn} (Z = 30)$ and $^{76}\text{Sr} (Z = 38)$ in the $N = 38$ isotone chain up to $N = Z = 38$. Note that the deformation energy curve in the $N = Z = 38$ nucleus $^{76}\text{Sr}$ has a well-developed deformed minimum at around $\beta \sim 0.4$.

Figure 8 shows a plot of the neutron Nilsson diagram in $^{76}\text{Sr}$. (The proton Nilsson diagram is not shown here as it is very similar to the neutron’s except for an overall energy shift due to the Coulomb potential.) Comparing the neutron Nilsson diagrams in Fig. 8 and Fig. 5(a), we see that the presence of the deformed $N = 38$ gap is common to both cases. The $N = 38$ deformed gap at $\beta \sim 0.4$ is universal in the sense that it exists in both the proton- and neutron-rich regions. This confirms that the deformation mechanism in the neutron-rich Cr and Fe isotopes is intimately

![Figure 7. Quadrupole deformation energy curves in $N = 38$ isotones obtained with SkM*.](image-url)
related to that in the $N = Z \sim 38$ region.

In spite of the above similarity, however, there is small but clear differences between the neutron Nilsson diagrams in the proton-rich $N = Z \sim 38$ region and in the neutron-rich Cr-Fe region. Looking closely at the $N = 38$ deformed shell gap, we see that the relevant level crossing of the downsloping $\nu g_{7/2} \Omega = \frac{3}{2}$ orbit and the upsloping orbit from $\nu f_{5/2}$ and $\nu p_{1/2}$ occurs at a smaller deformation $\beta \sim 0.20$ in neutron-rich $^{62}$Cr than in $^{76}$Sr, where the crossing takes place at $\beta \sim 0.26$. It is also seen that the $N = 40$ spherical gap at $\beta \sim 0$ is smaller in the neutron-rich $^{62}$Cr than in $^{76}$Sr. Both features are helpful in producing a largely deformed minimum at $\beta \sim 0.27$ in the deformation energy curve of $^{62}$Cr even though the deformation driving effect due to the proton configuration is weaker in $^{62}$Cr than in $^{76}$Sr. Also note that the deformed shell gap at $N = 40$ at around $\beta \sim 0.45$ observed in $^{76}$Sr is barely observed in $^{62}$Cr. Another difference is also seen in the $N = 34$ oblate gap which is large in the proton-rich region (cf. Fig. 8), leading to an oblate ground state in $^{68}$Se ($\beta = -0.21$). However, the $N = 34$ oblate gap is much weaker in neutron-rich Cr isotopes (Fig. 5(a)), and hence the deformation energy curve in $^{58}$Cr (Fig. 4) shows no very strong tendency toward oblate deformation.

### 3.4. Interaction dependence

As we have seen above, the Skyrme-HFB model using the parameter set SkM* produces the onset of a large quadrupole deformation in the $N \sim 38$–40 region of the Cr isotopes, being in qualitative agreement with the experimental observations. Note, however, that the calculations using other parameter sets such as SLy4, SkP and BSk do not show largely deformed minima in the same isotopes. Let us discuss how the onset of deformation depends on the Skyrme parameter sets by comparing results that we obtain using SLy4 as well as SkM*. The calculation for SLy4 is the same as above except for the use of different Skyrme parameters. We show in Fig. 9 the deformation energy curve in $^{62}$Cr obtained with the parameter...
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Fig. 9. Deformation energy curve obtained with SLy4 in $^{62}$Cr, plotted with the solid curve. The one for SkM* is also shown with the dotted curve for comparison.

set SLy4. The deformation energy curve for SLy4 does not have a well-deformed minimum, and it is stiff with respect to the quadrupole deformation. We show the neutron Nilsson diagram for SLy4 in Fig. 5 (c). By comparing with the Nilsson diagram for SkM* (Fig. 5 (a)), we see a large difference in the position of the $\nu g_{\frac{9}{2}}$ orbit. The $N = 40$ subshell gap at the spherical point is larger in the case of SLy4 than SkM* by about 2 MeV. The higher position of $\nu g_{\frac{9}{2}}$ also shifts the position of the $N = 38$ deformed single-particle gap at larger deformation $\beta > 0.35$ in the SLy4 case. These features apparently favor the stability of the spherical shape in contrast to the case of SkM*. All these observations indicate that the position of the $g_{\frac{7}{2}}$ orbit plays a central role in the onset of quadrupole deformation in neutron-rich Cr and Fe isotopes at around $N = 38$. The precise position of the $\nu g_{\frac{9}{2}}$ orbit and the size of the $N = 40$ subshell gap depend on the Skyrme parameter set. In other words, the deformation properties in the neutron-rich Cr region provide us with a rather strong constraint for the proper choice of the Skyrme parameter set. It is important to explore the best Skyrme parameter set in this connection, but it requires a quantitative description of the first $2^+$ state among other things. Such an analysis is beyond the scope of this study, and we leave it for future investigation.

§4. Conclusions

We have developed an axially symmetric Skyrme-HFB code based on the 2D mesh representation in the cylindrical coordinate system in order to describe the quadrupole deformation of unstable nuclei. Our code has sufficient accuracy to analyse the deformation property as tested by comparisons with calculations using the THO and B-Spline methods.

We applied the code to neutron-rich Cr, Fe and Ti isotopes around a possible new region of deformation with $N \gtrsim 38$. The quadrupole deformation energy curve obtained with the Skyrme parameter set SkM* indicates an onset of deformation
in the isotopes with $N \sim 38$–42. The deformation energy curve is soft although the deformation of the minimum reaches $\beta \sim 0.25$ for $N = 38$ and 40; hence, nuclei in this region are expected to exhibit a strong quadrupole collectivity having a transitional character rather than that associated with a well-developed stable deformation. These results are in qualitative agreement with the trends of the presently available experimental data. The SkM* model also describes Fe isotopes in the same mass region as transitional nuclei while Ti isotopes as spherical nuclei with a stiffer quadrupole deformation energy curve. By inspecting the neutron Nilsson diagram, we discussed that the deformed $N = 38$ gap emerging at $\beta \gtrsim 0.25$ as well as the position of $\nu g_{\frac{2}{7}}$ orbit play important role in the onset of quadrupole deformation. We have also shown that, in contrast to SkM*, the parameter set SLy4 cannot reproduce the onset of deformation. The sensitivity to the Skyrme parameter set arises from the fact that the deformation in this region emerges as a consequence of a delicate competition between spherical and deformed configurations, for which the position of $\nu g_{\frac{2}{7}}$ orbit plays an essential role.

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