HFODD
(v2.40h)

User’s Guide
Abstract

We describe the input data and installation procedures of the code HFODD (v2.40h). The present write-up contains complete and comprehensive information that has originally been given in six independent publications. It is enhanced by the subject index and indexes of variables, input-data keywords, subroutines, and files that are used in this user guide.

Keywords

Hartree-Fock; Hartree-Fock-Bogolyubov; Skyrme interaction; self-consistent mean field; nuclear many-body problem; superdeformation; quadrupole deformation; octupole deformation; pairing; nuclear radii; single-particle spectra; nuclear rotation; high-spin states; three-dimensional rotation; chiral symmetry in nuclei; gauge symmetry; moments of inertia; level crossings; harmonic oscillator; Coulomb field; pairing; point-group symmetries. Yukawa interaction; angular-momentum projection; generator coordinate method; Schiff moments
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1. INTRODUCTION

The code **HFODD** (v2.40h) solves the nuclear Skyrme-Hartree-Fock or Skyrme-Hartree-Fock-Bogolyubov problem by using the Cartesian deformed harmonic-oscillator basis. It is a result of a long-term project that is developed at the Institute of Theoretical Physics, University of Warsaw and in many other collaborating institutions. The code is one of the main solvers that are developed within the UNEDF collaboration ([http://unedf.org/](http://unedf.org/)). The code has been published and is available from the Computer Physics Communications Program Library ([http://www.cpc.cs.qub.ac.uk/cpc/](http://www.cpc.cs.qub.ac.uk/cpc/)). The description of the code, and how to use it, has been published in the Computer Physics Communications in the form of six independent publications, which are below referred to as I [1], II [2], III [3], IV [4], V [5], and VI [6].

The present user’s guide summarizes articles I-VI and provides practical details presented in the form that is suitable for a rapid reference on how to run the code. It also contains details updated to those corresponding to version (v2.40h). Information pertaining to the physics issues and numerical methods are not repeated here, and the user is referred to the original publications and to the references given therein.

Together with consulting the present user’s guide, the reader is invited to visit the HFODD home page ([http://www.fuw.edu.pl/~dobaczew/hfodd/hfodd.html](http://www.fuw.edu.pl/~dobaczew/hfodd/hfodd.html)), where many useful files are available for downloading and which contains information on future versions and extensions being developed.

The present user’s guide overrides the previous version published in Ref. [7], which is now obsolete.
2. **INPUT DATA FILE**

The code reads the input data from the standard FORTRAN input file, and a general structure of the input data file is defined by the following rules:

1. Input data file is an ASCII file composed of independent input items.

2. An item is composed of the keyword line, and of the data line which follows immediately the keyword line. Two items contain no data lines, see point 6 below.

3. The keyword line contains in columns 1 through 10 a keyword which is a specific text defining the item. If the keyword has less than 10 characters it has to be obligatorily padded with appropriate number of trailing spaces. Columns beyond 10 are ignored and can be used to place arbitrary comments or texts.

4. The data line contains a prescribed number of data values which are read in the free FORTRAN FORMAT. The type of data (REAL, INTEGER, or CHARACTER) should match the definition of the given data line. The CHARACTER data should be provided starting from the 13-th column of the data line.

5. Items can be separated by an arbitrary numbers of comment lines. A line is treated as a comment and ignored provided it does not contain in columns 1 through 10 any of the valid keywords.

6. Two items contain no data lines. The first one is defined by the keyword EXECUTE, and starts a calculation for the currently defined input parameters. The second one is defined by the keyword ALL_DONE, and terminates the program. The latter item is not required if the compiler is able to properly recognize the end of input data file. When the end of input data file is encountered, the program terminates as if the keyword ALL_DONE was found.

7. A given item may occur any number of times in different places of the input data file. Only the last one of the same items occurring before a given EXECUTE keyword is taken into account.

8. The items appearing between two consecutive items EXECUTE define the data set, i.e, the set of input parameters, for which the calculation will start at the moment when the latter of the two such items is found. Between two consecutive items EXECUTE, the order of other items is arbitrary.

9. All input parameters have the default values defined in the code (subroutine PREDEF). Therefore, if the input data file contains only the item EXECUTE, and no other lines, a calculation for the default values is performed. In the present version, this results in performing 50 iterations for the superdeformed state of $^{152}$Dy at the angular frequency of $\hbar\omega=0.5\text{ MeV}$.

10. Only those items which define the values of input parameters which are different from the default values have to be included in the input data file. The values of input parameters
defined by any item stay in effect till another occurrence of the same item, or till the code terminates. This rule is valid irrespective of how many EXECUTE items follow the given item.

In the following subsections we list all the valid keywords and their corresponding data lines. Titles of the subsections are introduced only to organize the keywords into groups pertaining to specific categories, but are otherwise irrelevant. The default values are given in data lines following the keyword lines. In the data lines we also show names of the corresponding variables, which are referred to in the text.
2.1. General data

This section lists keywords pertaining to definitions of particle numbers, iterations, and phase space.

2.1.1. Keyword: **NUCLIDE**

86, 66 = **IN_FIX**, **IZ_FIX**

Numbers of neutrons (**IN_FIX**) and protons (**IZ_FIX**) in the nucleus under consideration. Calculations for odd and odd-odd nuclei can be done only either with **IROTAT**=1 or with **IPAIRI**=1. In the latter case, the odd and odd-odd nuclei are described within the false-vacuum approximation unless the quasiparticle blocking approximation is used for **IPAHFB**=1, see Secs. 2.7–2.7. For **IPABCS**=1, the blocking approximation is not yet implemented. For **IN_FIX**=0 or **IZ_FIX**=0, calculations are performed for one type of particles only, which allows to treat the atomic gases.

2.1.2. Keyword: **ITERATIONS**

50 = **NOITER**

For **NOITER**>0, the specified number of iterations is performed. Unless **ICONTI**=1 or **IREAWS**=1, the code starts with iteration number 0 by constructing the initial mean fields based on the Nilsson potential. Specifying **NOITER**=0 requests only this initial phase. If the iteration is restarted from the previously recorded potentials (**ICONTI**=1), then the counting of iterations continues from the number of iterations performed in the previous run. Along with requesting the initial $D_{2h}^T$ transformations (**INIINV**>0 or **INIKAR**>0) or initial rotation (**INIROT**=1) one must set **NOITER**=1.

2.1.3. Keyword: **ITERAT_EPS**

0.0 = **EPSITE**

2.1.4. Keyword: **MAXANTIOSC**

1 = **NULAST**

These two parameters govern the termination of the HF iterations according to the achieved stability of solutions. The stability of the HF energy has been defined in (I-37) as the difference between the total energies calculated from the single-particle energies and from the Skyrme functional. The HF iterations continue until the absolute value of the stability is smaller than **EPSITE** (in MeV) over **NULAST** consecutive iterations. When this condition is fulfilled, iteration procedure terminates and the final results are printed. This allows for an automated adjustment of the number of iterations that are required to achieve a given level of convergence. The number of iterations **NOITER**, can now be set to a large value, at which the iterations terminate if a stable solution is not found.
2.1. General data

The default value of $\text{EPSITE}=0.0$ deactivates this option, and then the code continues up to $\text{NOITER}$ iterations regardless of the achieved stability. If a non-zero value of $\text{EPSITE}$ is used, a non-zero value of $\text{NULAST}$ has to be used too. In practice, a value of $\text{NULAST}=5$ prevents an accidental termination of iterations in all cases when the stability energy gradually goes through zero, but the solution is not yet self-consistent.

2.1.5. Keyword: PING-PONG

$0.0, 3 = \text{EPSPNG, NUPING}$

The code is able to detect the “ping-pong” divergence described in Sec. III-2.6, i.e., the situation when the HF iteration procedure gives oscillating results in every second iteration. Upon continuing the iteration, both sequences of results, i.e., those which correspond to the iteration numbers being even and odd, stay different but perfectly stable, and hence the correct self-consistent solution is never attained.

The code recognizes such a situation by calculating the averages and variances of the stability energy (I-37), separately in the even and in the odd sequences of results, over the last $\text{NUPING}$ pairs of iterations. The “ping-pong” divergence condition occurs when both variances become a factor $\text{EPSPNG}$ smaller than the absolute value of the difference of the corresponding averages, i.e., when

$$
\Delta(\delta E)_{\text{even}} < \text{EPSPNG} \times |\overline{\delta E}_{\text{even}} - \overline{\delta E}_{\text{odd}}|, \\
\Delta(\delta E)_{\text{odd}} < \text{EPSPNG} \times |\overline{\delta E}_{\text{even}} - \overline{\delta E}_{\text{odd}}|,
$$

(1a, 1b)

where

$$
\overline{\delta E}_{\text{even}} = \left( \frac{\sum_{p=0}^{\text{NUPING}-1} \delta E_{n-2p}}{\text{NUPING}} \right) / \text{NUPING},
$$

(2a)

$$
\overline{\delta E}_{\text{odd}} = \left( \frac{\sum_{p=0}^{\text{NUPING}-1} \delta E_{n-2p-1}}{\text{NUPING}} \right) / \text{NUPING},
$$

(2b)

and

$$
\Delta(\delta E)_{\text{even}} = \left( \frac{\sum_{p=0}^{\text{NUPING}-1} (\delta E_{n-2p} - \overline{\delta E}_{\text{even}})^2}{\text{NUPING}} \right)^{1/2} / \text{NUPING},
$$

(3a)

$$
\Delta(\delta E)_{\text{odd}} = \left( \frac{\sum_{p=0}^{\text{NUPING}-1} (\delta E_{n-2p-1} - \overline{\delta E}_{\text{odd}})^2}{\text{NUPING}} \right)^{1/2} / \text{NUPING}.
$$

(3b)

Here, $n$ denotes the number of the last accomplished HF iteration, and $\delta E_n$ denotes the stability energy (I-37) obtained in the $n$-th iteration.

The default value of $\text{EPSPNG}=0.0$ deactivates this option, and then the code continues up to $\text{NOITER}$ iterations regardless of the “ping-pong” divergence. If a non-zero value of $\text{EPSPNG}$ is used, a value of $\text{NUPING}>1$ has to be used too. In practice, values of $\text{EPSPNG}=0.01$ and $\text{NUPING}=3$ allow for an efficient detection of the “ping-pong” divergence condition.
Upon discovering the “ping-pong” divergence, the HF iterations are terminated and a table of absolute values of maximum differences of single-particle observables between the two sequences of iterations is printed, see Sec. III-2.6. These maximum differences are determined for states in each of the charge–parity–signature, charge–simplex, parity, or charge blocks, depending on the conserved symmetries, and separately for particle and hole states. Whenever such a maximum difference is found for a particle state and for a hole state with adjacent indices, such a pair is proposed as a candidate for the diabatic blocking calculation.

2.1.6. Keyword: CHAOTIC

\(0 = \text{NUCHAO}\)

The code is able to detect the “chaotic” divergence which occurs when the HF iterations give results which chaotically vary from one iteration to another one. The code recognizes such a divergence by finding the local maxima \(M_k, k=1,2,\ldots\), in the sequence of absolute values of the stability energies (I-37), obtained in the entire series of the HF iterations performed. The “chaotic” divergence condition occurs when the code finds NUCHAO positive differences \(M_k - M_{k-1}\). When this condition occurs, iteration procedure terminates and the final results are printed.

For NUCHAO=0 (the default value) the code does not check whether the “chaotic” divergence occurs or not. In practice, a value of NUCHAO=5 allows for an efficient detection of the “chaotic” divergence condition. However, for a small value of NUCHAO and a small value of EPSPNG, the “ping-pong” divergence can sometimes be mistaken for the “chaotic” divergence. If one is interested in the diabatic-blocking data, printed after the “ping-pong” divergence, the recommended value of NUCHAO=5 should be increased to 10 or more.

2.1.7. Keyword: PHASESPACE

\(0, 0, 0, 0 = \text{NUMBSP}(0,0), \text{NUMBSP}(1,0), \text{NUMBSP}(0,1), \text{NUMBSP}(1,1)\)

Numbers of the lowest mean-field eigenstates which are kept after the diagonalization of the mean-field Hamiltonians in the four charge–simplex blocks: \((s,q)=(+i,n), (-i,n), (+i,p), (-i,p)\). All other eigenstates are discarded. If any of these numbers is equal to zero (the default value), the code sets it equal to the number of neutrons IN_FIX (for \(q=n\)) or protons IZ_FIX (for \(q=p\)). When no symmetry is conserved, the numbers of states kept in charge blocks are determined by sums \(\text{NUMBSP}(0,0) + \text{NUMBSP}(1,0)\) and \(\text{NUMBSP}(0,1) + \text{NUMBSP}(1,1)\).

For calculations without pairing, i.e. for IPAIRI=0, the user is responsible for using values of NUMBSP large enough to accommodate all wave functions which might be useful for the required vacuum and particle-hole configurations, see Sec. II-3.4. In practice, the use of the default values described above is recommended as a safe option. The size of the matrices defined by the NDSTAT parameter can be reduced by the user when small values of NUMBSP are used.

For calculations with the BCS pairing, i.e. for IPAIRI=1 and IPAHF=0, values of NUMBSP define the pairing window in which the BCS equations are solved.
For calculations with the HFB pairing, i.e. for $\text{IPAIRI}=1$ and $\text{IPAHFB}=1$, values of $\text{NUMBSP}$ define the numbers of canonical states kept after diagonalizing density matrices. They are irrelevant for the pairing window, which is then defined by the cutoff energy $\text{ECUTOF}$. 
2. INPUT DATA FILE

2.2. Interaction

This section lists keywords pertaining to definitions of coupling constants and interaction parameters.

2.2.1. Keyword: SKYRME-SET

\[ \text{SKM}^* = \text{SKYRME} \]

CHARACTER*4 acronym of the Skyrme force parameter set. Must start at the 13-th column of the data line. In version (v2.40h), valid acronyms are SII, SIII, SV, SVI, SKM*, SKP, SKMP, SKII, SKO, SKOP, SLY4, SLY5, SLY6, SLY7, MSK1, MSK2, MSK3, MSK4, MSK5, MSK6, SKX, SKXC. Other sets of parameters can easily be included in the subroutine PARAMS.

2.2.2. Keyword: SKYRME-STD

\[ 0, 1, 0, 0, 0 = \text{ISTAND, KETA}_J, \text{KETA}_W, \text{KETACM}, \text{KETA}_M \]

Parameters of several standard Skyrme forces are encoded within the program. Calculation for a given standard force can be requested by specifying in the input data file its acronym SKYRME. Along with the force parameters, for each force there is encoded information on how the given force should be used, i.e., with which value of the parameter \( \frac{h^2}{2m} \), and with which treatment of tensor, spin-orbit, and center-of-mass terms. For ISTAND=1, calculations are performed with these features set in the way specific for the given force, and the rest of the switches read on the same line is ignored. For ISTAND=0, the switches define nonstandard features in the following way:

- For KETA.J=1 the code takes into account in the functional, and for KETA.J=0 neglects, the so-called tensor \( J^2 \) terms. The second option is equivalent to setting in Eq. (I-12) coupling constants \( C_i^J=0 \) and \( C_i^T=0 \).
- For KETA.W=0 or 1 the code uses the traditional \( (W'_0 \equiv W_0) \) or generalized \( (W'_0 \neq W_0) \) spin-orbit term, respectively, where

\[
\begin{align*}
C_0^{\nabla J} &= C_0^{\nabla j} = -\frac{1}{2}W_0 - \frac{1}{4}W'_0, \\
C_1^{\nabla J} &= C_1^{\nabla j} = -\frac{1}{4}W'_0.
\end{align*}
\]  

(4a)  

(4b)

For forces that use generalized spin-orbit term, option KETA.W=0 sets \( W'_0 \) equal to \( W_0 \), while for forces that use traditional spin-orbit, option KETA.W=1 has no effect. For KETA.W=2, strengths \( W_0 \) and \( W'_0 \) are set equal to the values of W0_INP and W0_PINP, respectively, which are read under the keyword of SPIN_ORBIT. Note that if KETA.W=2 is used, and keyword SPIN_ORBIT is not specified in the input data file, the default values of W0_INP and W0_PINP supersede those that are encoded within the program for the given Skyrme force.
• For $\text{KETACM}=0$ the code uses the traditional one-body center-of-mass correction before variation,

$$E_{\text{c.m.}} \simeq E_{\text{c.m.}}^{\text{dir}} = -\frac{1}{A} \langle \hat{T} \rangle,$$

(5)

where $\hat{T} = -\frac{\hbar^2}{2m} \sum_{i=1}^{A} \nabla_i^2$ is the one-body kinetic-energy operator. For $\text{KETACM}=1$ the code uses the two-body center-of-mass correction after variation,

$$E_{\text{c.m.}} = -\frac{1}{2mA} \langle \hat{P}^2 \rangle,$$

(6)

where $\hat{P} = -i\hbar \sum_{i=1}^{A} \nabla_i$ is the total linear momentum operator. Value of $\text{KETACM}=2$ is reserved for a future implementation of the two-body center-of-mass correction before variation. For $\text{KETACM}=3$ the center-of-mass correction is neglected.

• For $\text{KETA.M}=0$ the code uses the value of $\frac{\hbar^2}{2m} = 20.73620941 \text{ MeV fm}^2$, which was encoded in version (v1.75r). For $\text{KETA.M}=1$ the code uses the value specific for the given Skyrme force. For $\text{KETA.M}=2$ the code uses the value specified in the input data file under keyword $\text{HBAR20VR2M}$.

### 2.2.3. Keyword: HBAR20VR2M

20.73620941 = HBMINP

Value of the $\frac{\hbar^2}{2m}$ parameter, which is used if $\text{KETA.M}=2$ is set under keyword $\text{SKYRME-STD}$, and ignored otherwise.

### 2.2.4. Keyword: SPIN.ORBIT

120.0, 120.0 = W0.INP, W0PINP

Strengths $W_0$ and $W'_0$ of the generalized spin-orbit interaction (4), which are used if $\text{KETA.W}=2$ is set under keyword $\text{SKYRME-STD}$, and ignored otherwise.

### 2.2.5. Keyword: LANDAU

000, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0 =LANODD, XO_LAN, X1_LAN, GO_LAN, G0PLAN, G1_LAN, G1PLAN

Three-digit steering switch $\text{LANODD}$ is used to specify the type of operations performed in order to define selected time-odd coupling constants based on values of the Landau parameters. The switch is followed by values of $x_0$, $x_1$, $g_0$, $g'_0$, $g_1$, and $g'_1$, as given by equations:

$$x_0 = \frac{C_0^s[0]}{C_0^s[\rho_{\text{sat}}]}$$

(7a)

$$x_1 = \frac{C_1^s[0]}{C_1^s[\rho_{\text{sat}}]}$$

(7b)
\[ g_0 = N_0(2C_0^s[\rho_{\text{sat}}] + 2C_0^T \beta \rho_{\text{sat}}^{2/3}), \quad (7c) \]
\[ g_0' = N_0(2C_1^s[\rho_{\text{sat}}] + 2C_1^T \beta \rho_{\text{sat}}^{2/3}), \quad (7d) \]
\[ g_1 = -2N_0 C_0^T \beta \rho_{\text{sat}}^{2/3}, \quad (7e) \]
\[ g_1' = -2N_0 C_1^T \beta \rho_{\text{sat}}^{2/3}, \quad (7f) \]

where \( \beta = (3\pi^2/2)^{2/3} \) and

\[ N_0 = \pi^{-2} \left( \frac{\hbar^2}{2m} \right)^{-1} \left( \frac{m^*}{m} \right) \left( \frac{3\pi^2 \rho_{\text{sat}}}{2} \right)^{1/3}. \quad (8) \]

For LANODD=000, coupling constants are not defined by the Landau parameters, and the rest of parameters read on the same data line is ignored. For LANODD=111, Eqs. (7) are solved, and coupling constants \( C_0^s[0], C_0^s[\rho_{\text{sat}}], C_1^s[0], C_1^s[\rho_{\text{sat}}], C_0^T, \) and \( C_1^T \) are determined from the values of \( x_0, x_1, g_0, g_0', g_1, \) and \( g_1' \). For other values of LANODD, the following three steps are performed in sequence:

1. **Step one:** If the rightmost digit of LANODD is equal to 1 then the coupling constants \( C_0^T \) and \( C_1^T \) are determined from \( g_1 \) and \( g_1' \), Eqs. (7c) and (7f); otherwise these two coupling constants are determined from the Skyrme force parameters.

2. **Step two:** If the middle digit of LANODD is equal to 1 then the coupling constants \( C_0^s[\rho_{\text{sat}}] \) and \( C_1^s[\rho_{\text{sat}}] \) are determined from \( g_0 \) and \( g_0' \), Eqs. (7c) and (7d); otherwise these two coupling constants are determined from the Skyrme force parameters.

3. **Step three:** If the leftmost digit of LANODD is equal to 1 then the coupling constants \( C_0^s[0] \) and \( C_1^s[0] \) are determined from \( x_0 \) and \( x_1 \), Eqs. (7a) and (7b); otherwise these two coupling constants are determined from the Skyrme force parameters.

All combinations of zeros and ones are allowed in LANODD.

**2.2.6. Keyword: LANDAU-SAT**

\[-1.0, -1.0, -1.0 = \text{HBMSAT, RHOSAT, EFFSAT} \]

Values of parameters \( \hbar^2/2m, \rho_{\text{sat}}, \) and \( m^*/m, \) respectively, which are used when solving Eq. (7). If a negative number is read for any of these parameters, then the program uses the corresponding value calculated from parameters of the given Skyrme force.

**2.2.7. Keyword: EVE_SCA_TS**

1., 1., 1., 1., 1., 1., 1., 1., 1., 1.
\[ \text{SRHO}_T, \text{SRHO}_S, \text{SRHODT}, \text{SRHODS}, \text{SLPR}_T, \text{SLPR}_S, \text{STAU}_T, \text{STAU}_S, \text{SSCU}_T, \text{SSCU}_S, \text{SDIV}_T, \text{SDIV}_S \]

By using this item, the coupling constants corresponding to a given Skyrme parameter set can be arbitrarily scaled. This allows calculations with modified Skyrme functionals. The time-even
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Coupling constants in the total-sum representation,

\[ C_{\text{tot}}^\rho = C_0^\rho - C_1^\rho, \quad (9a) \]
\[ C_{\text{sum}}^\rho = 2C_1^\rho, \quad (9b) \]

are multiplied by the 12 numbers from \texttt{SRHO\_T} to \texttt{SDIV\_S}. Variables with names ending with \_\texttt{T} and \_\texttt{S} multiply the “total” and “sum” coupling constants, respectively. Variables with names containing the acronyms \texttt{RHO}, \texttt{LPR}, \texttt{TAU}, \texttt{SCU}, and \texttt{DIV}, multiply the coupling constants with superscripts \( \rho \), \( \Delta \rho \), \( \tau \), \( J \), and \( \nabla J \), respectively, and those with \texttt{RHOD} multiply the density-dependent part of \( C^\rho \). Similar name convention is used for many other variables in the code \texttt{HFODD}.

2.2.8. Keyword: \texttt{ODD\_SCA\_TS}

1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.
\texttt{SSPI\_T, SSPI\_S, SSPIDT, SSPIDS, SLPS\_T, SLPS\_S},
\texttt{SCUR\_T, SCUR\_S},
\texttt{SKIS\_T, SKIS\_S},
\texttt{SROT\_T, SROT\_S}

Same as above but for the time-odd coupling constants. The acronyms \texttt{SPI}, \texttt{LPS}, \texttt{CUR}, \texttt{KIS}, and \texttt{ROT} correspond to coupling constants with superscripts \( s \), \( \Delta s \), \( T \), \( J \), and \( \nabla j \), respectively, and those with \texttt{SPID} correspond to the density-dependent part of \( C^s \).

2.2.9. Keyword: \texttt{EVE\_SCA\_PM}

1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.
\texttt{SRHO\_P, SRHO\_M, SRHODP, SRHODM, SLPR\_P, SLPR\_M},
\texttt{STAU\_P, STAU\_M},
\texttt{SSCU\_P, SSCU\_M},
\texttt{SDIV\_P, SDIV\_M}

Same as above but for the time-even coupling constants in the isoscalar-isovector representation,

\[ C_0^\rho = \frac{1}{2}C_{\text{sum}}^\rho + C_{\text{tot}}^\rho, \quad (10a) \]
\[ C_1^\rho = \frac{1}{2}C_{\text{sum}}^\rho. \quad (10b) \]

Variables with names ending with \texttt{P} and \texttt{M} multiply the isoscalar and isovector coupling constants, respectively. The total-sum scaling factors are used first, and the isoscalar-isovector scaling factors are used afterwards.
2.2.10. Keyword: **ODD_SCA_PM**

```
1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.
SSPI_P, SSPI_M, SSSIDP, SSSIDM, SLPS_P, SLPS_M,
  SCUR_P, SCUR_M,
  SKIS_P, SKIS_M,
  SROT_P, SROT_M
```

Same as above but for the time-odd coupling constants in the isoscalar-isovector representation.

2.2.11. Keyword: **EVE_ADD_TS**

```
0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.
ARHO_T, ARHO_S, ARHODT, ARHODS, ALPR_T, ALPR_S,
  ATAU_T, ATAU_S,
  ASCU_T, ASCU_S,
  ADIV_T, ADIV_S
```

By using this item, the coupling constants corresponding to a given Skyrme parameter set can be shifted by arbitrary values. The time-even coupling constants in the total-sum representation (I-14) are modified by adding the 12 numbers from **ARHO_T** to **ADIV_S**. By setting the scaling factors **SRHO_T** to **SDIV_S** equal to zero, see the keyword **EVE_SCA_TS**, one can input here a new set of the coupling constants. The name convention of variables is here the same as for many other variables in the code hfodd, see the keyword **EVE_SCA_TS**.

2.2.12. Keyword: **ODD_ADD_TS**

```
0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.
ASPI_T, ASPI_S, ASPIDT, ASPIDS, ALPS_T, ALPS_S,
  ACUR_T, ACUR_S,
  AKIS_T, AKIS_S,
  AROT_T, AROT_S
```

Same as above but for the time-odd coupling constants.

2.2.13. Keyword: **EVE_ADD_PM**

```
0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.
ARHO_P, ARHO_M, ARHODP, ARHODM, ALPR_P, ALPR_M,
  ATAU_P, ATAU_M,
  ASCU_P, ASCU_M,
  ADIV_P, ADIV_M
```

Same as above but for the time-even coupling constants in the isoscalar-isovector representation (10). The total-sum additive factors are used first, and the isoscalar-isovector additive factors
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are used afterwards.

2.2.14. Keyword: ODD_ADD_PM

0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.

ASPI_P, ASPI_M, ASPIDP, ASPIDM, ALPS_P, ALPS_M,
ACUR_P, ACUR_M,
AKIS_P, AKIS_M,
AROT_P, AROT_M

Same as above but for the time-odd coupling constants in the isoscalar-isovector representation [10].

2.2.15. Keyword: G_SCALING

1.0, 1.0 = FACTGN, FACTGP

For IPABCS=1 the code HFODD solves the BCS equations with the neutron and proton pairing strengths defined in Ref. [9]. These values can be modified by defining here the multiplicative factors FACTGN and FACTGP for neutrons and protons, respectively.

2.2.16. Keyword: PAIR_MATRI

1, 0, 0, 0 = IDESTA, IDEMID, IDESTO, IDEDIS

For IDESTA=1, the pairing matrix elements, required for the BCS pairing calculations with state-dependent pairing gaps (IPABCS=3), are calculated in the first iteration. In the present version (v2.40h), only the value of IDESTA=1 is allowed, because the option of storing the pairing matrix elements is not yet implemented. For IDEMID=1, the pairing matrix elements are calculated in the middle iterations (all between the first and the last one), for IDESTO=1 in the last iteration, and/or for IDEDIS=n, in every n-th iteration, counting from the first one.

2.2.17. Keyword: INI_FERMI

−8.0, −8.0 = FERINI(0), FERINI(1)

2.2.18. Keyword: INI_DELTA

1.0, 1.0 = DELINI(0), DELINI(1)

For ICONTI=0 or ICONTI=1 and IPCONT=0, the HFB calculations are started by using the initial values of the neutron and proton Fermi energies, FERINI(0) and FERINI(1), and pairing gaps, DELINI(0) and DELINI(1). For ICONTI=1, the initial values of pairing gaps overwrite the HFB pairing potentials with constant values of DELINI(0) and DELINI(1) for neutrons and protons, respectively. These constant potentials are ignored after the first iteration, i.e., in the
first iteration, the mixing of previous and current potentials (see keyword SLOW-PAIR) is not performed. A possibility of restarting calculations with nonzero pairing is very useful in case the pairing would have vanished in a former run. For ICONTI=0 or IPCONT=0, values of FERINI and DELINI are ignored.

2.2.19. **Keyword: FIXDELTA_N**

\[ 1.0, 0 = \text{DELFIN, IDEFIN} \]

For IDEFIN=1, the HFB pairing calculations (for IPAHFB=1) or BCS pairing calculations (for IPABCS=2) are performed with a fixed value of the neutron pairing gap equal to DELFIN. For IDEFIN=0, value of DELFIN is ignored and the zero-range density-dependent pairing force \(^{(11)}\) is used for neutrons. IDEFIN=1 requires IPAHFB=1 or IPABCS=2.

2.2.20. **Keyword: FIXDELTA_P**

\[ 1.0, 0 = \text{DELFIP, IDEFIP} \]

Same as above but for the proton pairing gap.

2.2.21. **Keyword: PAIRNFORCE**

\[ -200.0, 0.0, 1.0 = \text{PRHO}_N, \text{PRHODN}, \text{POWERN} \]

Parameters \( V_0, V_1, \) and \( \alpha \), respectively, of the zero-range density-dependent pairing force defined by the pairing form-factor:

\[
    f(r) = V_0 + V_1 \rho^\alpha(r) = V_0 \left( 1 - \left( \frac{\rho(r)}{\rho_0} \right)^\alpha \right),
\]

which is used in the HFB pairing or BCS pairing calculations for neutrons. In case the values of \( V_1 \) and \( \alpha \) allow it, the code calculates the value of the saturation density \( \rho_0 \) that gives the equivalent form of the pairing form-factor \(^{(11)}\). In case \( \rho_0 \) cannot be calculated, the codes set its value to 1; \( \rho_0 \) is calculated only for the purpose of information, while internally the code uses only the value of \( V_1 \). For IDEFIN=1, or for IPAHFB\( \neq \)1 and IPABCS\( \neq \)3, parameters PRHO\(_N\), PRHODN, and POWERN are ignored.

2.2.22. **Keyword: PAIRPFORCE**

\[ -200.0, 0.0, 1.0 = \text{PRHO}_P, \text{PRHODP}, \text{POWERP} \]

Same as above but for the proton pairing force.
2.2.23. **Keyword:** PAIR\_FORCE

\[-200.0, 0.0, 1.0 = PRHO\_T, PRHODT, POWERT\]

Same as above but for the neutron and proton pairing forces. This keyword is equivalent to using the two keywords simultaneously, PAIR\_NFORCE and PAIR\_PFORCE, with identical parameters for neutrons and protons.

2.2.24. **Keyword:** PAIR\_INTER

\[-200.0, 0.16, 1.0 = PRHO\_N, PRHOSN, POWERN\]

Parameters $V_0$, $\rho_0$, and $\alpha$, respectively, of the zero-range density-dependent pairing force \(^{11}\), which is used in the HFB pairing or BCS pairing calculations for neutrons. In case the values of $\rho_0$ and $\alpha$ allow it, the code calculates the value of $V_1$ that gives the equivalent form of the pairing form-factor \(^{11}\). In case $V_1$ cannot be calculated, the code stops. For $IDEF=1$, or for $IPAHFB\neq 1$ and $IPABCS\neq 3$, parameters $PRHO\_N$, $PRHOSN$, and $POWERN$ are ignored.

2.2.25. **Keyword:** PAIR\_PINTER

\[-200.0, 0.16, 1.0 = PRHO\_P, PRHOSP, POWERP\]

Same as above but for the proton pairing force.

2.2.26. **Keyword:** PAIR\_INTER

\[-200.0, 0.16, 1.0 = PRHO\_T, PRHOST, POWERT\]

Same as above but for the neutron and proton pairing forces. This keyword is equivalent to using the two keywords simultaneously, PAIR\_NINTER and PAIR\_PINTER, with identical parameters for neutrons and protons.

2.2.27. **Keyword:** CUTOFF

\[60.0 = ECUTOF\]

The cutoff energy $\bar{\varepsilon}_{max}$ for summing up contributions of the HFB quasiparticle states to density matrices, see Sec. IV-2.5. Ignored for $IPAHFB=0$.

2.2.28. **Keyword:** YUKA\_WATERM

\[0.7045, 4.7565, 1.0, 0.0, 0.0, 0.0, 1, 0\]

$PIMASS, PNMASS, YUKAGT, YUKAGO, YUKAG1, YUKAG2, IYUTYP, I\_YUKA$

For $I\_YUKA>0$, the code calculates the average values of the time-reversal- and parity-violating
Yukawa interaction (VI-59), with the pion mass \( m_\pi \) of PIMASS and the nucleon mass \( m_N \) of PNMAS.

If values of zero are read, variables PIMASS and PNMAS remain unchanged. Variables YUKAGT, YUKAGO, YUKAG1, and YUKAG2 correspond, respectively, to the coupling constants \( g \), \( \bar{g}_0 \), \( \bar{g}_1 \), and \( \bar{g}_2 \), see Eq. (VI-59). For \( \text{LYUKA}=2 \) or 3, the direct matrix elements of the Yukawa interaction (VI-59) are, in addition, added to the self-consistent mean field. For \( \text{LYUKA}=2 \) or 4, the exchange matrix elements are added. For \( \text{IYUTYP}=1 \), expression (VI-61) is used, while for \( \text{IYUTYP}=2 \), an analogous six-Gaussian expression is used without the short-range correction (VI-58), that is, for \( f(r) = 1 \). For \( \text{LYUKA}=0 \), all these input data are ignored and the Yukawa interaction is not taken into account.

Figures 1 and 2 show the actual CPU times required in calculations using the Skyrme and Yukawa interactions, respectively. At \( N_0 = 10 \), the latter take more than two orders of magnitude longer and, moreover, their CPU times scale like \( N_0^7 \) rather than \( N_0^4 \). A local EDF clearly makes for easier computing.

![Figure 1: The hfodd CPU times required for calculations that use the standard Skyrme EDF, shown as a function of the number of HO shells \( N_0 \). The doubly logarithmic scale in the Figure, shows that these times scale as \( N_0^4 \).](image)

**2.2.29. Keyword: COULOMBPAR**

\( 7, 1, 1 = \text{ICOTYP}, \text{ICOUDI}, \text{ICOUEX} \)

For \( \text{ICOUDI}=0, 1, \) or 2, the Coulomb direct energy and Coulomb direct mean field are neglected, calculated by using the Green-function method, see Section I-5, or calculated by using the Gaussian-expansion method, see Section VI-2.10, respectively. Similarly, for \( \text{ICOUEX}=0, 1, \) or 2, the Coulomb exchange energy and Coulomb exchange mean field are neglected, calculated by using the Slater approximation (I-19) or calculated exactly by using the Gaussian-expansion method, see Section VI-2.10, respectively. For the Gaussian-expansion method, that is, for \( \text{ICOUDI}=2 \) or \( \text{ICOUEX}=2 \), positive values of \( \text{ICOTYP} \) denote the numbers of Gauss-Legendre nodes used in the integral of Eq. (VI-103). For \( \text{ICOUDI}=2 \) or \( \text{ICOUEX}=2 \), the iteration can later be smoothly continued (\( \text{IFCONT}=1 \), see the keyword CONTFIELDS) only by saving the matrix.
Figure 2: Same as in Figure 1 but for calculations that use the Yukawa interaction. The CPU times scale as $N_0^7$.

Elements of the mean field, that is, by requesting IWRIFI=1, see the keyword FIELD_SAVE. Therefore, ICOUDI=2 or ICOUEX=2 and ICONTI=1 requires IFCONT=1.

In Fig. 3 the error in the exact Coulomb exchange energy is plotted as function of the number of Gauss-Legendre nodes $N_C$. A quite precise estimate is obtained for $N_C = 7$ Gauss-Legendre nodes and the machine precision is obtained by doubling this number (along with doubling the CPU time). For $N_C = 7$, these CPU times are shown in Fig. 4, which illustrates the fact that these times scale with the number of HO shells as $N_0^7$.

Figure 3: Errors in the exact Coulomb exchange energy plotted in function of the number of Gauss-Legendre nodes $N_C$. 
Figure 4: Same as in Figure 1 but for the calculations that determine the exact Coulomb exchange energies. The CPU times scale as $N_0^7$.

2.2.30. **Keyword**: INSERT_HO

\[ 0 = \text{IPOTHO} \]

For $\text{IPOTHO}=1$, an external HO potential is added to the self-consistent mean field. Parameters of the potential are identical to those defining the HO basis.
2.3. Symmetries

This section lists keywords pertaining to selection of conserved, broken, and restored symmetries.

2.3.1. Keyword: SIMPLEXY

\[ 1 = \text{ISIMPY} \]

For \( \text{ISIMPY} = 1 \), calculation with \( y \)-simplex conserved are performed, while for \( \text{ISIMPY} = 0 \) the simplex is broken. Value of \( \text{ISIMPY} \) must be consistent with switches \( \text{IPARTY}, \text{ISIGNY}, \text{ISIMTY}, \) and \( \text{IROTAT} \), see Tables 1 and 2.

2.3.2. Keyword: SIGNATUREY

\[ 1 = \text{ISIGNY} \]

For \( \text{ISIGNY} = 1 \), calculation with signature conserved are performed, while for \( \text{ISIGNY} = 0 \) the signature is broken. Value of \( \text{ISIGNY} \) must be consistent with switches \( \text{ISIMPY}, \text{IPARTY}, \text{ISIMTX}, \) and \( \text{ISIMTZ} \), see Tables 1 and 3.

2.3.3. Keyword: PARITY

\[ -1 = \text{IPARTY} \]

For \( \text{IPARTY} = 1 \), calculation with parity conserved are performed, while for \( \text{IPARTY} = 0 \) the parity is broken. Value of \( \text{IPARTY} \) must be consistent with switches \( \text{ISIMPY} \) and \( \text{ISIGNY} \), see Table 1. For \( \text{IPARTY} = -1 \) (the compatibility mode), the code sets \( \text{IPARTY} = \text{ISIGNY} \) and requires that \( \text{ISIMPY} = 1 \).

2.3.4. Keyword: ROTATION

\[ 1 = \text{IROTAT} \]

For \( \text{IROTAT} = 1 \), calculation with time-reversal breaking are performed, while for \( \text{IROTAT} = 0 \) the time-reversal symmetry is conserved. In the latter case the calculations are performed only for one value of the simplex, \( s = +i \), which gives almost twice shorter CPU times. \( \text{IROTAT} = 0 \) is incompatible with providing a non-zero value of the angular frequency or with attempting calculation for odd or odd-odd nuclei without pairing, \( \text{IPAIRI} = 0 \). \( \text{IROTAT} = 1 \) is incompatible with \( \text{IPABCS} > 0 \), i.e., the rotating solutions can be obtained for the HFB pairing but not for the BCS pairing.
Table 1: Primary set of conserved and nonconserved symmetries allowed in the code HFODD version (v2.40h).

| Option | Symmetries | Switches |
|--------|------------|----------|
|        | $\hat{S}_y$ | $\hat{R}_y$ | $\hat{P}$ | ISIMPY | ISIGNY | IPARTY |
| P1     | conserved  | conserved  | conserved | 1 | 1 | 1 |
| P2     | conserved  | nonconserved | nonconserved | 1 | 0 | 0 |
| P3     | nonconserved | conserved  | nonconserved | 0 | 1 | 0 |
| P4     | nonconserved | nonconserved | conserved  | 0 | 0 | 1 |
| P5     | nonconserved | nonconserved | nonconserved | 0 | 0 | 0 |

Table 2: Secondary set of conserved and nonconserved symmetries allowed in the code HFODD version (v2.40h).

| Option | Symmetries | Switches |
|--------|------------|----------|
|        | $\hat{S}_y$ | $\tilde{T}$ | $\hat{S}_y^T$ | ISIMPY | ITIREV | ISIMTY |
| S1     | conserved  | conserved  | conserved | 1 | 1 | 1 |
| S2     | conserved  | nonconserved | nonconserved | 1 | 0 | 0 |
| S3     | nonconserved | conserved  | nonconserved | 0 | 1 | 0 |
| S4     | nonconserved | nonconserved | conserved  | 0 | 0 | 1 |
| S5     | nonconserved | nonconserved | nonconserved | 0 | 0 | 0 |

Table 3: Ternary set of conserved and nonconserved symmetries allowed in the code HFODD version (v2.40h).

| Option | Symmetries | Switches |
|--------|------------|----------|
|        | $\hat{R}_y$ | $\tilde{S}_x^T$ | $\tilde{S}_z^T$ | ISIGNY | ISIMTX | ISIMTZ |
| T1     | conserved  | conserved  | conserved | 1 | 1 | 1 |
| T2     | conserved  | nonconserved | nonconserved | 1 | 0 | 0 |
| T3     | nonconserved | conserved  | nonconserved | 0 | 1 | 0 |
| T4     | nonconserved | nonconserved | conserved  | 0 | 0 | 1 |
| T5     | nonconserved | nonconserved | nonconserved | 0 | 0 | 0 |
2.3.5. Keyword: **TIMEREVERS**

\[ 0 = ITIREV \]

For $ITIREV=1$, calculation with time-reversal conserved are performed, while for $ITIREV=0$ this symmetry is broken. This switch is used only as a convenient replacement of switch $IROTAT$; $ITIREV=1$ is equivalent to $IROTAT=0$ and $ITIREV=0$ is equivalent to $IROTAT=1$.

---

2.3.6. Keyword: **TSIMPLEX_Y**

\[ -1 = ISIMTY \]

For $ISIMTY=1$, calculation with $y$-simplex$^T$ conserved are performed, while for $ISIMTY=0$ this symmetry is broken. Value of $ISIMTY$ must be consistent with switches $ISIMPY$ and $IROTAT$, see Table 2. For $ISIMTY=-1$ (the compatibility mode), the code sets $ISIMTY$ to $1-IROTAT$ and requires that $ISIMPY=1$.

---

2.3.7. Keyword: **TSIMPLEXES**

\[ 1, 1 = ISIMTX, ISIMTZ \]

For $ISIMTX=1$ and/or $ISIMTZ=1$, calculation with conserved symmetries given by $x$-simplex$^T$ and/or $z$-simplex$^T$ are performed, respectively. These symmetries are broken for $ISIMTX=0$ and $ISIMTZ=0$. Values of $ISIMTX$ and $ISIMTZ$ must be consistent with that of $ISIGNY$, see Table 3.

---

2.3.8. Keyword: **TSIMPLEX3D**

\[ 1, -1, 1 = ISIMTX, ISIMTY, ISIMTZ \]

This keyword allows to simultaneously input all the three switches that define the three $T$-simplexes. It is equivalent to using keywords **TSIMPLEXES** and **TSIMPLEX_Y** together.

---

2.3.9. Keyword: **PAIRING**

\[ 0 = IPAIRI \]

For $IPAIRI=0$, calculation without pairing correlations (pure HF) are performed, while for $IPAIRI=1$ the pairing correlations are included. In the latter case, for $IPAHFB=0$ or 1 pairing is included within the BCS or HFB method, respectively. $IPAIRI=1$ requires either $IPAHFB=1$ or $IPABCS>0$ and is incompatible with simultaneously setting $IPAHFB=1$ and $IPABCS>0$, i.e., the HFB pairing and BCS pairing cannot be used simultaneously. $IPAIRI=1$ is incompatible with $IROTAT=1$, unless $IPAHFB=1$, i.e., the rotating solutions can be obtained for the HFB pairing but not for the BCS pairing.
2.3.10. Keyword: HFB

\[ 0 = \text{IPAHFB} \]

For \( \text{IPAHFB}=1 \), calculation with pairing correlations included by solving the HFB equation are performed. \( \text{IPAHFB}=1 \) requires \( \text{IPAIRI}=1 \).

2.3.11. Keyword: BCS

\[ -1 = \text{IPABCS} \]

Parameter \( \text{IPABCS} \) defines the type of BCS pairing calculations. For \( \text{IPABCS}=0, 1, 2, \) or 3, the BCS pairing calculations are, respectively, not performed, performed with the seniority pairing force, performed with fixed pairing gaps, or performed with the state-dependent pairing gaps. Value of \( \text{IPABCS}=-1 \) is allowed for the sake of compatibility with earlier versions of the code, before (v2.13f). Then, \( \text{IPABCS}=0 \) is set for \( \text{IPAHFB}=1 \) and \( \text{IPABCS}=\text{IPAIRI} \) is set for \( \text{IPAHFB}=0 \).

For \( \text{IPABCS}=1 \) the code HFODD solves the BCS equations with the neutron and proton pairing strengths defined in Ref. [9]. These values can be modified by defining the multiplicative factors FACTGN and FACTGP for neutrons and protons, respectively. For \( \text{IPABCS}=2 \), the BCS pairing calculations are performed with fixed values of the neutron or proton pairing gaps equal to DELFIN or DELFIP, respectively. For \( \text{IPABCS}=3 \), the BCS pairing calculations are performed with state-dependent pairing gaps corresponding to the pairing matrix elements (see the keyword PAIRMATRI) calculated for the contact forces defined in the same way as for the HFB pairing calculations.

Positive values of \( \text{IPABCS} \) require \( \text{IPAIRI}=1 \) and \( \text{IPAHFB}=0 \) and are incompatible with rotations \( \text{IROTAT}=1 \) or broken simplex \( \text{ISIMPY}=0 \). \( \text{IPABCS}=2 \) requires \( \text{IDEFIN}=\text{IDEFIP}=1 \).

2.3.12. Keyword: FILSIG_NEU

\[ 2, 2, 2, 2, 1, 1, 1, 1, 0, 0, 0, 0 = \]
\[ \text{KPFILG}(0,0,0), \text{KPFILG}(0,1,0), \text{KPFILG}(1,0,0), \text{KPFILG}(1,1,0), \]
\[ \text{KHFIKG}(0,0,0), \text{KHFIKG}(0,1,0), \text{KHFIKG}(1,0,0), \text{KHFIKG}(1,1,0), \]
\[ \text{KOFILG}(0,0,0), \text{KOFILG}(0,1,0), \text{KOFILG}(1,0,0), \text{KOFILG}(1,1,0) \]

These parameters govern the filling approximation for the neutron single-particle parity–signature configurations. Matrices \( \text{KPFILG} \) contain the indices of particle states in the four parity–signature blocks denoted by \((+,+), (+,-), (-,+), \) and \((-,-), \) of given (parity,signature) combinations, i.e., \( (\pi, r) = (+,+,+), (+,-,-), (-,+,+), \) and \((-,-,-), \) respectively. Matrices \( \text{KHFIKG} \) contain analogous indices of hole states, and matrices \( \text{KOFILG} \) contain numbers of particles put into the states between \( \text{KHFIKG} \) and \( \text{KPFILG} \), by using for them partial occupation factors of \( \text{KOFILG}/(\text{KPFILG}–\text{KHFIKG}+1)/2 \). For \( \text{KOFILG}=0 \), in the given parity–signature block the filling approximation is inactive. The filling approximation is incompatible with pairing correlations, \( \text{IPAIRI}=1 \).
2.3.3. Symmetries

2.3.13. Keyword: **FILSIG** _PRO_

\[2, 2, 2, 2, 1, 1, 1, 0, 0, 0 = KPFILG(0,0,1), KPFILG(0,1,1), KPFILG(1,0,1), KPFILG(1,1,1),\]
\[KHFILG(0,0,1), KHFILG(0,1,1), KHFILG(1,0,1), KHFILG(1,1,1),\]
\[KOFIGL(0,0,1), KOFIGL(0,1,1), KOFIGL(1,0,1), KOFIGL(1,1,1)\]

Same as above but for the proton single-particle parity–signature configurations.

2.3.14. Keyword: **INI** _INVERS_

\[0, 0 = INIINV, INIKAR\]

Allowed values of **INI** _KAR_ = 0, 1, 2, or 3 and **INI** _INV_ = 0, 1, 2, or 3 correspond to the following initial \(D^{T}_{2h}\) transformations:

| INIINV  | INIKAR=0 | INIKAR=1 | INIKAR=2 | INIKAR=3 |
|---------|----------|----------|----------|----------|
| INIINV=0 | \(I\)   | \(R_x\)  | \(R_y\)  | \(R_z\)  |
| INIINV=1 | \(\hat{P}\)  | \(\hat{S}_x\)  | \(\hat{S}_y\)  | \(\hat{S}_z\)  |
| INIINV=2 | \(\hat{T}\)  | \(\hat{R}_x\)  | \(\hat{R}_y\)  | \(\hat{R}_z\)  |
| INIINV=3 | \(\hat{P}\)  | \(\hat{S}_x\)  | \(\hat{S}_y\)  | \(\hat{S}_z\)  |

where \(\hat{P}\) is the space inversion, \(\hat{T}\) is the time-reversal symmetry, \(\hat{R}_k\) is the signature (rotation by angle \(\pi\) about the \(k = x, y,\) or \(z\) axis), and \(\hat{R}_k^T = \hat{P}\hat{T}, \hat{S}_k = \hat{P}\hat{R}_k\) (simplex), \(\hat{T}_k = \hat{T}\hat{R}_k\) (\(k\)-signature\(^T\)), and \(\hat{S}_k^T = \hat{T}\hat{S}_k\) (\(k\)-simplex\(^T\)). For **INI** _KAR_ = **INI** _INV_ = 0, no transformation is performed and this option is inactive.

Transformations are performed at the level of the densities, after the first iteration. As a security measure, nonzero values of **INI** _KAR_ and **INI** _INV_ require **NOITER** = 1. Such values also require **SLOWEV** _SLOWOD_ _SLOWPA_ = 0.0, so as not to mix the old and new potentials corresponding to the original and transformed densities, respectively. They are also incompatible with **IPRGCm** _̸= 0_.

A given initial \(D^{T}_{2h}\) transformation must be accompanied by the correspondingly broken symmetries, that is, **INI** _INV_ = 1 or 3 requires **IROTAT** = 1 and **INI** _INV_ = 2 or 3 requires **IPARTY** = 0.

2.3.15. Keyword: **INI** _ROTAT_

\[0, 0, 0, 0, 0, 0 = ALPNI, BETI, GAINI, INIROT\]

For **INI** _ROTAT_ = 1, the wave functions are rotated by the Euler angles \(\alpha, \beta,\) and \(\gamma\) corresponding, respectively, to **ALPNI**, **BETI**, and **GAINI** (all in degrees). Transformations are performed at the level of the densities, after the first iteration. As a security measure, **INI** _ROTAT_ = 1 requires **NOITER** = 1. It also requires **SLOWEV** _SLOWOD_ _SLOWPA_ = 0.0, so as not to mix the old and new potentials corresponding to the original and transformed densities, respectively. **INI** _ROTAT_ = 1 is incompatible with **IPRGCm** _̸= 0_ and requires a spherical HO basis of \(\bar{h}\omega_x = \bar{h}\omega_y = \bar{h}\omega_z\).
A rotation about the z axis must be accompanied by the broken signature, that is, \textit{ALPINI} \neq 0 or \textit{GAMINI} \neq 0 requires \textit{ISIGNY}=0.

### 2.3.16. Keyword: \textit{PROJECTGCM}

\begin{align*}
0, 0, 1, 1, 0, 1, 1, 0 \\
\text{IPRGCM, IPROMI, IPROMA, NUAKNO, NUBKNO, KPROJE, IFRWAV, ITOWAV, IWRWAV}
\end{align*}

For \textit{IPRGCM}=1 and 2, the code calculates the diagonal and non-diagonal GCM kernels, respectively. In addition, for \textit{NUAKNO} \neq 1 or \textit{NUBKNO} \neq 1, the AMP kernels are calculated, as described in Section VI-2.1, although in the present version (v2.40h) this option is not yet available for non-diagonal kernels of \textit{IPRGCM}=2. The angular momentum projection (AMP) is performed for doubled angular momenta from \textit{IPROMI} to \textit{IPROMA} and requires a spherical HO basis of \( h\omega_x = h\omega_y = h\omega_z \). For even (odd) particle number \textit{IN\_FIX}+\textit{IZ\_FIX}, \textit{IPROMI}, \textit{IPROMA}, and \textit{KPROJE} must be even (odd). For \textit{IPRGCM}=1 and 2, the present version (v2.40h) also requires \textit{IROTAT}=1 and \textit{IPAIRI}=0.

The AMP has been tested up to the values of angular momenta of 70\( \hbar \), and therefore, \textit{IPROMA} must not be larger than 2\( \times \)70=140. After further tests, higher values could be used by increasing the parameter \textit{JMAX}=70 in function \textit{DSMALG}, which calculates the Wigner functions, see Eqs. (VI-1), (VI-4), and (VI-5).

\textit{NUAKNO} is the number of Gauss-Tchebyschev nodes, which are used to perform integrations over the \( \alpha \) and \( \gamma \) Euler angles. For \textit{NUAKNO}=1, these integrations are not performed (1D AMP) and the states are assumed to be axial with the doubled projection of the angular momentum on the z axis equal to \textit{KPROJE}. \textit{NUBKNO} is the number of Gauss-Legendre nodes, which are used to perform integrations over the \( \beta \) Euler angle. For \textit{NUAKNO}>1 and \textit{NUBKNO}>1, a full 3D AMP is performed and the value of \textit{KPROJE} is ignored. \textit{NUAKNO}>1 requires \textit{ISIMPY}=0 and \textit{ISIGNY}=0. \textit{IPROMA} must be larger than the absolute value of \textit{KPROJE}.

For \textit{IPRGCM}=2, the code calculates the GCM kernels between the states labeled by three-digit indices from "000" to "999". Indices of the "left" states vary between \textit{IFRWAV} and \textit{ITOWAV}, and these states are read from the disc. The index of the "right" state equals to \textit{ITOWAV}, and this state is equal to the current state. In addition, for \textit{IWRWAV}=1, the current state is saved on the disc with the index of \textit{ITOWAV}. This allows for a simultaneous calculation of the "right" state along with calculating its kernels with all previously calculated and stored "left" states. The states can also be stored on disc without calculating kernels in the given run, that is, by setting the value of \textit{ITOWAV} along with \textit{IWRWAV}=1 and \textit{IPRGCM}=0. Names of files on the disc are composed by concatenating the three-digit index, ",-", and \textit{FILWAV}.

### 2.3.17. Keyword: \textit{SAVEKERNEL}

\begin{align*}
0 = \text{ISAKER}
\end{align*}
For \( \text{ISAKER}=1 \), the code attempts reading the kernel files \( Nxxx-Lyyy-Rzzz-//\text{FILKER} \), where // denotes concatenated strings. The three-digit indices are:

- \( xxx \) is the consecutive index of the kernel file,
- \( yyy \) is the index of the left wave function,
- \( zzz \) is the index of the right wave function.

In the work directory, the file names for all indices \( xxx \) are scanned, starting from 001. The kernels stored in these files are read into memory and are not recalculated. The kernels that have not been found in the kernel files are calculated and stored in the kernel file with the lowest available index \( xxx \). In this way, one can submit many parallel jobs, see the keyword \text{PARAKERNEL} \), that calculate kernels for different values of the Euler angles \( \alpha, \beta, \text{and} \gamma \). The results are then collected in different kernel files with indices \( xxx \) attributed automatically. If any of the jobs is terminated before completing its task, the same input data can be resubmitted and the calculation automatically continues from the point where it has been interrupted. Once all the kernels will have been calculated, which requires a large CPU time, the AMP can be performed within a very small CPU time by reading, again automatically, all the created kernel files. \( \text{ISAKER}=1 \) requires \( \text{IPRGCM}>0 \)

### 2.3.18. Keyword: \text{CHECKERNEL}

\[ 1 = \text{ICHKER} \]

The names of kernel files are saved within these files. As a security measure, when reading the kernel files, their names are cross-checked against the saved information. This cross-checking can be deactivated by using \( \text{ICHKER}=0 \). This option is useful whenever the kernel files have been renamed for any reason.

### 2.3.19. Keyword: \text{PARAKERNEL}

\[ 0, 1, 1, 1, 1 = \text{IPAKER}, \text{NUASTA}, \text{NUASTO}, \text{NUGSTA}, \text{NUGSTO} \]

For \( \text{IPAKER}=1 \), the code only calculates kernels for different values of the Euler angles \( \alpha, \beta, \text{and} \gamma \) and the AMP is suspended. Calculations are performed for the Gauss-Tchebyschev nodes in the Euler angle \( \alpha \) from \( \text{NUASTA} \) to \( \text{NUASTO} \), for those in the Euler angle \( \gamma \) from \( \text{NUGSTA} \) to \( \text{NUGSTO} \), and for all the Gauss-Legendre nodes in the Euler angle \( \beta \), that is, from 1 to \( \text{NUBKNO} \). For \( \text{IPAKER}=1 \), to save memory, the code can be compiled with \( \text{IPARAL}=1 \). \( \text{IPAKER}=1 \) requires \( \text{IPRGCM}>0 \) and \( \text{ISAKER}=1 \). Values of \( \text{NUASTA}, \text{NUASTO}, \text{NUGSTA}, \text{NUGSTO} \) must all be between 1 and \( \text{NUAKNO} \) and must be ordered as \( \text{NUASTA} \leq \text{NUASTO} \) and \( \text{NUGSTA} \leq \text{NUGSTO} \).

### 2.3.20. Keyword: \text{TRANSITION}

\[ 2, 1, 0 = \text{NMURED}, \text{NMARED}, \text{NSIRED} \]

Maximum numbers of transition electric, transition magnetic, and transition surface or Schiff moments, respectively, for which proton kernels and reduced matrix elements are calculated,
printed, and stored in the kernel files. \texttt{NMARED} and \texttt{NSIRED} must not exceed \texttt{NMURED}. For \texttt{NMURED}=0, \texttt{NMARED}=0, or \texttt{NSIRED}, the corresponding proton kernels and reduced matrix elements are not calculated.

2.3.21. **Keyword:** \texttt{CUTOVERLAP}

\[0, 10^{-10}, 1. = \texttt{ICUTOV, CUTOVE, CUTOVF}\]

For \texttt{ICUTOV}=0, parameters \texttt{CUTOVE} and \texttt{CUTOVF} are ignored and the collective states for the \(K\)-mixing calculation, Eq. (VI-10), are selected by their norm eigenvalues \(n_m\) being larger than the negative of the smallest norm eigenvalue \(Ovemin\). For \texttt{ICUTOV}=1, the collective states are selected by their norm eigenvalues being larger than \texttt{CUTOVE+CUTOVF*Ovemin}.

2.3.22. **Keyword:** \texttt{LIPKIN}

\[0, 0 = \texttt{LIPKIN, LIPKIP}\]

For \texttt{LIPKIN}=1 and/or \texttt{LIPKIP}=1, the Lipkin-Nogami corrections are included for neutrons and/or protons, respectively, see Section VI-29. In the present version (v2.40h), \texttt{LIPKIN}=1 or \texttt{LIPKIP}=1 requires \texttt{IPAHFB}=1.

2.3.23. **Keyword:** \texttt{INI\_LIPKIN}

\[0.1, 0.1 = \texttt{FE2INI}(0), \texttt{FE2INI}(1)\]

For \texttt{IPCONT}=0, or \texttt{IPCONT}=1 and \texttt{ILCONT}=0, the Lipkin-Nogami calculations are started by using the initial values of the neutron and proton Lipkin-Nogami parameters \(\lambda_2\) (VI-98), \texttt{FE2INI}(0) and \texttt{FE2INI}(1), respectively. For \texttt{IPCONT}=1 and \texttt{ILCONT}=1, values of \texttt{FE2INI} are ignored.

2.3.24. **Keyword:** \texttt{FIXLAMB2\_N}

\[0.1, 0 = \texttt{FE2FIN}, \texttt{IF2FIN}\]

For \texttt{IF2FIN}=1, the neutron Lipkin-Nogami calculations are performed by using the fixed value of the neutron Lipkin-Nogami parameter \(\lambda_2\) (VI-98) equal to \texttt{FE2FIN}. \texttt{IF2FIN}=1 requires \texttt{LIPKIN}=1.

2.3.25. **Keyword:** \texttt{FIXLAMB2\_P}

\[0.1, 0 = \texttt{FE2FIP}, \texttt{IF2FIP}\]

Same as above but for the proton Lipkin-Nogami calculations.
2.3.26. Keyword: SLOWLIPKIN

\[ 0.5 = \text{SLOWLI} \]

\text{SLOWLI} gives the value of the mixing fraction \( \epsilon \) used for the Lipkin-Nogami parameter \( \lambda_2 \) (VI-98), in analogy to the \text{SLOWEV}, \text{SLOWOD} and \text{SLOWPA} parameters.

2.3.27. Keyword: FIXFERMI\_N

\[ -8.0, 0 = \text{FERFIN, IFEFIN} \]

For IFEFIN=1, the HFB pairing calculations are performed with a fixed value of the neutron Fermi energy equal to \text{FERFIN}. In the present version (v2.40h), IFEFIN=1 requires IPAHFB=1.

2.3.28. Keyword: FIXFERMI\_P

\[ -8.0, 0 = \text{FERFIP, IFEFIP} \]

Same as above but for the proton HFB pairing calculations.
2.4. Configurations with no conserved symmetries

This section lists keywords pertaining to definitions of configurations in the case when no symmetries are conserved, and the single-particle or single-quasiparticle space is divided into two charge blocks (neutrons and protons).

2.4.1. Keyword: `PHNONE_NEU`

\[ 1, 00, 00 = \text{NUPAHO}, \text{KPNONE}, \text{KHNONE} \]

Neutron particle-hole excitations pertaining to the situation when all neutrons are in one common block (no simplex, signature, or parity is conserved). `NUPAHO` is the consecutive number from 1 to 5 (up to five sets of excitations can be specified in separate items). Particles are removed from the `KHNONE`-th state and put in the `KPNONE`-th state. At every stage of constructing excitations the Pauli exclusion principle has to be respected (particle removed from an occupied state and put in an empty state). Values equal zero have no effect. Note that for all neutrons sitting in one common block the reference configuration from which the particle-hole excitations are counted is defined by the total number of neutrons. These particle-hole excitations are ignored unless `ISIMPY=0, IPARTY=0, and IPAIRI=0`.

2.4.2. Keyword: `PHNONE_PRO`

\[ 1, 00, 00 = \text{NUPAHO}, \text{KPNONE}, \text{KHNONE} \]

Same as above but for the proton particle-hole excitations.

2.4.3. Keyword: `DIANON_NEU`

\[ 2, 1, 0 = \text{KPFLIZ}, \text{KHFLIZ}, \text{KOFLIZ} \]

The diabatic blocking of neutron single-particle configurations in the situation when all neutrons are in one common block. The rules to define the blocking are analogous to those described for the conserved parity, keyword `DIAPAR_NEU`.

2.4.4. Keyword: `DIANON_PRO`

\[ 2, 1, 0 = \text{KPFLIZ}, \text{KHFLIZ}, \text{KOFLIZ} \]

Same as above but for the diabatic blocking of proton single-particle configurations in the situation when all protons are in one common block.

2.4.5. Keyword: `BLOCKSIZ_N`

\[ 1, 0 = \text{INSIZN}, \text{IDSIZN} \]
2.4. Configurations with no conserved symmetries

For $|IDSIZN|=1$, the code performs the neutron quasiparticle blocking calculations in the case when no symmetries are conserved, see Section VI-2.7. For $IDSIZN=+1$ or $-1$, the blocked quasiparticle state is selected by having the largest overlap with the $INSIZN$-th neutron single-particle eigenstate of the HFB mean-field Routhian or with its time-reversed partner, respectively. Note that for rotating states, the time-reversed eigenstate is not necessarily an eigenstate of the Routhian. $|IDSIZN|=1$ requires $ISIMPY=0$, $IPARTY=0$, $IPAHFB=1$, and $IROTAT=1$.

2.4.6. Keyword: BLOCKSIZ_P

$1, 0 = INSIZP, IDSIZP$

Same as above but for the proton quasiparticle blocking. For odd-odd nuclei, neutron and proton quasiparticles can be simultaneously blocked.
2.5. Configurations with conserved simplex

This section lists keywords pertaining to definitions of configurations in the case when simplex is conserved, and the single-particle or single-quasiparticle space is divided into four charge-simplex blocks (neutrons and protons with simplexes \( s=\pm i \)).

2.5.1. Keyword: \texttt{VACSIM\_NEU}

\[ 43, 43 = \texttt{KVASIM}(0), \texttt{KVASIM}(1) \]

Numbers of lowest neutron states occupied in the two simplex blocks, denoted by \( (+) \) and \( (-) \), of given simplexes, \( s=+i \) and \( s=-i \), respectively. These numbers define the simplex reference configuration from which the particle-hole excitations are counted. The definitions of simplex reference configuration and excitations are ignored unless \( \texttt{ISIMPY}=1, \texttt{ISIGNY}=0, \texttt{IPAIRI}=0 \).

2.5.2. Keyword: \texttt{VACSIM\_PRO}

\[ 33, 33 = \texttt{KVASIM}(0), \texttt{KVASIM}(1) \]

Same as above but for the numbers of proton states.

2.5.3. Keyword: \texttt{PHSIMP\_NEU}

\[ 1, 00, 00, 00, 00 = \texttt{NUPAHO}, \texttt{KPSIMP}, \texttt{KPSIMM}, \texttt{KHSIMP}, \texttt{KHSIMM} \]

Neutron particle-hole excitations in the simplex blocks. \texttt{NUPAHO} is the consecutive number from 1 to 5 (up to five sets of excitations can be specified in separate items). Particles are removed from the \texttt{KHSIMP}-th state in the \( (+) \) block and from the \texttt{KHSIMM}-th state in the \( (-) \) block, and put in the \texttt{KPSIMP}-th state in the \( (+) \) block and in the \texttt{KPSIMM}-th state in the \( (-) \) block. At every stage of constructing excitations the Pauli exclusion principle has to be respected (particle removed from an occupied state and put in an empty state). Values equal zero have no effect. In practice, reasonable excitations can only be constructed by consulting the printed lists of single-particle states with their consecutive numbers in given blocks. These particle-hole excitations are ignored unless \( \texttt{ISIMPY}=1, \texttt{ISIGNY}=0, \texttt{IPAIRI}=0 \).

2.5.4. Keyword: \texttt{PHSIMP\_PRO}

\[ 1, 00, 00, 00, 00 = \texttt{NUPAHO}, \texttt{KPSIMP}, \texttt{KPSIMM}, \texttt{KHSIMP}, \texttt{KHSIMM} \]

Same as above but for the proton particle-hole excitations.
2.5.5. Keyword: DIASIM_NEU

\[2, 2, 1, 1, 0, 0 = \text{KPFLIM}(0,0), \text{KPFLIM}(1,0), \]
\[\text{KHFLIM}(0,0), \text{KHFLIM}(1,0), \]
\[\text{KOFLIM}(0,0), \text{KOFLIM}(1,0)\]

The diabatic blocking of neutron single-particle simplex configurations. Matrices KPFLIM contain the indices of the particle states in the two simplex blocks denoted by (+) and (−), of given simplex values, i.e., \(s=+i\) and \(−i\), respectively. Matrices KHFLIM contain analogous indices of the hole states, and matrices KOFLIM define types of blocking in analogy to those shown in Table 4.

2.5.6. Keyword: DIASIM_PRO

\[2, 2, 1, 1, 0, 0 = \text{KPFLIM}(0,1), \text{KPFLIM}(1,1), \]
\[\text{KHFLIM}(0,1), \text{KHFLIM}(1,1), \]
\[\text{KOFLIM}(0,1), \text{KOFLIM}(1,1)\]

Same as above but for the diabatic blocking of proton single-particle simplex configurations.

2.5.7. Keyword: BLOCKSIM_N

\[1, 0, 0 = \text{INSIMN}, \text{IRSIMN}, \text{IDSIMN}\]

For \(|\text{IDSIMN}|=1\), the code performs the neutron quasiparticle blocking calculations in the case when simplex is conserved, see Section VI-2.7. For \(\text{IDSIMN}=+1\) or \(−1\), the blocked quasiparticle state is selected by having the largest overlap with the \(\text{INSIMN}\)-th neutron single-particle eigenstate of the HFB mean-field Routhian in a given simplex block or with its time-reversed partner, respectively. The simplex of the state, \(+i\) or \(−i\), is defined by \(\text{IRSIMN}=0\) or 1, respectively. \(|\text{IDSIMN}|=1\) requires \(\text{ISIMPY}=1\), \(\text{IPARTY}=0\), \(\text{IPAHFB}=1\), and \(\text{IROTAT}=1\).

2.5.8. Keyword: BLOCKSIM_P

\[1, 0, 0 = \text{INSIMP}, \text{IRSIMP}, \text{IDSIMP}\]

Same as above but for the proton quasiparticle blocking. For odd-odd nuclei, neutron and proton quasiparticles can be simultaneously blocked.
2. INPUT DATA FILE

2.6. Configurations with conserved parity

This section lists keywords pertaining to definitions of configurations in the case when parity is conserved, and the single-particle or single-quasiparticle space is divided into four charge–parity blocks (neutrons and protons with parities \( \pi = \pm 1 \)).

2.6.1. Keyword: \texttt{VACPAR\_NEU}

\[ 44, 42 = KVASIQ(0), KVASIQ(1) \]

Numbers of lowest neutron states occupied in the two parity blocks, denoted by \(+1\) and \((-1)\), of given parities, \(\pi = +1\) and \(\pi = -1\), respectively. These numbers define the parity reference configuration from which the particle-hole excitations are counted. The definitions of parity reference configuration and excitations are ignored unless \(\text{IPARTY}=1\), or \(\text{IPARTY}=-1\) and \(\text{ISIMPY}=\text{ISIGNY}=1\). They are also ignored for \(\text{ISIMPY}=1\) and \(\text{IPAIRI}=1\).

2.6.2. Keyword: \texttt{VACPAR\_PRO}

\[ 32, 34 = KVASIQ(0), KVASIQ(1) \]

Same as above but for the numbers of proton states.

2.6.3. Keyword: \texttt{PHPARI\_NEU}

\[ 1, 00, 00, 00, 00 = \text{NUPAHO}, \text{KPSIQP}, \text{KPSIQM}, \text{KHSIQP}, \text{KHSIQM} \]

Neutron particle-hole excitations in the parity blocks. \texttt{NUPAHO} is the consecutive number from 1 to 5 (up to five sets of excitations can be specified in separate items). Particles are removed from the \texttt{KHSIQP}-th state in the \(+1\) block and from the \texttt{KHSIQM}-th state in the \((-1)\) block, and put in the \texttt{KPSIQP}-th state in the \(+1\) block and in the \texttt{KPSIQM}-th state in the \((-1)\) block. At every stage of constructing excitations the Pauli exclusion principle has to be respected (particle removed from an occupied state and put in an empty state). Values equal zero have no effect. These particle-hole excitations are ignored unless \(\text{ISIMPY}=0\), \(\text{IPARTY}=1\), and \(\text{IPAIRI}=0\).

2.6.4. Keyword: \texttt{PHPARI\_PRO}

\[ 1, 00, 00, 00, 00 = \text{NUPAHO}, \text{KPSIQP}, \text{KPSIQM}, \text{KHSIQP}, \text{KHSIQM} \]

Same as above but for the proton particle-hole excitations.
2.6. Configurations with conserved parity

2.6.5. Keyword: **DIAPAR_NEU**

\[ 2, 2, 1, 1, 0, 0 = \begin{align*}
&\text{KPFLIQ}(0,0), \text{KPFLIQ}(1,0), \\
&\text{KHFLIQ}(0,0), \text{KHFLIQ}(1,0), \\
&\text{KOFLIQ}(0,0), \text{KOFLIQ}(1,0)
\end{align*} \]

The diabatic blocking of neutron single-particle parity configurations. Matrices \text{KPFLIQ} contain the indices of the particle states in the two parity blocks denoted by (+1) and (−1), of given parities, i.e., \(\pi=+1\) and \(\pi=-1\), respectively. Matrices \text{KHFLIQ} contain analogous indices of the hole states, and matrices \text{KOFLIQ} define the type of blocking according to definitions shown in Table 4.

Table 4: Values of parameter \text{KOFLIQ} that specify type of blocking in case of conserved parity. Analogous values define type of blocking for other conserved symmetries.

| \text{KOFLIQ} | Definition |
|---------------|------------|
| 0             | No diabatic blocking in the given parity block. |
| +1            | The state which has the *larger* y-alignment is occupied. |
| −1            | The state which has the *smaller* y-alignment is occupied. |
| +2            | The state which has the *larger* y-intrinsic spin is occupied. |
| −2            | The state which has the *smaller* y-intrinsic spin is occupied. |
| +3            | The state which has the *larger* x-alignment is occupied. |
| −3            | The state which has the *smaller* x-alignment is occupied. |
| +4            | The state which has the *larger* x-intrinsic spin is occupied. |
| −4            | The state which has the *smaller* x-intrinsic spin is occupied. |
| +5            | The state which has the *larger* z-alignment is occupied. |
| −5            | The state which has the *smaller* z-alignment is occupied. |
| +6            | The state which has the *larger* z-intrinsic spin is occupied. |
| −6            | The state which has the *smaller* z-intrinsic spin is occupied. |
| +7            | The state which has the *larger* o-alignment is occupied. |
| −7            | The state which has the *smaller* o-alignment is occupied. |
| +8            | The state which has the *larger* o-intrinsic spin is occupied. |
| −8            | The state which has the *smaller* o-intrinsic spin is occupied. |
| +9            | The state which has the *larger* multipole moment \(Q_{20}\) is occupied. |
| −9            | The state which has the *smaller* multipole moment \(Q_{20}\) is occupied. |
| +10           | The state which has the *larger* multipole moment \(Q_{22}\) is occupied. |
| −10           | The state which has the *smaller* multipole moment \(Q_{22}\) is occupied. |

Here, the \(x\)-, \(y\)-, and \(z\)-alignments or intrinsic spins denote projections of the total angular momentum or spin, respectively, on the \(x\), \(y\), and \(z\) axes. Similarly, the \(o\)-alignment or \(o\)-intrinsic spin denotes analogous projections on the direction of the angular frequency \(\omega_J\).

Within the diabatic blocking procedure one does not predefine whether the particle or the hole state is occupied (as is the case when the particle-hole excitations are defined, see Section 3.4 of II). In each iteration the code calculates the average alignments (or average intrinsic spins, or average quadrupole moments) of both states (those defined by \text{KPFLIM} and \text{KHFLIM}), and occupies that state for which a larger, or a smaller value is obtained. Therefore, the order...
of both states in the Routhian spectrum is irrelevant.

The user is responsible for choosing the particle-state indices (in $\text{KPFLIM}$) only among those corresponding to empty single-particle states, and the hole-state indices (in $\text{KHFLIM}$) only among those corresponding to occupied single-particle states.

2.6.6. **Keyword: DIAPAR.PRO**

\[2, 2, 1, 1, 0, 0 = \text{KPFLIQ}(0,1), \text{KPFLIQ}(1,1),\]
\[\text{KHFLIQ}(0,1), \text{KHFLIQ}(1,1),\]
\[\text{KOFLIQ}(0,1), \text{KOFLIQ}(1,1)\]

Same as above but for the diabatic blocking of proton single-particle parity configurations.

2.6.7. **Keyword: BLOCKSIQ_N**

\[1, 0, 0 = \text{INSIQN}, \text{IPSIQN}, \text{IDSIGN}\]

For $|\text{IDSIGN}|=1$, the code performs the neutron quasiparticle blocking calculations in the case when parity is conserved. For $\text{IDSIGN}=+1$ or $-1$, the blocked quasiparticle state is selected by having the largest overlap with the $\text{INSIQN}$-th neutron single-particle eigenstate of the HFB mean-field Routhian in a given parity block or with its time-reversed partner, respectively. The parity of the state, $+1$ or $-1$, is defined by $\text{IPSIQN}=0$ or 1, respectively. $|\text{IDSIGN}|=1$ requires $\text{ISIMPY}=0$, $\text{IPARTY}=1$, $\text{IPAHFB}=1$, and $\text{IROTAT}=1$.

2.6.8. **Keyword: BLOCKSIQ_P**

\[1, 0, 0 = \text{INSIQP}, \text{IPSIQP}, \text{IDSIQP}\]

Same as above but for the proton quasiparticle blocking. For odd-odd nuclei, neutron and proton quasiparticles can be simultaneously blocked.
2.7. Configurations with conserved parity and signature

This section lists keywords pertaining to definitions of configurations in the case when parity and signature are conserved, and the single-particle or single-quasiparticle space is divided into eight charge–parity–signature blocks (neutrons and protons with parities $\pi=\pm 1$ and signatures $r=\pm i$).

2.7.1. Keyword: VACSIG_NEU

$\begin{align*}
22, 22, 21, 21 &= \text{KVASIG}(0,0), \text{KVASIG}(0,1), \text{KVASIG}(1,0), \text{KVASIG}(1,1) \\
\end{align*}$

Numbers of lowest neutron states occupied in the four parity–signature blocks, denoted by $(+,+), (+,-), (-,+), \text{ and } (-,-), \text{ of given (parity,signature) combinations, i.e., } (\pi, r) = (+1,+i), (+1,-i), (-1,+i), \text{ and } (-1,-i), \text{ respectively. These numbers define the parity–signature reference configuration from which the particle-hole excitations are counted. The definitions of parity–signature reference configuration and excitations are ignored unless ISIMPY}=1, \text{ ISIGNY}=1, \text{ and } \text{IPAIRI}=0.

2.7.2. Keyword: VACSIG_PRO

$\begin{align*}
16, 16, 17, 17 &= \text{KVASIG}(0,0), \text{KVASIG}(0,1), \text{KVASIG}(1,0), \text{KVASIG}(1,1) \\
\end{align*}$

Same as above but for the numbers of proton states.

2.7.3. Keyword: PHSIGN_NEU

$\begin{align*}
1, 00,00,00,00, 00,00,00,00 &= \text{NUPAHO}, \text{ KPPPSP}, \text{ KPPPSM}, \text{ KPPMSP}, \text{ KPPMSM}, \text{ KHPPSP}, \text{ KHPPPSM}, \text{ KHPMSP}, \text{ KHPMSM} \\
\end{align*}$

Neutron particle-hole excitations in the parity–signature blocks. Basic principles are the same as for the excitations in the parity blocks. Particles are removed from the KHPMSP-th state in the $(+,+) \text{ block, from the KHPPSP-th state in the } (-,+) \text{ block, and from the KHPPMS-th state in the } (-,+), \text{ and put in the KPPPSP-th state in the } (+,+) \text{ block, in the KPPPSM-th state in the } (+,+) \text{ block, in the KPPMSP-th state in the } (-,+), \text{ and in the KPPMSM-th state in the } (-,+) \text{ block. These particle-hole excitations are ignored unless ISIMPY}=1, \text{ ISIGNY}=1, \text{ and } \text{IPAIRI}=0.
2.7.4. **Keyword:** `PHSIGN_PRO`

```
1, 00,00,00,00, 00,00,00,00 = NUPAHO,  
KPPPSP, KPPPSM, KPPMSP, KPPMSM,  
KHPGPS, KHPSPS, KHPMSP, KHPMSM
```

Same as above but for the proton particle-hole excitations.

2.7.5. **Keyword:** `DIASIG_NEU`

```
2, 2, 2, 2, 1, 1, 1, 1, 0, 0, 0, 0 =  
KPFLIG(0,0,0), KPFLIG(0,1,0), KPFLIG(1,0,0), KPFLIG(1,1,0),  
KHFLIG(0,0,0), KHFLIG(0,1,0), KHFLIG(1,0,0), KHFLIG(1,1,0),  
KOFLIG(0,0,0), KOFLIG(0,1,0), KOFLIG(1,0,0), KOFLIG(1,1,0)
```

The diabatic blocking of neutron single-particle parity–signature configurations. Matrices `KPFLIG` contain the indices of particle states in the four parity–signature blocks denoted by (+,+), (−,+), (−,−), and (+,−), of given (parity,signature) combinations, i.e., \((\pi, r) = (+1, +i), (1,−i), (−1, +i), (−1,−i)\) respectively. Matrices `KHFLIG` contain analogous indices of hole states, and matrices `KOFLIG` define the type of blocking according to Table 4. Other rules described for the parity case apply here analogously.

2.7.6. **Keyword:** `DIASIG_PRO`

```
2, 2, 2, 2, 1, 1, 1, 1, 0, 0, 0, 0 =  
KPFLIG(0,0,1), KPFLIG(0,1,1), KPFLIG(1,0,1), KPFLIG(1,1,1),  
KHFLIG(0,0,1), KHFLIG(0,1,1), KHFLIG(1,0,1), KHFLIG(1,1,1),  
KOFLIG(0,0,1), KOFLIG(0,1,1), KOFLIG(1,0,1), KOFLIG(1,1,1)
```

Same as above but for the diabatic blocking of proton single-particle parity–signature configurations.

2.7.7. **Keyword:** `BLOCKSIG_N`

```
1, 0, 0, 0 = INSIGN, IPSIGN, ISSIGN, IDSIGN
```

For \(|IDSIGN| = 1\), the code performs the neutron quasiparticle blocking calculations in the case when parity and signature are conserved. For \(IDSIGN = +1\) or \(-1\), the blocked quasiparticle state is selected by having the largest overlap with the `INSIGN`-th neutron single-particle eigenstate of the HFB mean-field Routhian in a given parity–signature block or with its time-reversed partner, respectively. The parity of the state, \(+1\) or \(-1\), is defined by `IPSIGN = 0` or `1`, respectively. The signature of the state, \(+i\) or \(-i\), is defined by `ISSIGN = 0` or `1`, respectively. \(|IDSIGN| = 1\) requires `ISIMPY = 1`, `IPARTY = 1`, `IPAHFB = 1`, and `IROTAT = 1`. 
2.7.8. Keyword: \texttt{BLOCKSIGP}

\[ 1, 0, 0, 0 = \text{INSIGP, IPSIGP, ISSIGP, IDSIGP} \]

Same as above but for the proton quasiparticle blocking. For odd-odd nuclei, neutron and proton quasiparticles can be simultaneously blocked.
2.8. Configurations

This section lists keywords pertaining to definitions of configurations in the case when any combination of parity and signature symmetry is conserved.

2.8.1. Keyword: BLOCKFIX_N

\[ 0, 0 = \text{IFIBLN}, \text{INIBLN} \]

For \( \text{IFIBLN}=1 \), the neutron quasiparticle blocking is based on calculating overlaps with a fixed single-particle wave function. The method is based on beginning the iteration by defining the number of the single-particle state, that is, \( \text{INSIGN}, \text{INSIMN}, \text{INSIQN}, \) or \( \text{INSIZN} \), depending on the selected symmetry conditions. Then, for \( \text{INIBLN}=1 \) this one single-particle wave function is stored in memory and on the record file, and in consecutive iterations the overlaps are calculated with respect to this fixed single-particle wave function. Therefore, subsequent changes in the ordering and structure of single-particle states do not affect the blocking mechanism. For \( \text{INIBLN}=0 \), in the first iteration this fixed single-particle wave function is not initialized, but it is read from the record file. \( \text{IFIBLN}=1 \) requires \( |\text{IDSIGN}|=1, |\text{IDSIMN}|=1, |\text{IDSIQN}|=1, \) or \( |\text{IDSIZN}|=1, \) depending on the selected symmetry conditions. \( \text{IFIBLN}=1 \) and \( \text{INIBLN}=0 \) requires \( \text{ICONTI}=1. \)

2.8.2. Keyword: BLOCKFIX_P

\[ 0, 0 = \text{IFIBLP}, \text{INIBLP} \]

Same as above but for the proton quasiparticle blocking.
2.9. Miscellaneous parameters

This section lists keywords pertaining to definitions of parameters specifying various numerical conditions of the code execution.

2.9.1. Keyword: MAX_MULTIP

\[ 2, 4, 4 = \text{NMUCON, NMUCOU, NMUPRI} \]

Maximum multipolarities \( \lambda \) of multipole moments used in the code for the constraints, Eq. (15), surface term of the Coulomb mean field, and printed on the output, respectively. Values not larger than \( \lambda=9 \) are currently allowed. In case of the conserved parity, only even multipoles are used in the Coulomb mean field.

2.9.2. Keyword: MAX_SURFAC

\[ 0, 0 = \text{NSICON, NSIPRI} \]

Maximum multipolarities \( \lambda \) of surface multipole moments, used in the code for the constraints, Eq. (15), and printed on the output, respectively. Values not larger than \( \lambda=7 \) are currently allowed.

2.9.3. Keyword: MAX_MAGNET

\[ 0, 0 = \text{NMACON, NMAPRI} \]

Same as above but for the magnetic moments. In version (v2.40h) constraints on magnetic moments are not yet implemented, which requires \( \text{NMACON}=0 \). Values not larger than \( \lambda=9 \) are currently allowed.

2.9.4. Keyword: COULOMB

\[ 80, 79, 0.25 = \text{NUMCOU, NUMETA, FURMAX} \]

\( \text{NUMCOU} \) gives the number of points \( N_{\text{Coul}} \), Eq. (I-100), used when summing up the Coulomb Green function. The dimensionless parameter \( d \) defining the size of the Coulomb parallelepiped, Eqs. (I-102) and (I-96), is given by \( \text{NUMCOU} \times \text{FURMAX} \). \( \text{NUMETA} \) gives the order of the Simpson integration of the solid harmonics on the faces of the parallelepiped, see Sec. I-5.

2.9.5. Keyword: SLOW-DOWN

\[ 0.5, 0.5 = \text{SLOWEV, SLOWOD} \]

The standard prescription to calculate the HF potential in the next iteration is to mix a given fraction \( \epsilon \) of the HF potentials from the previous iteration, with the fraction \( 1-\epsilon \) of potentials
calculated in the current iteration. \texttt{SLOWEV} and \texttt{SLOWOD} give the values of the mixing fractions $\epsilon$, separately for the time-even and time-odd potentials. This mixing slows down the convergence, and is necessary for the convergence of the iterative procedure.

### 2.9.6. Keyword: \texttt{SLOW-PAIR}

\[ 0.5 = \texttt{SLOWPA} \]

Similarly as in the particle-hole channel, \texttt{SLOWPA} gives the value of the mixing fraction $\epsilon$ used in the pairing channel, in analogy to \texttt{SLOWEV} and \texttt{SLOWOD}.

### 2.9.7. Keyword: \texttt{EPS\_HERMIT}

\[ 1.0\times10^{-14} = \texttt{EPSHER} \]

Numerical precision requested for determining values of Hermite polynomials.

### 2.9.8. Keyword: \texttt{OPTI\_GAUSS}

\[ 1 = \texttt{IOPTGS} \]

For \texttt{IOPTGS=1} and \texttt{IREAWS=0}, expression $L_\mu = 2N_\mu + 2$ is used to calculate the order of the Gauss-Hermite integration $L_\mu$ from the maximum number $N_\mu$ of HO quanta in the direction $\mu=x$, $y$, or $z$, and the input parameters \texttt{NXHERM}, \texttt{NYHERM}, and \texttt{NZHERM} are ignored.

### 2.9.9. Keyword: \texttt{GAUSHERMIT}

\[ 18, 18, 32 = \texttt{NXHERM}, \texttt{NYHERM}, \texttt{NZHERM} \]

Orders $L_x$, $L_y$, and $L_z$ of the Gauss-Hermite integration in three Cartesian directions. Must be even. Ignored if \texttt{IOPTGS=0} or \texttt{IREAWS=1}.

### 2.9.10. Keyword: \texttt{BROYDEN}

\[ 0, 7, 0.8, 1000. = \texttt{IBROYD}, \texttt{N\_ITER}, \texttt{ALPHAM}, \texttt{BROTRI} \]

For \texttt{IBROYD=1}, the Broyden method is used to accelerate the convergence, see Section VI-2.8. For \texttt{IBROYD=0}, or \texttt{IBROYD=1} and \texttt{N\_ITER=0}, variables \texttt{N\_ITER}, \texttt{ALPHAM}, and \texttt{BROTRI}, which are read on this line, are ignored, that is, the previous values are kept. \texttt{N\_ITER} is the number of iterations used to approximate the inverse Jacobian, \texttt{ALPHAM} is the value of the parameter $\alpha$ of the linear mixing to which is added the Broyden correction, and \texttt{BROTRI} triggers an automatic switch to the Broyden method, that is, when the absolute value of the stability energy becomes lower than \texttt{BROTRI}, iterations are changed to the Broyden scheme. A large value of \texttt{BROTRI} ensures that the Broyden method is used from the very first iteration. \texttt{IBROYD=1} is incompatible
with $I_{YUKA}>0$, $ICOUDI=2$, or $ICOUEX=2$. The Broyden method is implemented only in the FORTRAN-90 version of HFODD.
2. INPUT DATA FILE

2.10. Parameters of the HO basis

This section lists keywords pertaining to definitions of parameters of the HO basis.

2.10.1. Keyword: **BASIS_SIZE**

\[ 15, 301, 800.0 = \text{NOSCIL, NLIMIT, ENECUT} \]

The HO basis is composed of states having not more than \( N_0 = \text{NOSCIL} \) quanta in either of the Cartesian directions, and not more than \( M = \text{NLIMIT} \) states in total. The states are added to the basis according to the increasing energy of the deformed harmonic oscillator,

\[
\epsilon_{n_x n_y n_z} = \hbar \omega_x (n_x + \frac{1}{2}) + \hbar \omega_y (n_y + \frac{1}{2}) + \hbar \omega_z (n_z + \frac{1}{2}).
\]  

(12)

In case of degenerate HO states (e.g., for an axially deformed HO) the complete multiplets are included, so the actual number of states \( \text{LDBASE} \) can be slightly larger than \( \text{NLIMIT} \). If \( \text{NLIMIT}=0 \), it is set to the number of states up to \( \text{NOSCIL} \) spherical HO shells, that is, \( \text{NLIMIT} = ((\text{NOSCIL}+1) * (\text{NOSCIL}+2) * (\text{NOSCIL}+3))/6 \). If \( \text{NLIMIT} \geq 0 \), the cutoff energy \( \text{ENECUT} \) is ignored; otherwise all states having HO energy smaller then \( \text{ENECUT} \) are included in the basis, and \( \text{NLIMIT} \) is ignored.

2.10.2. Keyword: **HOMEGAZERO**

\[ 1.2 = \text{FCHOM0} \]

The code uses the standard value of the spherical HO frequency \( \hbar \omega_0 = 41 \text{ MeV}/A^{1/3} \) multiplied by the scaling factor \( f = \text{FCHOM0} \).

2.10.3. Keyword: **SURFAC_PAR**

\[ 86, 66, 1.23 = \text{INNUMB, IZNUMB, ROPARM} \]

The code \texttt{HFODD} calculates parameters of the HO basis, and the zero-iteration Nilsson potential, by defining the standard nuclear surface \( \Sigma \),

\[
\Sigma : R(\theta, \phi) = c(\alpha) \left[ 1 + \sum_{\lambda=0}^{\lambda_{max}} \sum_{\mu=-\lambda}^{\lambda} \alpha_{\lambda \mu} Y_{\lambda \mu}(\theta, \phi) \right],
\]  

(13)

corresponding to the volume \( \frac{4}{3} \pi \alpha^3 \text{ROPARM}^3 (\text{INNUMB} + \text{IZNUMB}) \), where \( c(\alpha) \) is a function of \( \alpha_{\lambda \mu} \) such that the volume enclosed by the surface \( \Sigma \) does not depend on \( \alpha \), i.e., in particular \( c(0) = R_0 = \text{ROPARM} (\text{INNUMB} + \text{IZNUMB})^{1/3} \).
2.10.4. Keyword: **SURFAC\_DEF**

\[ 2, 0, 0.61 = \text{LAMBDA, MIU, ALPHAR} \]

The code defines frequencies of the deformed HO in three directions by using relation \( \omega_x R_x = \omega_y R_y = \omega_z R_z \), where \( R_\mu \) are the lengths of principal axes of the nuclear surface \( \Sigma \) \[13\] defined by real deformation parameters \( \alpha_\lambda \mu = \text{ALPHAR} (\text{LAMBDA, MIU}) \). The overall factor is defined by \((\omega_x \omega_y \omega_z)^{1/3} = \omega_0 \).
2.11. Constraints on angular momentum

This section lists keywords pertaining to definitions of constraints on angular momentum. The complete cranking term in the energy density functional is given by:

\[ E_{\text{cran}} = \sum_{a=x,y,z} \left[ -\omega_{J0a} \langle \hat{J}_{0a} \rangle + C_Ja \left( \langle \hat{J}_{0a} \rangle - \bar{J}_{0a} \right)^2 - \omega_{J1a} \langle \hat{J}_{1a} \rangle \right] + C_A \left( \frac{\omega_{J0} \times \langle \hat{J}_0 \rangle}{\omega_{J0}} \right)^2. \]  \hspace{1cm} (14)

2.11.1. Keyword: OMEGAY

0.5 = OMEGAY

Isoscalar angular frequency \( \omega_{J0y} \) in the \( y \) direction, see Eq. (14). A non-zero value of OMEGAY requires IROTAT=1 and cannot be used for the BCS pairing, i.e., for IPAIRI=1 and IPAHFB=0.

2.11.2. Keyword: OMISOY

0.00 = OMISOY

Same as above for the isovector angular frequency \( \omega_{J1y} \) in the \( y \) direction.

2.11.3. Keyword: OMEGA_XYZ

0.00, 0.00, 0.00, 0 = OMEGAX, OMEGAY, OMEGAZ, ITILAX

For ITILAX=1, values of the three Cartesian components of the isoscalar angular frequency vector \( \omega_{J0} \), see Eq. (14). For ITILAX=0 these values are ignored. ITILAX=1 requires IROTAT=1, ISIMPY=0, and IPAIRI=0. A non-zero value of OMEGAX, OMEGAY, or OMEGAZ requires broken symmetry ISIMTX=0, ISIMTY=0, or ISIMTZ=0, respectively.

2.11.4. Keyword: OMEGA_RTP

0.00, 0.00, 0.00, 0 = OMERAD, OMETHE, OMEPHI, ITILAX

Same as above but for values of the standard spherical components of the isoscalar angular frequency, i.e., \( \omega_{J0r} \), \( \omega_{J0\theta} \), and \( \omega_{J0\phi} \).

2.11.5. Keyword: OMISO_XYZ

0.00, 0.00, 0.00, 0 = OMISOX, OMISOY, OMISOZ, ITISAX

For ITISAX=1, values of the three Cartesian components of the isovector angular frequency vector \( \omega_{J1} \), see Eq. (14). For ITISAX=0 these values are ignored. ITISAX=1 requires IROTAT=1,
2.11. Constraints on angular momentum

**ISIMPY**=0, and **IPAIRI**=0. A non-zero value of **OMISOX**, **OMISOY**, or **OMISOZ** requires broken symmetry **ISIMTX**=0, **ISIMTY**=0, or **ISIMTZ**=0, respectively.

### 2.11.6. Keyword: OMEGA_TURN

\[ 0 = \text{IMOVA}_X \]

For **IMOVA**=1 or \(-1\), the isoscalar angular frequency vector \( \omega J_0 \) is in each iteration set in the direction of the total angular momentum \( J_0 \), or opposite to this direction, respectively, while its length is kept equal to that fixed by the sum of squares of **OMEGAX**, **OMEGAY**, and **OMEGAZ**. For **IMOVA**=0, vector \( \omega J_0 \) is not changed during the iteration. **IMOVA**=1 or \(-1\) requires **ITILAX**=1, **ITISAX**=0, and **IFLAGA**=0.

### 2.11.7. Keyword: SPINCONSTR

\[ 0.0, 0.0, 0 = \sigma^{(2)}, a^{(2)}, i^{(2)} \]

For **IFLAGI**(2)=1, the quadratic constraint on spin is used together with the linear constraint. Values of **STIFFI**(2) and **ASKEDI**(2) correspond respectively to \( C_{J_0y} \) and \( \bar{J}_{0y} \) in Eq. (14). For **IFLAGI**(2)=0, there is no quadratic constraint on spin. This keyword is maintained only for compatibility reasons; in version (v2.40h) of the code HFODD it has been replaced by **SPICON_XYZ**.

### 2.11.8. Keyword: SPICON_XYZ

\[ 0.0, 0.0, 0 = \sigma^{(1)}, a^{(1)}, i^{(1)}, \sigma^{(2)}, a^{(2)}, i^{(2)}, \sigma^{(3)}, a^{(3)}, i^{(3)} \]

Same as above but for quadratic constraints in the \( x \), \( y \), and \( z \) directions corresponding to **IFLAGI**(1)=1, **IFLAGI**(2)=1, and **IFLAGI**(3)=1, respectively. **IFLAGI**(1)=1, **IFLAGI**(2)=1, or **IFLAGI**(3)=1 requires broken symmetry **ISIMTX**=0, **ISIMTY**=0, or **ISIMTZ**=0, respectively.

### 2.11.9. Keyword: SPICON_OME

\[ 0.0, 0.0, 0 = \sigma^{(1)}, a^{(1)}, i^{(1)}, \sigma^{(2)}, a^{(2)}, i^{(2)}, \sigma^{(3)}, a^{(3)}, i^{(3)} \]

For **IFLAGA**=1, the quadratic constraint on the angle between the angular frequency and angular momentum vectors, see Eq. (14). In version (v2.40h) the angle is constrained to zero. Value of **STIFFA** corresponds to \( C_A \) in Eq. (14). Value of **ASKEDA** must be set to 0; this variable is reserved for a future implementation of the constraint to a non-zero angle. For **IFLAGA**=0, there is no quadratic constraint on the angle. **IFLAGA**=1 requires **ISIMPY**=0, **IROTAT**=1, **ITILAX**=1, **ITISAX**=0, **IFLAGI**(1)=0, **IFLAGI**(2)=0, **IFLAGI**(3)=0, and a non-zero value of sum of squares of **OMEGAX**, **OMEGAY**, and **OMEGAZ**.
2.11.10. **Keyword: **`NORBCONSTR`

    0 = **NO.ORB**

For **NO.ORB**=1, constraints on the intrinsic spin only are used and the orbital part of the angular momentum is not constrained. **NO.ORB**=1 requires **IROTAT**=1.
2.12. Constraints on multipole moments

This section lists keywords pertaining to definitions of constraints on multipole moments and surface multipole moments. The complete multipole constraint term in the energy density functional is given by:

$$\mathcal{E}_{\text{mult}} = \sum_{\lambda\mu} C_{\lambda\mu} \left( \langle \hat{Q}_{\lambda\mu} \rangle - \bar{Q}_{\lambda\mu} \right)^2 + \sum_{\lambda\mu} C^S_{\lambda\mu} \left( \langle \hat{Q}^S_{\lambda\mu} \rangle - \bar{Q}^S_{\lambda\mu} \right)^2. \tag{15}$$

The multipole and surface multipole moments are defined as

$$Q_{\lambda\mu}(r) = a_{\lambda\mu} r^\lambda Y^*_{\lambda\mu}(\theta, \phi), \tag{16}$$

and

$$Q^S_{\lambda\mu}(r) = a_{\lambda\mu} r^{\lambda+2} Y^*_{\lambda\mu}(\theta, \phi), \tag{17}$$

respectively, where $Y_{\lambda\mu}$ are the standard spherical harmonics in the convention of Ref. [10]. For $\lambda \leq 2$, factors $a_{\lambda\mu}$ are listed in Table 5 while for $\lambda > 2$ $a_{\lambda\mu} = 1$.

Table 5: Adopted definitions of the normalization factors $a_{\lambda\mu}$ and the corresponding multipole moments $Q_{\lambda\mu}$.

| $\lambda$ | $\mu$ | $a_{\lambda\mu}$ | $Q_{\lambda\mu}$ |
|-----------|-------|-----------------|----------------|
| 0         | 0     | $\sqrt{4\pi}$  | 1              |
| 1         | 0     | $\sqrt{4\pi}/3$| $z$            |
| 1         | 1     | $-\sqrt{8\pi}/3$| $x - iy$       |
| 2         | 0     | $\sqrt{16\pi}/5$| $2z^2 - x^2 - y^2$ |
| 2         | 1     | $-\sqrt{8\pi}/15$| $zx - izy$     |
| 2         | 2     | $\sqrt{32\pi}/5$| $\sqrt{3}(x^2 - y^2 - 2ixy)$ |

2.12.1. Keyword: MULTCONSTR

2, 0, 0.01, 42.0, 1 = LAMBDA, MIU, STIFFQ, QASKED, IFLAGQ

For IFLAGQ=1, the total multipole moment of the given multipolarity $\lambda$ and $\mu$ is constrained. Values of LAMBDA, MIU, STIFFQ, and QASKED correspond respectively to $\lambda$, $\mu$, $C_{\lambda\mu}$, and $Q_{\lambda\mu}$ in Eq. (15). For IFLAGQ=0, there is no constraint in the given multipolarity.

2.12.2. Keyword: SURFCONSTR

2, 0, 0.0, 0.0, 0 = LAMBDA, MIU, STIFFS, SASKED, IFLAGS
For $\text{IFLAGS}=1$, the total surface multipole moment of the given multipolarity $\lambda$ and $\mu$ is constrained. Values of $\text{LAMBDA}$, $\text{MIU}$, $\text{STIFFS}$, and $\text{SASKED}$ correspond respectively to $\lambda$, $\mu$, $C_{\lambda\mu}^S$, and $\bar{Q}_{\lambda\mu}^S$ in Eq. (15). For $\text{IFLAGS}=0$, there is no constraint in the given multipolarity. For $\text{IFLAGS}=2$ or 3, only the neutron or proton, respectively, surface multipole moments are constrained. For all constrained multiplicities, values of $\text{IFLAGS}$ must be the same.

## 2.12.3. Keyword: MULTCONSCA

$1, 0., 0., 0 = \text{LAMBDA}$, $\text{STIFFG}$, $\text{GASKED}$, $\text{IFLAGG}$

For $\text{IFLAGG}=1$, the total scalar multipole moment of the given multipolarity $\lambda$ is constrained. Values of $\text{LAMBDA}$, $\text{STIFFG}$, and $\text{GASKED}$ correspond, respectively, to $\lambda$, $C_{\lambda}$, and $\bar{Q}_{\lambda}$ in Eq. (VI-80). For $\text{IFLAGG}=0$, there is no scalar constraint in the given multipolarity. The constrained multipolarity $\text{LAMBDA}$ cannot be equal to 0 or exceed $\text{NMUCON}$. For conserved parity $\text{IPARTY}=1$, only even moments can be constrained.

## 2.12.4. Keyword: BOHR_BETAS

$4, 0, 1 = \text{NEXBET}$, $\text{IPRIBE}$, $\text{IPRIBL}$

For a given set of electric multipole moments, the code calculates and prints the corresponding first-order (for $\text{IPRIBL}=1$) and/or exact (for $\text{IPRIBE}=1$) Bohr deformation parameters, see Section VI-2.5. For $\text{IPRIBE}=1$, in case the code fails to find the exact values, the first-order values are printed irrespective of the value of $\text{IPRIBL}$. The exact values are sought for multiplicities up to $\text{NEXBET}$, which must not be greater than $\text{NMUPRI}$. The approximate values are printed up to multipolarity of $\text{NMUPRI}$.

## 2.12.5. Keyword: SCHIFF_MOM

$0 = \text{ISCHIF}$

For $\text{ISCHIF}=1$, the surface multipole moments are everywhere in the code replaced by the Schiff moments, see Section VI-2.6.
2.13. Output-file parameters

This section lists keywords pertaining to definitions of parameters specifying character of information printed on the output file.

2.13.1. Keyword: PRINT-ITER

1, 0, 1 = IPRSTA, IPRMID, IPRSTO

The code prints results for the first, middle, and/or last iteration if the corresponding parameters IPRSTA, IPRMID, and IPRSTO equal 1.

2.13.2. Keyword: PRINT-MOME

1, 1, 1 = IPRI_N, IPRI_P, IPRI_T

The code prints values of the neutron, proton, and total moments (multipole moments, surface multipole moments, or magnetic moments) only if the corresponding parameters IPRI_N=1, IPRI_P=1, and IPRI_T=1, respectively.

2.13.3. Keyword: PRINT-INTR

1 = INTRIP

The code prints the values of moments (multipole moments, surface multipole moments, or magnetic moments) and angular momenta in the intrinsic frame only if INTRIP=1.

2.13.4. Keyword: EALLMINMAX

-12.0, 0.0 = EMINAL, EMAXAL

The code prints tables of single-particle properties for states with values of the single-particle Routhians between EMINAL and EMAXAL. No table is printed unless EMINAL ≤ EMAXAL.

2.13.5. Keyword: EQUASI_MAX

10.0 = EMAXQU

The code prints tables of quasiparticle properties for the HFB states with values of the quasiparticle energies smaller than EMAXQU. No table is printed unless EMAXQU>0.
2.13.6. Keyword: **HFBMEANFLD**

\[ 0 = IMFHFB \]

For \( IMFHFB = 1 \), eigenvalues of the HFB mean-field single-particle Hamiltonian or Routhian are printed. \( IMFHFB = 1 \) requires \( IPAHFB = 1 \).

2.13.7. Keyword: **PRINT** _AMP_

\[ 0, 999, 1, 1, 1, 0, 0 \]

\[ ISLPRI, ISUPRI, IENPRI, ISRPRI, IMIPRI, IKEPRI, IRMPRI \]

These parameters govern the printing of the AMP results. If not restricted by the values of the doubled angular momenta for which the calculations are performed, \( IPROMI \) and \( IPROMA \), the results are printed only for the doubled angular momenta between \( ISLPRI \) and \( ISUPRI \). For \( IENPRI = 1 \), the AMP energies are printed. In addition, for \( IENPRI = 2 \), the AMP kernels are also printed. For \( ISRPRI = 1 \), the sum rules are printed and compared with the HF average values. For \( IMIPRI = 1 \), the energies of the \( K \)-mixed states are printed. For \( IKEPRI = 1 \) and/or \( IRMPRI = 1 \), the proton reduced kernels and/or reduced matrix elements, respectively, are printed.

2.13.8. Keyword: **TRANCUTPRI**

\[ 0., 0., 0., = QMUCUT, QMACUT, QSICUT \]

Values of the proton kernels and reduced matrix elements for the transition electric, transition magnetic, and transition surface or Schiff moments are printed only if their absolute values are larger than, respectively, \( QMUCUT \), \( QMACUT \), and \( QSICUT \). This option is meant to avoid printing long lists of very small or zero values.

2.13.9. Keyword: **ONE** _LINE_

\[ 1 = I1LINE \]

For \( I1LINE \neq 0 \), a one-line convergence report is printed at each iteration. For \( I1LINE = 1 \), the code prints the values of deformation \( \gamma \), total angular momentum, total angular frequency \( \omega \), and angle between vectors of angular momentum and frequency. For \( I1LINE = 2 \), the code prints the values of neutron and proton pairing gaps and Lipkin-Nogami parameters \( \lambda_2 \).

2.13.10. Keyword: **PRINT_VIOL**

\[ 0 = IVIPRI \]

For \( IVIPRI = 1 \), the code prints integrals of several symmetry-violating terms. \( IVIPRI = 1 \) requires \( IROTAT = 1 \).
2.13.11. Keyword: **NILSSONLAB**

\[ 3 = \text{NILXYZ} \]

This option used for **NILXYZ**=1, 2, or 3, allows for printing the Nilsson labels defined with respect to the \( x \), \( y \), or \( z \) axis, respectively. This feature is useful when the axial symmetry axis of a nucleus and its angular momentum are aligned along the \( x \) or \( y \) axis and not along the \( z \) axis, for which the standard Nilsson labels are defined. This is particularly important for analyzing configurations of band heads of odd nuclei within the conserved \( y \)-signature-symmetry limit.
2.14. Files

This section lists keywords that define files used by the code.

2.14.1. Keyword: REVIEWFILE

HFODD.REV = FILREV

CHARACTER*68 file name of the review file. Must start at the 13-th column of the data line. The ASCII review file is written after calculating every data set (i.e., once per every EXECUTE item), provided IREVIE > 0. The file is not rewound, so the results for several data sets can be accumulated in a single file. This is so provided the filename FILREV is not changed between the EXECUTE items. The file contains all relevant parameters and results of calculation in a form suitable for reading by another program. It is meant as an interface to programs which analyze and/or plot the results. The file contains sections defined by keywords (different than keywords used in the input data file described here). The detailed structure of the review file is not documented in the present write up, and can be inferred from inspecting the specimen produced by the sample run, and from the subroutine REVIEW.

2.14.2. Keyword: REVIEW

2 = IREVIE

The review file is not written if IREVIE=0. For IREVIE=2, the table of single-particle properties is included in the review file in addition to other results, which are written for IREVIE=1.

2.14.3. Keyword: REPLAYFILE

HFODD.REP = FILREP

CHARACTER*68 file name of the replay file. Must start at the 13-th column of the data line. The binary replay file with the name defined in FILREP must exist if ICONTI=1, and will be read. If the filenames FILREP and FILREC are identical, the replay file will be subsequently overwritten as a new record file. These feature is implemented to facilitate chaining of jobs which follow one another.

2.14.4. Keyword: RECORDFILE

HFODD.REC = FILREC

CHARACTER*68 file name of the record file. Must start at the 13-th column of the data line. If IWRIRE=1, binary record file is written after each HF iteration. It contains complete information which allows restarting the iteration in another run of the code. To restart, one has to specify ICONTI=1 and provide the name of the file by defining FILREP. In case of the computer crash, or upon a successful completion of the given input data set, the record file contains the results
of the last performed iteration. The file is always rewound before it is written, so the results for consecutive iterations do not pile up.

2.14.5. Keyword: RECORDSAVE

\[ 1 = \text{IWRIRE} \]

For \text{IWRIRE} = 1, the record file is saved on disc after each iteration is completed. For \text{IWRIRE} = 0, it is saved only once, after all iterations are completed. This option is useful on systems where the speed of writing large amounts of data to disc could hamper the system performance. For \text{IWRIRE} = -1, the record file is never saved, and the run cannot be later continued.

2.14.6. Keyword: WOODSAFILE

\text{WOODS.WFN} = \text{FILWOO}

\text{CHARACTER*68} file name of the Woods-Saxon file. Must start at the 13-th column of the data line. This file is read provided \text{IREAWS} = 1. The binary Woods-Saxon file constitutes an interface between the Woods-Saxon code and the code \text{HFODD}. It contains the Woods-Saxon wave functions and numerous other parameters which define the current calculation. \text{The parameters read from the Woods-Saxon file overwrite the values provided in the input data file.} Since the current version of the Woods-Saxon code will be published separately, the feature of starting the iteration from the Woods-Saxon results is not documented in the present write up.

2.14.7. Keyword: COULOMFILE

\text{HFODD.COU} = \text{FILCOU}

\text{CHARACTER*68} file name of the Coulomb file containing auxiliary data for a faster calculation of the Coulomb mean field. Must start at the 13-th column of the data line. Parameters \text{NUMCOU}, \text{NUMETA}, and \text{FURMAX} which define the calculations of the Coulomb direct potential (see Secs. I-5 and II-3.5) are usually kept unchanged for the whole series of calculations in one region of nuclei. Therefore, many Coulomb auxiliary results can be calculated only once, and stored in the file \text{FILCOU}. Handling of this file is determined by the input parameters \text{ICOULI} and \text{ICOULO}.

2.14.8. Keyword: COULOMSAVE

\[ 0,0 = \text{ICOULI, ICOULO} \]

Input parameters \text{ICOULI} and \text{ICOULO} determine actions pertaining to reading and/or writing of the Coulomb file \text{FILCOU}, according to the following table:
2. INPUT DATA FILE

| ICOULI | ICOULO | Action                          |
|--------|--------|---------------------------------|
| 0      | 0      | neither read nor write the Coulomb file |
| 1      | 0      | read, but do not write the Coulomb file |
| 0      | 1      | do not read, but write the Coulomb file |
| 1      | 1      | use automated handling of the Coulomb file |

The default values of $\text{ICOULI}=\text{ICOULO}=0$ ensure that the code $\text{HFODD (v2.40h)}$ behaves as that in version (v1.60r). However, unless it is required by special circumstances, a use of the automated handling of the Coulomb file ($\text{ICOULI}=\text{ICOULO}=1$) is recommended. Within the automated mode, the code checks whether the Coulomb file exists, and whether it contains data which match the current values of the input parameters $\text{NUMCOU}$, $\text{NUMETA}$, and $\text{FURMAX}$. If this is the case, the code reads the data from the Coulomb file. If this is not the case, the code calculates the Coulomb auxiliary results and stores them in the Coulomb file $\text{FILCOU}$. In the automated mode, the user is informed by appropriate messages printed on the output file about what type of the action has been taken in the given run of the code.

2.14.9. Keyword: **WAVEF_FILE**

$\text{HFODD.WFN = FILWAV}$

 CHARACTER*68 file name of the wave function file. Must start at the 13-th column of the data line. The binary wave function files must exist if $\text{IPRGCM}=2$, and will be read, see the keyword $\text{PROJECTGCM}$.

2.14.10. Keyword: **KERNELFILE**

$\text{HFODD.KER = FILKER}$

 CHARACTER*68 file name of the kernel file. Must start at the 13-th column of the data line. The binary kernel files are written and read if $\text{ISAKER}=1$, see the keyword $\text{SAVEKERNEL}$.

2.14.11. Keyword: **YUKAWASAVE**

$1 = \text{IWRIYU}$

For $\text{IWRIYU}=1$ and $\text{I_YUKA} \geq 2$, the Yukawa file is saved on disc after each iteration is completed. The file contains the matrix elements of the Yukawa mean field. For $\text{IWRIYU}=0$ and $\text{I_YUKA} \geq 2$, the file is saved only once, after all iterations are completed. For $\text{IWRIYU}=-1$, the file is never saved. The Yukawa calculations can be restarted by using the Yukawa file. Therefore, $\text{IYCONT}=1$ requires setting $\text{IWRIYU}=0$ or 1 in the run that is to be continued. Equivalently, the Yukawa calculations can be restarted by using the field file, which requires setting $\text{IWRIFI}=0$ or 1 in the run that is to be continued.

2.14.12. Keyword: **REPYUKFILE**

$\text{HFODD.YUP = FILYUP}$
2.14. Files

CHARACTER*68 file name of the Yukawa file. Must start at the 13-th column of the data line. The binary Yukawa file with the name defined in FILYUP must exist if IYCONT=1, and will be read. If the filenames FILYUP and FILYUC are identical, the Yukawa file will be subsequently overwritten as a new Yukawa file.

2.14.13. Keyword: RECYUKFILE

    HFODD.YUC = FILYUC

CHARACTER*68 file name of the Yukawa file. Must start at the 13-th column of the data line. If IWRIYU=1, binary Yukawa file is written after each HF iteration. It contains complete information that allows restarting the Yukawa calculations in another run of the code. To restart, one has to specify IYCONT=1 and provide the name of the file by defining FILYUP.

2.14.14. Keyword: LIPKINSAVE

    1 = IWRILI

For IWRILI=1 and LIPKIN=1 or LIPKIP=1, the Lipkin-Nogami file is saved on disc after each iteration is completed. The file contains the matrix elements of the particle density matrices. For IWRILI=0 and LIPKIN=1 or LIPKIP=1, the file is saved only once, after all iterations are completed. For IWRILI=−1, the file is never saved. The Lipkin-Nogami calculations can be restarted by using the Lipkin-Nogami file. Therefore, ILCONT=1 requires setting IWRILI=0 or 1 in the run that is to be continued. Equivalently, the Lipkin-Nogami calculations can be restarted by using the field file, which requires setting IWRIFI=0 or 1 in the run that is to be continued.

2.14.15. Keyword: REPLIPFILE

    HFODD.LIP = FILLIP

CHARACTER*68 file name of the Lipkin-Nogami file. Must start at the 13-th column of the data line. The binary Lipkin-Nogami file with the name defined in FILLIP must exist if ILCONT=1, and will be read. If the filenames FILLIP and FILLIC are identical, the Lipkin-Nogami file will be subsequently overwritten as a new Lipkin-Nogami file.

2.14.16. Keyword: RECLIPFILE

    HFODD.LIC = FILLIC

CHARACTER*68 file name of the Lipkin-Nogami file. Must start at the 13-th column of the data line. If IWRILI=1, binary Lipkin-Nogami file is written after each HF iteration. It contains complete information that allows restarting the Lipkin-Nogami calculations in another run of the code. To restart, one has to specify ILCONT=1 and provide the name of the file by defining FILLIP.
2.14.17. **Keyword:** FIELD\_SAVE

\[ -1 = \text{IWRIFI} \]

For \( \text{IWRIFI}=1 \), the field file, is saved on disc after each iteration is completed. The file contains the matrix elements of the mean field. For \( \text{IWRIFI}=0 \), the file is saved only once, after all iterations are completed. For \( \text{IWRIFI}=-1 \), the file is never saved. To restart calculations of the exact Coulomb exchange energy, the field file must exist. \( \text{IFCONT}=1 \) requires setting \( \text{IWRIFI}=0 \) or 1 in the run that is to be continued.

2.14.18. **Keyword:** FIELD\_OLD

\[ 0 = \text{IWRIOL} \]

For \( \text{IWRIOL}=1 \), in the last iteration the mean fields are not updated, that is, the mixing fractions \( \epsilon \) are set equal to 1, irrespective of values of the SLOWEV, SLOWOD and SLOWPA parameters. In this way, information stored on the record file corresponds to the last but one iteration. Only then, restarting of the calculation from the field file leads to a smooth continuation of iterations.

2.14.19. **Keyword:** REP\_FIELDS

\[ \text{HFODD.FIP} = \text{FILFIP} \]

CHARACTER*68 file name of the field file. Must start at the 13-th column of the data line. The binary field file with the name defined in FILFIP must exist if \( \text{IFCONT}=1 \), and will be read. If the filenames FILFIP and FILFIC are identical, the field file will be subsequently overwritten as a new field file.

2.14.20. **Keyword:** REC\_FIELDS

\[ \text{HFODD.FIC} = \text{FILFIC} \]

CHARACTER*68 file name of the field file. Must start at the 13-th column of the data line. If \( \text{IWRIFI}=1 \), binary field file is written after each HF iteration. It contains complete information that allows restarting the calculations from the matrix elements of fields. To restart, one has to specify \( \text{IFCONT}=1 \) and provide the name of the file by defining FILFIP.
2.15. Starting the iteration

This section lists keywords that pertain to starting and restarting the code.

2.15.1. Keyword: **RESTART**

\[ 0 = \text{ICONTI} \]

For \text{ICONTI}=1, results stored in the replay file (written as a record file in a previous run) are used to start the iteration. The code assumes (without checking) that the parameters of the HO basis are the same as those used in the previous run. The replay file name should be provided by defining \text{FILREP}. If the previous run was done with \text{IREAWS}=1, the current run must also use \text{IREAWS}=1, and the same Woods-Saxon file must be provided. This so because the Woods-Saxon file contains not only the information about the starting potential (which is ignored for \text{ICONTI}=1) but also defines the HO basis.

2.15.2. Keyword: **CONT\_PAIRI**

\[ 0 = \text{IPCONT} \]

For \text{IPCONT}=1, results stored in the replay file are used to define the HFB pairing properties in the first iteration; otherwise values read in matrices \text{FERINI} and \text{DELINI} are used. When the HFB pairing correlations are taken into account (i.e., for \text{IPAHFB}=1), and if a smooth restart and continuation of iterations from previously stored results is required, value of \text{IPCONT}=1 must be used. \text{IPCONT}=1 is incompatible with either of \text{IPAHFB}=0 or \text{ICONTI}=0.

2.15.3. Keyword: **CONT\_OMEGA**

\[ 0 = \text{IOCONT} \]

For \text{IOCONT}=1, the angular momentum vector \( J_0 \) stored in the replay file is used to define in the first iteration the direction of the angular frequency vector \( \omega_J \), see Eq. [14]; otherwise values read in \text{OMEGAX}, \text{OMEGAY}, and \text{OMEGAZ} are used (see keyword \text{OMEGA\_XYZ}). \text{IOCONT}=1 requires \text{IMOVAX}=1 or \text{IMOVAX}=-1.

2.15.4. Keyword: **READ\_WOODS**

\[ 0 = \text{IREAWS} \]

For \text{IREAWS}=1, the results stored by the previously performed Woods-Saxon calculation are used to start the iteration and to define the HO basis. For \text{ICONTI}=1 and \text{IREAWS}=1 the Woods-Saxon file must also be provided, and is used only to define the HO basis.
2.15.5. Keyword: *NILSSONPAR*

\[0, -1.175, -0.247, -1.175, -0.352, 11.17, 11.17, 6.28 = \]
\[\text{NILDAT, CNILSN, DNILSN, CNILSP, DNILSP, HBANIX, HBANIY, HBANIZ}\]

For \texttt{IREAWS}=0 and \texttt{ICONTI}=0, the code starts the calculation from the Nilsson potential. For \texttt{NILDAT}=1 or \texttt{NILDAT}=2, the Nilsson parameters \(C\) and \(D\) [Ref. [11], Eq. (2.89)] are for neutrons given by \texttt{CNILSN} and \texttt{DNILSN} and for protons by \texttt{CNILSP} and \texttt{DNILSP}. For \texttt{NILDAT}=1, frequencies of the deformed HO are defined by \texttt{HBANIX}, \texttt{HBANIY}, and \texttt{HBANIZ}, while for \texttt{NILDAT}=2 they are the same as those of the HO basis defined under keyword \texttt{SURFAC_DEF}. If \texttt{NILDAT}=0, the Nilsson parameters \(C\) and \(D\) are defined by Eq. (2.91) and Table 2.3 of Ref. [11], while frequencies of the deformed HO are the same as those of the HO basis defined under keyword \texttt{SURFAC_DEF}. For \texttt{NILDAT}=0, the Nilsson parameters read from the input file are ignored.

2.15.6. Keyword: *CONTYUKAWA*

\[0 = \text{IYCONT}\]

For \texttt{IYCONT}=1, results stored in the Yukawa file are used to define the Yukawa fields in the first iteration; otherwise the Yukawa fields are set equal to zero. When the Yukawa fields are taken into account (i.e., for \texttt{I_YUKA}=2), and if a smooth restart and continuation of iterations from previously stored results is required, value of \texttt{IYCONT}=1 must be used. \texttt{IYCONT}=1 is incompatible with either of \texttt{I_YUKA}<2 or \texttt{ICONTI}=0.

2.15.7. Keyword: *CONTLIPKIN*

\[0 = \text{ILCONT}\]

For \texttt{ILCONT}=1, results stored in the Lipkin-Nogami file are used to define the density matrix required for the Lipkin-Nogami calculations in the first iteration; otherwise the required density matrix is set equal to zero. For the Lipkin-Nogami calculations (i.e., for \texttt{LIPKIN}=1 or \texttt{LIPKIP}=1), and if a smooth restart and continuation of iterations from previously stored results is required, value of \texttt{ILCONT}=1 must be used. \texttt{ILCONT}=1 is incompatible with either of \texttt{LIPKIN}=LIPKIP=0 or \texttt{IPCONT}=0.

2.15.8. Keyword: *CONTFIELDS*

\[0 = \text{IFCONT}\]

For \texttt{IFCONT}=1, results stored in the field file are used to define the matrix elements of fields in the first iteration; otherwise the matrix elements are recalculated. For the Gaussian-expansion method used to calculate the Coulomb energy and Coulomb mean field, that is for \texttt{ICOUDI}=2 or \texttt{ICOUEX}=2, and if a smooth restart and continuation of iterations from previously stored results is required, value of \texttt{IFCONT}=1 must be used. \texttt{IFCONT}=1 is incompatible with \texttt{ICONTI}=0.
3. OUTPUT FILE

The code writes results on standard FORTRAN output file. The output file begins with the information pertaining to the general parameters of the calculation, then gives information about the starting point of the iteration, provides the convergence report, and finally contains the results calculated at the last iteration. Structure of the output file strongly depends on the type of calculation that are requested in the given run; especially on the assumed conserved and broken symmetries. As a rule, only the information relevant for the specific run is printed. Descriptions and comments printed on the output file are in most cases self-explanatory. In this section we list only those explanations that are not explicitly included in the output file.

- **Section CLASSICAL NUCLEAR SURFACE** lists deformation parameters used to define the nuclear surface from which the basis parameters are derived, see keyword SURFAC_DEF. It also gives the basis parameters such as the OSCILLATOR FREQUENCIES: HBAROX, HBAROY, and HBAROZ corresponding to \( h\omega_x, h\omega_y, \) and \( h\omega_z \).

- **Section PHYSICAL CONSTANTS** gives values of \( \hbar c \) in MeV fm (H_BARC), of \( \hbar c/e^2 \) (HBCOE2), of the neutron and proton masses in MeV/c\(^2\) (XMASSN and XMASSP), of the kinetic-energy coefficient \( \hbar^2/2m \) before (HBMASS) and after the center-of-mass correction (HBMRPA), of the elementary charge squared \( e^2 \) in MeV fm (ECHAR2), and of the coefficient preceding the integral in the Coulomb exchange energy (COULEX). For details see the comments in the SETBAS subroutine.

- **Section OSCILLATOR LENGTHS, CONSTANTS, and FREQUENCIES** gives the values of \( 1/b_\mu, b_\mu, \) and \( \hbar\omega_\mu \), respectively, which characterize the HO basis in three Cartesian directions, \( \mu=x, y, z. \)

- **Section BASIS CUT-OFF CONTROL PARAMETERS** gives maximum numbers of the HO quanta in three directions NXMAXX, NYMAXX, and NZMAXX corresponding to \( N_x, N_y, \) and \( N_z \), as well as the orders of the Gauss-Hermite quadratures NXHERM, NYHERM, and NZHERM, corresponding to \( L_x, L_y, \) and \( L_z \), see keyword OPTI_GAUSS. It also gives the number \( M \) of the HO states included in the basis as requested in the input file (NLIMIT) and as used in the calculation (LDBASE).

- **Section SHAPE OF THE OSCILLATOR–BASIS DIAMOND** gives the numbers of the HO quanta in a given direction for fixed numbers of the HO quanta in both remaining directions. The output is arranged in such a way that the shape of the grid of points \( n_xn_yn_z \) is clearly visualized by projections in every of the three directions.

- **Section SKYRME FORCE DEFINITION** lists the name and parameters of the Skyrme force, together with parameters KETA_J, KETA_W, KETACM, and KETA_M that define the way the given force should be used (see keyword SKYRME_STD).

- **Section COEFFICIENTS DEFINING THE SKYRME FUNCTIONAL** gives values of the coupling constants in the Skyrme functional. These values take into account scaling factors, which are printed in the section SCALING_FACTORS, unless they are all equal to 1.
Section **CALCULATIONS WITH THE TILTED-AXIS CRANKING** gives values of components of the angular frequency vector and its length. For switches IMOVAX=1 or -1 and IOCONT=0, these values are used only in the first iteration, and later ignored, because the angular frequency vector is in each iteration readjusted to be aligned or anti-aligned with the angular momentum vector.

Sections **PARITY/SIGNATURE**, **SIMPLEX**, or **PARITY CONFIGURATIONS** give the vacuum and particle-hole configurations requested in the input file for the corresponding symmetry.

Section **CONVERGENCE REPORT** gives the list of performed iterations. For each iteration, one line is printed showing the energy, stability energy, average values of the intrinsic quadrupole moment $Q$ and $\gamma$ deformation, total angular momentum, angular frequency, angle between the angular frequency and angular momentum vectors, and total pairing energy.

Section **SINGLE-PARTICLE PROPERTIES** lists the single-particle states calculated for the Nilsson, Woods-Saxon, or Hartree-Fock Routhian operators. For every state one line is printed which gives the value of the single-particle Routhian, the consecutive numbers in the parity–signature block or simplex block, the quantum numbers $[N, n_z, \Lambda]\Omega$ of the Nilsson asymptotic state which has the largest component in the given state, the average value of the parity operator (in %), the average values of projections of the intrinsic and total angular momenta (in $\hbar$), and their ratio called the $g$-factor. For broken simplex symmetry, three projections of the total angular momentum and intrinsic spin are printed in the first and second line, respectively, for each single-particle state.

Section **DENSITY INTEGRALS IN THE SKYRME FUNCTIONAL** gives integrals of products of densities, which appear in the Skyrme functional. Terms in the functional are identified by the acronyms described under keywords EVE, SCA, and ODD.

Section **CONTRIBUTIONS TO ENERGY IN THE SKYRME FUNCTIONAL** gives the values of various terms which appear in the Skyrme functional. These contributions are the products of the coupling constants and of the density integrals described above. The sums of time-even and time-odd contributions are also printed.

Section **EULER ANGLES OF THE PRINCIPAL-AXES FRAME** gives the standard Euler angles $\alpha$, $\beta$, and $\gamma$ in degrees, which define the orientation of the intrinsic frame (principal-axes frame) of reference with respect to the original frame.

Section **MULTIPOLE MOMENTS** gives values of neutron, proton, or mass multipole moments with respect to the original frame of reference. In particular, the $\lambda=0$ moment corresponds to the number of particles. Similarly, section **MULTIPOLE MOMENTS [UNITS: (10 FERMI)^LAMBDA] [INTRINSIC FRAME]** gives analogous values with respect to the intrinsic frame of reference. Whenever the parity symmetry is broken, yet another analogous section gives information on values of multipole moments with respect to the center-of-mass reference frame.

Sections **ROOT-MEAN-SQUARE AND GEOMETRIC SIZES** gives the rms average values of the radius and of the $x$, $y$, and $z$ coordinates. In order to better visualize the size of the
nucleus, the geometric sizes are also calculated by multiplying the rms radius by $\sqrt{5/3}$ and the rms coordinates by $\sqrt{5}$.

- Sections **MAGNETIC MOMENTS** [MAGNETON*FERMI^-(LAMBDA-1)] and **MAGNETIC MOMENTS** [MAGNETON*FERMI^-(LAMBDA-1)] [INTRINSIC FRAME] give values of magnetic moments with respect to the original and intrinsic frame, respectively.

- Section **ANGULAR MOMENTA** gives for $ISIMPY=1$ the average values of the total and intrinsic neutron, proton, and total angular momentum (in $\hbar$). It also gives the corresponding values and contributions to the first moment of inertia $J^{(1)}=I/\omega$ (in $\hbar^2$/MeV). For $ISIMPY=0$, this section gives values of neutron, proton, and total projections of the total angular momentum and intrinsic spin on the three Cartesian axes in the original and intrinsic frame, respectively.

- Sections **NEUTRON CONFIGURATIONS** and **PROTON CONFIGURATIONS** give a visual representation of states occupied in the parity–signature blocks, simplex blocks, or parity blocks. The lines denoted by **CONF**: give the configurations requested in the input data set, while those denoted by **VACC**: give the configurations characterizing the given HF state. By comparing the two sets one can verify whether the requested configuration has been obtained, and eventually devise a new configuration to be calculated. The consecutive numbers printed in the horizontal direction correspond to the consecutive numbers in blocks printed in the section **SINGLE-PARTICLE PROPERTIES**. By comparing the two sections one can effectively associate the Nilsson labels with the calculated configurations and also prepare the configuration input data.

- Section **ENERGIES** gives a summary of the energies calculated for the HF state. The kinetic energy, single-particle energy, and pairing energy are printed for neutrons (NEU), protons (PRO), and all particles (TOT). Then, pairing rearrangement energy $P$-REARR, pairing gap $PAIRGAP$, and Fermi energy $E$-FERMI are printed. The Coulomb direct energy (DIR) and Coulomb exchange energy (EXC) are printed together with their sum (TOT). The multipole (MULT), surface multipole (SURF), and cranking (SPIN) constraint energies, are printed together with the corresponding corrections energies (CORR.). Then the rearrangement energy is printed followed by the values of the Routhian and the spin-orbit and Skyrme energies, the latter two split in the time-even (EVE) and time-odd (ODD) contributions. Finally, the total energies are printed as (SP) and (FUN), respectively, while their difference is printed as the stability (STAB).

- Section **CODE COMPILED WITH THE...** lists the values of the most important array dimensions and switches declared in the **PARAMETER** statements, fixed at the compilation stage.

- Sections **BOHR DEFORMATIONS** (EXACT MULTIPOLe MOMENTS) give values of the Bohr deformation parameters, determined as described in Section VI-2.5.

- Section **KERNELS AND AVERAGE VALUES...** gives values of the diagonal norm kernels $N_{KK}$ (VI-5) and average AMP energies $H_{KK}/N_{KK}$ for different values of $I$ and $K$. Real and imaginary parts of $N_{KK}$ are both printed, although all imaginary parts should be equal to zero when the numerical precision is sufficiently good.
• Section **SUM RULES**... compares real and imaginary parts of the sum rules (VI-49) and (VI-50) with the corresponding HF average values. Results are printed for the norm kernels $N_{KK}^I$, which must sum up to 1. This condition is a primary test of whether a sufficient number of the angular momenta are included in the sum of Eq. (VI-48). In the example of the file `ge064-a.out`, the sum rule for the norm kernel `NORM= 0.3248` indicates a much too small value of $I_{max}$ and too small numbers of the Gauss-Tchebyschev and Gauss-Legendre integration nodes.

• Sections **REDUCED KERNELS**... give values of the reduced kernels (VI-56) of electric and magnetic transition operators.

• Sections **RESULTS OF THE K-MIXING**... give values of the energies $E_i$ of $K$-mixed states, see Eq. (VI-3) and values of norm eigenvalues $n_m$, see Eq. (VI-9).

• Sections **REDUCED MAT.ELEMS**... give values of the reduced matrix elements (VI-57) of electric and magnetic transition operators calculated for the $K$-mixed states.

• Section **NUMBERS OF CALLS TO SUBROUTINES** gives the statistics of calls to subroutines, which together with the section **EXECUTION TIMES IN SUBROUTINES** illustrates the work flow of the code.
4. FORTRAN SOURCE FILE

FORTRAN source of code HFODD (v2.40h) is provided in the file hfodd.f and can be modified in several places, as described in this section.

4.1. Dimensions of arrays

The code HFODD uses the arrays’ dimensions declared through the PARAMETER statements. This allows changing the dimensions and adapting the size of the reserved memory to the problem being solved. Whenever too small a dimension is defined, the code aborts with a message indicating the dimension that should be increased. Substantial amount of memory is required only for arrays depending on the following PARAMETER values:

PARAMETER (NDMAIN=21)
Corresponds to the maximum number of the HO quanta. Should be larger or equal to the input parameter NOSCIL defined under keyword BASIS_SIZE.

PARAMETER (NDBASE=507)
Corresponds to the maximum number of the HO basis states. Should be larger or equal to the input parameter NLIMIT defined under keyword BASIS_SIZE. It should also be larger or equal to the actual size of the HO basis LDBASE, which can be larger than NLIMIT in case of degenerate HO states.

PARAMETER (NDXRM=33, NDYRM=33, NDZRM=45)
Corresponds to the maximum numbers of the HO Gauss-Hermite integration nodes in three Cartesian directions. Should be larger or equal to the input parameters NXHERM, NYHERM, and NZHERM, respectively, that are defined under keyword GAUSHERMIT or determined in an optimal way, see keyword OPTI_GAUSS.

PARAMETER (NDSTAT=181)
Corresponds to the maximum numbers of the single-particle states or quasiparticle states, which are kept after diagonalization. Should be larger or equal to the input parameters NUMBSP(0,0) + NUMBSP(1,0) and NUMBSP(0,1) + NUMBSP(1,1), see keyword PHASESPACE.

On vector machines, parameters NDBASE, NDXRM, NDYRM, NDZRM, and NDSTAT should be odd integers in order to minimize the risk of bank memory conflicts. By the same token, parameter NDMAIN should be even, because it defines the array dimensions beginning with 0.

4.2. Vectorization properties

As discussed in Sec. I-4.3, the code HFODD has to operate by using seven-fold nested short loops, and this part does not perform well in a vector processor. However, it turns out that the loops can be artificially made longer in such a way that the final CPU time in a vector processor actually becomes much shorter. All the places where this trick has been applied can be identified in the source file by finding the lines beginning with CVVECTOR and CSCALAR, for example:

CVVECTOR

DO KZ=0,LAZOXY(NX,NY)+LAZOXY(MX,MY)
The line beginning with `CSCALAR` should be made active on a scalar or superscalar machine. The line immediately below the line which begins with `CVECTOR` should be active on a vector machine. The results of calculation do not depend on which version of loops is activated.

### 4.3. FORTRAN-90 version

The code `HFODD` version (v2.40h) is written in FORTRAN-77. However, on several platforms, several tested FORTRAN-77 compilers did not perform well with respect to the memory management. In particular, they often distributed large arrays on computer’s stack and heap in a wasteful way, and then the available memory could be insufficient for the code to execute, especially for a large HO basis. Therefore, crucial parts of the code have been promoted to FORTRAN-90, with a use of an explicit memory allocation and deallocation. In the FORTRAN source code provided in the file `hfodd.f`, all these FORTRAN-90 features are commented out and inactive. However, very simple modifications of the source code can easily be performed to transform code `HFODD` to FORTRAN-90. To this end, the user should run an automated editor script which performs the following two operations:

1. Replace all strings "C F90" by spaces, and
2. Remove two lines of code (or three lines of the file) after lines marked by the string: "C IN F90 VERSION PLEASE REMOVE THE TWO FOLLOWING LINES".

The FORTRAN-90 version should be compiled with the "fixed form" non-standard option of the FORTRAN-90 compiler.

A set of c-shell and ex-editor scripts is provided within the `HFODD` distribution file, and allows performing the above modifications of the FORTRAN source code.

The present version of the code `HFODD` version (v2.40h) is the last one that works under FORTRAN-77; future releases will only use FORTRAN-90 programming.

### 4.4. Library subroutines

#### 4.4.1. BLAS

The code `HFODD` requires an implementation of the BLAS (Basic Linear Algebra Subprograms) interface for common dense vector and matrix computations. A reference implementation of these subroutines can be downloaded from

[http://www.netlib.org/blas/blas.tgz](http://www.netlib.org/blas/blas.tgz)

but for peak performance it is recommended that an optimized version of these routines should be installed. Optimized machine-specific BLAS (such as Sun Performance Library and Intel Math Kernel Library) are available from most hardware vendors, and there are also third-party optimized implementations such as GOTO and ATLAS available for various architectures.

The BLAS subroutines are in the `REAL*8/COMPLEX*16` version, and should be compiled without promoting real numbers to the double precision. On the other hand, the code `HFODD`
itself does require compilation with an option promoting to double precision. Therefore, the
code and the BLAS package should be compiled separately, and then should be linked together.

4.4.2. Diagonalization subroutines

The code hfodd requires an external subroutine that diagonalizes complex hermitian matrices. Version (v1.60r) (see II) has been prepared with an interface to the NAGLIB subroutine \texttt{f02axe}, version (v1.75r) (see III) with an interface to the LAPACK subroutine \texttt{zhpev}, and version (v2.08i) (see IV) with an interface to the LAPACK subroutine \texttt{zhpevx}. In the present version (v2.40h), all these interfaces remain supported and can be activated as described in II–IV. However, the recommended interface is now to the LAPACK subroutine \texttt{zheevr}, as described in this section below.

In version (v2.08i) we have implemented interface to the LAPACK subroutine \texttt{zhpevx}, which can be downloaded (with dependencies) from
\url{http://netlib2.cs.utk.edu/cgi-bin/netlibfiles.pl?filename=/lapack/complex16/zhpevx.f}
This subroutine finds not all, but only the lowest eigenvectors, and hence performs calculations in less CPU time; the gain is particularly significant for a large HO basis. Numbers of eigenvectors to be found are defined by the size of the phasespace, see keyword \texttt{PHASESPACE}.

Subroutine \texttt{zhpevx} and its dependencies are in the \texttt{REAL*8/COMPLEX*16} version, and should be compiled without promoting real numbers to the double precision. Therefore, the code and the \texttt{zhpevx} package should be compiled separately, and then should be linked together.

In order to activate the interface to the LAPACK \texttt{zhpevx} subroutine, the following modifications of the code hfodd (v2.40h) have to be made:

1. Change everywhere the value of parameter \texttt{ICRAY}=1 into \texttt{ICRAY}=0.
2. Change everywhere the value of parameter \texttt{IZHPEV}=0 into \texttt{IZHPEV}=2.
3. If your compiler does not support undefined externals, or subroutines called with different parameters, remove calls to subroutines \texttt{cgemm}, \texttt{f02axe}, \texttt{zhpev}, and \texttt{zheevr}.

In version (v2.40h) we have implemented interface to the LAPACK subroutine \texttt{zheevr}, which can be downloaded (with dependencies) from
\url{http://www.netlib.org/cgi-bin/netlibfiles.pl?filename=/lapack/complex16/zheevr.f}
This subroutine works with unpacked matrices and hence performs calculations in less CPU time at the expense of using a larger memory. Alternatively, the entire LAPACK library can be downloaded from
\url{http://www.netlib.org/lapack/lapack.tgz}

Subroutine \texttt{zheevr} and its dependencies are in the \texttt{REAL*8/COMPLEX*16} version, and should be compiled without promoting real numbers to the double precision. Therefore, the code and the \texttt{zheevr} package should be compiled separately, and then should be linked together.

In order to activate the interface to the LAPACK \texttt{zheevr} subroutine, the following modifications of the code hfodd (v2.40h) have to be made:

1. Change everywhere the value of parameter \texttt{ICRAY}=1 into \texttt{ICRAY}=0.
2. Change everywhere the value of parameter \texttt{IZHPEV}=0 into \texttt{IZHPEV}=3.
3. If your compiler and linker do not support undefined externals, or subroutines called with
derived parameters, remove calls to subroutines CGEMM, F02AXE, ZHPEV, and ZHPEVX.

4.4.3. Matrix inversion subroutines

The code HFODD requires external subroutines that invert complex matrices and calculate their
determinants. In version (v2.40h) we have implemented interfaces to the LINPACK subroutines
ZGEDI and ZGECO, which can be downloaded from
http://www.netlib.org/linpack/zgedi.f, and
http://www.netlib.org/linpack/zgeco.f, respectively, together with
http://www.netlib.org/linpack/zgefa.f

These subroutines are in the REAL*8/COMPLEX*16 version, and should be compiled without
promoting real numbers to the double precision. Therefore, the code and these subroutines
should be compiled separately, and then should be linked together.

4.5. Printing the execution times

After successful completion of execution, the code HFODD prints the table of CPU times spent
in principal subroutines, as well as the total execution time. Since implementation of the
time-checking functions widely varies between compilers and platforms, in the file hfodd.f all
references to these functions are commented out and inactive. However, very simple modific-
ations of the source code can easily be performed to activate one of the following options:

1. Replace all strings "CCPUT" by spaces in order to activate a call to the FORTRAN-90
   subroutine CPU_TIME, which returns CPU execution times.

2. Replace all strings "CETIM" by spaces in order to activate a call to function ETIME, which
   returns CPU execution times.

3. Replace all strings "CUNIX" by spaces in order to activate a call to the UNIX function
   TIME, which returns wall clock execution times.

4. Replace all strings "CSAL" by spaces in order to activate a call to the Salford FORTRAN subroutine
   DCLOCK, which returns wall clock execution times.

5. Replace all strings "CF32" by spaces in order to activate a call to the Microsofi FORTRAN subroutine
   GETTIM, which returns wall clock execution times.

Other time-checking functions, available to the user, can be analogously called in the subroutine
CPUTIM.
5. TEST RUNS

Several examples of input and output files are provided with the released versions (v1.60r), (v1.75r), (v2.08i), and (v2.40h) of the program hfodd, or added in this user’s guide, as listed in Table 6. The input data files dy152-a.dat through dy152-f.dat present the valid input items of each version and the default or recommended values of the input parameters. The input data files tb151-a.dat through tb151-d.dat are distributed with version (v1.75r), and provide examples of calculations with diabatic blocking. The input data files la132-a.dat and la132-b.dat are specific for version (v2.08i) and later, and illustrate various symmetry options of the code. The files pb128-a.dat and sn120-a.dat are added in this user’s guide and give examples of calculations of the spherical HF and HFB calculations, respectively. The input data files ge064-a.dat through ge064-c.dat and sn120-b.dat are specific for version (v2.40h) and later, and illustrate the AMP calculations and Lipkin-Nogami method, respectively.

Table 6: Input data files supplied with versions (v1.60r), (v1.75r), (v2.08i), and (v2.40h) of the program hfodd or added in this user’s guide. Each output file listed has been obtained by running the version of the code specific for the given input data file.

| Distribution | Input     | Contents                                      | Output  |
|--------------|-----------|-----------------------------------------------|---------|
| (v1.60r)     | dy152-a.dat | Only keyword EXECUTE                         | dy152-a.out |
|              | dy152-b.dat | Example of superdeformed HF calculations     | dy152-b.out |
|              |            | All input items of (v1.60r), default values of input items |         |
| (v1.75r)     | dy152-c.dat | All input items of (v1.75r), default values of input items | dy152-c.out |
|              | dy152-d.dat | Input items added in (v1.75r), recommended values of input items | dy152-d.out |
|              | tb151-a.dat | Example of adiabatic calculations            | tb151-a.out |
|              | tb151-b.dat | Example of adiabatic calculations            | tb151-b.out |
|              | tb151-c.dat | Example of diabatic blocking                 | tb151-c.out |
|              | tb151-d.dat | Example of diabatic blocking                 | tb151-d.out |
| (v2.08i)     | dy152-e.dat | All input items of (v2.08i), default values of input items | dy152-e.out |
|              | la132-a.dat | Example of tilted-axis-cranking calculations | la132-a.out |
|              | la132-b.dat | Example of tilted-axis-cranking calculations | la132-b.out |
| (v2.40h)     | dy152-f.dat | All input items of (v2.40h), default values of input items | dy152-f.out |
|              | ge064-a.dat | Example of AMP calculations                  | ge064-a.out |
|              | ge064-b.dat | Example of AMP calculations                  | ge064-b.out |
|              | sn120-b.dat | Example of Lipkin-Nogami method              | sn120-b.out |
| User’s guide | pb128-a.dat | Example of spherical HF calculations         | pb208-a.out |
|              | sn120-a.dat | Example of spherical HFB calculations        | sn120-a.out |
5. TEST RUNS

5.1. Descriptions of the test runs

5.1.1. Files dy152-a.dat through dy152-f.dat

As explained in Section 2., all the input data parameters of the code have their default values, which are assumed if the relevant input items are absent in the input data file. Each parameter introduced in a given version is also valid in all later versions, and its default value remains unchanged. Later versions introduce new parameters, but their default values are such that the new features are not active. Thus, the results of running a later version are identical to those of running an earlier version, provided that the values of those new parameters are left at the default. In particular, running each version with its default data set corresponds to identical conditions and gives the same solution. All the input items valid for a given version are also recognized and read by the subsequent ones. In general, running a later version with an input data file prepared for an earlier version leads to the same solution. However, the structure of the output file may be modified from version to version; in particular because later versions may calculate more observables.

Running the code with the default values results in performing 50 iterations for the superdeformed state in $^{152}$Dy at the angular frequency of $\hbar \omega = 0.5$ MeV. The pairing correlations are not taken into account. The HO basis is defined by an axially symmetric (with respect to the $z$ axis) nuclear surface with physical deformation typical for superdeformed bands in the $A \sim 150$ region. The parity, $y$-signature, $x$-simplex $^T$ (and their products) are imposed as conserved symmetries, while the time-reversal symmetry is broken in order to describe rotation (about the $y$ axis). The run starts from the Nilsson potential, and an appropriate weak constraint on the quadrupole moment $\langle \hat{Q}_{20} \rangle$ is used to ensure that the iterations fall into the superdeformed minimum.

The input data files dy152-a.dat through dy152-f.dat define either the default or recommended values of the input parameters for the released versions of the code. They contain either all or some of the valid input items, as described in Table 6. File dy152-a.dat contains only keyword EXECUTE, and when used as input for any version of the code it results in performing calculations with the default data set. Files dy152-b.dat, dy152-c.dat, dy152e.dat, and dy152f.dat contain all the valid input items of versions (v1.60r), (v1.75r), (v2.08i), and (v2.40h), respectively, and the input data are identical to the default values. File dy152-d.dat contains only the input items introduced in version (v1.75r), and the corresponding new parameters are set to recommended values, which differ from the default ones in the following way. The default values are such that the code works identically to version (v1.60r). The parameters EPSITE, NULAST, EPSPNG, and NUCHAO, control the termination of the iterations. By default, they are set so that always the number of iterations specified by NOITER is performed. The recommended values define an optimal level, at which convergence, “chaotic” divergence, or “ping-pong” divergence are detected to stop the iterations earlier. The differences between the default and recommended values of the variables governing the diabatic blocking are irrelevant because the diabatic blocking is disabled by default. Also by default, the Coulomb file is neither read from nor written to disc. With the recommended values of the parameters ICOULI and ICOULO, its reading and writing is handled automatically, which saves the CPU time.

Files dy152-a.dat through dy152-f.dat serve only as suitable patterns to modify the input parameters. However, it should be a good practice to include in the input data file only those input items which modify the input parameters with respect to the default values.
5.1. Descriptions of the test runs

Figure 5: Negative-parity neutron single-particle Routhians in $^{151}$Tb calculated for the [761]3/2($r=+i$) (a) and [514]9/2($r=+i$) (b) neutron diabatic configuration. Solid and dashed curves denote the $r=+i$ and $r=-i$ signatures, respectively. The arrows denote the angular frequencies where the converged solutions near the crossing points could not be found.

way, the danger of accidentally modifying some intricate numerical parameters of the code is minimized.

5.1.2. Files $\text{tb151-a.dat}$ through $\text{tb151-d.dat}$

Files $\text{tb151-a.dat}$ through $\text{tb151-d.dat}$ provide data for calculations in which single-particle configurations corresponding to two crossing bands in $^{151}$Tb are followed either adiabatically or diabatically. The pairing correlations are not taken into account. The parity, $y$-signature, $x$-simplex $T$ (and their products) are imposed as conserved symmetries, while the time-reversal symmetry is broken in order to describe rotation (about the $y$ axis). The angular frequency range from $\hbar \omega = 0.50$ to $0.80$ MeV is scanned with the step of $0.05$ MeV. Calculations at $\hbar \omega = 0.50$ are started from the Nilsson potential, and iterations for each subsequent frequency are restarted from the solution obtained at the preceding frequency. The two considered bands are based on excited physical configurations, in which the last neutron occupies either the [514]9/2($r=+i$) or [761]3/2($r=+i$) Nilsson level. At $\hbar \omega = 0.50$ MeV the level [514]9/2($r=+i$) is lower in energy, and has number 23$-+$ (23rd state of $\pi=-1$ and $r=+i$), while the level [761]3/2($r=+i$) has number 24$-+$. These two levels cross in the concerned frequency interval so that at $\hbar \omega = 0.80$ MeV the situation is the opposite. This is illustrated in Figure 5 which is explained in detail below.
In the files \texttt{tb151-a.dat} and \texttt{tb151-b.dat} it is required that always the level $23\,^-\,+ 0$ or $24\,^-\,+ 0$ be occupied, respectively, which amounts to following the configuration adiabatically. If, say, the level $23\,^-\,+ 0$ is occupied, the solutions at low and high frequencies correspond to physical configurations $[514]9/2(r=+i)$ and $[761]3/2(r=+i)$, respectively, while in the vicinity of the crossing no solution can be found, because the so-called “ping-pong” divergence occurs. This means that the physical states $[514]9/2(r=+i)$ and $[761]3/2(r=+i)$ change their energy order every second iteration, so that each of them once becomes the level $23\,^-\,+$. Thus, putting the neutron always on the level $23\,^-\,+$ results in occupying alternately the very different physical states $[514]9/2(r=+i)$ and $[761]3/2(r=+i)$, which cannot lead to convergence.

The code detects the “ping-pong” divergence, stops the iterations, and prints a table that helps identify the crossing orbitals. Such a table is reproduced in Table 7 for the $23\,^-\,+$ adiabatic configuration at $\bar{\hbar}\omega = 0.65\text{ MeV}$. For both protons and neutrons, in each parity–signature block, and separately for the particle and hole states, the code finds the level for which the difference in the angular momentum or intrinsic spin alignment (on the $y$ axis) between the last and last but one iteration is the largest. The indices of those levels in the parity–signature blocks, and the absolute values of the differences are printed in the upper part of the table, independently for the angular momentum and intrinsic spin. If in some symmetry block, the indices of the particle and hole states found in this way differ by one, then it is probable that these two levels cross and cause the “ping-pong” divergence. When such pairs exist, they are listed in the lower part of the table. In the given example, the pair of states $23\,^-\,+ 0$ and $24\,^-\,+ 0$ is properly recognized on the basis of both the angular momentum and intrinsic spin. The crossing orbitals, $[514]9/2(r=+i)$ and $[761]3/2(r=+i)$, have markedly different alignments of about $-0.46\hbar$ and $+2.23\hbar$, respectively, which corresponds to the values $2.820$ and $2.807\hbar$ given in the table.

If one wishes to follow, say, the configuration $[761]3/2(r=+i)$ diabatically, one should request that, of the levels $23\,^-\,+ 0$ and $24\,^-\,+ 0$, the one with physical properties of the state $[761]3/2(r=+i)$ be occupied. One can chose, for instance, the state with higher angular momentum alignment, independent of whether it is lower or higher in energy. In order to diabatically follow the configuration $[514]9/2(r=+i)$, one can chose the state with lower alignment. The corresponding runs are defined in the files \texttt{tb151-c.dat} and \texttt{tb-151-d.dat}. Indeed, in each case solutions corresponding to the same physical configuration is found at each angular frequency. Moreover, the “ping-pong” divergence does not occur, even very close to the crossing frequency. Figure 5 shows the negative-parity neutron single-particle Routhians obtained from the calculations of files \texttt{tb151-c.dat} and \texttt{tb-151-d.dat}.

### 5.1.3. Files \texttt{la132-a.dat} and \texttt{la132-b.dat}

File \texttt{la132-a.dat} defines two consecutive runs, which lead to a planar solution [13] in the triaxially deformed nucleus $^{132}\text{La}$ for $\hbar\omega = 0.25\text{ MeV}$. The pairing correlations are not taken into account. Since the calculations involve the tilted-axis cranking, a spherically invariant HO basis (with the three HO frequencies equal and comprising only entire HO shells) is used in order not to favor any orientation of the solution in space. The first run is performed at $\hbar\omega = 0$ with the parity, $y$-signature, $x$-simplex$^T$ (and their products) conserved, and with the time-reversal broken in order to describe odd numbers of neutrons and protons. Due to the presence of the odd nucleons, even for $\hbar\omega=0$ one obtains a non-zero angular momentum, which is oriented along the $y$ axis. The run starts from the Nilsson potential, and in 94 iterations finds
Table 7: Example of the output printed when the “ping-pong” divergence is found, see text.

******************************************************************************
* TABLE BELOW GIVES THE MAXIMUM ABSOLUTE VALUES OF DIFFERENCES OF ALIGNMENT *
* BETWEEN THE LAST TWO ITERATIONS. IT MAY SERVE AS A GUIDE TO SELECT STATES *
* WHICH EXCHANGE WAVE FUNCTIONS IN EVERY SECOND ITERATION. SUCH STATES MAY *
* BE CANDIDATES FOR A CALCULATION WITH DIABATICALLY BLOCKED CONFIGURATIONS *
******************************************************************************

| BLOCKS | ANGULAR MOMENTUM ALIGNMENT | INTRINSIC SPIN ALIGNMENT |
|--------|-----------------------------|--------------------------|
| ISO. PAR. SIG. | PARTICLES | HOLES | PARTICLES | HOLES | PARTICLES | HOLES | PARTICLES | HOLES |
| NEUT + + | 38 | 0.221 | 13 | 0.018 | 24 | 0.023 | 13 | 0.016 |
| NEUT + - | 28 | 0.163 | 7 | 0.041 | 33 | 0.014 | 7 | 0.032 |
| NEUT - - | 39 | 0.095 | 13 | 0.198 | 44 | 0.015 | 14 | 0.150 |
| NEUT - + | 24 | 2.820 | 23 | 2.807 | 24 | 0.164 | 23 | 0.167 |
| PROT + + | 24 | 0.255 | 13 | 0.149 | 25 | 0.129 | 14 | 0.122 |
| PROT + - | 27 | 1.733 | 13 | 0.062 | 21 | 0.319 | 8 | 0.020 |
| PROT - - | 32 | 0.119 | 10 | 0.530 | 32 | 0.029 | 10 | 0.065 |
| PROT - + | 24 | 2.649 | 15 | 0.082 | 24 | 0.153 | 10 | 0.030 |

******************************************************************************
* FOLLOWS THE LIST OF CANDIDATE CONFIGURATIONS FOR THE DIABATIC BLOCKING *
******************************************************************************

* NEUT - + | 24 | 2.820 | 23 | 2.807 |
* NEUT - + | 24 | 0.164 | 23 | 0.167 |

a triaxial solution, whose shape is forced by using appropriate constraints for the quadrupole moments $\langle \hat{Q}_{20} \rangle$ and $\langle \hat{Q}_{22} \rangle$. The constraints are set so that this solution nearly corresponds to the unconstrained minimum, and are used only to prevent the iterations from falling into other local minima. These constraints are chosen so that the short, medium, and long axes of the mass distribution coincide with the $y$, $x$, and $z$ axes, respectively. For the concerned solution, the single-particle configuration defined in the input data file in terms of numbers of particles in the parity–signature blocks physically corresponds to the odd proton particle occupying the lowest substate of the $h_{11/2}$ orbital and the odd neutron hole left on the highest $h_{11/2}$ substate.

The second run starts from the solution obtained in the first run, and performs calculations with all symmetries broken except parity, with multipole constraints released, and for the angular frequency of $\hbar \omega = 0.25 \text{MeV}$. The single-particle configuration specified in terms of parity blocks is obtained from the configuration for the first run simply by adding the numbers
of particles in the two signature sub-blocks of each parity block. All the three components of the initial angular frequency vector are non-zero, \( \bar{\hbar}\omega_x = \bar{\hbar}\omega_y = \bar{\hbar}\omega_z = (0.25/\sqrt{3}) \text{ MeV} \), which breaks all symmetries except parity in the first iteration, thus making the calculations otherwise symmetry-unrestricted. If a symmetry was not broken in the first iteration, it would artificially remain conserved as governed by the theorem about self-consistent symmetries [11].

The Kerman-Onishi condition [14] states that the angular momentum and angular frequency vectors must be parallel in self-consistent solutions. Standard iteration, with \( IMOVAX=0 \), requires several thousand iterations for the nucleus to turn appropriately in space to achieve the alignment of these vectors below the angle of 0.01°. On the other hand, iteration with \( IMOVAX=1 \), as shown in the example of file la132-a.dat, achieves the alignment of 0.000001° within 92 iterations. In the solution resulting from the second run, the angular momentum vector has non-zero components only on the \( y \) and \( z \) axes of the intrinsic frame, which are the short and long axes of the triaxial mass distribution. The calculations of the file la132-a.dat are performed in two steps to get a better control over what is going on and to avoid divergence or falling into undesired minima.

The input data provided in the file la132-b.dat are similar to those of the file la132-a.dat, except that the second run is performed with the \( x \)-simplex\( ^T \) conserved. In this way, the angular momentum and angular frequency vectors are confined within the plane \( y-z \), which is also a principal plane of the mass distribution. After the first run, this plane contains the short and long axes. The components of the initial angular frequency vector are set to \( \bar{\hbar}\omega_y = \bar{\hbar}\omega_z = (0.25/\sqrt{3}) \text{ MeV} \) and \( \bar{\hbar}\omega_x=0 \). Since the planar solution in question corresponds to non-equal projections of the angular momentum on the short and long axes, in order to satisfy the Kerman-Onishi condition, the nucleus still has to turn in space about the \( x \) axis. For \( IMOVAX=0 \), this process is also very slow, while for \( IMOVAX=1 \), as in file la132-b.dat, it takes again only 92 iterations. The \( x \)-simplex\( ^T \)-imposing solution obtained by using the file la132-b.dat differs from the symmetry-unrestricted result of the file la132-a.dat only by orientation in space; apart from that, the values of all observables are identical. This shows that in the considered self-consistent solution the \( x \)-simplex\( ^T \) symmetry is spontaneously conserved.

5.1.4. File pb208-a.dat

The input data file pb208-a.dat defines two consecutive runs to perform precise calculations for the spherical ground state of the doubly-magic nucleus \(^{208}\text{Pb}\) in a large basis of 26 HO shells. The pairing correlations are not taken into account. Conservation of all the symmetries considered in the code (the group \( D_{2h}^T \)) is imposed. For the spherical shape, the specified parity–signature configuration corresponds to occupation of the entire magic shells, up to the proton and neutron magic numbers 82 and 126, respectively. A spherical basis is used, i.e., with all the three characteristic HO frequencies equal (\( \bar{\hbar}\omega_x=\bar{\hbar}\omega_y=\bar{\hbar}\omega_z=\bar{\hbar}\omega_0 \)) and comprising only the entire HO shells. The so-called physical value of \( \bar{\hbar}\omega_0 = f \times 41 \text{ MeV}/A^{1/3} \) with \( f = 1.2 \) is taken, following the default settings of the code. To speed up the calculations, the program HFODD uses a diagonalization algorithm that can reduce the computational effort by finding less eigenstates than the matrix size (the lowest ones). In the present example, in each charge–simplex block only one extra state is calculated as compared to the number of occupied states in that block, as governed by the input parameter \( NUMBSP \). This is far less than the code’s default, and such a way of proceeding is possible only because no particle-hole excitations into higher
5.1. Descriptions of the test runs

5.1. States are required. Also for the sake of saving time, a solution in a small basis of $N_0=12$ HO shells is obtained first, starting from the Nilsson potential, and then serves as a good starting point for the time-consuming calculations with $N_0=26$. The number of states in the spherical basis comprising the HO shells from 0 to $N_0$ equals $M=(N_0+1)(N_0+2)(N_0+3)/6$, and hence the numbers of the HO basis states (for each projection of the intrinsic spin) equal $M=455$ and $M=3654$, respectively for $N_0=12$ and $N_0=26$. Since the code HFODD can restart iterations only if the number of Gauss-Hermite integration nodes is preserved, both runs are performed with 54 points in each of the Cartesian directions, which is excessive for $N_0=12$, but optimal for $N_0=26$. For $N_0=26$, the 54 points ensure exact integration of all matrix elements apart from those of the Coulomb interaction and density-dependent term.

The energies of $^{208}$Pb obtained from calculations with $N_0=12$ and $N_0=26$ equal $-1630.638$ and $-1635.531$ MeV, respectively. The latter value is very close to the result of $-1635.666$ MeV obtained by using a very precise one-dimensional spherical code working in spatial coordinates [15]. Although the $N_0=12$ HO basis is evidently too small for a precise determination of the energy, other observables may not be so sensitive to the HO basis size. For instance, the mass root-mean-square radii obtained for $N_0=12$ and $N_0=26$ equal 5.5540 and 5.5554 fm, respectively, the result of coordinate-space calculations being 5.5550 fm.

5.1.5. File sn120-a.dat

The input data file sn120-a.dat provides an example of the HFB calculations for the spherical ground state in $^{120}$Sn. All symmetries considered in the code (the group $D_{2h}^3$) are imposed, except the particle-number symmetry, which is broken in order to describe the pairing correlations. A spherical basis is used. The pairing correlations are included within the full HFB method, and the zero-range density-dependent interaction given by the pairing form-factor [11] is used in the particle-particle channel. The particle and pairing densities are obtained by summing up contributions from the quasiparticle states with the equivalent-spectrum energies not exceeding $\bar{\epsilon}_{\text{max}}=60$ MeV, which is the code’s default pairing window. In the pairing form-factor [11], the power $\alpha=1$ and the saturation density $\rho_0=0.32$ fm$^{-3}$ are taken. The interaction strength, $V_0=-285.88$ MeV fm$^3$, was adjusted for the given cutoff energy, $\bar{\epsilon}_{\text{max}}$, to reproduce the value of $\Delta_N=1.245$ MeV for the average neutron pairing gap in $^{120}$Sn. The same values of $\alpha$, $\rho_0$ and $V_0$ are taken for both neutrons and protons. The Fermi energy of $-8$ MeV and the pairing gap of 1 MeV are used in the first iteration to construct the HFB Hamiltonian, while the initial mean field is given by the Nilsson potential.

Since $^{120}$Sn is a proton-magic nucleus, the proton pairing decreases during the iteration and vanishes in the HFB solution. As expected, one obtains a significant thickness of the neutron skin (difference between the neutron and proton root-mean-square radii), which in the present case equals 0.14 fm.

5.1.6. Files ge064-a.dat and ge064-b.dat

File ge064-a.dat contains the input data that allow for determining the rotating triaxial state in the nucleus $^{64}$Ge and then performing a 3D AMP of this state. This input data file comprises four runs of the code: (i) starting from the Nilsson initial potential, the code performs 20 iterations with constrained values of quadrupole moments $Q_{20}$ and $Q_{22}$, such that the initial deformation and orientation of the nucleus is determined, (ii) after releasing the constraints, the
5. TEST RUNS

A triaxial minimum is converged, (iii) the rotating solution for $I = 6$ is converged by setting the angular frequency of $\hbar \omega = 0.575$ MeV, and (iv) the AMP of the rotating solution is performed. Small numbers of the Gauss-Tchebyschev (10) and Gauss-Legendre nodes (10), see Section VI-2.1, which are used in this run, do not allow for a precise AMP resolution of high angular momenta. This input data file is only meant to provide an example of a rapid calculation.

File `ge064-b.dat` contains the input data that allow for a correct AMP, with higher numbers of the Gauss-Tchebyschev (40) and Gauss-Legendre nodes (40), but its execution requires a CPU time which is $4^3 = 64$ times longer (about 200h). Alternatively, one can run in parallel 40 jobs by executing the input data files `ge064-c.dat` with characters NUASTA replaced by integers from 1 to 40.

5.1.7. File `sn120-b.dat`

File `sn120-b.dat` contains the input data that allow for determining the ground state in the nucleus $^{120}$Sn with the Lipkin-Nogami corrections taken into account.
6. ACKNOWLEDGMENTS

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