Nuclear DFT calculations - a practitioner's intro

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Brief description of formalism

Goal: Solve $H|\Psi\rangle = E|\Psi\rangle$ starting from $H = T + V$

with $V = \sum V_{12}$ and V_{12} a nuclear two-body interaction, in practice either a **Skyrme** (below), or a Gogny

Central — Momentum-dependent terms simulating finite range

$$V_{12} = t_0(1 + x_0 P_\sigma)\delta + \frac{1}{2}t_1(1 + x_1 P_\sigma)(\mathbf{k}'^2\delta + \delta\mathbf{k}^2) + t_2(1 + x_2 P_\sigma)\mathbf{k}' \cdot \delta\mathbf{k}$$

$$+ \frac{1}{6}t_3(1 + x_3 P_\sigma)\rho^\gamma\delta + iW_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{k}' \times \delta\mathbf{k}), \qquad \boldsymbol{\delta} = \boldsymbol{\delta}(\mathbf{r_1} - \mathbf{r_2})$$

Density-dependent term simulating 3-body effects — Spin-orbit term

With $t_{0\text{-}3}$ and $x_{0\text{-}3}$, W_0 and γ parameters of the interaction and all the others

$$\mathbf{k} = \mathbf{k_1} - \mathbf{k_2} \quad (\longrightarrow)$$

$$\mathbf{k}' = \mathbf{k_1} - \mathbf{k_2} \quad (\longleftarrow)$$

Momentum operator: $\mathbf{k_{1,2}} = \frac{\boldsymbol{i}}{\mathbf{2}}\boldsymbol{\nabla_{1,2}}$

$\mathbf{P_\sigma}$ Spin exchange operator

D. Vautherin, D.M. Brink, Phys. Rev. C 5, 626 (1972)
K. Bennaceur, J. Dobaczewski, Comp. Phys. Commun. 168, 96 (2005)

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Use variational principle: Minimize $\langle\Psi|H|\Psi\rangle$ with a specific class of $|\Psi\rangle$

Hartree-Fock: $|\Psi\rangle$ is a Slater determinant of single-particle wavefunctions

In this case: $\langle\Psi|H|\Psi\rangle = \mathcal{E}[\rho]$ (functional of the density)

Density functional theory: postulate that this is the case also for the exact wavefunction

- This means one can optimize directly $E[\rho]$ as a function of ρ
- For electron systems in Coulomb potential: proven mathematically to be true
- In nuclei: no formal proof

The basic difference:

Hartree-Fock-(Bogoliubov/BCS)

$$\frac{\delta\langle\Psi|H|\Psi\rangle}{\delta|\Psi\rangle} = 0$$, for a given class of $|\Psi\rangle$

Density Functional Theory

$$\frac{\delta\mathcal{E}[\rho]}{\delta\rho} = 0$$ varying ρ

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$$\begin{aligned}\mathcal{E}_{\text{Skyrme}} = &\frac{1}{2}t_0\left[\left(1+\frac{x_0}{2}\right)\rho^2 - \left(x_0+\frac{1}{2}\right)\sum_q \rho_q^2\right] \\ &+ \frac{t_1}{4}\left\{\left(1+\frac{x_1}{2}\right)\left[\rho\tau + \frac{3}{4}(\nabla\rho)^2\right] - \left(x_1+\frac{1}{2}\right)\sum_q\left[\rho_q\tau_q + \frac{3}{4}(\nabla\rho_q)^2\right]\right\} \\ &+ \frac{t_2}{4}\left\{\left(1+\frac{x_2}{2}\right)\left[\rho\tau - \frac{1}{4}(\nabla\rho)^2\right] + \left(x_2+\frac{1}{2}\right)\sum_q\left[\rho_q\tau_q - \frac{1}{4}(\nabla\rho_q)^2\right]\right\} \\ &- \frac{1}{16}(t_1x_1 + t_2x_2)J^2 + \frac{1}{16}(t_1 - t_2)\sum_q J_q^2 \\ &+ \frac{1}{12}t_3\rho^\gamma\left[\left(1+\frac{x_3}{2}\right)\rho^2 - \left(x_3+\frac{1}{2}\right)\sum_q \rho_q^2\right] \\ &+ \frac{1}{2}W_0\left(J\nabla\rho + \sum_q J_q\nabla\rho_q\right).\end{aligned}$$

For a Skyrme

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$\frac{\delta\langle\Psi|H|\Psi\rangle}{\delta|\Psi\rangle} = 0$, for $|\Psi\rangle$ a Slater determinant

If one actually performs this differentiation, one sees that it is equivalent to an eigenvalue problem for a one-body Hamiltonian *h:*

$$h_{ij} = t_{ij} + \Gamma_{ij} = t_{ij} + \sum_{l,k} \bar{v}_{ikjl}\rho_{lk}$$

$$\rho_{ij} = \langle\phi|a_j^\dagger a_i|\phi\rangle$$

The one-body density matrix

$$\sum_j h_{ij}D_{jk} = \epsilon_k D_{ik}$$

Diagonal in the same basis as h_{ij} ***(canonical basis)***

$$\rho_{ij} = \sum_{k=1}^{A} D_{ik}D_{jk}^*$$

Notations:

$|i\rangle$ One-body wavefunction (e.g. harmonic oscillator)

$$A_{ij} = \langle i|A|j\rangle$$

$$A_{ijkl} = \langle ij|A|kl\rangle$$

$$\bar{A}_{ijkl} = \langle ij|A|kl\rangle - \langle ij|A|lk\rangle$$

$$a_i^\dagger|-\rangle = |i\rangle$$
$$a_i|i\rangle = |-\rangle$$

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Brief description of formalism: quasiparticles

The BCS idea: instead of Slater determinant,

$$|\phi\rangle = \prod_{i=1}^{A} a_i^\dagger |-\rangle$$

use this ansatz:

$$|BCS\rangle = \prod_{k>0} (u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle$$

Theorem: one can define

$$\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\bar{k}}$$

then

$$|BCS\rangle \propto \prod_k \alpha_k |-\rangle$$

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Theorem: one can define

$$\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\bar{k}} \qquad \beta_k^\dagger = \sum_l U_{lk} a_l^\dagger + V_{lk} a_l$$

then

$$|BCS\rangle \propto \prod_k \alpha_k |-\rangle \qquad |\phi_{HFB}\rangle = \prod_k \beta_k |-\rangle$$

Bogoliubov: Let's generalize the definition, not making directly pairs from basis states

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The BCS idea: instead of Slater determinant,

$$|\phi\rangle = \prod_{i=1}^{A} a_i^\dagger |-\rangle$$

This form only in the basis that diagonalizes the one-body density matrix: mean field chooses what states will pair

use this ansatz:

$$|BCS\rangle = \prod_{k>0} (u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle$$

Theorem: one can define

$$\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\bar{k}} \qquad \beta_k^\dagger = \sum_l U_{lk} a_l^\dagger + V_{lk} a_l$$

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Hartree-Fock-Bogoliubov equations

$$\begin{pmatrix} \hat{h} - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}^* - \lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} E_k$$

Think of it as state mixing with a cross-diagonal term which is only non-zero if particles are paired

Hartree-Fock field

$$\begin{cases} h_{ij} = t_{ij} + \Gamma_{ij} = t_{ij} + \sum_{l,k} \bar{v}_{ikjl} \rho_{lk} \\ \rho_{ij} = \langle \phi_{HFB} | a_j^\dagger a_i | \phi_{HFB} \rangle \end{cases}$$

Pairing field

$$\Delta_{ij} = \frac{1}{2} \sum_{l,k} \bar{v}_{ijlk} \kappa_{lk},$$

$$\kappa_{lk} = \langle \phi_{HFB} | a_k a_l | \phi_{HFB} \rangle$$

Exactly the same as for pure Hartree-Fock, but $|\phi\rangle = |\phi_{HFB}\rangle$

Pairing tensor

$$\rho = V^* V^T$$

$$\kappa = V^* U^T$$

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Exactly the same as for pure Hartree-Fock, but $|\phi\rangle = |\phi_{HFB}\rangle$

Pairing tensor

$$\rho = V^* V^T$$

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The numerical algorithm mostly proceeds like in the HF case

Input file

```
&HFBTHO_GENERAL
 number_of_shells = 16,
 oscillator_length = -1.0,
 basis_deformation = 0.0,
 proton_number = 36, neutron_number = 62, type_of_calculation = -1 /
&HFBTHO_INITIAL
 beta2_deformation = 0.0, beta4_deformation = 0.0 /
&HFBTHO_ITERATIONS
 number_iterations = 500, accuracy = 1.E-7, restart_file = 1 /
&HFBTHO_FUNCTIONAL
 functional = "UNE0", add_initial_pairing = F,
 type_of_coulomb = 2/
&HFBTHO_PAIRING
 user_pairing = F, vpair_n = -300.0, vpair_p = -300.0,
 pairing_cutoff = 60.0, pairing_feature = 0.5 /
&HFBTHO_CONSTRAINTS
 lambda_values = 1, 2, 3, 4, 5, 6, 7, 8,
 lambda_active = 0, 1, 0, 0, 0, 0, 0, 0,
 expectation_values = 0.0,-9.50 , 0.0, 0.0, 0.0, 0.0, 0.0, 0.0 /
&HFBTHO_BLOCKING
 proton_blocking = 0, 0, 0, 0, 0, neutron_blocking = 0, 0, 0, 0, 0 /
&HFBTHO_PROJECTION
 switch_to_THO = 0, projection_is_on = 0,
 gauge_points = 1, delta_Z = 0, delta_N = 0 /
&HFBTHO_TEMPERATURE
 set_temperature = F, temperature = 0.0 /
&HFBTHO_FEATURES
 collective_inertia = F, fission_fragments = F, pairing_regularization = F,
 localization_functions = F /
&HFBTHO_NECK
 set_neck_constrain = F, neck_value = 0.5  /
&HFBTHO_DEBUG
 number_Gauss = 40, number_Laguerre = 40, number_Legendre = 80,
 compatibility_HFODD = F, number_states = 500, force_parity = T,
 print_time = 0 /
```

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```

Wavefunctions expanded in a Harmonic Oscillator basis

Larger means more accurate representation, but longer computation time: use 10 for today's exercise. Normally this parameter is gradually increased until convergence.

The length parameter of the oscillator (equivalently, the oscillator frequency) needs to scale with mass in order to avoid truncation errors: -1 means standard scaling hω as 1,2 x 41/$A^{1/3}$

The oscillator basis can be axially quadrupole deformed: this helps converge faster (with fewer shells) very deformed states. Keep it spherical for today.

Type of calculation (HFB or HFB with Lipkin-Nogami corrections for breaking particle number conservation). -1 means HFB-LN, which we will use.

Type of functional:
'SIII','SKM*','SKP','SLY4','SLY5','SLY6','SLY7','SKI3','SKO','SKX','HFB9',**'UNE0'**,'UNE1','UNE2','N0LO','N1LO','N2LO','FITS','D1','D1p','D1S','D1N','T0X0'

Type of calculation of Coulomb potential: use 2 (full approximate calculation)

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```
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```

Generally, pairing interaction defined by 2 parameters:

- A strength (V_0) which can be different for protons and neutrons
- A coefficient defining how much « volume » or « surface » it is:
  - α = 0 → pure volume force
  - α = 1 → pure surface force
  - α = 1/2 → mixed volume/surface
- If *user_pairing* = F, the pairing force is set by default to what the functional prescribed (use this at the beginning)
- If *user_pairing* = T, the pairing force is defined by the *vpair_n* and *vpair_p* (which fix V_0 for protons and neutrons), and *pairing_feature* (which fixes the value of α); you can use this (for example α = 0) to play with the pairing strength and see what this does to the results.

$$V_{\text{pair}}^{\text{n,p}}(\boldsymbol{r}) = V_0^{\text{n,p}} \left(1 - \alpha \frac{\rho(\boldsymbol{r})}{\rho_c}\right) \delta(\boldsymbol{r} - \boldsymbol{r'})$$

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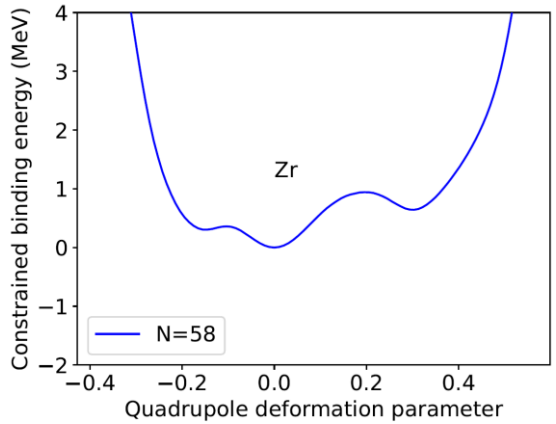
```

Allows applying a constraint to a multipole moment of the nucleus and determining how the energy varies with shape (allows producing a « deformation plot ») like shown below.

lambda_values simply lists what moments (dipole, quadrupole, octupole, hexadecapole, … 2^lamba_value-pole) can be constrained, *lambda_active* shows which ones are actually constrained (put 1 at the appropriate position) and *expectation_values* sets to which values they should be constrained (in the example, you can see what one should input for a constraint on the quadrupole moment to -9,5 barn).

To produce the plot below, 101 calculations were performed, each constraning the shape to a slightly different value of the quadrupole moment, scanning the range between -10 b and +15 b.



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 compatibility_HFODD = F, number_states = 500, force_parity = T,
 print_time = 0 /
```

Allows computing an odd nucleus by the « blocking » prescription, which performs a 1-quasiparticle excitation starting from a fully paired HFB solution of the Z-1 or N-1 even neighbour. **To block neutrons in Z = 50 and N = 71, set *proton_number* = 50, *neutron_number* = 70 and *neutron_blocking* = 1,0,0,0,0.** This is an automatic choice which blocks one after the other quasiparticle states having maximum wavefunction overlap with the single-particle states within 2 MeV from the Fermi level. For each trial state, one full calculation and one full output is generated. At the end, the user should assign the ground state to the result with minimal energy.

In the .sum file, one will have a line of results for the reference calculation performed in the neighbouring even isotope (in my example Z = 50 and N = 70) and then a line of results for each blocked candidate state in the odd one (Z = 50, N = 71 in this case), of which the lowest in energy should be picked as the ground state.

If one can infer from experimental data the Nilsson quantum numbers of a state, then one can specify a single state to block. In this exercise, we will use the automatic search for the optimal state to block.

Running the code

To run a single calculation:

- Create an input file, ideally without any extension (to avoid double extension of the output files)
- In the terminal (being in the « source » folder), run ./hfbtho_main [input_file]
- The code will run and show the output in the terminal
- The output will be written in the file [input_file].out
- A summary of the output will be written in the file **[input_file].sum**
  - The file contains the following values: **[constrained value of Q_{20}],[binding energy], [charge radius], [quadrupole deformation parameter beta_20], [convergence]**
- The hfbtho_solver.f90 can be modified and recompiled to write other outputs tot he summary file (search for string *lsumm*, which is the label of the output file, to find the line where the values are written to file)

A bash script *create_inputs.sh* can be used to automatically generate inputs with one parameter varies (like the Q_{20} constraint), which can then be run in series using another bash script.

Key elements of output file

```
---------------------------------------
        UNEDF Module Version: 17
      M.Kortelainen & M.Stoitsov
---------------------------------------

UNE0 functional
---------------------------------------
Crho(0)=    -706.382928878428856    ; Crho(1)=     240.049520427681131
CDrho(0)=    868.871771539645351    ; CDrho(1)=   -69.0518957481631617
Ctau(0)=    -12.9172408208016112    ; Ctau(1)=    -45.1894169426759476
CrDr(0)=    -55.2605999999999966    ; CrDr(1)=    -55.6225999999999985
CrdJ(0)=    -79.5307999999999993    ; CrdJ(1)=     45.6302000000000021
CJ(0)=       0.0000000000000000     ; CJ(1)=       0.0000000000000000
CpV0(0)=    -170.373999999999995    ; CpV0(1)=    -199.201999999999998
CpV1(0)=    0.500000000000000000    ; CpV1(1)=    0.500000000000000000
sigma=      0.321955989588264435    ; hbzero=      20.7355300000000007
e^2 chrg=    1.43997840859651305    ; CExPar=      1.0000000000000000
c.m. correction: T, chr. density in direct Coul: F
use tensor terms: F

Coupling constants in natural units
---------------------------------------
Crho_nu(0)=  -0.795471888366726554    ; Crho_nu(1)=    0.270324547082873012
CDrho_nu(0)=  0.906309849094393161    ; CDrho_nu(1)= -0.720272142163200374E-01
Ctau_nu(0)=  -0.183103357231201552    ; Ctau_nu(1)=  -0.640565122870490944
CrDr_nu(0)=  -0.783325287728328767    ; CrDr_nu(1)=  -0.788456678885096074
CrdJ_nu(0)=   -1.12735813207355995    ; CrdJ_nu(1)=   0.646813272821887275
CJ_nu(0)=      0.0000000000000000     ; CJ_nu(1)=      0.0000000000000000
CpV0_nu(0)=  -0.191861555493390873    ; CpV0_nu(1)=  -0.224325340588320099
CpV1_nu(0)=   0.443851127103029534E-03; CpV1_nu(1)=   0.443851127103029534E-03
fpi_nu=        93.0000000000000000    ; Lambda_nu=     700.000000000000000

Nuclear matter properties
---------------------------------------
E_NM=       -16.0558999999999656    ; K_NM=         229.999999999999460
P_NM=      0.244129189051514750E-15; RHO_NM=     0.160525999999999752
ASS_NM=      30.5428999999999569    ; LASS_NM=     45.0803999999999689
SMASS_NM=  0.900000000000000133    ; VMASS_NM=    1.24983799999999956

Associated (t,x)-coupling constants
---------------------------------------
t0=       -1883.68781034247695     ; x0=       0.974374651612197606E-02
t1=        277.500212238931113     ; x1=       -1.77784394560870229
t2=        608.430905591534383     ; x2=       -1.67699034528797575
t3=        13901.9483446343256     ; x3=      -0.380790414633100260
b4=        125.161000000000001     ; b4p=      -91.2604000000000042
te=       -184.461552003853939     ; to=       -118.275413333333319
sigma=    0.321955989588264435     ; hbzero=    20.7355300000000007
```

Coupling constants of the energy density functional

Equivalent coupling constants of the Skyrme interaction

Key elements of output file

```
-------------------------------------
     Characteristics of the run
-------------------------------------
Output file .............:     7
Nucleus .................:   Zr 100
Number of HO shells .....:    16
HO length b0 (fm) .......:     1.97798662217975
Basis deformation .......:  beta0=   0.000 q=   1.000
HO: b0,1/b0,bp,bz,q .....:   0.19779866E+01  0.50556459E+00  0.19779866E+01  0.19779866E+01  0.10000000E+01
h**2/(2m_n), cmc, e**2 ..:   0.20735530E+02  0.20528175E+02  0.14399784E+01
h**2/(2m_p), cmc, e**2 ..:   0.20735530E+02  0.20528175E+02  0.14399784E+01
hom=f*41.0_pr*A^{-1/3}, f...:   0.10599819E+02  0.12000000E+01
THO basis is ............:  OFF
Maximal number of iterations:   500
Initial mixing parameter ...:  0.300
Initial w.f. ............:  from spherical scratch
Energy functional .......:    UNE0
  with direct and exchange Coulomb
Lipkin-Nogami procedure is .:   ON
PAV procedure is ........:  OFF
Constraint calculation is ..:   ON
  Constraint 1 ..........: lambda=2 Ql=   7.500
Temperature T ...........:   0.00 MeV
Pairing regularization is ..:  OFF
Collective inertia is ......:  OFF
Fission fragments are ......:  OFF
Restart indicator .......:   1
Broyden mixing (#iterations):   7
```

Summary of the calculation options in natural language

Key elements of output file

```
--------------------------------------
     Harmonic Oscillator Basis
--------------------------------------
NUV, NQP:                         47241     969
Comparison with bookkeeping spherical basis:
n00:                                 16      16  Maximal number of shells
nbx, 2*n00+1:                        33      33  Maximal number of K-blocks
ntx, (n00+1)*(n00+2)*(n00+3)/6      969     969  Max.num. p/n levels
nzx, n00:                            16      16  Maximal nz-quantum number
nrx, n00/2  :                         8       8  Maximal nr-quantum number
nlx, n00:                            16      16  Maximal ml-quantum number
ndx, (n00+2)*(n00+2)/4:              81      81  Maximal dim. of one k-block

Actual basis used
Number of blocks: nb .......:   33
Number of levels: nt .......:  969
Maximal 2*omega : nom ......:   33
Maximal nz:       nzm ......:   16
Maximal nr:       nrm ......:    8
Maximal ml:       nlm ......:   16
Maximal N=nz+2*nr+nl .......:   16
2 x biggest block dim. .....:  162
Non-zero elements of h .....:    24105
Number of Broyden elements .:    96420

--------------------------------------
        Integration Meshes
--------------------------------------
Number of Gauss-Hermite mesh points ngh ....:  40
Number of Gauss-Laguerre mesh points ngl ...:  40
Number of Gauss-Legendre mesh points nleg ..:  80
Integration boundaries
  Hermite   - from xh(1)  =  0.12379686 to xh(ngh)   = 11.88786356
  Laguerre  - From xl(1)  =  0.03570039 to xl(ngl)   =142.28004447
  Legendre  - From xleg(1)=  0.00978669 to xleg(nleg)=  0.99988775
Max.dev.in:     Orthogonality            Normalization
Hermite     8.1015979368012488E-015   1.0991207943789050E-014
Laguerre    7.2721983928999130E-015   1.3544720900426910E-014

Scratch initialization for the nucleus: Zr  60  40


Initial potentials of Saxon-Woods shape
v0ws   =  -71.28000000
kappa  =    0.46160000
vs0    =   11.11750000   11.11750000
r0     =    1.23340000    1.23340000
a      =    0.61500000    0.61500000
r0-so  =    1.14430000    1.14430000
a-so   =    0.64760000    0.64760000
b2_ws  =    0.00000000
b4_ws  =    0.00000000
```

Parameters of the Harmonic Oscillator basis used for the computation

Numerical parameters for integrations

Parameters of the initial solutions used to start the calculations

Key elements of output file

```
### REGULAR STAGE (reflection symmetry imposed)
|HFB+HO> iterations(b0=  1.978, Nsh= 16, inin=  1, N= 60, Z= 40)...
-------------------------------------------------------------------------------------------------------------------------------
i          si     mix   beta      Etot       A       rn      rp         En      Dn      Ep      Dp        Ln      Lp     time  time(Gog.)
-------------------------------------------------------------------------------------------------------------------------------
 1L  90.35027967 0.30  0.000     0.000000    0.0   0.000   0.000 |   -2.000   1.000  -2.000   1.000 |   -7.000  -7.000   0.000   0.000
                       f: ala2(n,p)=   0.123   0.299 #eln(n,p,t)=    -0.740    -0.595    -1.334 #del+ala2=   0.608   0.628
 2B  67.64928848 0.10 -0.000  -641.042019  100.0   4.275   3.940 |   -6.948   0.608  -3.715   0.628 |  -13.757 -27.749  32.556   0.000
                       f: ala2(n,p)=   0.140   0.160 #eln(n,p,t)=    -0.867    -0.828    -1.695 #del+ala2=   0.698   0.700
 3B 217.40670759 0.10  1.115  -299.541504  100.0   7.381   6.852 |   -5.036   0.698  -3.595   0.700 |  -15.413 -20.593   2.329   0.000
                       f: ala2(n,p)=   0.381   1.233 #eln(n,p,t)=    -1.237    -1.628    -2.865 #del+ala2=   0.805   1.605
 4B  36.82296625 0.11  0.038  -812.081791  100.0   4.475   4.249 |   -2.814   0.805  -1.452   1.605 |   -4.629 -11.253   2.222   0.000
                       f: ala2(n,p)=   0.237   0.830 #eln(n,p,t)=    -0.944    -1.343    -2.287 #del+ala2=   0.729   1.247
 5B  22.06677896 0.13  0.210  -658.821055  100.0   4.593   4.185 |   -2.666   0.729  -1.429   1.247 |   -4.510  -9.275   1.403   0.000
                       f: ala2(n,p)=   0.173   0.184 #eln(n,p,t)=    -0.831    -0.868    -1.700 #del+ala2=   0.679   0.794
 6B   9.21400779 0.14  0.222  -826.749908  100.0   4.582   4.343 |   -2.851   0.679  -2.919   0.794 |   -4.573  -9.999   2.040   0.000
                       f: ala2(n,p)=   0.179   0.229 #eln(n,p,t)=    -0.843    -0.919    -1.761 #del+ala2=   0.702   0.826
 7B   5.07735569 0.16  0.256  -842.609436  100.0   4.592   4.328 |   -2.965   0.702  -2.830   0.826 |   -4.867 -10.302   2.343   0.000
                       f: ala2(n,p)=   0.181   0.239 #eln(n,p,t)=    -0.841    -0.916    -1.757 #del+ala2=   0.709   0.830
 8B   3.73206178 0.18  0.276  -845.149448  100.0   4.596   4.355 |   -2.985   0.709  -2.764   0.830 |   -5.150 -10.478   2.134   0.000
                       f: ala2(n,p)=   0.251   0.276 #eln(n,p,t)=    -0.967    -0.961    -1.928 #del+ala2=   0.776   0.872
 9B   4.41088128 0.10  0.314  -845.619716  100.0   4.611   4.360 |   -2.896   0.776  -2.813   0.872 |   -5.810 -11.292   2.304   0.000
                       f: ala2(n,p)=   0.206   0.378 #eln(n,p,t)=    -0.906    -1.073    -1.979 #del+ala2=   0.768   0.960
10B   9.17173480 0.10  0.341  -846.315476  100.0   4.615   4.418 |   -3.299   0.768  -2.655   0.960 |   -6.190 -11.946   2.139   0.000
                       f: ala2(n,p)=   0.205   0.251 #eln(n,p,t)=    -0.926    -0.942    -1.868 #del+ala2=   0.776   0.872
11B   6.50478134 0.11  0.328  -849.597709  100.0   4.607   4.390 |   -3.383   0.776  -3.039   0.872 |   -6.112 -11.922   1.541   0.000
                       f: ala2(n,p)=   0.194   0.253 #eln(n,p,t)=    -0.896    -0.951    -1.847 #del+ala2=   0.757   0.866
12B   3.29051270 0.13  0.308  -850.499104  100.0   4.597   4.377 |   -3.326   0.757  -2.970   0.866 |   -5.791 -11.607   1.874   0.000
                       f: ala2(n,p)=   0.189   0.243 #eln(n,p,t)=    -0.900    -0.951    -1.851 #del+ala2=   0.774   0.879
13B   2.94201069 0.14  0.310  -849.457240  100.0   4.591   4.382 |   -3.559   0.774  -3.195   0.879 |   -5.885 -11.753   2.455   0.000
                       f: ala2(n,p)=   0.183   0.247 #eln(n,p,t)=    -0.893    -0.966    -1.858 #del+ala2=   0.779   0.893
14B   1.89384856 0.16  0.301  -849.069955  100.0   4.589   4.373 |   -3.711   0.779  -3.283   0.893 |   -5.846 -11.784   2.491   0.000
                       f: ala2(n,p)=   0.175   0.239 #eln(n,p,t)=    -0.889    -0.973    -1.862 #del+ala2=   0.785   0.899
15B   1.23827203 0.18  0.297  -850.288033  100.0   4.590   4.365 |   -3.888   0.785  -3.423   0.899 |   -5.795 -11.796   2.698   0.000
                       f: ala2(n,p)=   0.169   0.232 #eln(n,p,t)=    -0.879    -0.968    -1.846 #del+ala2=   0.784   0.900
16B   0.61036197 0.21  0.293  -850.557154  100.0   4.585   4.370 |   -3.943   0.784  -3.508   0.900 |   -5.808 -11.781   2.558   0.000
                       f: ala2(n,p)=   0.170   0.231 #eln(n,p,t)=    -0.885    -0.971    -1.856 #del+ala2=   0.788   0.904
```

Print-out of the result of each HFB iteration (Etot being the binding energy), with some additional check parameters. The iterations stop when the energy difference between consecutive steps is below what was set in the input file as « accuracy »

Key elements of output file

```
#quasiparticle energies neutrons
--------------------------------
 eqp(k) -> q.p. energy
 e(k)   -> referent s.p. energy
 p(k)   -> occ.probability
 del(k) -> referent s.p. gap
 fermi energy alast=  -5.8457130432870885
 #k  block#    eqp(k)     e(k)       (1-2N)E      decay        p(k)         del(k)    overl      labels
  1    1     0.714806   -5.381524    0.464189   1.130639   0.17530460   0.5436   0.6926  1+[ 4, 1, 1]
  2    1     1.538994   -7.230905   -1.385192   1.199559   0.95003159   0.6706   0.6048  1+[ 4, 3, 1]
  3    1     1.869578   -4.050552    1.795161   1.226114   0.01990210   0.5222   0.8481  1+[ 4, 0, 0]
  4    1     3.218747   -8.997599   -3.151886   1.329002   0.98961381   0.6526   0.5289  1+[ 4, 4, 0]
  5    1     6.371161    0.486417    6.332130   1.542890   0.00306305   0.7041   0.5284  1+[ 6, 6, 0]
  6    1     7.065377  -12.845303   -6.999590   1.586121   0.99534435   0.9619   0.5935  1+[ 4, 4, 0]
  7    1     8.832814    2.951810    8.797523   1.691204   0.00199768   0.7888   0.4698  1+[ 6, 4, 0]
  8    1    10.411049    4.550391   10.396104   1.779803   0.00071774   0.5576   0.4406  1+[ 6, 3, 1]
  9    1    10.629665    4.773412   10.619125   1.791730   0.00049576   0.4732   0.3517  1+[ 6, 2, 0]
 10    1    12.122995    6.268074   12.113787   1.871170   0.00037978   0.4724   0.4845  1+[ 6, 2, 0]
 11    1    12.366970    6.513314   12.359027   1.883830   0.00032112   0.4432   0.4501  1+[ 6, 1, 1]
 12    1    13.947406  -19.773145  -13.927432   1.963866   0.99928396   0.7462   0.9243  1+[ 2, 0, 0]
 13    1    15.550603    9.693596   15.539309   2.041852   0.00036314   0.5926   0.4847  1+[ 6, 3, 1]
 14    1    16.243797  -22.066650  -16.220936   2.074664   0.99929633   0.8615   0.8596  1+[ 2, 1, 1]
 15    1    16.977705   11.123378   16.969091   2.108847   0.00025370   0.5408   0.4404  1+[10,10, 0]
 16    1    18.401141   12.537360   18.383074   2.173615   0.00049094   0.8152   0.3142  1+[ 6, 5, 1]
 17    1    19.258775   -9.109275   -3.263562   2.211722   0.58472923  18.9802   0.6186  1+[ 2, 2, 0]
 18    1    19.327355   -2.542789    3.302924   2.214741   0.41455314  19.0430   0.5196  1+[ 2, 2, 0]
 19    1    20.301358   14.450442   20.296155   2.257181   0.00012816   0.4596   0.3308  1+[ 8, 6, 0]
 20    1    20.595340   14.741222   20.586935   2.269835   0.00020405   0.5883   0.5465  1+[ 6, 1, 1]
 21    1    21.214167   15.362048   21.207761   2.296243   0.00015099   0.5213   0.6199  1+[ 6, 0, 0]
 22    1    22.371846   16.522089   22.367802   2.344847   0.00009039   0.4254   0.2343  1+[ 6, 3, 1]
 23    1    23.883505   18.032302   23.878015   2.406836   0.00011492   0.5120   0.4031  1+[ 8, 4, 0]
 24    1    27.489405   21.642767   27.488480   2.548624   0.00001682   0.2255   0.2711  1+[ 8, 5, 1]
 25    1    28.492014  -34.329834  -28.484121   2.586667   0.99986148   0.6706   0.9483  1+[ 0, 0, 0]
 26    1    29.722710   23.872769   29.718482   2.632614   0.00007114   0.5014   0.5504  1+[ 8, 8, 0]
 27    1    30.724554   24.874893   30.720606   2.669432   0.00006425   0.4925   0.3848  1+[ 8, 6, 0]
 28    1    31.641465   25.790840   31.636553   2.702690   0.00007762   0.5575   0.4370  1+[ 8, 4, 0]
 29    1    32.473349   26.623564   32.469277   2.732513   0.00006270   0.5142   0.4206  1+[ 8, 7, 1]
 30    1    33.046854   27.197937   33.043651   2.752885   0.00004847   0.4602   0.5812  1+[ 8, 2, 0]
```

Energies of neutron quasiparticle states

Key elements of output file

```
#canonical s.p. energies neutrons
---------------------------------


 labels -> {2*omega}{parity}[nn=nz+2*nr+nl,nz,nl]
 cqpe   -> canonical q.p. energies
 ce     -> canonical s.p. energies
 fermi energy=  -5.8457130432870885
 average cdelt=  0.64232686612821188
 k0      ceqp        ce         v*v        u*v        cdel     overl      labels
  2   58.146509   58.146371   0.00000000   0.00000000   0.1328   0.5529  1+[14, 6, 0]
  3   58.205771   58.205570   0.00000000   0.00000000   0.1606   0.5241  1+[14, 0, 0]
  6   59.096943   59.096770   0.00000000   0.00000000   0.1499   0.4066  1+[14, 2, 0]
 12   56.296896   56.296791   0.00000000   0.00000000   0.1144   0.6095  1+[14, 1, 1]
 17   57.890810   57.890620   0.00000000   0.00000000   0.1555   0.4279  1+[14, 4, 0]
 18   55.340940   55.340774   0.00000000   0.00000000   0.1426   0.3707  1+[16,12, 0]
 21   59.337930   59.337830   0.00000000   0.00000000   0.1143   0.4128  1+[14, 3, 1]
 24   57.595074   57.594807   0.00000000   0.00000000   0.1840   0.6302  1+[14, 8, 0]
 35   55.732280   55.731717   0.00000015   0.00039365   0.2634   0.3199  1+[16, 3, 1]
 36   59.440481   59.439731   0.00000018   0.00042183   0.3129   0.3662  1+[16, 0, 0]
 37   47.163826   47.163455   0.00000019   0.00043572   0.1983   0.3400  1+[14,14, 0]
 38   59.005791   59.004942   0.00000023   0.00047489   0.3319   0.3568  1+[16, 0, 0]
 39   56.788883   56.787941   0.00000025   0.00050162   0.3435   0.3652  1+[12, 5, 1]
 40   50.705115   50.704217   0.00000029   0.00054297   0.3186   0.4299  1+[12, 8, 0]
 41   41.432682   41.431957   0.00000036   0.00059608   0.2618   0.5464  1+[12, 9, 1]
 43   34.509208   34.508608   0.00000058   0.00076151   0.2201   0.6045  1+[12,12, 0]
 44   59.560920   59.559094   0.00000099   0.00099697   0.4887   0.4045  1+[12, 9, 1]
 45   46.124574   46.123577   0.00000167   0.00129332   0.3220   0.4906  1+[10, 0, 0]
 46   44.866858   44.865807   0.00000204   0.00142878   0.3265   0.5003  1+[10, 1, 1]
 47   44.251288   44.250134   0.00000282   0.00168022   0.3400   0.5276  1+[10, 2, 0]
 48   43.840165   43.838853   0.00000399   0.00199836   0.3610   0.5958  1+[10, 3, 1]
 49   43.661435   43.659869   0.00000580   0.00240878   0.3938   0.6118  1+[10, 4, 0]
 50   51.629398   51.627894   0.00000662   0.00257220   0.4158   0.4836  1+[12,12, 0]
 51   43.477508   43.475694   0.00000823   0.00286854   0.4230   0.5358  1+[10, 5, 1]
 52   42.712640   42.710464   0.00001170   0.00342028   0.4597   0.5117  1+[10, 7, 1]
 53   42.519123   42.516592   0.00001609   0.00401177   0.4948   0.6218  1+[10, 8, 0]
 54   47.427008   47.423790   0.00001948   0.00441340   0.5855   0.6773  1+[10, 9, 1]
 55   35.958304   35.956002   0.00002254   0.00474734   0.4387   0.7607  1+[ 8, 0, 0]
 56   41.782111   41.778863   0.00002483   0.00498310   0.5562   0.7433  1+[10,10, 0]
 57   35.802057   35.799321   0.00002820   0.00530998   0.4774   0.7455  1+[ 8, 1, 1]
 58   34.534880   34.531617   0.00003636   0.00603014   0.5133   0.7408  1+[ 8, 2, 0]
 59   34.306283   34.302346   0.00004584   0.00677017   0.5623   0.6932  1+[ 8, 3, 1]
 60   40.543438   40.538651   0.00004875   0.00698178   0.6664   0.4060  1+[10, 8, 0]
 61   31.049537   31.044887   0.00006036   0.00776875   0.5858   0.6482  1+[ 8, 4, 0]
 62   29.264635   29.259318   0.00007333   0.00856279   0.6110   0.5906  1+[ 8, 6, 0]
```

Energies of canonical single-particle basis states for neutrons

Key elements of output file

#quasiparticle energies protons

eqp(k) -> q.p. energy
e(k) -> referent s.p. energy
p(k) -> occ.probability
del(k) -> referent s.p. gap
fermi energy alast= -11.809344645049283

#k	block#	eqp(k)	e(k)	(1-2N)E	decay	p(k)	del(k)	overl	labels
1	1	1.528856	-13.187050	-1.377705	1.612143	0.95056750	0.6628	0.5703	1+[4, 4, 0]
2	1	2.492987	-9.399593	2.409752	1.669392	0.01669390	0.6388	0.5296	1+[4, 4, 0]
3	1	4.533144	-7.322190	4.487154	1.784489	0.00507256	0.6441	0.6439	1+[4, 3, 1]
4	1	7.760188	-4.091927	7.717418	1.952743	0.00275574	0.8136	0.8631	1+[4, 1, 1]
5	1	8.426524	-20.182446	-8.373101	1.985710	0.99683009	0.9474	0.9100	1+[2, 0, 0]
6	1	10.940357	-14.675955	-2.866610	2.105439	0.63101082	10.5581	0.6749	1+[2, 1, 1]
7	1	10.961337	-8.927274	2.882071	2.106410	0.36853469	10.5757	0.7440	1+[4, 0, 0]
8	1	13.263823	1.436620	13.245965	2.210342	0.00067319	0.6881	0.4860	1+[6, 4, 0]
9	1	14.413240	-26.200294	-14.390949	2.260438	0.99922672	0.8013	0.7862	1+[2, 2, 0]
10	1	18.421749	6.603752	18.413097	2.427067	0.00023484	0.5645	0.5721	1+[6, 6, 0]
11	1	20.592728	8.776718	20.586062	2.512703	0.00016186	0.5239	0.6371	1+[6, 5, 1]
12	1	21.797708	9.981653	21.790998	2.558999	0.00015391	0.5408	0.4576	1+[6, 2, 0]
13	1	23.065342	11.251945	23.061289	2.606814	0.00008786	0.4324	0.4055	1+[6, 0, 0]
14	1	23.301983	11.487731	23.297075	2.615643	0.00010530	0.4782	0.5009	1+[6, 1, 1]
15	1	24.556059	-36.347248	-24.537903	2.661945	0.99963032	0.9441	0.9417	1+[0, 0, 0]
16	1	25.587481	13.772439	25.581783	2.699431	0.00011135	0.5400	0.4677	1+[6, 3, 1]
17	1	27.844453	16.031728	27.841073	2.779695	0.00006069	0.4338	0.4672	1+[10,10, 0]
18	1	29.121946	17.309517	29.118861	2.824116	0.00005296	0.4239	0.3118	1+[10, 9, 1]
19	1	30.009565	18.196946	30.006291	2.854573	0.00005455	0.4433	0.3537	1+[6, 2, 0]
20	1	30.783782	18.970734	30.780079	2.880876	0.00006015	0.4775	0.4536	1+[8, 6, 0]
21	1	31.618684	19.805435	31.614779	2.908974	0.00006175	0.4969	0.6020	1+[6, 1, 1]
22	1	32.572927	20.759505	32.568850	2.940760	0.00006258	0.5153	0.7014	1+[6, 0, 0]
23	1	33.558640	21.747807	33.557152	2.973237	0.00002218	0.3161	0.2326	1+[10, 9, 1]
24	1	33.711827	21.900588	33.709933	2.978253	0.00002810	0.3574	0.3689	1+[8, 4, 0]
25	1	39.254161	27.444052	39.253396	3.154352	0.00000973	0.2449	0.3081	1+[8, 5, 1]
26	1	40.828037	29.016269	40.825614	3.202595	0.00002968	0.4448	0.5488	1+[8, 8, 0]
27	1	41.789267	29.978721	41.788065	3.231704	0.00001437	0.3169	0.2951	1+[12,10, 0]
28	1	43.014922	31.203086	43.012430	3.268445	0.00002897	0.4630	0.3572	1+[8, 4, 0]
29	1	43.878866	32.066937	43.876282	3.294098	0.00002944	0.4762	0.4016	1+[8, 7, 1]
30	1	44.531177	32.719642	44.528986	3.313334	0.00002459	0.4417	0.5647	1+[8, 2, 0]
31	1	45.381793	33.570174	45.379519	3.338253	0.00002506	0.4544	0.4790	1+[8, 1, 1]

Energies of proton quasiparticle states

Key elements of output file

	neutrons	protons	total
Requested part.numbs.	60.000000	40.000000	100.000000
UnPj(av) part.numbs .	60.000000	40.000000	100.000000
b0, bz, bp	1.977987	1.977987	1.977987
lambda (ala)	-5.845713	-11.809345	
Lambda (alast)	-5.845713	-11.809345	
delta(n,p), pwi	0.642327	0.706494	60.000000
pairing energy	-4.291083	-3.917031	-8.208114
LN lambda_2 ... ala2	0.171767	0.229923	
LN energies	-0.920565	-1.012320	-1.932885
delta(n,p)+ala2	0.814094	0.936416	
Geff(n,p)	-0.096149	-0.127426	
rms-radius	4.586471	4.370413	4.581292
charge-radius, r0 ...		4.441661	5.569907
deformation beta2....	0.284161	0.308692	0.293411
dipole moment[fm] ...	0.000000	0.000000	0.000000
quadrupole moment[b]	4.524631	2.975369	7.500000
octupole moment	0.000000	0.000000	0.000000
hexadecapole moment .	0.127094	0.084295	0.211390
q5	0.000000	0.000000	0.000000
q6	0.018185	0.010424	0.028609
q7	0.000000	0.000000	0.000000
q8	0.003634	0.001482	0.005116
kinetic energy	1149.833004	664.567872	1814.400876
volume energy			-2987.621520
rho_tau			-151.437884
rho_rho			-2836.183637
surface energy			150.829343
rho_DELTA_rho			150.829343
(NABLA_rho)^2			0.000000
spin-orbit energy ...			-52.525055
rho_NABLA_J ...			-52.525055
NABLA_rho_J ...			0.000000
coulomb energy			234.338584
direct			249.470293
exchange			-15.131708
tensor energy			0.000000
direct Hartree E ...			0.000000
Extra E			0.000000
External field E			0.000000
Entropy	0.000000	0.000000	0.000000
tEnergy: ehfb (qp)...			-848.785885
tEnergy: ehfb(qp)+LN			-850.718770

Main calculations results

Charge radius without Lipkin-Nogami corrections (larger than proton rms radius due to contribution from the radius of a single proton)

Quadrupole moment obtained in the calculation without LN corrections (usually equal exactly to the one which was constrained)

Hexadecapole moment obtained in the calculation without LN corrections

Binding energy in the calculation without LN corrections (if *type_of_calculation* = *1* meaning standard HFB, only this will appear)

Binding energy in the calculation with LN corrections (appears only if *type_of_calculation* = *-1* meaning calculations with LN corrections).

Key elements of output file

Main calculations results

```
  With Lipkin-Nogami Corrections
================================
  rms-radius ..........      4.587257      4.372526      4.502594
  charge-radius, r0 ...                    4.443741      5.569907
  deformation beta ....      0.288599      0.315317      0.298678
  quadrupole moment[b]       4.596871      3.042164      7.639035
  hexadecapole moment .      0.137810      0.088924      0.226734
================================
```

If calculations are performed with LN corrections (*type_of_calculation* = *-1*), this additional set of results will appear, since the charge radii, quadrupole moment and deformation parameters will be also impacted. If LN corrections are active, these results should be chosen rather than the ones without corrections (together with the corresponding binding energy).

Calculations with LN corrections are considered to be more accurate (obtained binding energy is lower).

Note: HFBTHO manuals for full information
arXiv:1210.1825v3 and arXiv:1704.03945v1