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Computation of the Skyrme–Hartree–Fock equations in the Cartesian deformed harmonic-oscillator basis

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Abstract

We present the modified version of the code HFODD which solves the nuclear Skyrme–Hartree–Fock problem using the Cartesian deformed harmonic-oscillator basis. The modified code gives (i) the general parameters for starting point of the iteration, that provides the convergence report (ii) maximum numbers of the HO quanta in three directions, (iii) the vacuum and particle-hole configurations for the case of the parity symmetry, (iv) the corresponding values of the coupling constants in the Skyrme functionals, (v) the average values of the total and intrinsic neutron, proton, and total angular momentum, it (vi) the corresponding values and contributions to the first moment of inertia and (vii) a summary of the energies calculated for the HF state. Items (ii) and (iv) we not obtainable using the original program.

1.0 Introduction

The nuclear mean-field and an analysis of its symmetries in realistic cases are the main ingredients of a description of nuclear states. Within the Local Density Approximation, or for a zero-range velocity-dependent Skyrme interaction, the nuclear mean-field is local and velocity dependent. The locality allows for an effective and fast solution of the self-consistent Hartree–Fock equations, even for heavy nuclei, and for various nucleonic (*n*-particle *n*-hole) configurations, deformations, excitation energies, or angular momenta.

The program uses the Cartesian harmonic oscillator basis to expand single-particle wave functions of neutrons and protons interacting by means of the Skyrme effective interaction. The expansion coefficients are determined by the iterative diagonalization of the mean field Hamiltonians or Routhians which depend nonlinearly on the local neutron and proton densities. Suitable constraints are used to obtain states corresponding to a given configuration, deformation or angular momentum.

1.1 Cartesian harmonic oscillator basis

The set of Hartree-Fock (HF) equations is solved by expanding the single-particle wave functions $\psi_i(\boldsymbol{r}\sigma)$ onto the deformed Harmonic Oscillator (HO) wave functions $\psi_{n_x n_y n_z}(\boldsymbol{r}\sigma)$ in the Cartesian coordinates, [1] i.e

$$\psi_i(\boldsymbol{r}\sigma) = \sum_{n_x=0}^{N_x}\sum_{n_x=0}^{N_x}\sum_{n_x=0}^{N_x}\sum_{s_z=-\frac{1}{2},\frac{1}{2}} A_i^{n_x n_y n_z, s_z}\psi_{n_x n_y n_z, s_z}(\boldsymbol{r}\sigma) \qquad (1.1)$$

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Here *Nx, Ny*, and *Nz* are the maximum numbers of the *HO* quanta corresponding to the three Cartesian directions. However, the three parameters $\hbar\omega_x$, $\hbar\omega_y$, $\hbar\omega_z$ defining the *HO* frequencies in three Cartesian directions and on the number *M* of the *HO* states are included in the basis. In the code HFODD we use the standard prescription [2, 3] to choose the *HO* states included in the basis, namely, the *M* states with the lowest *HO* single-particle energies. The sums over nx, ny, and nz are performed over the grid of points which form a pyramid rather than a cube.

The *HO* wave functions have the standard form

$$\psi_{n_x n_y n_z}(\mathbf{r}\sigma) = \psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z)\delta_{s_z\sigma}, \tag{1.2}$$

where, $\psi_{n_\mu}(\mu) = b_\mu^{\frac{1}{2}} H^{(0)}_{n_\mu}(\xi_\mu) e^{-\frac{1}{2}\xi_\mu^2}$, and $\xi_\mu = b_\mu x_\mu$ are dimensionless variables scaled by the oscillator constants,

$$b_\mu = \sqrt{m\omega_\mu/\hbar} \tag{1.3}$$

Polynomials $H_n^{(0)}(\xi)$ are proportional to the standard Hermite orthogonal polynomials $H_n(\xi)$ [4],

$$H_n^{(0)}(\xi) = \left(\sqrt{\pi}\,2^n n!\right)^{-\frac{1}{2}} H_n(\xi) \tag{1.4}$$

and normalized as,

$$\int_{-\infty}^{\infty} d\xi H_n^{(0)}(\xi) H_{n'}^{(0)}(\xi) e^{-\xi^2} = \delta_{nn'} \tag{1.5}$$

When convenient, we also use the standard bra-ket notation:

$$. \left| n_x n_y n_z, s_z \right\rangle \equiv \psi_{n_x n_y n_z, s_z}(\mathbf{r}\sigma) \tag{1.6}$$

1.2 The Simplex basis

The *y*-simplex symmetry operator $\hat{S}_y = \hat{P}\exp(-i\pi\hat{J}_y)$ transforms the HO states Eq. (1.6) in the following way

$$\hat{S}_y \left| n_x n_y n_z, s_z \right\rangle = (-1)^{n_y + \frac{1}{2} - s_z} \left| n_x n_y n_z, s_z \right\rangle. \tag{1.7}$$

Since in the present implementation of the code HFODD, the simplex symmetry is always assumed, it is convenient to use the HO basis composed of states which belong to a given simplex, i.e.,

$$\left| n_x n_y n_z, s = +i \right\rangle = \frac{1}{\sqrt{2}} \left(i^{n_y} \left| n_x n_y n_z, \tfrac{1}{2} \right\rangle - i^{n_y+1} \left| n_x n_y n_z, -\tfrac{1}{2} \right\rangle \right), \tag{1.8a}$$

$$\left| n_x n_y n_z, s = +i \right\rangle = \frac{1}{\sqrt{2}} \left(-i^{n_y+1} \left| n_x n_y n_z, \tfrac{1}{2} \right\rangle + i^{-n_y} \left| n_x n_y n_z, -\tfrac{1}{2} \right\rangle \right), \tag{1.8b}$$

for which

$$\hat{S}_y \left| n_x n_y n_z, s = \pm i \right\rangle = (\pm i) \left| n_x n_y n_z, s = \pm i \right\rangle. \tag{1.9}$$

Since the HO wave functions are real, the time-reversal operator $\hat{T} = -i\sigma_y \hat{K}_0$, $\hat{T}^2 = (-1)^A$ where $\hat{K}_0$ is the complex conjugation in coordinate space, transforms them in the following way

$$\hat{T} \left| n_x n_y n_z, s_z \right\rangle = (-1)^{\frac{1}{2} - s_z} \left| n_x n_y n_z, s_z \right\rangle \tag{1.10}$$

The relative phases of states (1.8a) and (1.8b) have been chosen in such a way that the time reversal simply flips the simplex:

$$\hat{T} \left| n_x n_y n_z, s = \pm i \right\rangle = \pm \left| n_x n_y n_z, s = \mp i \right\rangle. \tag{1.11}$$

Having the relative phases established, we may still arbitrarily choose the absolute phases of, say, the $s = +i$ simplex eigenstates. The choice in (1.8a) is made by considering the antiunitary

operator $\hat{K}$, $$\hat{K} = \hat{T} i\sigma_z, \hat{K}^2 = 1. \quad (1.12)$$

This operator does not act on the space coordinates and therefore conserves quantum numbers $n_x n_y n_z$. Since it is an antilinear operator with the square equal to one, the phases in the spin space can always be chosen [5] in such a way that all the basis states are its eigenstates with the eigenvalues being equal to 1. Since $\hat{K}$ commutes with $\hat{T}$, such a choice of phase convention made in (1.8a) applies in fact to both simplexes, i.e.,

$$\hat{K} \left| n_x n_y n_z, s = \pm i \right\rangle = \left| n_x n_y n_z, s = \pm i \right\rangle \quad (1.13)$$

One should stress that $\hbar\omega_x, \hbar\omega_y, \hbar\omega_z$ is not a conserved symmetry, and therefore the HF single-particle states do not have any particular symmetry with respect to this operator.

2.0 Description of the code HFODD

The original code HFODD written in FORTRAN program was obtained from the CPC Program Library, Queen's University of Belfast, *N*. Ire-land. The computers for which the program was designed and others on which it has been tested are CRAY C-90, SG Power Challenge L, and IBM RS/6000. The Operating systems on which it was run are UNIX, UNICOS, IRIX, AIX and the Programming language used was FORTRAN-77. The memory requirement to execute with typical data was 10 Mwords Number of bits in a word was 64 Number of lines and the distributed program was 19 438 (of which 8354 are comments and separators) [6]

Modification was made to the code to make and operate under Windows and Visual Fortran. Initially we encountered different errors some more subroutines were added, which included: CGEMM, ZHPEV, ZDSCAL, ZHPTRD, DSTERF, ZUPGTR, ZSTEQR e.t.c, number of lines for the original code was 19438 with number of characters 814761. with the added subroutines the code line now becomes 24536.

In addition, we have implemented an interface to the LAPACK subroutine ZHPEV, which was downloaded (with the dependencies) from http://netlib2.cs.utk.edu/cgi-bin/netlibfile. 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 large HO bases. Numbers of eigenvectors to be found are defined by the size of the HO phasespace, Subroutine ZHPEV and its dependencies 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 ZHPEV package were compiled separately and then linked together. CGEMM performs one of the matrix-matrix operations, ZHPTRD reduces a complex Hermitian matrix A stored in packed form to real symmetric tridiagonal form *T* by a unitary similarity, ZLARFG generates a complex elementary reflector *H* of order *n*, such that H' * (alpha) = (beta), H' * H = I, ZHPMV performs the matrix-vector operation *y* := alpha*A**x* + beta**y*, where alpha and beta are scalars, *x* and *y* are *n* element vectors and *A* is an *n* by *n* hermitian matrix, supplied in packed form, ZHPR2 performs the hermitian rank 2 operation A := alpha**x*conjg(*y*') + conjg(alpha)**y*conjg(*x*') + A, where alpha is a scalar, *x* and y are n element vectors and A is an *n* by *n* hermitian matrix, supplied in packed form.and so on.

3.0 Numerical tests

Accuracy of the solution of the HF equations with the wave functions expanded onto the Cartesian HO basis, (1.1) depends on the three parameters $\hbar\omega_x, \hbar\omega_y, \hbar\omega_z$ defining the HO

frequencies in three Cartesian directions, and on the number M of the HO states included in the basis. In the code HFODD we use the standard prescription [2, 3] to choose the HO states included in the basis, namely, the M states with the lowest HO single-particle energies,

$$\in_{n_x n_y n_z} = \hbar\omega_x(n_x + \tfrac{1}{2}) + \hbar\omega_y(n_y + \tfrac{1}{2}) + \hbar\omega_z(n_z + \tfrac{1}{2}), \qquad (3.1)$$

are selected among those which have $n_x \le N_0$, $n_y \le N_0$ and $n_z \le N_0$ where *N0* is the fixed maximum number of *HO* quanta. It should be noted that in general both M and N0 have to be specified to define the basis. Only for large *N0*, the basis is defined solely by M and does not depend on *N0*. In this case, the grid of points (*nx, ny, nz*) defining the states included in the basis forms a pyramid in three dimensions, with the inclined face delimited by the condition $\in_{n_x n_y n_z} \le const$. On the other hand, only for small values of N0 the basis is defined solely by *N0* and does not depend on the energy cut-off. In this case the corresponding grid of point's *nxnynz* forms a cube of the size *N0*. In all intermediate cases the shape of the basis corresponds to a pyramid with the corners cut off, or to a cube with the corners cut off. Usually *N0* is chosen large enough so that all the states allowed by the energy cut-off are included in the basis. The *HO* basis is composed of states having not more than *N0 = NOSCIL* quanta in either of the Cartesian directions, and not more than *M = NLIMIT* states in total, the states are added to the basis according to the increasing energy of the deformed harmonic oscillator.

The code HFODD calculates parameters of the *HO* basis, and the zero-iteration Nilsson potential [7], by defining the standard nuclear shape defined by the surface Σ , $\Sigma: R(\theta,\phi) = c(\alpha)\sum_{\lambda=0}^{\lambda_{\max}} \sum_{\mu=-\lambda}^{\lambda} \alpha\lambda_\mu Y_{\lambda\mu}(\theta,\phi)$, where c(α) is a function of $\alpha_{\lambda\mu}$ such that the volume enclosed by the surface Σ does not depend on α. Due to the assumed y-simplex symmetry, all multipole deformations $\alpha_{\lambda\mu}$ are real, and only those with μ=0 are used in the code HFODD because then $\alpha_{\lambda,-\mu} = (-1)^\mu \alpha_{\lambda\mu}$. The lengths of principal axes of the volume enclosed in the surface Σ can be defined as $R_x = R(\pi/2, 0)$, $R_y = R(\pi/2, \pi/2)$ and $R_z = R(0,0)$. All calculations below have been performed for the Skyrme parametrization SkM* with the coupling in the energy functional $H_{t_t}^{even}(\mathbf{r}) \equiv C_t^\rho \rho_t^2 + C_t^{\Delta\rho} \rho_t \Delta\rho_t + C_t^\tau \rho_t \tau_t + C_t^J \vec{J}^2{}_t + C_t^{\Delta J} \rho_t \nabla.\mathbf{J}_t$.

3.1 Spherical nuclei

We begin with the results obtained for a spherical nucleus ^{208}Pb for which the spherical basis is used, *q* = 1, and the results are studied in function of $\hbar\omega_0$. The physical value for this nucleus is $\hbar\omega_0 = 8.304 MeV$, and is represented in Figures 3.1 and 3.2. The energies of ^{208}Pb, shown in Figure 3.1, converge rather slowly to the exact value of -1635.956MeV. Figure 3.2 shows the corresponding results of calculations for the root-mean-square (rms) radii of ^{208}Pb.

3.2 Deformed nuclei

In order to study the properties of the optimization of the deformation of the basis, we have performed a series of calculations for the non-rotating superdeformed state in ^{152}Dy ($\hbar\omega_0 = 0$) with $\hbar\omega_0$ fixed at the physical value, and for several different values of q and M. one

obtains [8], respectively, the total energies E = -1234.611, -1230.769, or -1230.104MeV and the proton quadrupole moments Qp = 42.316b, 44.369b, and 46.376b. These values of energies were obtained by using the finite difference expressions for derivatives, which are less precise than the Fourier expressions [9]. Such a procedure yields [10] for Δx=0.7 fm the value of *E*= -1229.365.

Figure 3.3 shows the total energies in ^{152}Dy calculated by the code HFODD for M=300, 600, 900, or 1200. Keeping a fixed number *M* of states with varying q means that a given HO orbital may cross the boundary $n_x n_y n_z = const$. However, the energy gain from optimizing the value of *q* is very small. For *M* = 900 the optimal and physical values of *q* are close to one another, but the minimum of energy is hardly visible. For *M* = 1200 we obtain *E*=.1229.383 in a very good agreement with the exact result. Figure 3.4 shows the values of proton quadrupole moment calculated by the code HFODD.

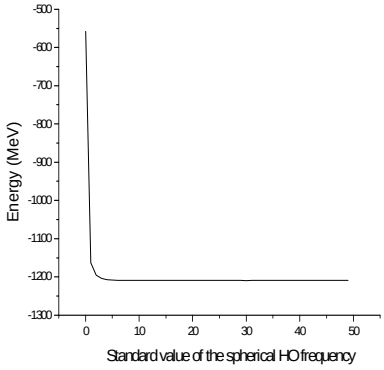

Figure 3.1: Ground-state energies of 208Pb calculated as functions of $\hbar\omega_0$ for several values of the number N0 of HO shells included in the basis.

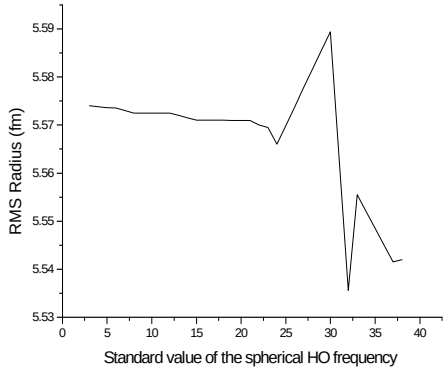

Figure 3.2: Same as in Figure 2.1 but for the rms radii of 208Pb.

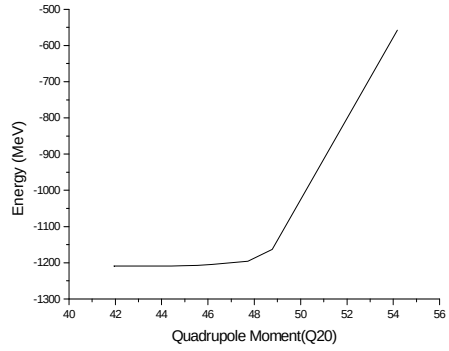

Figure 3.3: Energies of superdeformed state in ^{152}Dy calculated at $\hbar\omega_0 = 0$ as functions of the basis deformation parameter *q* for several values of the number *M* of states included in the HO basis.

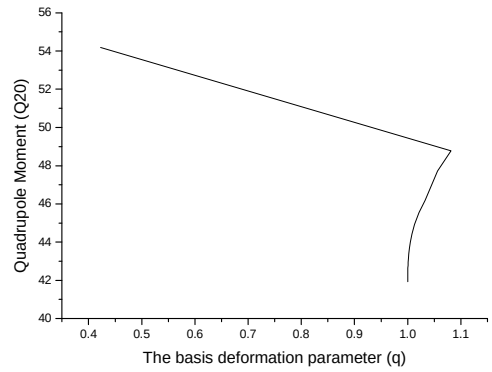

Figure 3.4: Same as in Figure 3.3 but for the proton quadrupole moments Qp of superdeformed^{152}Dy at $\hbar\omega_0 = 0$.

4.0 Output

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. The sample output is as follows

CLASSICAL NUCLEAR SURFACE DEFINED FOR: N = 86 Z = 66
AL10 = ZERO AL11 = ZERO.

AL20 = 0.610 AL21 = ZERO AL22 = ZERO.
AL30 = ZERO AL31 = ZERO AL32 = ZERO AL33 = ZERO.
AL40 = 0.100 AL41 = ZERO AL42 = ZERO AL43 = ZERO AL44 = ZERO
HOMEGA= 9.2190 FCHOM0= 1.2000
OSCILLATOR FREQUENCIES: HBAROX= 11.1998 HBAROY= 11.1998 HBAROZ= 6.2464
MOMENTS OF INERTIA: XMOMFC= 90.2596 YMOMFC= 90.2596 ZMOMFC= 42.8300
CENTRES OF MASS: CMSXFC= 0.0000 CMSYFC= 0.0000 CMSZFC= 0.0000
OSCILLATOR LENGTHS: X= 1.9243099 Y= 1.9243099 Z= 2.5766958
OSCILLATOR CONSTANTS: X= 0.5196668 Y= 0.5196668 Z= 0.3880939
OSCILLATOR FREQUENCIES: X=11.1997759 Y=11.1997759 Z= 6.2464470
BASIS CUT-OFF CONTROL PARAMETERS: NXMAXX= 8 NYMAXX= 8 NZMAXX= 15
OPTIMUM NUMBERS OF GAUSS POINTS: NXHERM= 18 NYHERM= 18 NZHERM= 32 NLIMIT= 301 LDBASE= 306 MCOUNT= 4096 ENECUT= 800.0000 ELIMIT= 112.7539
SHAPE OF THE OSCILLATOR-BASIS DIAMOND
NZ ===>>> 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
MAX.NX => 8 8 7 7 6 6 5 4 4 3 3 2 2 1 0 0
NX= 0 (15) | 8 8 7 7 6 6 5 4 4 3 3 2 2 1 0 0
NX= 1 (13) | 7 7 6 6 5 5 4 3 3 2 2 1 1 0
NX= 2 (12) | 6 6 5 5 4 4 3 2 2 1 1 0 0
NX= 3 (10) | 5 5 4 4 3 3 2 1 1 0 0
NX= 4 (8) | 4 4 3 3 2 2 1 0 0
NX= 5 (6) | 3 3 2 2 1 1 0
NX= 6 (5) | 2 2 1 1 0 0
NX= 7 (3) | 1 1 0 0
NX= 8 (1) | 0 0
PARAMETER SET SKM*: T0= -2645.00 T1= 410.00 T2= -135.00 T3= 15595.00
POWER=0.1667 W=130 X0= 0.09000 X1= 0.00000 X2= 0.00000 X3= 0.00000 COEFFICIENTS DEFINING THE SKYRME FUNCTIONAL

	TOTAL(T)	SUM(S)	ISOSCALAR(P)	ISOVECTOR(M)
CRHO_ =	-1382.012500	780.275000	-991.875000	390.137500
CRHOD =	1299.583333	-649.791667	974.687500	-324.895833
CLPR_ =	-85.312500	34.218750	-68.203125	17.109375
CTAU_ =	68.750000	-68.125000	34.687500	-34.062500
CSCU_ =	0.000000	68.125000	34.062500	34.062500
CDIV_ =	-65.000000	-65.000000	-97.500000	-32.500000
CSPI_ =	-59.512500	661.250000	271.112500	330.625000
CSPID =	0.000000	-649.791667	-324.895833	-324.895833
CLPS_ =	0.000000	34.218750	17.109375	17.109375
CCUR_ =	-68.750000	68.125000	-34.687500	34.062500
CKIS_ =	0.000000	-68.125000	-34.062500	-34.062500
CROT_ =	-65.000000	-65.000000	-97.500000	-32.500000

PARITY/SIGNATURE CONFIGURATIONS:

	V A C U U M				P A R T I C L E S				H O L E S			
	(++)	(+-)	(-+)	(--)	(++)	(+-)	(-+)	(--)	(++)	(+-)	(-+)	(--)
NEUTRONS:	22	22	21	21	0	0	0	0	0	0	0	0
PROTONS:	16	16	17	17	0	0	0	0	0	0	0	0

CONVERGENCE REPORT
ITER ENERGY STABILITY Q20 Q22 SPIN OMEGA RATIO OF E

0	-559.936804	-759.775974	54.178	-0.027	98.777	0.500	0.424287
1	-1163.385944	88.001030	48.812	0.025	53.243	0.500	1.081832
48	-1208.769024	0.000468	41.807	0.067	49.581	0.500	1.000000
49	-1208.768731	0.000400	41.806	0.067	49.581	0.500	1.000000

SINGLE-PARTICLE PROPERTIES: HARTREE-FOCK NEUTRONS

NO) ENERGY (++,+-,-+,--) | N,nz,/\,OMEG> <P> JY SY GFACT

76) -11.743	(0, 0,21, 0)	5, 3, 2, 3/2>	-100	0.103	-0.092	-0.896
77) -11.728	(0, 0, 0,20)	5, 3, 2, 3/2>	-100	0.209	-0.101	-0.485
78) -11.433	(19, 0, 0, 0)	4, 1, 1, 1/2>	100	0.007	-0.182	-3.E+01
79) -11.334	(0,19, 0, 0)	4, 1, 3, 5/2>	100	-0.129	-0.040	0.307
80) -11.241	(20, 0, 0, 0)	4, 1, 3, 5/2>	100	-0.100	-0.189	1.885
81) -11.137	(21, 0, 0, 0)	6, 5, 1, 1/2>	100	1.119	-0.176	-0.157
82) -11.069	(0,20, 0, 0)	6, 5, 1, 1/2>	100	0.984	0.084	0.086
83) -10.881	(0,21, 0, 0)	4, 1, 1, 1/2>	100	-0.112	-0.201	1.784
84) -10.379	(22, 0, 0, 0)	6, 4, 2, 5/2>	100	-0.155	-0.064	0.414
85) -10.365	(0,22, 0, 0)	6, 4, 2, 5/2>	100	0.007	-0.024	-3.300
86) -9.557	(0, 0, 0,21)	7, 6, 1, 3/2>	-100	2.517	0.041	0.016
87) -7.880	(0, 0,22, 0)	5, 2, 1, 3/2>	-100	0.903	0.201	0.222
88) -7.840	(0, 0, 0,22)	5, 2, 1, 3/2>	-100	0.442	0.217	0.490
89) -7.738	(23, 0, 0, 0)	4, 0, 2, 5/2>	100	-0.247	0.161	-0.650
90) -7.732	(0,23, 0, 0)	4, 0, 2, 5/2>	100	-0.235	0.162	-0.690
91) -7.562	(0, 0,23, 0)	5, 2, 1, 3/2>	-100	1.068	0.153	0.144
92) -7.221	(0, 0, 0,23)	5, 1, 4, 9/2>	-100	-0.337	0.028	-0.083
93) -7.221	(0, 0,24, 0)	5, 1, 4, 9/2>	-100	-0.337	0.028	-0.083
94) -7.096	(0, 0, 0,24)	7, 7, 0, 1/2>	-100	-0.134	-0.167	1.252
95) -7.076	(0,24, 0, 0)	6, 4, 0, 1/2>	100	1.232	0.328	0.266
96) -6.350	(0,25, 0, 0)	4, 0, 0, 1/2>	100	0.078	0.455	5.825
97) -6.284	(24, 0, 0, 0)	6, 3, 3, 7/2>	100	0.140	-0.044	-0.313

MULTIPOLE MOMENTS IN UNITS OF (10 FERMI) **LAMBDA
Q00 =152.0000, Q10 = ZERO, Q11 = ZERO,Q20 = 41.8059,Q21 = ZERO
Q22 = 0.0675, Q30 = ZERO, Q31 = ZERO, Q32 = ZERO, Q33 = ZERO
Q40 = 4.7902, Q41 = ZERO, Q42 = 0.0058, Q43 = ZERO, Q44 = -0.0011

ROOT-MEAN-SQUARE AND GEOMETRIC SIZES IN FERMIS TOTAL
R_RMS = 5.5420 X_RMS = 2.3844 Y_RMS = 2.3712 Z_RMS = 4.4052
R_GEO = 7.1547 X_GEO = 5.3318 Y_GEO = 5.3022 Z_GEO = 9.8504

DENSITY INTEGRALS IN THE SKYRME FUNCTIONAL

	TOTAL(T)	SUM(S)	ISOSCALAR(P)	ISOVECTOR(M)
DRHO_ =	17.566618	8.912767	17.566618	0.258917
DRHOD =	12.488132	6.334617	12.488132	0.181102
DLPR_ =	-3.719401	-1.886188	-3.719401	-0.052976
DTAU_ =	15.598603	7.983209	15.598603	0.367815
DSCU_ =	0.119929	0.064074	0.119929	0.008219
DDIV_ =	0.823496	0.419204	0.823496	0.014912
DSPI_ =	0.018303	0.010522	0.018303	0.002740
DSPID =	0.013147	0.007544	0.013147	0.001941
DLPS_ =	-0.037372	-0.023155	-0.037372	-0.008937
DCUR_ =	0.060724	0.031580	0.060724	0.00243
DKIS_ =	0.029460	0.015277	0.029460	0.001094
DROT_ =	0.007844	0.004322	0.007844	0.000799

CONTRIBUTIONS TO ENERGY IN THE SKYRME FUNCTIONAL

	TOTAL(T)	SUM(S)	ISOSCALAR(P)	ISOVECTOR(M)
ERHO_ =	-24277.285107	6954.409417	-17423.888833	101.013143
ERHOD =	16229.367796	-4116.181326	12172.025847	-58.839377
ELPR_ =	317.311377	-64.543010	253.674755	-0.906388
ETAU_ =	1072.403924	-543.856103	541.076525	-12.528704
ESCU_ =	0.00000	0.365047	4.085077	0.279970

```
EDIV_ = -53.527218          -27.248236          -80.290827          -0.484627
SUM EVEN: -6711.729227      2206.945789         -4533.317455        28.534017
ESPI_ = -1.089276           6.957479            4.962258            0.905945
ESPID = 0.000000            -4.901833           -4.271249           -0.630584
ELPS_ = 0.000000            -0.792320           -0.639413           -0.152907
ECUR_ = -4.174748           2.151393            -2.106350           0.082995
EKIS_ = 0.000000            -1.040747           -1.003485           -0.037261
EROT_ = -0.509892           -0.280907           -0.764838           -0.025961
SUM ODD: -5.773917          2.093065            -3.823078           0.142226

ANGULAR MOMENTA AND THE FIRST MOMENTS OF INERTIA FOR OMEGA = 0.500000 MEV
                        SPINS                                   J(1)
                        ORBITAL INTRINSIC TOTAL         ORBITAL INTRINSIC TOTAL
NEUTRONS 28.21798   1.21125     29.42923    56.43596    2.42250     58.85846


 PROTONS  19.29890   0.85368     20.15257    38.59779    1.70736     40.30515
 TOTAL    47.51687   2.06493     49.58181    95.03375    4.12986     99.16361

 NEUTRON CONFIGURATIONS
 ======================
            P S 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32
 CONF: + +  1 1  1  1  1  1  1  1  1 1  1  0  0  0  0  0  0  0  0  0  0
 VACC: + +  1 1  1  1  1  1  1  1  1 1  1  0  0  0  0  0  0  0  0  0  0

CONF: + -   1 1  1  1  1  1  1  1  1 1  1  0  0  0  0  0  0  0  0  0  0
 VACC: + -  1 1  1  1  1  1  1  1  1 1  1  0  0  0  0  0  0  0  0  0  0

 CONF: - +  1 1  1  1  1  1  1  1  1  1  0 0  0  0  0  0  0  0  0  0  0
 VACC: - +  1 1  1  1  1  1  1  1  1  1  0 0  0  0  0  0  0  0  0  0  0

CONF: - -    1 1  1  1  1  1  1  1  1  1  0  0 0  0  0  0  0  0  0  0  0
VACC: - -    1  1  1  1  1  1  1  1  1  1  0  0 0 0  0   0  0  0  0  0  0

ENERGIES (MEV)
KINETIC: (NEU)= 1652.730622 (PRO)= 1107.885480 (TOT)= 2760.616103
 SUM EPS: (NEU)= -2034.973323 (PRO)= -1133.181733 (TOT)= -3168.
 PAIRING: (NEU)= 0.000000 (PRO)= 0.000000 (TOT)= 0.000000
 COULOMB: (DIR)= 564.434280 (EXC)= -25.354572 (TOT)= 539.
 CONSTR. (MULT)= 0.000377 SLOPE= -0.003881 CORR.= -0.081133
CONSTR. (SPIN)= -24.790903 SLOPE= 0.500000 CORR.= -12.39545
 REARRANGEMENT ENERGY FROM THE SKYRME DENSITY-DEPENDENT TERMS= 1009.023720
 ROUTHIAN (TOTAL ENERGY PLUS MULTIPOLE AND SPIN CONSTRAINTS) = -1233.
 SPIN-ORB (EVE) = -80.775454 (ODD)= -0.790799 (TOT)= -81.566253
SKYRME: (EVE) = -4504.783438 (ODD)= -3.680852 (TOT)= -4508.464290
TOTAL: (STAB) = 0.000343 (SP)= -1208.768136 (FUN)= -1208.768479
```

5.0 Conclusion

The motivation to construct the Skyrme-Hartree-Fock code using the Cartesian Harmonic Oscillator basis is based on the necessity to obtain a tool which would allow rapid computation for the nuclear superdeformed or hyperderformed rotating states for which the deformation is relatively well known. The method we employed in this research gives a fast, robust, and simple algorithm that can be used to solve physical problems relating to nuclear deformation computations. The modified HFODD developed produced, in additions to the results obtained by the original code, the maximum numbers of the HO quanta in three directions and; the corresponding values of the coupling constants in the Skyrme functional

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