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THREE NUMERICAL METHODS FOR THE COMPUTATION OF THE ELECTROSTATIC ENERGY

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Abstract

The FORTRAN programs for computation of the electrostatic energy of a body with axial symmetry by Lawrence, Hill-Wheeler and Beringer methods are presented in detail. The accuracy, time of computation and the required memory of these methods are tested at various deformations for two simple parametrizations: two overlapping identical spheres and a spheroid. On this basis the field of application of each method is recomended.

1. Introduction

In the liquid drop model of fission, the deformation energy is composed from the surface energy and the electrostatic (Coulomb) energy of an uniformly charged drop with sharp surface.

Generally speeking, the surface energy is not difficult to compute, but the Coulomb energy, E_c , is defined as a six-fold integral [1-4]:

$$E_c = \rho_e^2 \iiint \frac{d\vec{r}_1 \, d\vec{r}_2}{|\vec{r}_1 - \vec{r}_2|} \qquad (1)$$

where ρ_e is the volume density of the electric charge..

One prefers to find the ratio of this quantity to the electrostatic energy E_{co} of a sphere with radius R_o and the same volume. It is known that:

$$E_{co} = \frac{3q^2}{5R_o} = 16\pi^2 R_o^5 \rho_e^2 / 15 \qquad (2)$$

By definition

$$B_c \equiv E_c / E_{co} = \frac{15}{16\pi^2 R_0^5} \iiint\!\!\iiint \frac{d\vec{r}_1\, d\vec{r}_2}{|\vec{r}_1 - \vec{r}_2|} \qquad (3)$$

In this work we will confine only to the shapes possesing axial and reflexion symmetry.

2. Three methods of computation.

Usually the eq.(3) can not be integrated analyticaly, and the numerical integration of a six-fold integral with the required accuracy (4 or 5 significant digits) is very time consuming. For these reasons, some methods were developed in order to decrease the problem complexity. For shapes with axial symmetry, three of these methods are frequently used, namely:

1° Lawrence method [5], in which B_c is expressed as a three fold integral;

2° Hill-Wheeler method [6], in which B_c is a two fold integral;

3° Beringer method [7], in which B_c formula contains only a sum of terms.

These methods are based on the fact that the electrostatic energy of a drop can be calculated in terms of the self energies and the interaction energies of the smaller parts the body was divided into.

The relationships for B_c in the three cases mentioned before, are given by the following (4), (5) and respectively (9) eqs.:

$$B_c = 120\left(\frac{z''-z'}{2R_c}\right)^5 \int_0^1 \rho_1^2 z\, dz \int_0^1 \rho_2^2\, dy \int_0^1 \frac{\sin^2(\pi w)\, dw}{z(1-y)+\left[z^2(1-y)^2+\rho_1^2+\rho_2^2-2\rho_1\rho_2\cos(\pi w)\right]^{1/2}} \qquad (4)$$

where (z"-z') is the drop length along the symmetry axis, $\rho_1 = \rho_1(z)$ is the surface equation in cylindrical coordinates, with ρ_1 and z so normalised that the intersection of the surface with the symmetry axis is 0 and 1, $\rho_2 = \rho_1(zy)$.

$$B_c = \frac{3}{8\pi}\left(\frac{z''-z'}{2R_0}\right)^5 \int_{-1}^{1} dx \left[\rho^2(x) - \frac{x}{2}\frac{\partial\rho^2(x)}{\partial x}\right] \cdot$$

$$\cdot \int_{-1}^{1} dy \left\{E(a,k) + \left[\rho'^2(y) - \rho^2 + (x-y)\left(\frac{\partial\rho'^2}{\partial y} - (x-y)\right)\right] F(a,k)\right\} \quad (5)$$

where $\rho = \rho(x)$ is the surface eq. in cylindrical coordinates, having the intersection with the symmetry axis -1 and +1; $\rho' = \rho(y)$, and:

$$E(a,k) = a\,\mathcal{F}(k) \quad , \quad F(a,k) = \mathcal{E}(k)/a \quad (6)$$

in which $\mathcal{E}$ and $\mathcal{F}$ are the elliptic integrals of first and second kind:

$$\mathcal{E}(k) = \int_0^{\pi/2} (1-k^2\sin^2 t)^{-1/2}\,dt \; ; \; \mathcal{F}(k) = \int_0^{\pi/2} (1-k^2\sin^2 t)^{1/2}\,dt \quad (7)$$

of argument

$$k = (2\sqrt{\rho\rho'}/a) < 1 \quad ; \quad a^2 = (x-y)^2 + (\rho+\rho')^2 \quad (8)$$

when x = y it follows that $\rho = \rho'$, k = 1 and we get an indetermination of the type $0\cdot\infty$ in the function to be integrated in eq. (5, because $\mathcal{E} \to \infty$ in this case. This indetermination is removed, making $\mathcal{E}$ finite quantity.

In the Beringer method [7], the drop is divided into N slices of the some thickness Δ, and each slice is replaced by one cylinder with the height Δ and the radius ρ_c (derived from the condition that the two equivalent bodies have the same volume). In this case B_c is calculated with the relationship:

$$E_c = \Delta^2 \left(E^S + 3.75\, E^{int} \right) \quad ; \quad \Delta = \frac{2''-2'}{N} \tag{9}$$

where E^S is proportional to the sum of self energies of small cylinders, which due to the reflexion symmetry can be computed with the following formula:

$$E^S = 2\sum_{i=1}^{m} E_i^S + E_{m+1}^S \quad ; \quad m = (N-1)/2 \quad ; \quad N - \text{odd} \tag{10}$$

where E_i^S is approximated by a semiempirical relationship:

$$E_i^S = \rho_{ci}^3 \left\{ 0.79577472 + \frac{\Delta}{\rho_{ci}} \left[\frac{\Delta}{\rho_{ci}} \left(0.10883945 - 0.04851281 \ln \frac{\Delta}{\rho_{ci}} \right) - 0.3125 \right] \right\} \tag{11}$$

with which we get errors smaller than 5.10^{-5} if $(\Delta/\rho_{ci}) < 0.5$ [7].

E^{int} is proportional to the sum of interaction energies between cylinders. Due to the reflexion symmetry, we have

$$E^{int} = \sum_{i=1}^{m} \left(2\sum_{j=i+1}^{m+1} E_{ij}^{int} + \sum_{j=m+2}^{N} E_{ij}^{int} \right) \tag{12}$$

where

$$E_{ij}^{int} = \rho_{ci}^3 \left\{ q_{ij}^2 \left[(1+k_{ij}^2)^{1/2} - k_{ij} \right] 0.5 + \sum_{n=1}^{\infty} C_{2n} P_{2n}(0) \frac{q_{ij}^{2n}}{(1+k_{ij}^2)^{2n}} \left[\frac{q_{ij}^2}{2n+2} - \right.\right.$$

$$\left.\left. - \frac{n}{6} \left(\frac{\Delta}{\rho_{ci}} \right)^2 \right] (1+k_{ij}^2)^{1/2} F(-n, -n+1, 1/2 ; -k_{ij}^2) \right\} \tag{13}$$

and

$$q_{ij} = (\rho_{cj}/\rho_{ci}) < 1 \quad ; \quad k_{ij} = (j-i)\Delta/\rho_{ci} \tag{14}$$

The terms C_{2n} and $P_{2n}(0)$ are determined by using the relationships:

$$C_{2n} = \frac{(2n-1)!!}{2^{n}\,n!}\,(-1)^{n}, \qquad P_{2n}(0) = \frac{1-2n}{2n}\,P_{2(n-1)}(0) \qquad (15)$$

$$C_0 = P_0(0) = 1$$

and the hypergeometric series F is calculated with the relationship:

$$F = 1 + \sum_{i=1}^{n-1} T_i \quad ; \quad T_i = T_{i-1}\,\frac{(n-i+1)(i-n)}{(i-0.5)\,i} \quad ; \quad T_0 = 1 \qquad (16)$$

The integrals from the eqs.(4) and (5) are calculated numerically by using Gauss-Legendre method, which for example, in the case of eq.(4) leads to a relationship of the following form:

$$\int_0^1 dx \int_0^1 dy \int_0^1 dz\; g(x,y,z) = \sum_{i=1}^{p}\sum_{j=1}^{p}\sum_{k=1}^{p} w_i w_j w_k\, g(x_i, x_j, x_k) \qquad (17)$$

where the abscissae $\{x_i\}$ and the weighting factors $\{w_i\}$ for various number of points, p, are tabulated in ref.[8]. A similar relationship is used for the eq.(5) in which IBM subroutines allow to compute the elliptic integrals. The listing of the FORTRAN programs are given at the end.

3. Application for two connected spheres and for a spheroid.

Two parametrisations of the nuclear shape were selected for checking the methods, namely: two overlapping spheres (with a cusp) and the spheroid which allows to obtain very elongated shapes.

3.1. Two identical connected spheres (precission) with radius R and the separation of centers $2z_1$. We have for the Lawrence method

$$\rho_1^2(z) = \begin{cases} z\,(a_2 - z) & , z \le 0.5 \\ (1-z)(a_2 - 1 + z) & , 0.5 < z \le 1 \end{cases} \quad ; \quad a_2 = \frac{R}{R + z_1} \qquad (18)$$

$$\frac{z'' - z'}{2R_0} = \frac{\bar{R} + \bar{z}_1}{\bar{R}_0} \qquad (19)$$

in which for a given z_1, R is found from the condition of volume conservation:

$$2\bar{R}^3 + 3z_1\bar{R}^2 - z_1^3 = 2\bar{R}_0^3 \qquad (20)$$

The quantities of interest for the Hill-Wheeler method have the following expressions:

$$\rho^2(x) = \begin{cases} a_z^2 - (x+\zeta_1)^2, & x < 0 \\ a_z^2 - (x-\zeta_1)^2, & x \geq 0 \end{cases} \quad , \quad \zeta_1 = \frac{z_1}{R+z_1} \qquad (21)$$

$$\frac{\partial \rho^2(x)}{\partial x} = -2 \begin{cases} (x+\zeta_1), & x < 0 \\ (x-\zeta_1), & x \geq 0 \end{cases} \qquad (22)$$

For the Beringer method we have:

$$\rho_{ci}^2 = \Delta[r(2i-1) - \Delta(i^2 - i + 1/3)] \qquad (23)$$

$$\rho_{cm+1}^2 = \Delta[rN + \zeta_1(1-N) - \Delta/6]/2 \; ; \; m = (N-1)/2 \qquad (24)$$

$$\Delta = 2(r+\zeta_1)/N \; ; \; r = R/R_0 \; ; \; \zeta_1 = z_1/R_0 \qquad (25)$$

3.2. <u>Spheroid</u> with the ratio of semiaxis d = c/a > 1. The condition of volume conservation leads to

$$a^2 c = R_0^3 \qquad (26)$$

and the above formulae became:

$$\rho_1^2(z) = z(1-z)/d^2 \quad ; \quad \frac{z''-z'}{2R_o} = \frac{c}{R_o} = d^{2/3} \tag{27}$$

$$\rho^2(x) = (1-x)(1+x)/d^2 ; \quad \frac{\partial \rho^2}{\partial x} = -2x/d^2 \tag{28}$$

$$\rho_{ci}^2 = \frac{\Delta}{d}\left\{(2i-1)d^{-1/3} - \frac{\Delta}{d}[i(i-1)+1/3]\right\}; \quad \Delta = 2d^{2/3}N^{-1} \tag{29}$$

The analytical relationships [9] for the spheroid

$$B_c = \frac{1}{2e}(1-e^2)^{1/3}\ln\left(\frac{1+e}{1-e}\right) \tag{30}$$

where

$$e = \sqrt{1-d^{-2}} \tag{31}$$

allows us to check the methods at various deformations.

For every shape, the number of divisions, N, can be estimated from the condition $(\Delta/\rho_{ci}) \leq 0.5$, or

$$\rho_{ci}^2/\Delta^2 \geq 4 \tag{32}$$

By substituting in this relationship the eqs.(24)-(26) for two overlapped identical spheres, we obtain

$$\frac{\rho_{ci}^2}{\Delta^2} = \frac{rN}{r+z_1}(i-0.5) - i^2 + i - 1/3 \geq 4 \tag{33}$$

$$\frac{\rho_{c\,m+1}^2}{\Delta^2} = \frac{rN^2}{4(r+z_1)} + \frac{(1-N)Nz_1}{4(r+z_1)} - \frac{1}{12} \geq 4 \tag{34}$$

and one can see that the most severe condition (for two tangent spheres $r = z_1 = 2^{-1/3}$) is $N \geq 32$ following from the eq.(34).

In the case of a spheroid, from eqs. (29) and (32) we have

$$\frac{\rho_{c_i}^2}{\alpha^2} = \frac{1}{\alpha^2}\left[\left(i-0.5\right)N - \left(i-1\right) - N^2\right] \geq 0 \qquad (35)$$

and for i = 1, we get

$$N \geq \alpha^2 + 2.3 \qquad (36)$$

In this way, for very elongated shapes (for example $\alpha = 10$) $N \geq 300$!

4. Results and concluding remarks.

The order of magnitude of E_{co} for actinide nuclei is 1000 MeV, and consequently in order to reach an accuracy of 100 keV, the maximum bound of error for B_c must be lower than 10^{-4}.

By analyzing the results presented in tables 1 and 2, we can see that each of the three methods has some advantages, either from the accuracy - or from the computation speed point of view.

As it was expected, the error for Lawrence and Hill-Wheeler method rises very sharply with deformation. This is due to the fact that the approximation of the nuclear surface by a p-order polynomial is better for the sphere and is less suitable when the deformation increases. In this way, for two connected spheres, it was not possible to obtain an error lower than 10^{-4} with none of these two methods, even by using Hill-Wheeler method with 64 x 64 integration points.

It is important to point out that by using Cardan formula it was necessary to solve the eq.(20) (condition of volume conservation for two overlapping spheres) in double precision, even for simple precision calculations.

Generally speaking, for the same number of integration points, in double precision computations the Lawrence method is more accurate than the Hill-Wheeler method, but this accuracy is payed for by an increase of the computation time. The difference between the errors for the two methods is very pronounced in the case of the spheroid (see table 2).

The Beringer method allows us to obtain an error independent of deformation, but for the undistorted sphere, the error is higher than for the two preceeding cases. Also for very elongated shapes, this method requires very high number of division points.

Therefore, for very distorted shapes, with cusp, but for which the ratio Δ/ξ_{ci} preserves small value with a reasonable number of division points N, the Beringer method is most suitable one, especially when various accuracies are needed.

For small deformations, very accurate is the Lawrence method, but for moderate precision the Hill-Wheeler method is more convenient due to its lower computation time. Only the Hill-Wheeler method [2,3] was generalized for shapes without axial symmetry.

Concerning the memory places, the order of predilection of the three methods is: Lawrence, Hill-Wheeler and Beringer. The differences between the first and second methods are not very high, the total memory being in the range 18 - 21 k. We have used two versions of the Beringer method: one, which is resumed in the table 1, requesting only 22 k memory places, and the improved version listed at the end, with which we performed the calculations given in table 2. The high core memory needed for the latter version is about 50 k.

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Table 1 Comparison of different methods of computation of the electrostatic energy for two overlapping symmetric spheres

Center seperation z_1 (in units of R_0)			0.	0.05	0.1	0.2	0.4	$2^{-1/3}$	Computation time		Total memory (bytes)
$(B_c)_{exact}$			1.00000	.99975	.99902	.99580	.97992	.89244	$\frac{T-C}{6}$ [sec]	$\frac{Exec}{6}$ (sec)	
	p	Method	$\varepsilon = (B_c)_{exact} - B_c$								
Simple precision	24	L [a]	2.10^{-3}	10^{-3}	2.10^{-3}	3.10^{-3}	-8.10^{-4}	-3.10^{-3}	46	37.33	18007
		H-W [a]	4.10^{-5}	-2.10^{-5}	-7.10^{-5}	-2.10^{-4}	-7.10^{-4}	-4.10^{-4}	18.33	5.89	20840
	32	L	4.10^{-3}	$+4.10^{-3}$	4.10^{-3}	2.10^{-3}	3.10^{-4}	4.10^{-4}	94.16	87.77	18159
			5.10^{-5}	10^{-4}	-10^{-5}	-10^{-4}	-4.10^{-4}	-2.10^{-3}	22.5	9.85	20840
	35		3.10^{-4}	2.10^{-4}	2.10^{-4}	3.10^{-4}	3.10^{-4}	2.10^{-4}	21.83	12.93	19255
	81	B	3.10^{-4}	2.10^{-4}	2.10^{-4}	2.10^{-4}	10^{-4}	10^{-4}	86.66	78.09	19255
Double precision	24	L	10^{-7}	-10^{-4}	-2.10^{-4}	-5.10^{-4}	-10^{-3}	-2.10^{-3}	73.66	61.81	18815
		H-W	8.10^{-6}	-5.10^{-5}	-10^{-4}	-2.10^{-4}	-8.10^{-4}	-4.10^{-3}	21.33	9.30	21013
	32	L	5.10^{-9}	-7.10^{-5}	-10^{-4}	-2.10^{-4}	-7.10^{-4}	-2.10^{-3}	157.83	148.76	19035
		H-W	3.10^{-6}	-4.10^{-5}	-6.10^{-5}	-10^{-4}	-5.10^{-4}	-2.10^{-3}	28.16	16.09	21013
	64	H-W	4.10^{-7}	-2.10^{-5}	-3.10^{-5}	-5.10^{-5}	-10^{-4}	-5.10^{-4}	69	56.99	21039
	35	B	2.10^{-4}	2.10^{-4}	2.10^{-4}	2.10^{-4}	2.10^{-4}	2.10^{-4}	41.16	32.10	21695
	81	B	4.10^{-5}	2.10^{-5}	2.10^{-5}	3.10^{-5}	2.10^{-5}	3.10^{-5}	224.17	209.28	21695

[a] L - Lawrence; H-W - Hill-Wheeler; B - Beringer

[b] T - total; C - compilation

Table 2 Comparison of different methods of computation of the electrostatic energy for a spheroid

	Ratio of semiaxes r=c/a	1.	1.2	2.	4.	8.	10.	Computation time $\frac{T-C^{***)}}{\epsilon}$ (sec)	Computation time $\frac{Exec}{6}$ (sec)	Total memory (bytes)
	$(B_c)_{exact}$	1.0000000	.9970360	.9579759	.8457310	.6976366	.6481190			
p	Method	$\mathcal{E} = (B_c)_{exact} - B_c$								
Simple precision 24	L*)	2.10^{-3}	6.10^{-4}	10^{-3}	8.10^{-4}	6.10^{-4}	10^{-3}	48.33	37.39	17687
Simple precision 24	H-W*)	4.10^{-5}	4.10^{-5}	2.10^{-5}	-8.10^{-5}	-6.10^{-4}	-10^{-3}	17.33	5.06	19871
Simple precision 32	L	4.10^{-3}	10^{-3}	3.10^{-3}	2.10^{-3}	2.10^{-3}	2.10^{-3}	98.5	87.98	17875
Simple precision 32	H-W	5.10^{-5}	5.10^{-5}	2.10^{-5}	2.10^{-5}	-2.10^{-4}	-4.10^{-4}	20.83	8.26	19871
Double precision 24	L	10^{-7}	2.10^{-7}	2.10^{-7}	10^{-6}	4.10^{-7}	10^{-6}	73.33	62.29	18479
Double precision 24	H-W	7.10^{-6}	10^{-5}	-10^{-5}	-10^{-4}	-5.10^{-4}	-10^{-3}	19.67	7.94	19743
Double precision 32	L	10^{-7}	2.10^{-7}	10^{-7}	2.10^{-7}	2.10^{-7}	2.10^{-7}	158.33	147.08	18735
Double precision 32	H-W	3.10^{-6}	2.10^{-6}	-5.10^{-6}	-5.10^{-5}	-3.10^{-4}	-5.10^{-4}	25.5	13.67	19743
Double precision 64	H-W	4.10^{-7}	3.10^{-7}	-5.10^{-7}	-6.10^{-6}	-3.10^{-5}	-6.10^{-5}	66.17	54.63	20599
Double precision Var.	B	8.10^{-4}	10^{-3}	10^{-4}						49631
		17	21	65						

***) Number of division points

```
C                                  MAIN LAWRENCE
CC                                 ***************
C
      REAL*8 BC,AZ,X,Y,WI,WJ,ZO,R13,D
      REAL*8 Z1V(6)/0.000,0.0500,0.100,0.200,0.400,0.7900/
      REAL*8 AZV(6)/0.1D1,0.95124973307[illegible]0,0.90499562573766300,
     1 0.81992476645142800,0.67873397996933300,0.5D0/
      REAL*8 ZV(6)/0.1D1,0.10256354099747301,0.10525831128982401,
     1 0.11106592360160701,0.12450740976646601,0.15874010519682001/
      REAL*8 XN(32),WN(32)
        COMMON /F/ AZ
C
CC    COMPUTES (DOUBLE PRECISION) THE ELECTROSTATIC ENERGY 'BC' OF TWO
C     SYMMETRICAL SPHERES (PRESCISSION) BY USING THE LAWRENCE METHOD IN
C     CONNECTION WITH 32*32*32 POINTS GAUSS-LEGENDRE QUADRATURE. 'AZ'=
C     R/(R+Z1).
C
        R13=0.1D1/(0.3D1)
      Z1V(6)=0.2D1**(-R13)
C
CC    HALF OF THE 32 INTEGRATION POINTS AND WEIGHTS
C
        XN(1)=.52415383284386915800
         XN(2)=.57223598079139825D0
        XN(3)=0.61964368112606854D0
        XN(4)=0.66593430114106394200
        XN(5)=0.71067563806531767D0
        XN(6)=0.75344995446611470D0
        XN(7)=0.79385787862038116D0
        XN(8)=0.83152213346510760D0
        XN(9)=0.86609105937014484D0
        XN(10)=0.89724189798397120D0
        XN(11)=0.92468380686628499D0
        XN(12)=0.94816057788302600 0
        XN(13)=0.96745303796886900
        XN(14)=0.98238112779375322D0
         XN(15)=0.99280575577263417D0
        XN(16)=0.99863193092474078D0
        WN(1)=0.48270044257363900D-1
        WN(2)=0.47819360039637430D-1
        WN(3)=0.46922199540402283D-1
        WN(4)=0.45586939347881942D-1
         WN(5)=0.43826046502201906D-1
        WN(6)=0.41655962113473378D-1
        WN(7)=0.39096947893535153D-1
        WN(8)=0.36172897054424253D-1
        WN(9)=0.32911111388180923D-1
        WN(10)=0.29342046739267774D-1
        WN(11)=0.25499029631188088D-1
        WN(12)=0.21417949011113340D-1
        WN(13)=0.17136931456510717D-1
        WN(14)=0.12696032654631030D-1
        WN(15)=0.81371973654528350D-2
        WN(16)=0.35093050047350483D-2
C
CC    THE OTHER POINTS CALCULATED BY PROPERTIES OF SYMMETRY
C
        KI=16
        KK=KI+KI
        KI1=KI+1
        KJ=KK+1
        DO 3 II=KI1,KK
        IJ=KJ-II
        WN(II)=WN(IJ)
 3      XN(II)=0.1D1-XN(IJ)
        DO 1 L=1,6
        D=Z1V(L)
        AZ=AZV(L)
        ZO=ZV(L)
C
CC    NUMERICAL INTEGRATION (GAUSS-LEGENDRE)
C
        BC=0.000
        DO 2 I=1,32
        X=XN(I)
        WI=WN(I)
         DO 2 J=1,32
        Y=XN(J)
        WJ=WN(J)
        DO 2 K=1,32
 2      BC=BC+WI*WJ*WN(K)*FCTRR(X,Y,XN(K))
         BC=0.12D3*BC*(ZO**0.5D1)
        WRITE(3,4)D,BC,ZO,AZ
 4      FORMAT(1H ,4D25.15)
 1      CONTINUE
```

```
      STOP
      END
C
C                                   FCTRR
C                                   *******
C
      REAL FUNCTION FCTRR*8(X,Y,Z)
      REAL*8 X,Y,Z,R01,R02,SZ,XY,R12,AZ,X1,C
      COMMON /F/ AZ
C
C   COMPUTES  THE  UNCTION TO BE INTEGRATED (LAWRENCE METHOD) IN THE CASE
C   OF TWO SYMMETRICAL SPHERES (PRESCISSION). 'AZ'=P/(R+Z1). ONLY 'R01'
C   AND 'R02' DEPENDS ON NUCLEAR SHAPE.
C
      C=0.31415926535897932D1*Z
      SZ=DSIN(C)
      IF(X.GT.0.5D0) GO TO 2
      R01=X*(AZ-X)
      GO TO 3
    2 X1=0.1D1-X
      R01=X1*(AZ-X1)
    3 XY=X*Y
      IF(XY.GT.0.5D0) GO TO 4
      R02=XY*(AZ-XY)
      GO TO 5
    4 XY=0.1D1-XY
      R02=XY*(AZ-XY)
    5 XY=X*(0.1D1-Y)
      R12=R01*R02
      FCTRR=R12*X*SZ*SZ/(XY+DSQRT(XY*XY+R01+R02-0.2D1*DSQRT(R12)*DCOS(C)
     1 ))
      RETURN
      END
```

```
C                              MAIN HILL-WHEELER
C                            ********************
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION XN(64),WN(64),ZIV(6)
      COMMON /F/R2
      DATA ZIV/0.1D1,0.12D1,0.2D1,0.4D1,0.8D1,0.10D2/
C
C    COMPUTES (DOUBLE PRECISION) THE ELECTROSTATIC ENERGY 'BC' OF A
C    SPHEROID BY USING THE HILL-WHEELER METHOD IN CONNECTION WITH GAUSS-
C    LEGENDRE QUADRATURE ('KI'**2 POINTS). 'AZ'=C/A(THE RATIO OF SEMIAXES)
C
      READ (1,110)KI
  110 FORMAT(I3)
      KK=KI*KI
      KII=KI+1
      KJ=KK+1
C
C    HALF OF THE    INTEGRATION POINTS AND WEIGHTS ARE READ
C
      READ(1,100)(XN(I),WN(I),I=1,KI)
  100 FORMAT(2F20.16)
      DO 3 II=KII,KK
      IJ=KJ-II
      WN(II)=WN(IJ)
    3 XN(II)=-XN(IJ)
      R103=0.102/0.3D1
      DO 1 L=1,6
      AZ=ZIV(L)
         R2=AZ*AZ
      Z5=AZ**R103
C
C    NUMERICAL INTEGRATION (GAUSS-LEGENDRE)
      SUM=0.000
      DO 2 I=1,KK
       X=XN(I)
      WI=WN(I)
      DO 2 J=1,KK
    2 SUM=SUM+WI*WN(J)*GFUNC(X,XR(J))
      BC=SUM*3.D0*Z5/(0.8D1*0.31415926535897931)
      WRITE(3,300)AZ,BC
  300 FORMAT(1H ,2D25.16)
    1 CONTINUE
      STOP
      END

C                                    GFUNC
C                                  *********
C
      FUNCTION GFUNC(X,Y)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /F/R2
C
C    COMPUTES THE FUNCTION TO BE INTEGRATED (HILL-WHEELER METHOD)
C
      CALL FD(X,FX,DFX)
      SFX=DSQRT(FX)
      IF(X.NE.Y) GO TO 3
      GFUNC=(FX-0.5D0*X*DFX)*(SFX+SFX)
      RETURN
    3 CALL FD(Y,FY,DFY)
      SFY=DSQRT(FY)
      SFXY=SFX+SFY
      XY=X-Y
      AF2=XY*XY+SFXY*SFXY
      AF=DSQRT(AF2)
      AK2=0.4D1*SFX*SFY/AF2
      AK=DSQRT(AK2)
      CALL DCEL1(F,AK,IER)
      IF(IER)5,10,5
   10 CALL DCEL2(E,AK,1.D0,1.D0-AK2  ,IER)
      IF(IER)5,11,5
    5 WRITE(3,100)X,Y
  100 FORMAT(1H ,'ELER',2D25.16)
      STOP
   11 F=F/AF
      E=E*AF
      GFUNC=(FX-0.5D0*X*DFX)*(E+F*(FY-FX+XY*(DFY-XY)))
      RETURN
      END
```

```
C                                       FD
C                                      ****
C
        SUBROUTINE FD(X,F,DF)
      IMPLICIT REAL*8(A-H,O-Z)
       COMMON /F/R2
C
C    THIS SUBROUTINE IS CALLED BY 'GFUNC'. COMPUTES THE FUNCTION 'F'=RO**2
C    AND THE DERIVATIVE 'DF'=D(RO**2)/DX IN THE CASE OF A SPHEROID
C
        F=(0.1D1-X*X)/R2
        DF=-(X+X)/R2
        RETURN
        END


C
C
C                                       DATA
C                                      ******
C
  32
 0.02435079266434244 0.04869095700913971
 0.07299312178779991 0.04857546744150341
 0.12146281929612051 0.04834476223480291
 0.16964442042399281 0.04799938859645831
 0.21742364374000711 0.04754016571483031
 0.26468716220876741 0.04696818281621
 0.31132287199021111 0.04628479658131441
  .3572201583376681   .0459491627927418
 0.40272701579639916 0.04459055816375661
 0.44636601725346411 0.04358372452939341
 0.48940314570705331 0.04247351512365361
 0.53127946401989451 0.04126256324262351
 0.57189564620263411 0.03995374113272031
 0.61115535517239321 0.03855015317861561
  .6489654712546573   .0370551285402411
 0.68523631305423321 0.03547221325688241
 0.71988185017161081 0.03380516183714161
 0.75281990726053191 0.03205792835485151
 0.78397235894334141 0.03023465707240251
 0.81326531512279761 0.02833967261425951
 0.84062929625258041 0.02637746971505471
 0.86599939815409281 0.02435270256871091
 0.88931544599511411 0.02227017380838321
 0.91052213707850281 0.02013482315353021
 0.92956917213193961 0.01795171577569731
 0.94641137485840281 0.01572603047602471
 0.96100879965205371 0.01346304789671861
 0.97332682778991101 0.01116813946013111
 0.98333625388462601 0.00884675982636391
 0.99101337147674431 0.00650445796897841
 0.99634011677195531 0.00414703326056251
 0.99930504173577211 0.00178328072169641
```

```
C
C                                  MAIN BERINGER
C                                  *************
C
      IMPLICIT REAL*8(A-H,O-Z)
       DIMENSION RC(801),RC2(801),CP(200)
C
C    DOUBLE PRECISION
C    COMPUTES THE ELECTROSTATIC ENERGY 'RC' OF A SPHEROID BY USING
C    BERINGER METHOD. 'Z1'=C/A
C    THE VOLUME IS DIVIDED IN 'N' CILINDERS WITH THE SAME HEIGHT '2'
C
       DO 70 JJ=1,6
      READ(1,100)Z1
  100  FORMAT(D8.1)
C
C    COMPUTATION OF THE SMALL CILINDER RADII 'RC' FROM THE CONDITION OF
C    VOLUME CONSERVATION. THE NUCLEAR SHAPE IS INTRODUCED ONLY IN THESE
C    QUANTITIES.
C
       ZN=Z1+Z1
       ZN=ZN*ZN
       N=IDINT(ZN)
        N=N+N
       N=N+N+1
       IF(N.GT.801)N=801
       M=(N-1)/2
       M1=M+1
       N1=N+1
       AN=DFLOAT(N)
       WRITE(3,400)N
  400  FORMAT(1H ,'N=',I4)
       Z13=Z1**(1.0D0/3.0D0)
       Z23=Z13*Z13
        D=Z23/AN
       D=D+D
       DR=D/Z1
        D2=D*D
       C1=DR/Z13
       C2=DR*DR
       DO 30 I=1,M
       AI=DFLOAT(I)
       AI1=AI-1.
       NI=N1-I
       RC2(I)=C1*(AI+AI1)-C2*(AI*AI1+0.3333333333333333D0)
       RC(I)=DSQRT(RC2(I))
         RC2(NI)=RC2(I)
   30  RC(NI)=RC(I)
       RC2(M1)=1.0D0/Z23-C2/1.2D1
       RC(M1)=DSQRT(RC2(M1))
C
C    'EI' IS PROPORTIONAL TO THE SELF ENERGY OF THE CILINDER 'I'.
C
       EI=0.0D0
       DO 1 I=1,M
       X=D/RC(I)
       EI=EI+RC2(I)*RC(I)*(0.7957747D0*X*(X*(0.1088394D0 -
     1  0.0485178D0*DLOG(X1)-0.3125D0))
    1  CONTINUE
         X=D/RC(M1)
```

```
      EI=EI+EI*RC2(M1)*RC(M1)*(0.75577471D0+X*(X*(0.1098394D0 -
     *  0.048512A1D0*DLOG(X))-0.3125D0))
C
C     COMPUTES THE COEFFICIENTS CP(I)
C
      CP(1)=-0.25D0
      CI=CP(1)
      DO 10 I=2,200
      AA=DFLOAT(I)
      P=0.5D0/AA
      P1=P+P
      P=P-0.1D1
      CI=CI*P*(P+P1)
      CP(I)=CI
10     CONTINUE
C
C     'EIJ' IS PROPORTIONAL TO THE INTERACTON  BETWEEN CILINDERS 'I' AND 'J'
C     'AK'=KIJ. 'G'=GIJ.  'K' IS THE SUMATION INDEX.
C
      EIJ=0.0D0
      DO 20 I=1,M
      I1=I+1
      DO 20 J=I1,N
      AJ=DFLOAT(J-I)
       IF(RC(I)-RC(J))2,2,3
2     X1=D/RC(J)
      G=RC(I)/RC(J)
      R1=RC(J)*RC2(J)
      GO TO 4
3     X1=D/RC(I)
      G=RC(J)/RC(I)
      R1=RC(I)*RC2(I)
4     AK=AJ*X1
      AK2=AK*AK
      AB=X1*X1/6.0D0
      AK21=1.0D0+AK2
      AK22=AK21*AK21
      SK=DSQRT(AK21)
      G2=G*G
      AK22=0.1D1/AK22
      S=0.0D0
      K=1
      A2K=0.1D1
      G2K=0.1D1
444   B=K
      B1=B+B
      G2K=G2K*G2
      A2K=A2K*AK22
      T=CP(K)*G2K*A2K
      SP=G2/(B1+2.0D0)-B*AB
      X=T*SP
      F=X
      IF(K.EQ.1) GO TO 222
      P=X
      K1=K-1
      DO 111 L=1,K1
      Q=DFLOAT(L)
      BL=Q-B
      P=(P/((Q-0.5D0)*Q1))*AK2*(0.1D1-BL)*BL
      ABP=DABS(P)
      IF(ABP.LT.(1.0D-8*DABS(F))) GO TO 222
111   F=F+P
```

```
222     S=S*F
        IF(DABS(F)-1.00-7*DABS(S)) 333,333,444
 334    IF(K-200)13,14,14
13      K=K+1
        GO TO 444
14      WRITE(3,200) F,S,I,J
200      FORMAT(1H ,*K=200*,5X,2D15.7,2I5)
333     S=S*SK
11      RR=(S+0.500*G2*(SK-AK))*R1
        IF(J.GT.M1) GO TO 22
        RB=RB+RR
22      EIJ=EIJ+RR
20      CONTINUE
        EIJ=3.7500*EIJ
        BC=02*(EI+EIJ)
         WRITE(3,300)Z1,BC,EI,EIJ,02,
300     FORMAT(1H ,5D15.7,I5)
70      CONTINUE
        STOP
        END
```

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