# ЯДЕРНА ФІЗИКА NUCLEAR PHYSICS 

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# THE INTERACTION ENERGY OF TWO UNIFORMLY CHARGED SPHEROIDS. EXAMPLE OF DEFORMED NUCLEI 


#### Abstract

We consider the question of calculations of the interaction energy of two uniformly charged spheroids. Three cases are realized in the software: the interaction of a uniformly charged spheroid with a point charge; interaction of two coaxial spheroids; and the general case of mutual position of spheroids. The presented programs are initially oriented for nuclear calculations. However, by a change of numerical coefficients, they can be used in the calculations of the interaction energy in any cases of spheroidal objects with the uniformly distributed charge or mass.

Keywords: Coulomb interaction, uniformly charged spheroids, potential of uniformly charged spheroids, interaction of uniformly charged spheroid and point charge, interaction of coaxial spheroids, interaction of arbitrarily placed spheroids.


## 1. Introduction

The potentials of uniform spheroidal and ellipsoidal charge distributions coincide functionally with the Newton potentials for homogeneous masses [1-3]. In [1], the potential of a spheroid with explicit dependence on the eccentricity is represented in the form of four separate expressions for interior and exterior domains in compressed and elongated spheroids. The analogous formulas in a somewhat other form were given in [2] based on the transition to the spheroidal limit in the general formulas for the potential of a triaxial ellipsoid [3].

The dependence of the potential on the eccentricity is equivalent to its dependence on the ratio of semiaxes $\beta=b / a$, which is the parameter characterizing the compression or elongation of a spheroid. The inclusion of the parameter $\beta$ in numerical algorithms reduces the number of representations of the potential of a spheroid to two ones, which are formally similar and are related to the interior and exterior domains.

In addition to Newton problems [1,3], plasma physics [2], and Coulomb clusters [4], the spheroidal
potential was applied to the estimation of a Coulomb contribution to the total interaction energy of deformed atomic nuclei (spheroids with uniformly distributed charge) and the comparison with the results obtained in multipole expansions of potential (see, e.g., [5] and references therein). The proposed package of programs is adapted namely for the solution of problems of nuclear physics.

In the algorithms, we used the following units for physical quantities accepted in nuclear physics: the charge of a nucleus is taken in units of the standard charge $e$; the quantities with the dimension of length are written in units of $R_{o}=10^{-15} \mathrm{~m}=1 \mathrm{Fm}$; potentials and the energy are presented, respectively, in units of $\Phi_{o}=e / 4 \pi \varepsilon_{o} R_{o} \cong 1.44 \mathrm{MeV}$, where $\varepsilon_{o}$ is the electrical constant, and $E_{o}=e \Phi_{o} \cong 1.44 \mathrm{MeV}$. The programs are written in Fortran-77.

## 2. Basic relations

The axisymmetric potential of a spheroid $\Phi$ at the internal points of the intrinsic reference system is parabolic

$$
\begin{equation*}
\Phi(\rho, z)=\frac{3}{2} \frac{Q}{a}\left\{S(\beta)-\frac{1}{2 a b}\left[\left(1+S^{\prime}(\beta)\right) \rho^{2}+\left(-2 S^{\prime}(\beta)\right) z^{2}\right]\right\} \tag{1}
\end{equation*}
$$

where $Q$ is the charge of a spheroid, $a$ are the lengths of semiaxes along the principal axes $x$ and $y, b$ is the semiaxis length along the rotation axis $z$, $\rho^{2}=x^{2}+y^{2}, \beta=b / a$.

The potential of a spheroid $\Phi(\rho, z)$ at external points corresponds to the right-hand side of (1), where the following changes should be carried out:

$$
\begin{gather*}
a \rightarrow a_{\lambda}=\sqrt{a^{2}+\lambda}, \quad b \rightarrow b_{\lambda}=\sqrt{b^{2}+\lambda} \\
\beta \rightarrow \beta_{\lambda}=b_{\lambda} / a_{\lambda} \tag{2}
\end{gather*}
$$

Here, $\lambda$ is a function of the coordinates of external points $\rho, z$ and the parameters $a, b$ and is determined as a positive root of the equation

$$
\begin{gather*}
\left(x^{2}+y^{2}\right) /\left(a^{2}+\lambda\right)+z^{2} /\left(b^{2}+\lambda\right)=1,  \tag{3}\\
\lambda=\frac{1}{2}\left(A+\sqrt{A^{2}+4 B}\right), A=\rho^{2}+z^{2}-a^{2}-b^{2}, \\
B=a^{2} b^{2}\left(\frac{\rho^{2}}{a^{2}}+\frac{z^{2}}{b^{2}}-1\right)>0 . \tag{4}
\end{gather*}
$$

The functions $S(\beta)$ and $S^{\prime}(\beta)$, like the case of the argument $\beta_{\lambda}$, are given by the relations

$$
\begin{gather*}
S(\beta<1)=\frac{\arccos (\beta)}{\sqrt{1-\beta^{2}}}, S(\beta=1)=1, \\
S(\beta>1)=\frac{\ln \left(\beta+\sqrt{\beta^{2}-1}\right)}{\sqrt{\beta^{2}-1}} ;  \tag{5}\\
S^{\prime}(\beta \neq 1)=\frac{\beta S(\beta)-1}{1-\beta^{2}}, \quad S^{\prime}(\beta=1)=-\frac{1}{3} . \tag{6}
\end{gather*}
$$

The function $S(\beta)>0$ and it decreases monotonically, as $\beta$ increases, by starting from $S(\beta=0)=\pi / 2$. Respectively, $S^{\prime}(\beta)<0$, and it increases monotonically, by starting from $S^{\prime}(\beta=0)=-1$. Potential (1) can be set with regard for only one of these functions, for example, $S(\beta)$ [4].

The interaction energy of two charge distributions, including two spheroidal ones, is given by the general equation

$$
\begin{equation*}
E_{\mathrm{int}}=\int \Phi_{1}(\vec{r}) \rho_{2}(\vec{r}) d \vec{r}, \tag{7}
\end{equation*}
$$

which includes the potential $\Phi_{1}$ depending on the electric field of one of the spheroids (first) and on the charge density $\rho_{2}$ of the second spheroid. The integration is performed over the volume of the second spheroid.

We admit the overlapping of spheroids. Below, we will give several exact formulas for the interaction energy of two spheroids with uniform density. Let the spheroids with charges $Q_{1}$ and $Q_{2}$ have the common rotation axis and the common central point. Let one of the spheroids be placed completely inside of the second one. We introduce the notations $\left(a_{<}, b_{<}\right)$and $\left(a_{>}, b_{>}\right)$for semiaxes and set $\beta_{<}=b_{<} / a_{<}, \beta_{>}=b_{>} / a_{>}$. In this case, the interaction energy of the spheroids takes the form
$E_{\text {int }}=\frac{3}{2} \frac{Q_{1} Q_{2}}{a_{>}}\left\{S\left(\beta_{>}\right)-\frac{1}{5}\left(\frac{a_{<}}{a_{>}}\right)^{2} \frac{1}{\beta_{>}}\left[1+\left(1-\beta_{<}^{2}\right) S^{\prime}\left(\beta_{>}\right)\right]\right\}$.

If the spheroids are concentric $\left(\beta_{<}=\beta_{>}=\beta\right)$, then

$$
\begin{equation*}
E_{\mathrm{int}}=\frac{3}{2} \frac{Q_{1} Q_{2}}{a_{>}} S(\beta)\left[1-\frac{1}{5}\left(\frac{a_{<}}{a_{>}}\right)^{2}\right] \tag{9}
\end{equation*}
$$

At the complete overlapping of spheroids $\left(a_{<}=a_{>}=a, b_{<}=b_{>}=b, \beta=b / a\right)$,

$$
\begin{equation*}
E_{\mathrm{int}}=\frac{6}{5} \frac{Q_{1} Q_{2}}{a} S(\beta) \tag{10}
\end{equation*}
$$

For the concentric spheroids-balls with radii $R_{<}$and $R_{>}$, Eqs. (8) - (10) take, respectively, the simple well-known form

$$
\begin{equation*}
E_{\mathrm{int}}=\frac{3}{2} \frac{Q_{1} Q_{2}}{R_{>}}\left[1-\frac{1}{5}\left(\frac{R_{<}}{R_{>}}\right)^{2}\right], \quad E_{\mathrm{int}}=\frac{6}{5} \frac{Q_{1} Q_{2}}{R} \tag{11}
\end{equation*}
$$

Relations (8) - (11) can be used for the testing of numerical algorithms.

We note that works [6] (see its Appendix) and [7] (two more economical options) present analytic formulas for the interaction energy of two uniformly charged balls centered at arbitrary spatial points.

## 3. Description of the SPP program

The SPP program allows one to calculate the interaction energy of a uniformly electrically charged spheroid with semiaxes $a$ and $b$ and a point charge. The point charge can be placed outside or inside of the spheroid. The spheroid center is at the coordinate origin. The location of the point charge relative to the spheroid center is determined by spherical coordinates $(\mathrm{r}, \theta, \varphi)$ (Fig. 1).


Fig. 1. The mutual arrangement of a point charge and a uniformly charged spheroid realized in the SPP program.

From the viewpoint of the used formulas, the integration over the volume of the second charged body is made with the $\delta$-function. Respectively, the interaction energy is represented by the potential created by the spheroid and multiplied by the charge of the point.

Input parameters:
Z1 - charge of a spheroid in units of the elementary charge;

Z2 - charge of the point in units of the elementary charge;
a - lengths of semiaxes of the spheroid along the axes $x$ and $y$ in Fm;
$b-$ semiaxis length of the spheroid along the axis $z$ in Fm;
rmin - minimum distance from the spheroid center to the point in Fm;
rmax - m ximum distance from the spheroid center to the point in Fm;
hr - increment in $r$ in Fm ;
tetmind - minimum value of the angle $\theta$ in degrees;
tetmaxd - maximum value of the angle $\theta$ in degrees;
htetd - increment in the angle $\theta$ in degrees;
fimind - minimum value of the angle $\varphi$ in degrees;
fimaxd - maximum value of the angle $\varphi$ in degrees;
hfid - increment in the angle $\varphi$ in degrees.
Eventually, the interaction energy of the point charge with the uniformly charged spheroid is assigned to the variable Eell and is calculated, by calling the subprogram Espherop(r,tetr,fir). The formal parameters of this subprogram are the variables r (distance from the spheroid center to the point), tetr (angle $\theta$ in radians), and fir (angle $\varphi$ in radians). The results of the calculations are recorded in the file 'Eell.dat'. In this case, the quantities ee $=1.44, \mathrm{Z} 1, \mathrm{Z} 2$, and $\mathrm{a}, \mathrm{b}$, respectively, are transferred from the basic program to the subprogram Espherop(r,tetr,fir) through the common blocks /ceez/ and /cab/.

To compare the results of calculations of the proposed program with those describing the interaction of a point charge with a uniformly charged ball, we introduce a subprogram Espherep(rsph,r), where rsph is the radius of a uniformly charged ball equivalent to the spheroid by volume, and $r$ is the distance from the ball center to the point charge. The result is assigned to the variable Esph and is recorded in the file 'Esph.dat'. The calculation of the interaction


Fig. 2. The mutual arrangement of two uniformly charged coaxial spheroids realized in the CoaxSpSp program.

Finally, the interaction energy of the spheroids is calculated by calling the subprogram Eellips(a1,b1, $2, \mathrm{~b} 2, \mathrm{R}$ ), where the formal parameters are the semiaxes of the first spheroid al and b1, semiaxes of the second spheroid a 2 and b 2 , and displacement between the centers of the spheroids R. The result is assigned to the variable Eell and is recorded in the file 'Esph.dat'. In this case, the number $\pi$, quantity ee $=1.44$, charges Z 1 and Z 2 , and accuracy of calculations of the external integral eps are transferred from the basic program to the subprogram Eellips(a1,b1,a2,b2,R) by means of the common blocks /cpi/pi/ceez/ee,Z1,Z2/ceps/eps. The accuracy of calculations of the internal integral eps1 is transferred from the basic program to the subpro-
gram $\mathrm{fz}(\mathrm{z})$ with the use of the common block /ceps1/eps1.

For the sake of comparison of the results of calculations by the proposed program with the results of calculations of the interaction of two uniformly charged balls, our program includes a subprogram Esphere(resph1,resph2,R), where resph1 - radius of the first ball; resph 2 - radius of the second ball; (the program operates with balls equivalent to spheroids by volume); R - the distance between the centers of the balls.

Here, we use the above-mentioned block /ceez/ee,Z1,Z2.

The interaction energy of two uniformly charged balls is calculated by the equation [7]
where $Q_{1}$ and $Q_{2}$ are the charges of the balls, $R_{1}$ and $R_{2}$ are the radii of the balls, and $R$ is the distance between the centers of the balls. In the presented record, the formula is valid for $R_{1} \geq R_{2}$, but this specific feature is easily compensated in calculations since the interaction energy of the balls is independent of their numbering.

## 5. Description of the program ComSPSP

The program ComSPSP is intended for the calculation of the interaction energy of two uniformly charged spheroids in the case of their arbitrary mutual arrangement. The spheroids can intersect each
other or be disjoint. The scheme presenting the clear idea of the parameters characterizing a mutual arrangement of the spheroids is given in Fig. 3. A similar parametrization of the mutual arrangement of spheroids is frequently used in nuclear physics. According to the equations in the Introduction, the program can integrate the potential created by the first spheroid in the volume of the second spheroid. The program makes integration over the volume of an equivalent ball with the help of the triple subsequent usage of the program DGAUSS taken from the CERN library, which calculates integrals in finite limits.


Fig. 3. The mutual arrangement of two uniformly charged spheroids realized in the program ComSPSP.

The input parameters of the program are as follows:

Z1 - charge of the first spheroid in units of the elementary charge;

Z2 - charge of the second spheroid in units of the elementary charge;
a1 - lengths of semiaxes of the first spheroid along the axes $x_{1}$ and $y_{1}$ in units of $F m$;
b1 - semiaxis length of the first spheroid along the axis $\mathrm{z}_{1}$ in units of Fm ;
a2 - lengths of semiaxes of the second spheroid along the axes $x_{2}$ and $y_{2}$ in units of $F m$;
b2 - semiaxis length of the second spheroid along the axis $z_{2}$ in units of Fm;
sZin - an initial shift of the center of the second spheroid relative to the center of the first spheroid along the axis z ;
sZfin - a final shift of the center of the second spheroid relative to the center of the first spheroid along the axis z ;

HsZ - shift increment along the axis z realized in a cycle;

Sx - a shift of the center of the second spheroid relative to the center of the first spheroid along the axis x ;

Sy - a shift of the center of the second spheroid relative to the center of the first spheroid along the axis y;
tet 1 d - rotation angle of the axis $\mathrm{z}_{1}$ of the intrinsic coordinate system of the first spheroid relative to the axis z (in degrees);
tet2din - starting angle between the axis $z_{2}$ of the intrinsic coordinate system of the second spheroid and the axis z (in degrees) in a cycle;
tet2dfin - the final angle between the axis $z_{2}$ of the intrinsic coordinate system of the second spheroid and the axis z (in degrees) in a cycle;
htet2d - an increment of the angle tet2d (in degrees) in a cycle;
psidin - starting rotation angle of the second spheroid around the axis $\mathrm{z}\left(\mathrm{z}^{\prime}\right.$ at the consideration of displacement along the axis x or y ) in degrees in a cycle;
psidfin - final rotation angle of the second spheroid around the axis $z\left(z^{\prime}\right.$ at the consideration of displacement along the axis x or y ) in degrees in a cycle;
hpsid - an increment of the angle psid (in degrees) in a cycle;
eps2 - the accuracy of calculations of the internal integral;
eps 1 - the accuracy of calculations of the mean integral;
eps - the accuracy of calculations of the external integral.

The final result of calculations is assigned to the
variable Eint at the call of a subprogram Ener(a1,b1, a2,b2,sX,sY,sZ,tet1,tet2,psi).

With the use of formal parameters, the subprogram Ener is supplied by the lengths of semiaxes of the spheroids a1,b1,a2,b2, shifts sX,sY,sZ of the second spheroid relative to the first one along the axes $\mathrm{x}, \mathrm{y}, \mathrm{z}$, and angles determining the mutual orientation of the spheroids tet1,tet2,psi, which are set in radians. In this case, we transfer the number $\pi$, quantity ee $=1.44$, charges Z1 and Z2, and accuracy of calculations of the external integral eps from the basic program to the subprogram Ener using the common blocks /cpi/pi/ceez/ee,Z1,Z2/ceps/eps. The accuracy of calculations of the internal integrals eps1 and eps2 is transferred from the basic program to the subprograms $\mathrm{fz}(\mathrm{z})$ and $\mathrm{fy}(\mathrm{y})$ with the use of the common blocks /ceps1/eps1 and /ceps2/eps2.

The results of calculations of the interaction energy of spheroids depending on the input parameters are recorded in the file 'Ener.dat'.

## 6. Calculation examples

Here are some examples of numerical calculation of interaction energy for uniformly charged spheroids. In the figures, beta characterizes the degree of spheroid deformation and is equal to $2 \cdot(b-a) /(b+a)$, where b is semi-axis of the sphe$\operatorname{roid} \mathrm{z}, \mathrm{a}$ and b - for x and y axes.

The spheroid is centered at the origin (Fig. 4). The point is moving closer to the spheroid along the Z axis (teta $=0$ ), at angle of 45 degrees relative to the Z axis $($ teta $=45)$ and at angle of 90 degrees to the Z axis, i.e. in the XY plane. For comparison, the interaction energy of a point charge with an isometric ball with the same charge is given depending on the distance from the center of the ball to the point.


Fig. 4. The interaction of point unit charge with spheroid.
Rotation occurs around the X axis (Fig. 5). Three cases are considered. The first case corresponds to
the situation in which the rotating point does not go beyond the spheroid border, being constantly inside ( $\mathrm{R}=2 \mathrm{Fm}$ ). The second case is when moving along a circular path $(\mathrm{R}=4 \mathrm{Fm})$ the charged point is located both inside of the spheroid and outside. And the third ( $\mathrm{R}=6 \mathrm{Fm}$ ) - the point is constantly outside of the spheroid.


Fig. 5. Rotation in XOZ plane of unit point charge around the spheroid center along spherical trajectories with different radiuses.

In the first case, two identical elongated charged spheroids with semiaxes shown in Fig. 6 are considered. For comparison, the energy of the interaction of two isometric balls is presented (two upper curves). A similar situation is presented for flattened spheroids (a pair of lower curves).


Fig 6. The interaction energy of two coaxial spheroids (elongated, flattened) and isometric spheres (see Fig. 2).

In Fig. 7 the axes of the first spheroid's coordinate system are aligned with the XYZ axes, and the Z2 own axis of the second spheroid is directed at angles of 0,45 and 90 degrees concerning the $Z$ axis. There is no rotation around the Z axis.


Fig 7. The interaction energy of two elongated spheroids for some mutual orientations.

The centers of spheroids are located on the Z axis (Fig. 8). The own axes of the spheroids Z1 and Z2 located at angles 90 degrees with the $Z$ axis. The rotation angle $\Psi$ of the second spheroid around $Z$ axis takes values of 0,45 and 90 degrees.


Fig. 8. The interaction energy of two elongated spheroids for some mutual orientations (see Fig. 3).


Fig. 9. Rotation around the Y axis of the second spheroid located at different distances from the first one (see Fig. 3).

In Fig. 9 the spheroid centers are located at Z . $\theta 1=0$ degrees and is a constant, the $\theta 2$ angle changes in a continuous manner. Herewith, the spheroid centers are located at different distances from each other.


Fig. 10. The interaction energy of two elongated spheroids in central and non-central collisions. $\Theta_{1}=\Theta_{2}=0$ (see Fig. 3).

In Fig. 10 the second spheroid moves relative to the first one in the direction opposite to the Z axis with an offset along the X axis, which is expressed in units of a.

## 7. Conclusion

By using the numerical methods, we have solved the problem of calculation of the interaction energy of two uniformly charged spheroids. The solution is presented in the form of three programs: SPP, CoaxSpSp, and ComSPSP. The first one involves the interaction of a uniformly charged spheroid with a point charge. The second and third programs consider, respectively, two coaxial spheroids and the general mutual arrangement of two uniformly charged spheroids.

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## ЕНЕРГІЯ ВЗАЄМОДЇ̈ ДВОХ РІВНОМІРНО ЗАРЯДЖЕНИХ СФЕРОЇДІВ. ПРИКЛАД ДЕФОРМОВАНОГО ЯДРА

Розглядається питання обчислення енергії взаємодії двох рівномірно заряджених сфероїдів. Програмно реалізовано три випадки: взаємодія рівномірно зарядженого сфероїда з точковим зарядом; взаємодія двох співвісних сфероїдів; загальний випадок взаємного розташування сфероїдів. Наведені програми з самого початку орієнтовані на проведення ядерних розрахунків. Однак заміною числових коефіцієнтів їх можна зробити корисними і для обчислення енергії взаємодії в будь-яких випадках, в яких фігурують сфероїдальні об'єкти з рівномірно розподіленим зарядом або масою.

Ключові слова: кулонівська взаємодія, рівномірно заряджені сфероїди, потенціал рівномірно заряджених сфероїдів, взаємодія рівномірно зарядженого сфероїда та точкового заряду, взаємодія співвісних сфероїдів, взаємодія довільно розміщених сфероїдів.

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 ПРИМЕР ДЕФОРМИРОВАННОГО ЯДРА}

Рассматривается вопрос вычисления энергии взаимодействия двух равномерно заряженных сфероидов. Программно реализованы три случая: взаимодействие равномерно заряженного сфероида с точечным зарядом; взаимодействие двух соосных сфероидов; общий случай взаимного расположения сфероидов. Приведенные программы изначально ориентированы на проведение ядерных расчетов. Однако заменой численных коэффициентов их можно сделать полезными и для вычисления энергии взаимодействия в любых случаях, в которых фигурируют сфероидальные объекты с равномерно распределенным зарядом или массой.

Ключевые слова: кулоновское взаимодействие, равномерно заряженные сфероиды, потенциал равномерно заряженных сфероидов, взаимодействие равномерно заряженного сфероида и точечного заряда, взаимодействие соосных сфероидов, взаимодействие произвольно расположенных сфероидов.

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