

## COULOMB ENERGY OF SPHERICAL NUCLEUS

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The analytical formula for calculating the Coulomb energy of spherical nucleus with Woods–Saxon charge distribution is refined by taking into account the higher-order terms of surface diffuseness. The obtained relative deviations are smaller than 0.05% from the results with numerical integration for almost all calculated nuclei.

*Keywords:* Woods–Saxon; Poisson equation; surface diffuseness; Coulomb energy.

The calculation of the Coulomb energy for nuclei or atoms with small computing effort and high accuracy is a great challenge in physics and quantum chemistry research.<sup>1–7</sup> For a complicated nuclear system, there exist serious difficulties in attempts to calculate the Coulomb energy.<sup>2</sup> As it is known, the Coulomb energy of a system with charge density distribution  $\rho(\mathbf{r})$  is written as

$$E_C = \frac{e^2}{2} \iint \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}'. \quad (1)$$

For a spherical nucleus with uniform charge distribution, the corresponding Coulomb energy is written as

$$E_C^{(0)} = \frac{3}{5} \frac{Z^2 e^2}{R}, \quad (2)$$

with the radius  $R$  of the nucleus and the charge number  $Z$ . For a system with Gaussian charge distribution  $\rho(r) = \rho_0 \exp(-\frac{r^2}{2\sigma^2})$ , the Coulomb energy is expressed as<sup>8</sup>

$$E_C^G = \frac{(2\pi\sigma^2)^{5/2}}{\sqrt{2}} \rho_0^2 e^2 = \frac{Z^2 e^2}{2\sqrt{\pi}\sigma}, \quad (3)$$

where  $\rho_0 = \frac{Z}{(2\pi\sigma^2)^{3/2}}$  is the central density, and  $\sigma$  is the width (standard deviation) of the Gaussian distribution. For a system with an arbitrary charge distribution,

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the Coulomb energy can be obtained numerically through Eq. (1). However, the six-dimensional integrals of Eq. (1) is very time-consuming. In the practical calculation, one needs to find an efficient approach to calculate the Coulomb energy at a high level of accuracy. Simple equations for calculating the Coulomb energies of various density distributions of nuclear system would therefore be useful. In the liquid-drop model, the Coulomb energy is roughly calculated under a uniform charge distribution approximation. But for light nuclei, the surface thickness is about 2 fm which is comparable to the corresponding nuclear radius. The contribution of the nuclear surface diffuseness to the Coulomb energy thus should not be neglected.

In this work, we attempt to propose an analytic expression for calculating the Coulomb energy of spherical nucleus with the nuclear surface diffuseness being taken into account. We first calculate the Coulomb potential of a spherical nucleus with Woods–Saxon charge distribution

$$\rho(r) = \frac{\rho_0}{1 + e^{\frac{r-R_0}{a}}} \quad (4)$$

by solving the Poisson equation. Where,  $\rho_0$ ,  $R_0$  and  $a$  are the central charge density, the half-density radius and the surface diffuseness, respectively. Then, we calculate the corresponding Coulomb energy with a numerical integration to the Coulomb potential. Finally, based on the calculated results, we propose an analytic expression for the Coulomb energy, with which the Coulomb energy of a spherical nucleus can be directly calculated with high accuracy.

The Coulomb energy of a nuclear system is calculated by

$$E_C = \frac{e}{2} \int \rho(\mathbf{r}) V_C(\mathbf{r}) d\mathbf{r}, \quad (5)$$

where  $V_C(\mathbf{r})$  is the Coulomb potential obtained by solving the Poisson equation

$$\nabla^2 V_C(\mathbf{r}) = -4\pi e\rho(\mathbf{r}). \quad (6)$$

The Poisson equation is solved by a code *hwscyl* (a Fortran subroutine in FISH-PACK<sup>9</sup>) which is an adaptive fast solver for solving a five-point finite difference approximation to the modified Helmholtz equation in cylindrical coordinates using a centered finite difference grid. We calculate the Coulomb potential in cylindrical coordinates within a region  $x = 0-40$  fm and  $z = -40-40$  fm (using a grid with step size 0.1 fm). It is known that when  $r \gg R$ , the asymptotic behavior of the Coulomb potential of a nucleus is  $V_C = eZ/r$ , which gives the boundary condition in solving the Poisson equation. The Coulomb energy of an arbitrary axially deformed nuclear system can be obtained with a two-dimensional integral (see Eq. (5)) to the Coulomb potential  $V_C(\mathbf{r})$  which can be calculated with the very fast solver for the Poisson equation mentioned above.

We first check the results of the numerical integration of Eq. (5). In Table 1, we list the Coulomb energies of some systems with Gaussian charge distribution. The width  $\sigma$  of the Gaussian distribution and the charge number  $Z$  of the systems in Table 1 are set arbitrarily.  $E_C^G$  denotes the exact Coulomb energy of the systems

Table 1. Coulomb energy of system with Gaussian charge distribution.

$Z$	8	20	40	50	82
$\sigma$ (fm)	1.5	2.5	3.0	5.5	7.1
$E_C^G$ (MeV)	17.3319	64.9946	216.6488	184.6439	384.7042
$E_C$ (MeV)	17.3345	64.9979	216.6573	184.6457	384.7066
$\frac{ E_C - E_C^G }{E_C^G} (\times 10^{-4})$	1.50	0.51	0.39	0.10	0.06

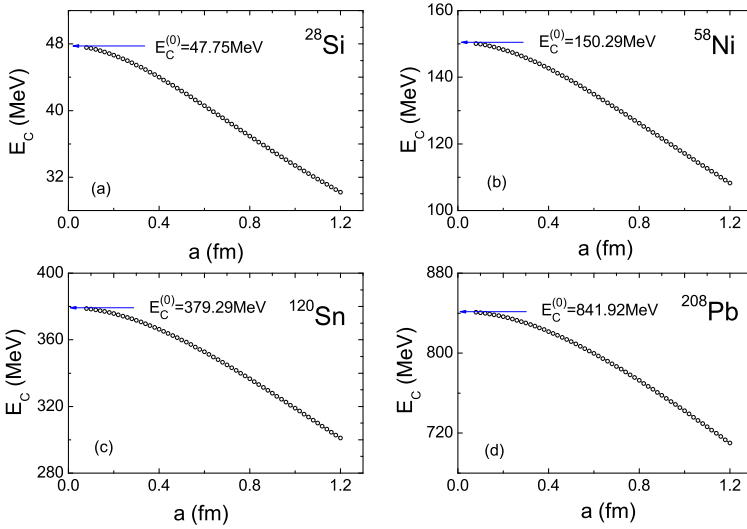


Fig. 1. The Coulomb energies of nuclei  $^{28}\text{Si}$ ,  $^{58}\text{Ni}$ ,  $^{120}\text{Sn}$ ,  $^{208}\text{Pb}$  as functions of nuclear surface diffuseness  $a$ . The arrows denote the corresponding values of  $E_C^{(0)}$  from Eq. (2). The open circles denote the results with numerical integration approach.

obtained with Eq. (3), and  $E_C$  denotes our results with numerical integration of Eq. (5). It shows that the obtained Coulomb energy  $E_C$  with our approach are very close to the exact value  $E_C^G$ , and the relative deviations  $|E_C - E_C^G|/E_C^G$  are about  $10^{-4}$ – $10^{-5}$ .

With the same numerical approach, we calculate the Coulomb energy of some nuclei with Woods–Saxon charge distribution. The central charge density of a nucleus is obtained with the Skyrme energy density functional together with the extended Thomas–Fermi (ETF) approach.<sup>10</sup> The nuclear surface diffuseness  $a$  varies from 0.1 to 1.2 fm in which the central charge density remains unchanged through the conservation of charge number and varying the half-density radius  $R_0$ . Figure 1 shows the calculated Coulomb energies of nuclei  $^{28}\text{Si}$ ,  $^{58}\text{Ni}$ ,  $^{120}\text{Sn}$ ,  $^{208}\text{Pb}$  as a function of nuclear surface diffuseness  $a$ . The arrows denote the corresponding Coulomb energy of uniform charge distribution  $E_C^{(0)}$ . With the decrease of  $a$ , the Coulomb

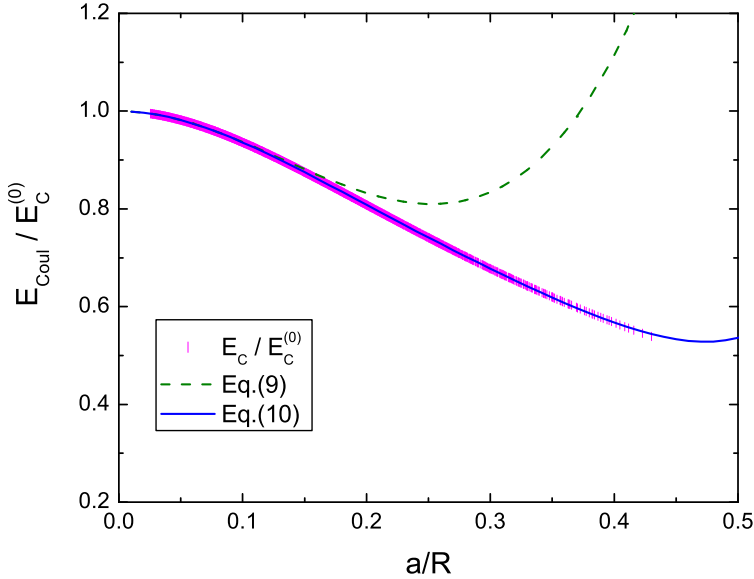


Fig. 2. The ratio of Coulomb energy to  $E_C^{(0)}$  for a number of nuclei with  $A = 16\text{--}300$ . The vertical dashes denote the results with numerical integration approach. The dashed and the solid curve denote the results of Eqs. (9) and (10), respectively.

energies approach to  $E_C^{(0)}$ . Table 1 and Fig. 1 indicate that our calculations are in good agreement with the exact values of the Coulomb energies for the two special cases mentioned above. From Fig. 1, one can see that the Coulomb energy of a nucleus gradually decreases with the surface diffuseness  $a$ , and could be written as

$$E_{\text{Coul}} = E_C^{(0)} F. \tag{7}$$

To obtain the expression of  $F$  as a function of the surface diffuseness  $a$ , we study the Coulomb energies of a number of nuclei from  $A = 16$  to 300 systematically. The calculated results through the numerical integration approach as a function of  $a/R$  are shown in Fig. 2 (the vertical dashes). It is known that the general expression in terms of a leptodermous expansion for the Coulomb energy of a uniform distribution with a diffuse surface is,<sup>8</sup>

$$E_{\text{Coul}} = E_C^{(0)} \left( 1 - \frac{5}{2} \beta^2 + \dots \right). \tag{8}$$

Where  $\beta = b/R$  (notation in Refs. 6 and 8) with  $b = \frac{\pi}{\sqrt{3}}a$  denotes the Süßmann's width<sup>8,11</sup> and  $R = [Z/(\frac{4\pi}{3}\rho_0)]^{1/3}$  is the corresponding radius of a spherical nucleus with uniform charge distribution. For a Woods–Saxon charge distribution, an expression for  $F(\beta)$  is previously proposed in Refs. 6 and 8 based on the leptodermous expansion,

$$F(\beta) = 1 - \frac{5}{2} \beta^2 + 3.0216 \beta^3 + \beta^4 + \dots, \tag{9}$$

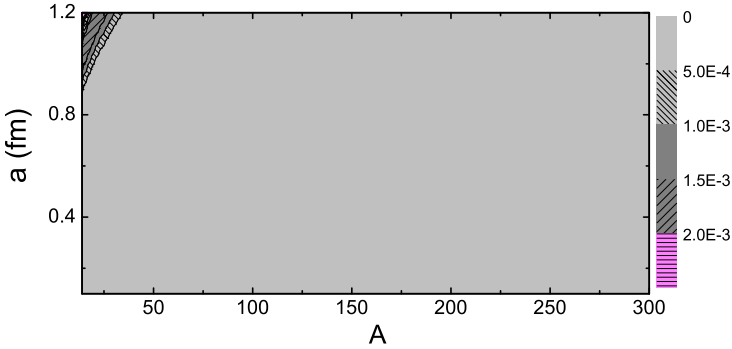


Fig. 3. Relative deviations  $|E_{\text{Coul}} - E_C|/E_C$  of the Coulomb energies from the numerical integration results.  $E_{\text{Coul}}$  denotes the calculated Coulomb energy with Eq. (10). The shades with light gray denote that the relative deviations are smaller than 0.05%.

in which the coefficients are directly obtained from the leptodermous expansion for a Woods–Saxon distribution so long as  $\exp(-R/a)$  is negligible. The results of Eq. (9) are shown in Fig. 2 (the dashed curve). One can see that for nuclei with  $a/R < 0.15$  the Eq. (9) gives nice results, which indicates that Eq. (9) is applicable for heavy nuclei at their ground state. With the increase of  $a/R$ , Eq. (9) deviates from the calculated results gradually, which is due to that the Coulomb energy of a nucleus is not converging very rapidly as a function of  $a/R$ , the higher-order terms should also be considered. For a better description of Coulomb energies of light nuclei (the corresponding value of  $a/R$  is about 0.2) or some exotic nuclear systems, the expression for  $F$  is refined by taking into account the influence of the higher-order terms of  $a/R$ . Because it is complicated to directly obtain the coefficients of all higher-order terms based on the leptodermous expansion, we attempt to obtain the coefficients by fitting the calculated Coulomb energies with numerical integration. Based on Eq. (9) and including the terms  $\beta^5$  and  $\beta^6$ , we get a refined expression for the ratio  $E_{\text{Coul}}/E_C^{(0)}$  by fitting the calculated Coulomb energies in Fig. 2 and the second and fourth terms remain fixed,

$$\frac{E_{\text{Coul}}}{E_C^{(0)}} = 1 - \frac{5}{2}\beta^2 + c_3\beta^3 + \beta^4 + c_5\beta^5 + c_6\beta^6 + \dots \quad (10)$$

with  $c_3 = 3.005$ ,  $c_5 = -4.822$ ,  $c_6 = 2.934$  and  $\beta = \frac{\pi}{\sqrt{3}} \frac{a}{R}$ . The results of Eq. (10) is also shown in Fig. 2 (the solid curve). One can see that Eq. (10) gives better results for nuclei with large  $a/R$  when the terms  $\beta^5$  and  $\beta^6$  are involved. Here, the contribution of other higher-order terms is approximately absorbed in the coefficients of Eq. (10). In Fig. 3, we show the relative deviations  $|E_{\text{Coul}} - E_C|/E_C$  of the Coulomb energies from the numerical results with Eq. (5).  $E_{\text{Coul}}$  denotes the calculated Coulomb energy with Eq. (10). From Fig. 3, one can see that the Coulomb energy obtained with the refined formula Eq. (10) is close to the calculated result with numerical integration. The relative deviations of the Coulomb energies with

Eq. (10) are smaller than 0.05% (denoted in light gray) for almost all calculated nuclei with the diffuseness  $a \leq 1.2$  fm.

In summary, the analytical formula for calculating the Coulomb energy of spherical nucleus with Woods–Saxon charge distribution has been refined by taking into account the higher-order terms of the surface diffuseness. We first calculate the corresponding Coulomb potential by numerically solving the Poisson equation. Then with an integral to the Coulomb potential, we obtain the Coulomb energy. We have checked the Coulomb energies of systems with Gaussian charge distributions. Our results are in good agreement with the exact values of the Coulomb energies. By fitting the calculated Coulomb energies with the numerical integration for a number of nuclei from  $A = 16$  to 300 with Woods–Saxon charge distribution, the analytical formula is finally obtained. The relative deviation of the Coulomb energy with the proposed formula is smaller than 0.05% for almost all calculated nuclei with surface diffuseness  $a \leq 1.2$  fm which is useful for study of nuclear structure. With the same approach, the Coulomb energy of an arbitrary axially deformed system can be reliably calculated with small computing effort. The study of the Coulomb energy for nuclear system with large deformation is in progress.

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### References

1. R. Beringer, *Phys. Rev.* **131**, 1402 (1963).
2. G. D. Adeev and P. A. Cherdantsev, *Rus. Phys. J.* **12**, 1617 (1969).
3. D. Kolb and R. Y. Cusson, *Z. Phys.* **253**, 282 (1972).
4. L. Füsti-Molnár and P. Pulay, *J. Molec. Struct.* **666**, 25 (2003).
5. J. A. Nolen and J. P. Schiffer, *Annu. Rev. Nucl. Sci.* **19**, 471 (1969).
6. W. D. Myers and W. J. Świątecki, *Phys. Rev. C* **58**, 3368 (1998).
7. F. R. Manby and P. J. Knowles, *Phys. Rev. Lett.* **87**, 163001 (2001).
8. R. W. Hasse and W. D. Myers, *Geometrical Relationships of Macroscopic Nuclear Physics* (Springer-Verlag, 1988), p. 33.
9. P. Swarztrauber and R. Sweet, Efficient FORTRAN Subprograms for the Solution of Elliptic Equations, NCAR Technical Report TN/IA-109, National Center for Atmospheric Research (1975), p. 138.
10. M. Liu, N. Wang, Z.-X. Li, X.-Z. Wu and E.-G. Zhao, *Nucl. Phys. A* **768**, 80 (2006).
11. G. Süßmann, *Z. Phys. A* **274**, 145 (1975).