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COULOMB ENERGY OF AXIALLY DEFORMED NUCLEUS

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We previously proposed a formula for calculating the Coulomb energy of spherical nucleus with Woods–Saxon charge distribution. In this work, the analytical formula is extended for description of the Coulomb energy of nucleus with β_2 and β_4 deformation.

Keywords: Coulomb energy; deformed nucleus; Poisson equation; Woods–Saxon.

The calculation of the Coulomb energy for complicated charged system with small computing effort and high accuracy is a great challenge in physics and quantum chemistry research.[1–3] For a system with an arbitrary charge distribution $\rho(\mathbf{r})$, the direct term of the Coulomb energy can be calculated with

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

However, the six-dimensional integration in Eq. (1) is very time-consuming and becomes a bottleneck in the large-scale calculations of potential energy surfaces of nuclear systems. In this work, we attempt to propose an analytic expression for calculating the Coulomb energy of nucleus with both the nuclear surface diffuseness and nuclear β_2 and β_4 deformation being taken into account. For reader's convenience, the approach to calculate the Coulomb energy of a nuclear system proposed in our previously work[1] is reviewed firstly, and then the analytical formula for calculating the Coulomb energy of spherical nucleus with Woods–Saxon density distribution will be extended for description of the Coulomb energy of nucleus with β_2 and β_4 deformation.

The Coulomb energy of an arbitrary nuclear system can be obtained by

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

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

$$\nabla^2 V_C(\mathbf{r}) = -4\pi e\rho(\mathbf{r})\,. \tag{3}$$

The charge distribution of a nucleus is usually described by a Woods–Saxon form,

$$\rho(r) = \frac{\rho_0}{1+\exp(\frac{r-\mathcal{R}}{a})}\,, \tag{4}$$

where ρ_0 and a denote the central charge density and the surface diffuseness, respectively. $\mathcal{R}$ defines the distance from the origin of the coordinate system to the point on the nuclear surface. For an axially deformed system, $\mathcal{R}$ is expressed as,

$$\mathcal{R}(\theta) = R_0[1+\beta_2 Y_{20}(\theta)+\beta_4 Y_{40}(\theta)+\cdots]\,. \tag{5}$$

In the calculation of Coulomb energy of nucleus as a function of nuclear deformation, we remain the central charge density ρ_0 of the nucleus unchanged by using the conservation of charge number and varying the half-density radius R_0 to consider the effect of incompressibility of nuclear matter in the nucleus.

The Poisson equation is solved by a code **hwscyl** (a Fortran subroutine in FISHPACK[4]) 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 $r \gg \mathcal{R}$, 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 integration[5] over the Coulomb potential $V_C(\mathbf{r})$ which can be calculated with the very fast solver for the Poisson equation mentioned above.

In our previous work,[1] we investigated the Coulomb energies of spherical nuclei with Woods–Saxon charge distributions. The central charge density of a nucleus is obtained with the Skyrme energy density functional together with the extended Thomas–Fermi (ETF) approach.[6] The nuclear surface diffuseness a varies from 0.1 to 1.2 fm in which the central charge density remains unchanged. We find that the Coulomb energies of spherical nuclei with Woods–Saxon charge distributions can be well described with an analytical expression based on the leptodermous expansion,[7]

$$E_{\rm Coul} = E_C^{(0)} F(\omega) \tag{6}$$

with[1]

$$F(\omega) = 1 - \frac{5}{2}\omega^2 + c_3\omega^3 + \omega^4 + c_5\omega^5 + c_6\omega^6 + \cdots\,, \tag{7}$$

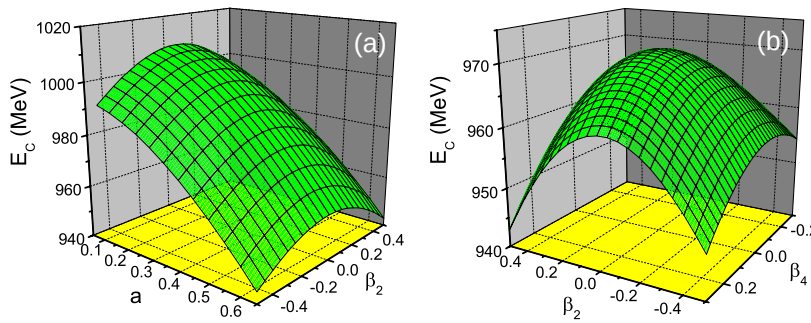

Fig. 1. (color online) Coulomb energies of ^{238}U as a function of nuclear surface diffuseness a and quadrupole deformation β_2 (a); and as a function of β_2 and β_4 (b).

where $\omega = \frac{\pi}{\sqrt{3}}\frac{a}{R}$ and $E_C^{(0)}$ denotes the Coulomb energy of a spherical nucleus with uniform charge distribution,

$$E_C^{(0)} = \frac{3}{5}\frac{Z^2e^2}{R}\,. \tag{8}$$

Z denotes the charge number of the nucleus and $R = [Z/(\frac{4\pi}{3}\rho_0)]^{1/3}$ is the corresponding radius of a spherical nucleus with uniform charge distribution. By fitting the calculated Coulomb energies with numerical integration for a number of spherical nuclei along the β-stability line, we obtained the coefficients $c_3 = 3.005$, $c_5 = -4.822$, $c_6 = 2.934$.

With the same approach, we investigate the Coulomb energies of deformed nuclei. In Fig. 1(a), we show the calculated Coulomb energy of ^{238}U as a function of nuclear surface diffuseness a and quadrupole deformation β_2, and show the corresponding Coulomb energy as a function of β_2 and β_4 (with $a = 0.55$ fm) in Fig. 1(b). One can see that the Coulomb energy decreases with the increase of the nuclear surface diffuseness and of the deformation. In this work, we write the Coulomb energy of a nucleus as

$$E_{\rm Coul} = E_C^{(0)} F(\omega) G(\omega, \beta)\,, \tag{9}$$

with a deformation factor $G(\omega, \beta) = G_2 G_4$ to consider the influence of nuclear β_2 and β_4 deformation. For nucleus with only β_2 deformation ($G_4 = 1$), we assume that the factor $G_2(\omega, \beta_2)$ has a form

$$G_2(\omega, \beta_2) = 1 - \frac{1}{4\pi}\beta_2^2 + b_1\omega\beta_2^2 + b_2\omega^2\beta_2^2 + b_3\beta_2^3 + b_4\beta_2^4 + \cdots\,, \tag{10}$$

where the term $-\frac{1}{4\pi}\beta_2^2$ is presented by Greiner and Maruhn in Ref. 8. By fitting the calculated Coulomb energies with Eq. (2) as a function of surface diffuseness ($a \leq 0.7$ fm) and quadrupole deformation ($|\beta_2| \leq 0.5$) for a number of nuclei along

Table 1. Values of $\omega = \frac{\pi}{\sqrt{3}}\frac{a}{R}$ for some nuclei by taking $a = 0.55$ fm and $R = 1.2A^{1/3}$ fm.

	^{16}O	^{40}Ca	^{90}Zr	^{144}Sm	^{208}Pb	^{238}U	^{298}114
ω	0.33	0.24	0.19	0.16	0.14	0.13	0.12

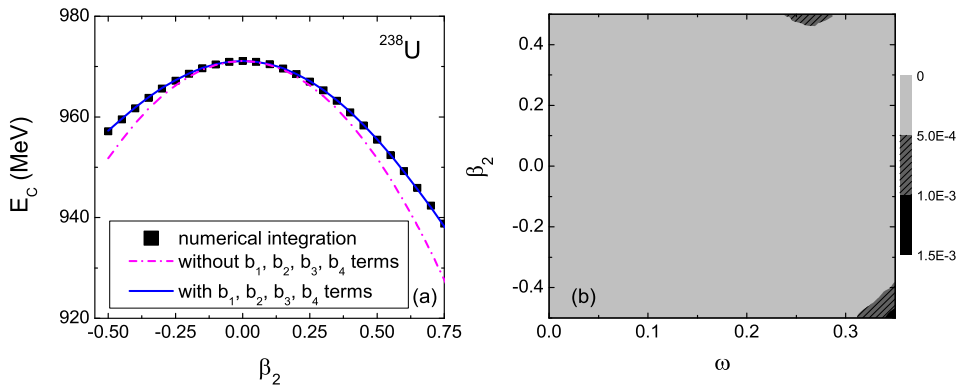

Fig. 2. (color online) (a) Coulomb energy of ^{238}U as a function of β_2 deformation (with $a = 0.55$ fm and $\beta_4 = 0$). The squares denote the results with numerical integration [with Eq. (2)]. The dot-dashed curve and the solid curve denote the results of Eq. (9) without and with the b_1, b_2, b_3 and b_4 terms being taken into account, respectively. (b) Relative deviations $|E_{\rm Coul} - E_C|/E_C$ of the Coulomb energies from the numerical integration results. $E_{\rm Coul}$ denotes the calculated Coulomb energy with Eqs. (9) and (10). The region with light gray denote that the relative deviations are smaller than 0.05%.

the β-stability line, we obtain the coefficients $b_1 = \frac{1}{4\pi}$, $b_2 = 0.188$, $b_3 = -0.007$ and $b_4 = 0.018$. We have also checked other combinations of β_2 and ω for the deformation factor with the same number of parameters, and found that the rms deviation of the Coulomb energies from the numerical integration results is smallest with the proposed form in Eq. (10).

In Fig. 2(a), we show the Coulomb energy of ^{238}U as a function of nuclear quadrupole deformation β_2. The squares denote the results with Eq. (2). The dot-dashed curve and the solid curve denote the results of Eq. (9) without and with the b_1, b_2, b_3 and b_4 terms being taken into account, respectively. One can see that the higher-order terms of deformation are still required for system with large deformation. In Fig. 2(b), we show the relative deviations $|E_{\rm Coul} - E_C|/E_C$ of the Coulomb energies from the numerical results for a number of nuclei $A = 16$–300 varying the surface diffuseness ($a \leq 0.7$ fm) and the quadrupole deformation ($|\beta_2| \leq 0.5$). $E_{\rm Coul}$ denotes the calculated Coulomb energy with Eqs. (9) and (10). From Fig. 2, one can see that the Coulomb energy obtained with the analytical formula Eq. (9) is close to the calculated results with numerical integration for most cases. In Table 1, we list some typical ω values of a series of nuclei from light to heavy. For interme-

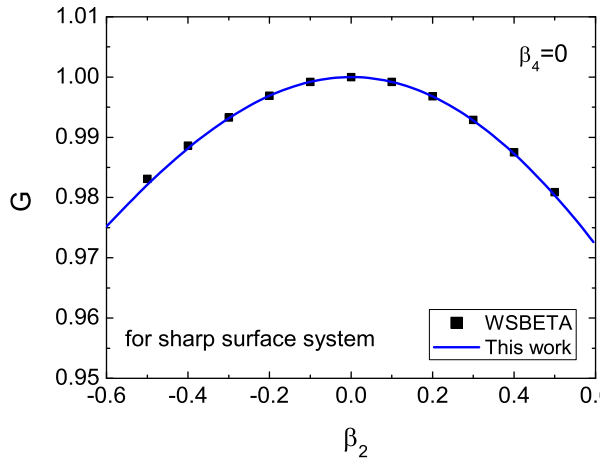

Fig. 3. (color online) Calculated deformation factor G of a charged liquid drop with two different approaches. The squares and the solid curve denote the results from Ref. 9 and this work, respectively. Here, we set $\beta_4 = 0$.

diate and heavy nuclei, ω has a value about 0.1–0.25, the corresponding relative deviations of the Coulomb energies with Eq. (9) are smaller than 0.05% [denoted by light gray in Fig. 2(b)] for almost all cases with $a \leq 0.7$ fm and $|\beta_2| \leq 0.5$. For light nuclei, the corresponding values of ω are larger than 0.25 in general and the relative deviations of the Coulomb energies with Eq. (9) slightly increase for some cases with strong deformations. It is known that the charge distributions of light nuclei are usually described by Gaussian functions rather than the Woods–Saxon form. The analytical expression of the Coulomb energy of a system with Gaussian charge distribution can be found in Refs. 1 and 7.

To further test the formula, we compare the Coulomb energy of nuclear system with sharp surface. In Ref. 9, the deformation factor G of a charged liquid drop is described with complete elliptic integrals of the first and second kinds and are evaluated numerically by the use of Gauss–Legendre quadratures. In Fig. 3, we show the calculated deformation factor $G(\beta_2)$ of a charged liquid drop with two different approaches. The squares denote the results from Ref. 9 (WSBETA). The solid curve denote the results with Eq. (10) and setting $\omega = 0$ and $\beta_4 = 0$. The results with two different approaches are close to each other.

For nuclei with β_4 deformations, we find that the deformation factor can be reasonably well described with a parametrized form

$$G_4(\omega, \beta_4) = 1 - 0.139\beta_4^2 + 0.243\omega\beta_4^2 - 0.070\beta_4^3 + \cdots \tag{11}$$

through fitting the numerical integration results in a region $a \leq 0.7$ fm, $|\beta_2| \leq 0.3$ and $|\beta_4| \leq 0.2$. In Fig. 4, we show the calculated deformation factor $G = G_2G_4$ of a charged liquid drop. The squares denote the results from Ref. 9 (WSBETA). The solid curve denotes the results with Eqs. (10), Eq. (11) and setting $\omega = 0$.

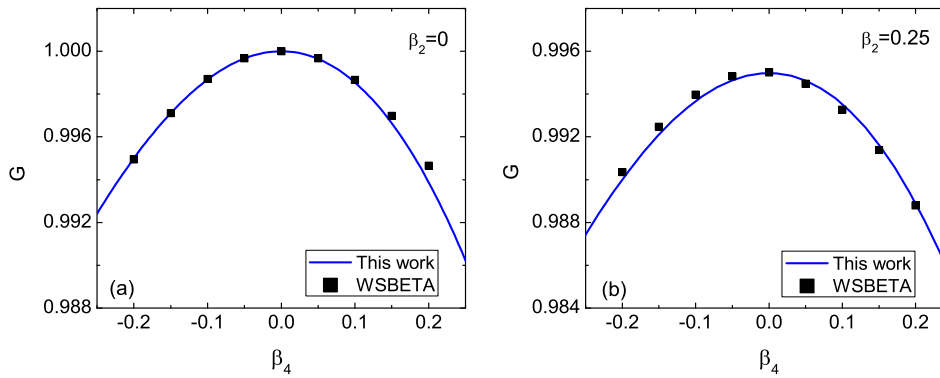

Fig. 4. (color online) The same as Fig. 3, but as a function of β_4.

From the comparison, one can see that the parametrized form in Eq. (11) is acceptable.

In summary, the Coulomb energy of axially deformed nucleus with Woods–Saxon charge distribution has been investigated. The Coulomb energy of a nuclear system was numerically calculated with a two-dimensional integration over the Coulomb potential which was obtained by solving the Poisson equation. By fitting the numerically calculated Coulomb energies for a number of nuclei from $A = 16$ to 300 with axially deformed Woods–Saxon charge distribution, an analytical formula, that is a function of nuclear β_2, β_4 deformation and surface diffuseness, is finally obtained. For intermediate and heavy nuclei with only β_2 deformations, the relative deviation of the Coulomb energy with the proposed formula is generally smaller than 0.05%. For nuclear system with $|\beta_2| > 0.5$, such as fissioning system, the proposed formula could not be applicable, and the two-dimensional numerical integration over the Coulomb potential has to be performed to obtain accurate results.

Acknowledgments

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