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Calculation of moments, potentials, and energies for an arbitrarily shaped diffuse-surface nuclear density distribution*

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We calculate several quantities of physical interest for an arbitrarily shaped diffuse-surface nuclear density distribution that is made diffuse by folding a short-range function over a uniform sharp-surface distribution of given shape. The quantities calculated include the moment of inertia about an arbitrary axis, generalized multipole moments, Coulomb and nuclear potentials, and Coulomb and nuclear energies. The expressions that are obtained in terms of volume integrals are converted into surface integrals by use of single and double divergence relations; these techniques are discussed for general functions. All of our methods and some of our results apply to arbitrary folding functions, although for definiteness most of our results are specialized to the case of a Yukawa folding function. The diffuseness of the nuclear surface increases the moment of inertia of light nuclei substantially, which increases the critical angular momentum at which compound nuclei can no longer be formed. The diffuseness correction to the Coulomb energy contains a term that is proportional to the surface area; this term increases the effective surface energy by approximately 2% for light nuclei and by approximately 1% for heavy nuclei.

NUCLEAR STRUCTURE Calculated quantities of physical interest for arbitrarily shaped diffuse-surface nuclear density distribution. Moment of inertia, generalized multipole moments, Coulomb and nuclear potentials, Coulomb and nuclear energies, Yukawa folding function, single and double divergence relations, applications to nuclear fission and heavy-ion reactions.

I. INTRODUCTION

It is often necessary to calculate quantities of physical interest for an arbitrarily shaped density distribution whose surface is diffuse rather than sharp. In nuclei, the distance[1] over which the density changes from 10% to 90% of its central value is approximately 2.4 fm. This distance is comparable to the nuclear radius for very light nuclei and is 30% of the nuclear radius for very heavy nuclei. The diffuseness corrections to certain quantities of physical interest should therefore be substantial, especially for very light nuclei.

Deformed density distributions are often made diffuse by generalizing a Fermi function to the deformed shape in some way. This leads to cumbersome expressions for the quantities of interest that must be evaluated numerically.[2,3] A much simpler method for generating a diffuse-surface distribution is to fold a short-range function (such as a Yukawa function) over a sharp distribution of the appropriate shape.[4-11] This method has been used recently to make the surfaces diffuse for the calculation of such special cases as the nuclear interaction energy of two semi-infinite distributions,[7] the moment of inertia,[11] generalized multipole moments,[8] the Coulomb self-energy of a sphere and Coulomb interaction energy of two spheres,[9] and the nuclear interaction energy of two spheres.[10]

Here we consider systematically the calculation of various quantities of physical interest for arbitrarily shaped distributions whose surfaces are made diffuse by folding a Yukawa function over a sharp-surface distribution of appropriate shape. In particular, we calculate the moment of inertia and generalized multipole moments of such distributions in Sec. II, the Coulomb and nuclear potentials in Sec. III, and the Coulomb and nuclear energies in Sec. IV.

All of our results have been derived by use of two separate methods. One of these involves the use of Fourier transforms and the other involves transforming the integration variables. In presenting the results here we use the former method in Secs. III and IV; the latter method is used in Sec. II and in an Appendix. The general formulas that we derive in terms of volume integrals are transformed into surface integrals by use of single and double divergence relations. These techniques for transforming volume integrals into surface integrals are discussed in two Appendixes for general functions. All of our methods and some of our results apply to arbitrary folding functions, although for definiteness most of our results are specialized to a Yukawa folding function.

Many of our results are of practical importance in the theory of nuclear fission and heavy-ion reactions. For example, the diffuse nuclear surface increases the moment of inertia of light nuclei substantially, which increases the critical angular momentum at which compound-nucleus formation is no longer possible. Also, the diffuseness correction to the Coulomb energy contains a term that is proportional to the surface area, which increases slightly the effective surface energy of nuclei. These and other applications are discussed at the appropriate places in the paper.

II. MOMENT OF INERTIA AND GENERALIZED MULTIPOLE MOMENTS

We assume throughout this paper that we are dealing with a diffuse density of the general form

$$\rho(\vec{r}_1)=\rho_0\int_V d^3r_2\, g(|\vec{r}_1-\vec{r}_2|)\,, \tag{2.1}$$

where the integration is over a given sharp-surface shape whose volume is V and where

$$\rho_0 V=\begin{cases} M & \text{for a mass density} \\ Ze & \text{for a charge density}\,. \end{cases} \tag{2.2}$$

The folding function g depends only on the magnitude of the vector $\vec{r}_{12}=\vec{r}_1-\vec{r}_2$ and is normalized so that

$$\int_\infty d^3r_{12}\, g(r_{12})=1\,, \tag{2.3}$$

where the integration is over all space. For definiteness we consider a folding function of Yukawa shape:

$$g(|\vec{r}_1-\vec{r}_2|)=\frac{1}{4\pi a^3}\,\frac{e^{-|\vec{r}_1-\vec{r}_2|/a}}{|\vec{r}_1-\vec{r}_2|/a}\,, \tag{2.4}$$

where a is the range of the Yukawa function. It will be clear from the general form of the equations in this paper how to specialize to other types of folding functions, e.g., those of Gaussian shape.

A. Moment of inertia

The first quantity that we consider is the rigid-body moment of inertia for rotation about an *arbitrary* axis, which we take to be the z axis:

$$\begin{aligned} I_z&=\int_\infty \rho(\vec{r}_1)(x_1^2+y_1^2)d^3r_1 \\ &=\rho_0\int_\infty d^3r_1\int_V d^3r_2\,(x_1^2+y_1^2)\,g(|\vec{r}_1-\vec{r}_2|)\,. \end{aligned} \tag{2.5}$$

The z axis need *not* pass through the center of mass of the body.

We evaluate this integral by redefining variables

$$\vec{r}_{12}=\vec{r}_1-\vec{r}_2$$

and by interchanging the order of integration. Equation (2.5) then becomes

$$I_z=I_z^{(1)}+I_z^{(2)}+I_z^{(3)}\,, \tag{2.6}$$

where

$$I_z^{(1)}\equiv\rho_0\int_V d^3r_2(x_2^2+y_2^2)\int_\infty d^3r_{12}\,g(r_{12})\,, \tag{2.7a}$$

$$I_z^{(2)}\equiv 2\rho_0\int_V d^3r_2\int_\infty d^3r_{12}(x_{12}x_2+y_{12}y_2)\,g(r_{12})\,, \tag{2.7b}$$

and

$$I_z^{(3)}\equiv\rho_0\int_V d^3r_2\int_\infty d^3r_{12}(x_{12}^2+y_{12}^2)\,g(r_{12})\,. \tag{2.7c}$$

Because g depends only on the magnitude of $\vec{r}_{12}$, $I_z^{(2)}$ vanishes and

$$I_z^{(3)}=\tfrac{2}{3}M\int_\infty d^3r_{12}\,r_{12}^2\,g(r_{12})\,, \tag{2.8}$$

where M is the total mass of the system. Then by use of Eq. (2.3) we find that

$$\begin{aligned} I_z^{(1)}&=\rho_0\int_V d^3r_2(x_2^2+y_2^2) \\ &\equiv I_z(\text{sharp})\,, \end{aligned} \tag{2.9}$$

the sharp-surface moment of inertia.

Equation (2.6) thus becomes

$$I_z=I_z(\text{sharp})+\tfrac{2}{3}M\int_\infty d^3r_{12}\,r_{12}^2\,g(r_{12})\,. \tag{2.10}$$

Note that the correction term (2.8) is completely independent of the shape of the sharp surface. For a Yukawa folding function, Eq. (2.10) reduces to

$$I_z=I_z(\text{sharp})+4Ma^2\,. \tag{2.11}$$

An alternative way of writing the general result [Eq. (2.10)] is obtained by realizing that the integral appearing in this equation is a measure of the width of the surface diffuseness that does not depend upon a specific choice of folding function. In particular,[11,12]

$$\int_\infty d^3r_{12}\,r_{12}^2\,g(r_{12})=3b^2\,,$$

where b is the root-mean-square width parameter of Myers defined in terms of surface moments.[11-14] Insertion of this result into Eq. (2.10) leads to[11]

$$I_z=I_z(\text{sharp})+2Mb^2\,.$$

For a sphere the moment of inertia for rotation about an axis that passes through the center is therefore given by

$$I_z^{\text{sphere}} = \tfrac{2}{5} MR_0^2 \left[1 + 10\left(\frac{a}{R_0}\right)^2\right]$$
$$= \tfrac{2}{5} MR_0^2 \left[1 + 5\left(\frac{b}{R_0}\right)^2\right],$$

where R_0 is the equivalent sharp-surface radius of the sphere. For nuclei throughout the Periodic Table R_0 is given approximately by[11,12,15]

$$R_0 = r_0 A^{1/3},$$

with

$$r_0 = 1.16 \text{ fm}.$$

The average width of experimental charge distributions for nuclei throughout the Periodic Table is reproduced by the value[11,12,16]

$$b = 1.0 \text{ fm}$$

or

$$a = 1.0 \text{ fm}/\sqrt{2} = 0.71 \text{ fm}.$$

Alternatively, in order to produce a density distribution which changes from 10% to 90% of its central value in a distance[1] of 2.4 fm by use of a Yukawa folding function, the Yukawa range a should have the value

$$a = \tfrac{1}{2}(2.4 \text{ fm})/\ln 5 = 0.75 \text{ fm}.$$

The diffuseness of the nuclear surface therefore increases the moment of inertia of a spherical nucleus substantially compared to the value for a uniform sharp-surface density distribution, especially for very light nuclei. For example, this increase is about 50% for a light nucleus with mass number 20 and is about 10% for a heavy nucleus with mass number 240. For a deformed shape the relative diffuseness correction to the moment of inertia for rotation about a minor axis is somewhat less.

The diffuseness correction to the moment of inertia should increase the critical angular momentum at which two colliding nuclei no longer fuse into a single compound nucleus, especially for very light nuclear systems. Taking into account this effect would therefore increase the calculated cross section for compound-nucleus formation relative to that calculated for a uniform sharp-surface density distribution.

As a particular example,[17] for the reaction ^{14}N + ^{27}Al at a ^{14}N laboratory bombarding energy of 262 MeV, the Bass model[18,19] predicts that the critical angular momentum for the production of ^{41}Ca is $39\hbar$ when the moments of inertia are calculated for uniform sharp-surface density distributions. When the moments of inertia are calculated for diffuse-surface density distributions the predicted critical angular momentum becomes $47.5\hbar$. This agrees with the experimental value[17] of $48 \pm 4\hbar$, whereas the result for uniform sharp-surface density distributions is in contradiction to the experimental result.

In Sec. II B we show that Eqs. (2.10) and (2.11) are special cases of relations for root-mean-square radii or multipole moments for bodies of nonspherical shape whose surfaces are made diffuse by use of a folding function.[8] Also, in Appendix A we show that the volume integral in Eq. (2.9) can be converted into the surface integral

$$I_z(\text{sharp}) = \tfrac{1}{3}\rho_0 \oint_S d\vec{S}_2 \cdot (x_2^3 \vec{e}_x + y_2^3 \vec{e}_y),$$

where $\vec{e}_x$ and $\vec{e}_y$ are unit vectors in the x and y directions, respectively. For axially symmetric shapes this reduces to a one-dimensional integral which can be easily evaluated by means of Gaussian-Legendre quadrature.

B. Generalized multipole moments

We define the generalized multipole moments $q_{LM}^{(k)}$ by

$$q_{LM}^{(k)} \equiv \int_\infty d^3r_1 r_1^{L+k} Y_{LM}(\theta_1, \phi_1)\rho(\vec{r}_1), \qquad (2.12)$$

where Y_{LM} is a spherical harmonic of degree L and order M. In our present discussion we restrict ourselves to *even* powers of k and derive explicit expressions only for $k = 0$ (the ordinary multipole moment) and $k = 2$.

For the evaluation of Eq. (2.12) it is convenient to use the solid-harmonic expansion[20]

$$r_1^L Y_{LM}(\theta_1, \phi_1) = \sum_{\lambda\mu} \left\{\frac{4\pi(2L+1)!}{(2\lambda+1)![2(L-\lambda)+1]!}\right\}^{1/2} r_2^{L-\lambda} Y_{L-\lambda, M-\mu}(\theta_2, \phi_2) r_{12}^\lambda Y_{\lambda\mu}(\theta_{12}, \phi_{12}) \langle L-\lambda, \lambda, M-\mu, \mu | LM\rangle, \qquad (2.13)$$

where $\langle ab\alpha\beta | c\gamma\rangle$ is a Clebsch-Gordan coefficient[20] and where

$$\vec{r}_1 = \vec{r}_2 + \vec{r}_{12}.$$

We first evaluate Eq. (2.12) for $k = 0$. This we do by substituting Eqs. (2.1) and (2.13) into Eq. (2.12) and interchanging the order of integration, as was done in Sec. II A. In the λ, μ summation only the $\lambda = \mu = 0$ term contributes. Then, by use of Eq. (2.3) we find that[8,11]

$$q_{LM}^{(0)}=\rho_0\int_V d^3r_1 r_1^L Y_{LM}(\theta_1,\phi_1)$$
$$\equiv q_{LM}^{(0)}(\text{sharp})\,. \tag{2.14}$$

Thus, the ordinary multipole moments for a diffuse-surface distribution obtained by folding are exactly equal to those for the equivalent sharp-surface distribution and are *completely independent* of the folding function. This is to be contrasted to the complicated relationship that exists between the multipole moments of a sharp-surface distribution and those for the corresponding diffuse-surface distribution obtained by generalizing a Fermi function.[2,3]

The evaluation of Eq. (2.12) for $k=2$ is much more complicated than for $k=0$ because of the extra factor

$$r_1^2=r_2^2+r_{12}^2+2\vec{r}_2\cdot\vec{r}_{12}$$

that appears in the integrand. The r_2^2 and r_{12}^2 terms lead to

$$J_1\equiv\rho_0\int_V d^3r_2 r_2^{L+2}Y_{LM}(\theta_2,\phi_2)\int_\infty d^3r_{12}\,g(r_{12})$$
$$=q_{LM}^{(2)}(\text{sharp}) \tag{2.15}$$

and

$$J_2\equiv\rho_0\int_V d^3r_2 r_2^L Y_{LM}(\theta_2,\phi_2)\int_\infty d^3r_{12}r_{12}^2 g(r_{12})$$
$$=q_{LM}^{(0)}(\text{sharp})\int_\infty d^3r_{12}r_{12}^2 g(r_{12})\,, \tag{2.16}$$

respectively.

The contribution from the $2\vec{r}_2\cdot\vec{r}_{12}$ term is

$$J_3\equiv 2\rho_0\left(\frac{4\pi}{3}\right)^{3/2}[L(2L+1)]^{1/2}\int_V d^3r_2 r_2^L K_{LM}(\vec{r}_2)\times\int_0^\infty dr_{12}r_{12}^4 g(r_{12})\,, \tag{2.17}$$

where

$$K_{LM}(\vec{r}_2)\equiv\sum_\mu\langle L-1,1,M-\mu,\mu|LM\rangle\times Y_{L-1,M-\mu}(\theta_2,\phi_2)Y_{1\mu}(\theta_2,\phi_2)\,. \tag{2.18}$$

The summation over μ in Eq. (2.18) can be performed explicitly,[20] which leads to

$$K_{LM}(\vec{r}_2)=\left[\frac{3L}{4\pi(2L+1)}\right]^{1/2}Y_{LM}(\theta_2,\phi_2)\,. \tag{2.19}$$

Upon substituting this result into Eq. (2.17) we find that

$$J_3=\frac{2L}{3}\rho_0\int_V d^3r_2 r_2^L Y_{LM}(\theta_2,\phi_2)\times\left[4\pi\int_0^\infty dr_{12}r_{12}^4 g(r_{12})\right]$$
$$=\frac{2L}{3}q_{LM}^{(0)}(\text{sharp})\int_\infty d^3r_{12}r_{12}^2 g(r_{12})\,. \tag{2.20}$$

By combining Eqs. (2.15), (2.16), and (2.20) we finally obtain[8]

$$q_{LM}^{(2)}=q_{LM}^{(2)}(\text{sharp})+\tfrac{1}{3}(2L+3)q_{LM}^{(0)}(\text{sharp})\times\int_\infty d^3r_{12}r_{12}^2 g(r_{12})$$
$$=q_{LM}^{(2)}(\text{sharp})+(2L+3)b^2 q_{LM}^{(0)}(\text{sharp})\,. \tag{2.21}$$

Equations (2.14) and (2.21) are identical to relations obtained by Satchler,[8] except that his expressions are in terms of the *individual* multipole coefficients of the density distribution. That his results are also valid for the entire distribution is not surprising since Eq. (2.12) projects out the L,M components of the generalized moments. Satchler[8] also derives a relation for the $k=4$ generalized multipole moments.

We now show that Eq. (2.10) can be derived from the generalized-multipole-moment formalism. We first note that $x_1^2+y_1^2$ can be rewritten as

$$x_1^2+y_1^2=r_1^2-z_1^2$$
$$=\tfrac{2}{3}(4\pi)^{1/2}\left[r_1^2Y_{00}(\theta_1,\phi_1)-\frac{1}{\sqrt{5}}r_1^2Y_{20}(\theta_1,\phi_1)\right]. \tag{2.22}$$

Upon substituting Eq. (2.22) into Eq. (2.5) and comparing with Eq. (2.12), we see that

$$I_z=\tfrac{2}{3}(4\pi)^{1/2}\left[q_{00}^{(2)}-\frac{1}{\sqrt{5}}q_{20}^{(0)}\right]. \tag{2.23}$$

Then by use of Eqs. (2.14) and (2.21), we find that

$$I_z=\tfrac{2}{3}(4\pi)^{1/2}\left[q_{00}^{(2)}(\text{sharp})-\frac{1}{\sqrt{5}}q_{20}^{(0)}(\text{sharp})+q_{00}^{(0)}(\text{sharp})\int_\infty d^3r_{12}r_{12}^2 g(r_{12})\right]$$
$$=I_z(\text{sharp})+\tfrac{2}{3}M\int_\infty d^3r_{12}r_{12}^2 g(r_{12})\,,$$

which is Eq. (2.10).

It is clear that Eq. (2.12) can always be expressed in terms of the sharp-surface integrals

$$q_{LM}^{(k)}(\text{sharp})=\rho_0\int_V d^3r_1 r_1^{L+k}Y_{LM}(\theta_1,\phi_1)\,, \tag{2.24}$$

as we see for example from Eqs. (2.14) and (2.21). In Appendix A we show that Eq. (2.24) can be transformed by use of the divergence theorem into the following two equivalent surface integrals:

$$q_{LM}^{(k)}(\text{sharp})=(k+2)^{-1}\left(\frac{2L+1}{L}\right)^{1/2}\rho_0\times\oint_S d\vec{S}_1\cdot[r_1^{L+k+1}\vec{\mathcal{Y}}_{LM}^{(L-1)}(\theta_1,\phi_1)]\,, \tag{2.25a}$$

$$q_{LM}^{(k)}(\text{sharp}) = -(2L+k+3)^{-1}\left(\frac{2L+1}{L+1}\right)^{1/2}\rho_0 \times \oint_S d\vec{S}_1\cdot[r_1^{L+k+1}\vec{\mathcal{Y}}_{LM}^{(L+1)}(\theta_1,\phi_1)], \tag{2.25b}$$

where $\vec{\mathcal{Y}}_{LM}^{(J)}(\theta,\phi)$ is a *vector* spherical harmonic.[20] As mentioned in Appendix A, for $L=0$ it is necessary to use Eq. (2.25b), whereas for $L>0$ it is more convenient to use Eq. (2.25a).

III. COULOMB AND NUCLEAR POTENTIALS

In this section we derive general formulas for the Coulomb and nuclear potentials for arbitrarily shaped diffuse-surface density distributions obtained by folding. We then specialize these results to the case of Yukawa folding functions. These formulas are in turn further specialized to spherical shapes.

A. Coulomb potential

The Coulomb potential is defined as

$$V_C(\vec{r}_1) = e\int_\infty d^3r_2\,\frac{1}{|\vec{r}_1-\vec{r}_2|}\rho(\vec{r}_2). \tag{3.1}$$

Upon inserting Eq. (2.1) and interchanging the order of integration we obtain

$$V_C(\vec{r}_1) = e\rho_0\int_V d^3r_3\int_\infty d^3r_2\,\frac{1}{|\vec{r}_1-\vec{r}_2|}g(|\vec{r}_2-\vec{r}_3|). \tag{3.2}$$

The faltung theorem[21] states that for arbitrary functions f and g,

$$\int_\infty d^3r_2 f(\vec{r}_1-\vec{r}_2)g(\vec{r}_2-\vec{r}_3) = \int_\infty d^3k\, f(\vec{k})g(\vec{k})e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_3)}, \tag{3.3}$$

where $f(\vec{k})$ and $g(\vec{k})$ are the Fourier transforms of $f(\vec{r}_{12})$ and $g(\vec{r}_{23})$, i.e.,

$$g(\vec{k}) = \frac{1}{(2\pi)^{3/2}}\int_\infty d^3r_{12}\,g(\vec{r}_{12})e^{-i\vec{k}\cdot\vec{r}_{12}}. \tag{3.4}$$

Upon applying this theorem to Eq. (3.2), we obtain

$$V_C(\vec{r}_1) = \frac{4\pi e\rho_0}{(2\pi)^{3/2}}\int_V d^3r_3\int_\infty d^3k\,\frac{1}{k^2}g(k)e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_3)}. \tag{3.5a}$$

Because g depends only on the magnitude of $\vec{k}$, this can be simplified to

$$V_C(\vec{r}_1) = 4(2\pi)^{1/2}e\rho_0\int_V \frac{d^3r_3}{|\vec{r}_1-\vec{r}_3|} \times\int_0^\infty dk\,\frac{g(k)}{k}\sin(k|\vec{r}_1-\vec{r}_3|), \tag{3.5b}$$

which is a *general* equation that is valid for any folding function. For most folding functions of physical interest, such as Yukawas, exponentials, and Gaussians, the Fourier transforms are relatively simple. Consequently, the single integral over k can ordinarily be readily performed, which reduces this equation to a three-dimensional volume integral over the sharp-surface shape.

For the Yukawa function defined by Eq. (2.4), the Fourier transform is

$$g(k) = \frac{1}{(2\pi)^{3/2}}\frac{1}{(1+a^2k^2)}, \tag{3.6}$$

which reduces Eq. (3.5b) to

$$V_C(\vec{r}_1) = \frac{\rho_0 e}{\pi a^2 i}\int_V d^3r_3\,\frac{1}{|\vec{r}_1-\vec{r}_3|}\int_{-\infty}^{\infty} dk\,\frac{e^{ik|\vec{r}_1-\vec{r}_3|}}{k(k^2+1/a^2)}. \tag{3.7}$$

The integral over k in Eq. (3.7) is evaluated by use of complex contour integration and the residue theorem. This gives

$$V_C(\vec{r}_1) = V_C(\vec{r}_1;\ \text{sharp}) + \Delta V_C(\vec{r}_1), \tag{3.8}$$

where $V_C(\vec{r}_1;\text{sharp})$ is the sharp-surface potential

$$V_C(\vec{r}_1;\text{sharp}) = \rho_0 e\int_V d^3r_2\,\frac{1}{|\vec{r}_1-\vec{r}_2|} \tag{3.9}$$

and where the correction term is given by

$$\Delta V_C(\vec{r}_1) = -\rho_0 e\int_V d^3r_2\frac{1}{|\vec{r}_1-\vec{r}_2|}e^{-|\vec{r}_1-\vec{r}_2|/a}. \tag{3.10}$$

Equations (3.9) and (3.10) can be converted from three-dimensional volume integrals to two-dimensional surface integrals by use of Gauss's divergence theorem. This leads to[5]

$$V_C(\vec{r}_1;\text{sharp}) = -\frac{\rho_0 e}{2}\oint_S[d\vec{S}_2\cdot(\vec{r}_1-\vec{r}_2)]|\vec{r}_1-\vec{r}_2|^{-1} \tag{3.11}$$

and

$$\Delta V_C(\vec{r}_1) = +\frac{\rho_0 e}{a}\oint_S[d\vec{S}_2\cdot(\vec{r}_1-\vec{r}_2)]\left(\frac{|r_1-r_2|}{a}\right)^{-3}\left[1-\left(1+\frac{|\vec{r}_1-\vec{r}_2|}{a}\right)e^{-|\vec{r}_1-\vec{r}_2|/a}\right]. \tag{3.12}$$

These integrals are evaluated efficiently by use of Gaussian-Legendre quadrature.[5]

A general method for converting any volume integral (for an analytic integrand of reasonable shape) into a surface integral is presented in Appendix A. This method should be useful for evaluating the Coulomb potential given by Eq. (3.5b) for folding functions other than the Yukawa.

For a *sphere* of radius R_0 one can show that[5]

$$V_C(r_1;\mathrm{sharp}) = \begin{cases} \frac{2\pi}{3}\rho_0 e R_0^{\,2}[3-(r_1/R_0)^2]\,, & r_1<R_0 \\ \frac{4\pi}{3}\rho_0 e R_0^{\,3}/r_1\,, & r_1>R_0 \end{cases} \tag{3.13}$$

and

$$\Delta V_C(r_1) = \begin{cases} -4\pi\rho_0 e a^2\left[1-\left(1+\frac{R_0}{a}\right)e^{-R_0/a}\frac{\sinh(r_1/a)}{(r_1/a)}\right], & r_1<R_0 \\ -4\pi\rho_0 e a^2\left[\frac{R_0}{a}\cosh\left(\frac{R_0}{a}\right)-\sinh\left(\frac{R_0}{a}\right)\right]\frac{e^{-r_1/a}}{(r_1/a)}, & r_1>R_0\,. \end{cases} \tag{3.14}$$

By use of Eqs. (2.1) and (2.4), we note that Eq. (3.10) is equivalent to

$$\Delta V_C(\vec{r}_1) = -4\pi a^2 e\rho(\vec{r}_1)\,.$$

The diffuseness correction to the Coulomb potential is therefore proportional to the square of the surface thickness and to the nuclear density. This means that the correction is nearly constant well inside the shape and is approximately zero well outside the shape. The negative sign arises because the effective charge density is reduced by making the surface diffuse.

As an order of magnitude estimate, we note that the diffuseness correction at the center of a spherical nucleus whose diffuseness is much smaller than its radius is given approximately by

$$\Delta V_C(0) \approx -4\pi a^2 e\rho_0 = -2\left(\frac{a}{R_0}\right)^2 V_C(0;\mathrm{sharp})\,. \tag{3.15}$$

The decrease in Coulomb potential is therefore about 10% for a light nucleus with mass number 20 and is about 2% for a heavy nucleus with mass number 240.

B. Nuclear potential

We use a spin-independent nuclear two-body potential of the form[4-6]

$$V(r_{12}) = -\frac{V_0}{4\pi\lambda^3}\frac{e^{-|\vec{r}_1-\vec{r}_2|/\lambda}}{|\vec{r}_1-\vec{r}_2|/\lambda}\,, \tag{3.16}$$

and calculate the spin-independent nuclear single-particle potential from

$$V_N(\vec{r}_1) = \int_\infty d^3r_2\, V(r_{12})\rho(\vec{r}_2)/\rho_0\,. \tag{3.17}$$

Upon Fourier transforming Eq. (3.17) and reversing the order of integrations, we obtain the *general* result

$$V_N(\vec{r}_1) = -\frac{V_0}{(2\pi)^{3/2}}\int_V d^3r_3\int_\infty d^3k\,\frac{g(k)}{1+\lambda^2k^2}e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_3)}\,. \tag{3.18a}$$

After performing the angular part of the integral over $\vec{k}$, this becomes

$$V_N(\vec{r}_1) = -\left(\frac{2}{\pi}\right)^{1/2}V_0\int_V\frac{d^3r_3}{|\vec{r}_1-\vec{r}_3|}\times\int_0^\infty dk\,k\frac{g(k)}{(1+\lambda^2k^2)}\sin(k|\vec{r}_1-\vec{r}_3|)\,, \tag{3.18b}$$

where $g(k)$ is the Fourier transform of the folding function. For most folding functions of physical interest, the integral over k can be performed explicitly.

For a Yukawa function we use Eq. (3.6) to obtain the *specialized* result

$$V_N(\vec{r}_1) = -\frac{V_0}{(2\pi)^2 i}\int_V\frac{d^3r_3}{|\vec{r}_1-\vec{r}_3|}\times\int_{-\infty}^{\infty}dk\,k\frac{e^{ik|\vec{r}_1-\vec{r}_3|}}{(1+\lambda^2k^2)(1+a^2k^2)}\,. \tag{3.19}$$

The range λ of the Yukawa effective two-nucleon interaction is assumed to be *different* from the range of the Yukawa folding function that generates the diffuse-surface density distribution.

In analogy with the case of the Coulomb potential, we reduce Eq. (3.19) by use of the residue theorem to obtain

$$V_N(\vec{r}_1) = V_N(\vec{r}_1;\mathrm{sharp}) + \Delta V_N(\vec{r}_1)\,, \tag{3.20}$$

where

$$V_N(\vec{r}_1;\mathrm{sharp}) = -\frac{V_0}{4\pi\lambda^3}\int_V d^3r_2\frac{e^{-|\vec{r}_1-\vec{r}_2|/\lambda}}{|\vec{r}_1-\vec{r}_2|/\lambda} \tag{3.21}$$

and

$$\Delta V_N(\vec{r}_1) = -\frac{a^2}{(a^2-\lambda^2)} V_N(\vec{r}_1;\text{sharp}) - \frac{V_0}{4\pi(a^2-\lambda^2)} \int_V d^3r_2 \frac{e^{-|\vec{r}_1-\vec{r}_2|/a}}{|\vec{r}_1-\vec{r}_2|}. \tag{3.22}$$

Equations (3.21) and (3.22) can be converted into the surface integrals[5,6]

$$V_N(\vec{r}_1;\text{sharp}) = +\frac{V_0}{4\pi\lambda^3} \oint_S [d\vec{S}_2\cdot(\vec{r}_1-\vec{r}_2)] \left(\frac{|r_1-r_2|}{\lambda}\right)^{-3} \left[1-\left(1+\frac{|\vec{r}_1-\vec{r}_2|}{\lambda}\right)e^{-|\vec{r}_1-\vec{r}_2|/\lambda}\right] \tag{3.23}$$

and

$$\Delta V_N(\vec{r}_1) = -\frac{a^2}{(a^2-\lambda^2)} V_N(\vec{r}_1;\text{sharp}) + \frac{V_0}{4\pi(a^2-\lambda^2)a} \oint_S [d\vec{S}_2\cdot(\vec{r}_1-\vec{r}_2)] \left(\frac{|r_1-r_2|}{a}\right)^{-3} \left[1-\left(1+\frac{|\vec{r}_1-\vec{r}_2|}{a}\right)e^{-|\vec{r}_1-\vec{r}_2|/a}\right], \tag{3.24}$$

which can be evaluated efficiently by means of Gaussian-Legendre quadrature.[5] Again, the general method presented in Appendix A for converting a volume integral into a surface integral should be very useful in simplifying Eq. (3.18b) for an arbitrary folding function.

For the special case in which $\lambda = a$, the integral over k in Eq. (3.19) can be performed by evaluating the residue of a double pole, or alternatively by setting $a=\lambda+\epsilon$ and taking the limit as $\epsilon\to 0$ in Eqs. (3.20)–(3.22). For this special case in which $\lambda = a$, we find that

$$V_N(\vec{r}_1) = -\frac{V_0}{8\pi\lambda^3}\int_V d^3r_2 e^{-|\vec{r}_1-\vec{r}_2|/\lambda}. \tag{3.25}$$

In Appendix A, it is shown how to convert the volume integral of an exponential function into a surface integral. Equation (3.25) for the special case in which $\lambda = a$ then becomes

$$V_N(\vec{r}_1) = \frac{V_0}{8\pi\lambda^3} \oint_S [d\vec{S}_2\cdot(\vec{r}_1-\vec{r}_2)] \left(\frac{|\vec{r}_1-\vec{r}_2|}{\lambda}\right)^{-3} \left[2 - e^{-|\vec{r}_1-\vec{r}_2|/\lambda}\left(2+\frac{2|\vec{r}_1-\vec{r}_2|}{\lambda}+\frac{|r_1-r_2|^2}{\lambda^2}\right)\right]. \tag{3.26}$$

For a *sphere* of radius R_0, Eq. (3.21) becomes[5,6]

$$V_N(r_1;\text{sharp}) = \begin{cases} -V_0\left[1-\left(1+\frac{R_0}{\lambda}\right)e^{-R_0/\lambda}\frac{\sinh(r_1/\lambda)}{(r_1/\lambda)}\right], & r_1 \le R_0 \\ -V_0\left[\frac{R_0}{\lambda}\cosh\left(\frac{R_0}{\lambda}\right)-\sinh\left(\frac{R_0}{\lambda}\right)\right]\frac{e^{-r_1/\lambda}}{(r_1/\lambda)}, & r_1 \ge R_0 \end{cases} \tag{3.27}$$

and Eq. (3.22) becomes

$$\Delta V_N(r_1) = -\frac{a^2}{(a^2-\lambda^2)} V_N(r_1;\text{sharp}) + \begin{cases} \frac{a^2V_0}{(\lambda^2-a^2)}\left[1-\left(1+\frac{R_0}{a}\right)e^{-R_0/a}\frac{\sinh(r_1/a)}{(r_1/a)}\right], & r_1 \le R_0 \\ \frac{a^2V_0}{(\lambda^2-a^2)}\left[\frac{R_0}{a}\cosh\left(\frac{R_0}{a}\right)-\sinh\left(\frac{R_0}{a}\right)\right]\frac{e^{-r_1/a}}{(r_1/a)}, & r_1 \ge R_0. \end{cases} \tag{3.28}$$

Similarly, for the special case in which $\lambda = a$, Eq. (3.25) simplifies for a sphere to

$$\Delta V_N(r_1) = \begin{cases} -\frac{V_0}{2}\left[2-3\left(1+\frac{R_0}{\lambda}\right)e^{-R_0/\lambda}\frac{\sinh(r_1/\lambda)}{(r_1/\lambda)} - \frac{R_0^2}{r_1\lambda}e^{-R_0/\lambda}\sinh(r_1/\lambda) + \left(1+\frac{R_0}{\lambda}\right)e^{-R_0/\lambda}\cosh(r_1/\lambda)\right], & r_1 \le R_0 \\ -\frac{V_0}{2}\frac{e^{-r_1/\lambda}}{(r_1/\lambda)}\left[\left(\frac{R_0}{\lambda}\cosh\frac{R_0}{\lambda}-\sinh\frac{R_0}{\lambda}\right)(3+r_1/\lambda)-(R_0/\lambda)^2\sinh(R_0/\lambda)\right], & r_1 \ge R_0. \end{cases} \tag{3.29}$$

IV. COULOMB AND NUCLEAR ENERGIES

In analogy with the previous section, we derive here general and various specialized formulas for the total Coulomb and nuclear energies. These energies include implicitly both self and interaction terms. Approximate expressions for the energies are derived for the case in which the range of the folding function is small compared to the nuclear radius. The expression for the Coulomb energy is compared with the second-order result obtained by Myers and Swiatecki.[22]

A. Coulomb energy

The Coulomb energy is given by

$$E_C=\frac{1}{2}\int_\infty\int_\infty d^3r_1d^3r_2\frac{1}{|\vec{r}_1-\vec{r}_2|}\rho(\vec{r}_1)\rho(\vec{r}_2). \tag{4.1}$$

By virtue of Eq. (2.1) this becomes

$$E_C=\frac{\rho_0^2}{2}\int_\infty\int_\infty d^3r_1d^3r_2\frac{1}{|\vec{r}_1-\vec{r}_2|}\times\int_V\int_V d^3r_3d^3r_4\,g(|\vec{r}_1-\vec{r}_3|)g(|\vec{r}_2-\vec{r}_4|). \tag{4.2}$$

The faltung theorem expressed by Eq. (3.3) can easily be generalized to three functions, which gives the relation[21]

$$\int_\infty\int_\infty d^3r_1d^3r_2 f(\vec{r}_1-\vec{r}_2)g(\vec{r}_1-\vec{r}_3)h(\vec{r}_2-\vec{r}_4)=(2\pi)^{3/2}\int_\infty d^3k f(\vec{k})g(-\vec{k})h(\vec{k})e^{i\vec{k}\cdot(\vec{r}_3-\vec{r}_4)}. \tag{4.3}$$

Upon reversing the order of integration in Eq. (4.2), applying theorem (4.3), and relabeling variables, we obtain

$$E_C=4\pi\frac{\rho_0^2}{2}\int_V\int_V d^3r_1d^3r_2\int_\infty d^3k\frac{1}{k^2}g^2(k)e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}. \tag{4.4a}$$

After performing the angular part of the three-dimensional integral over $\vec{k}$ this becomes

$$E_C=\frac{(4\pi)^2}{2}\rho_0^2\int_V\int_V\frac{d^3r_1d^3r_2}{|\vec{r}_1-\vec{r}_2|}\times\int_0^\infty dk\frac{g^2(k)}{k}\sin(k|\vec{r}_1-\vec{r}_2|), \tag{4.4b}$$

which is a *general* relation for the Coulomb energy. For simple folding functions the integral over k can easily be performed, which reduces this equation to two three-dimensional integrals over the sharp-surface shape.

In Appendix B we present a general method for converting double volume integrals to double surface integrals. This method then enables one to convert the sixfold integral in Eq. (4.4b) into a fourfold integral over the surface of the body. For axially summetric shapes this reduces to a triple integral, which can be evaluated easily by Gaussian-Legendre quadrature.[23]

We now *specialize* Eq. (4.4b) to a Yukawa folding function. Upon substituting Eq. (3.6) into (4.4b) we find that

$$E_C=\frac{\rho_0^2}{(2\pi)}\frac{1}{i}\int_V\int_V d^3r_1d^3r_2\frac{1}{|\vec{r}_1-\vec{r}_2|}\times\int_{-\infty}^\infty dk\frac{e^{ik|\vec{r}_1-\vec{r}_2|}}{k(1+a^2k^2)^2}. \tag{4.5}$$

Application of the residue theorem to the integral over k leads to

$$E_C=E_C(\text{sharp})+\Delta E_C, \tag{4.6}$$

where

$$E_C(\text{sharp})=\frac{\rho_0^2}{2}\int_V\int_V d^3r_1d^3r_2\frac{1}{|\vec{r}_1-\vec{r}_2|} \tag{4.7}$$

is the sharp-surface Coulomb energy and where

$$\Delta E_C=-\frac{\rho_0^2}{2}\int_V\int_V d^3r_1d^3r_2\frac{1}{|\vec{r}_1-\vec{r}_2|}\times e^{-|\vec{r}_1-\vec{r}_2|/a}\left(1+\frac{1}{2}\frac{|\vec{r}_1-\vec{r}_2|}{a}\right) \tag{4.8}$$

is the diffuse-surface correction.

In Appendix C we present an alternative method for deriving Eqs. (4.6)–(4.8) which involves various transformations of the integration variables.

By use of the double divergence relations[23,24] discussed in Appendix B, we convert Eqs. (4.7) and (4.8) from double volume integrals into the double surface integrals

$$E_C(\text{sharp})=-\frac{\rho_0^2}{12}\oint_S\oint_S\frac{[d\vec{S}_1\cdot(\vec{r}_1-\vec{r}_2)][d\vec{S}_2\cdot(\vec{r}_1-\vec{r}_2)]}{|\vec{r}_1-\vec{r}_2|}, \tag{4.9}$$

and

$$\Delta E_C = \frac{\rho_0^2}{2a} \oint_S \oint_S \frac{[d\vec{S}_1\cdot(\vec{r}_1-\vec{r}_2)][d\vec{S}_2\cdot(\vec{r}_1-\vec{r}_2)]}{(|\vec{r}_1-\vec{r}_2|/a)^4}\left[2\frac{|\vec{r}_1-\vec{r}_2|}{a} - 5 + \left(5 + 3\frac{|\vec{r}_1-\vec{r}_2|}{a} + \frac{1}{2}\frac{|\vec{r}_1-\vec{r}_2|^2}{a^2}\right)e^{-|\vec{r}_1-\vec{r}_2|/a}\right]. \tag{4.10}$$

For axially symmetric shapes these expressions can be evaluated efficiently by use of Gaussian-Legendre quadrature.[23]

We now explicitly evaluate Eqs. (4.7) and (4.8) for a *spherical* shape. The sharp-surface result is the usual spherical energy

$$E_C(\text{sharp}) = \tfrac{3}{5} Z^2 e^2/R_0, \tag{4.11}$$

where R_0 is the radius of the sphere. The first term in the integrand of Eq. (4.8) is a Yukawa function; this integral has been performed in Refs. 24 and 25. The second term in the integrand is an exponential function; this integral can be evaluated by complex contour integration. The final result is

$$\Delta E_C = -\frac{3Z^2e^2a^2}{R_0^3} \times \left\{1 - \frac{15}{8}\left(\frac{a}{R_0}\right) + \frac{21}{8}\left(\frac{a}{R_0}\right)^3 - \tfrac{3}{4}e^{-2R_0/a}\left[1 + \frac{9}{2}\left(\frac{a}{R_0}\right) + 7\left(\frac{a}{R_0}\right)^2 + \frac{7}{2}\left(\frac{a}{R_0}\right)^3\right]\right\}. \tag{4.12}$$

It is instructive[22] to separate Eq. (4.8) into terms that are of first order and second order in the quantity

$$\Delta\rho(\vec{r}_1) \equiv \rho(\vec{r}_1) - \rho_0(\vec{r}_1), \tag{4.13}$$

the deviation of the density from its sharp-surface values

$$\rho_0(\vec{r}_1) = \rho_0 \int_V d^3r_2\,\delta(\vec{r}_1-\vec{r}_2) = \begin{cases}\rho_0, & \vec{r}_1 \text{ within } V\\ 0, & \vec{r}_1 \text{ outside } V.\end{cases} \tag{4.14}$$

Upon substituting Eq. (4.13) into (4.1), we obtain the *general* result

$$\Delta E_C = \Delta E_C^{(1)} + \Delta E_C^{(2)}, \tag{4.15}$$

where

$$\Delta E_C^{(1)} = \int_\infty \int_\infty d^3r_1 d^3r_2 \frac{1}{|\vec{r}_1-\vec{r}_2|}\rho_0(\vec{r}_1)\Delta\rho(\vec{r}_2) \tag{4.16}$$

and

$$\Delta E_C^{(2)} = \frac{1}{2}\int_\infty \int_\infty d^3r_1 d^3r_2 \frac{1}{|\vec{r}_1-\vec{r}_2|}\Delta\rho(\vec{r}_1)\Delta\rho(\vec{r}_2). \tag{4.17}$$

For the delta folding function appearing in Eq. (4.14) the Fourier transform [see Eq. (3.4)] is given by

$$g_0(k) = \frac{1}{(2\pi)^{3/2}}. \tag{4.18}$$

By use of Eqs. (3.6), (4.13), and (4.18), we see that the folding function appropriate to $\Delta\rho$ has the Fourier transform

$$\Delta g(k) = -\frac{1}{(2\pi)^{3/2}}\frac{a^2k^2}{(1+a^2k^2)}. \tag{4.19}$$

In the usual way we reverse the order of integration in Eqs. (4.16) and (4.17), Fourier transform, and substitute Eqs. (4.18) and (4.19). After complex contour integration we then obtain

$$\Delta E_C^{(1)} = -\rho_0^2 \int_V \int_V d^3r_1 d^3r_2 \frac{e^{-|\vec{r}_1-\vec{r}_2|/a}}{|\vec{r}_1-\vec{r}_2|} \tag{4.20}$$

and

$$\Delta E_C^{(2)} = \frac{\rho_0^2}{4}\int_V \int_V d^3r_1 d^3r_2 \frac{e^{-|\vec{r}_1-\vec{r}_2|/a}}{|\vec{r}_1-\vec{r}_2|}\left(2 - \frac{|\vec{r}_1-\vec{r}_2|}{a}\right), \tag{4.21}$$

which apply to Yukawa folding functions.

We now derive a result that is valid when the range a of the folding function is small compared to the nuclear radius. In this case the major contributions to Eqs. (4.20) and (4.21) come from the regions where $|\vec{r}_1-\vec{r}_2| \lesssim a$. We can then approximate $\Delta E_C^{(1)}$ and $\Delta E_C^{(2)}$ by allowing *one* of the regions of integration to extend over *all* space. This gives for $\Delta E_C^{(1)}$ the approximate result

$$\Delta E_C^{(1)} \approx -\rho_0^2 \int_\infty d^3r_1 \int_V d^3r_2 \frac{e^{-|\vec{r}_1-\vec{r}_2|/a}}{|\vec{r}_1-\vec{r}_2|} = -4\pi a^2\rho_0 \int_\infty d^3r_1 \rho(\vec{r}_1) = -4\pi a^2 \rho_0 Ze = -3Z^2e^2a^2/R_0^3, \tag{4.22}$$

which is valid to second order in the surface diffuseness. Similarly, it can be shown that to second order

$$\Delta E_C^{(2)} \approx 0. \tag{4.23}$$

From Eqs. (4.15), (4.22), and (4.23) it then follows that the total second-order diffuseness correction to the Coulomb energy is

$$\Delta E_C \approx -3Z^2e^2a^2/R_0^3. \tag{4.24}$$

It should be mentioned that, when we refer to terms in ΔE_c which are second or third order in the diffuseness, we are implicitly neglecting all terms multiplied by exponential factors like $e^{-2R_0/a}$, as can be seen from Eq. (4.12). Strictly speaking, it is not mathematically possible to expand ΔE_C in only non-negative powers of (a/R_0). However, it is clear that the exponential terms can be neglected, except for very light systems. Thus, *after* neglecting such exponential terms, we loosely refer to corrections which are second or third order in the diffuseness or in (a/R_0).

The second-order diffuseness correction Eq. (4.24) lowers the Coulomb energy because the charge is spread over a greater effective volume when the surface is made diffuse. The magnitude of this effect is about 25% for a light nucleus with mass number 20 and is about 5% for a heavy nucleus with mass number 240. However, as was first observed by Myers and Swiatecki,[22] the second-order diffuseness correction to the Coulomb energy is independent of shape. It may therefore be disregarded when calculating the nuclear potential energy of deformation for use in the theory of fission and heavy-ion reactions, where only shape-dependent quantities need be considered.

Whereas the second-order diffuseness correction to the Coulomb energy is independent of shape, it is clear from the form[24,25] of Eq. (4.8) that the third-order correction is proportional to the surface area. By deducing the constant of proportionality from Eq. (4.12), we then obtain

$$\Delta E_C \approx -3Z^2e^2a^2/R_0{}^3 + \left[\frac{45}{8}\left(\frac{Z}{A}\right)^2\frac{e^2a^3}{r_0{}^4}\right]A^{2/3}B_s\,, \qquad (4.25)$$

where B_s is the ratio of the surface area of the deformed shape to the surface area of a sphere.

The overall term in square brackets that multiplies $A^{2/3}B_s$ in Eq. (4.25) varies slightly for nuclei throughout the Periodic Table. For a light nucleus with an equal number of neutrons and protons its value is about 0.4 MeV, whereas for a heavy actinide nucleus its value is about 0.2 MeV. Therefore, the diffuseness correction to the Coulomb energy increases the effective nuclear surface tension by approximately 2% for light nuclei and by approximately 1% for heavy nuclei.

For a given proton number Z, the term that multiplies $A^{2/3}B_s$ in Eq. (4.25) decreases with an increase in the mass number A. Therefore, the shape dependence of the third-order diffuseness correction to the Coulomb energy increases slightly the fissility of nuclei with the addition of neutrons. Although very small, this effect nevertheless hinders the production of heavy nuclei by means of the multiple capture of neutrons.

B. Nuclear energy

The nuclear energy is defined as[24,25]

$$E_N = \frac{1}{2}\int_\infty\int_\infty d^3r_1 d^3r_2 V(r_{12})\rho(\vec{r}_1)\rho(\vec{r}_2)/\rho_0{}^2\,, \qquad (4.26)$$

where, as in Sec. III B, we use Eq. (3.16) for $V(r_{12})$ and Eq. (2.1) for $\rho(\vec{r}_i)$. For this application, the quantity V_0 appearing in Eq. (3.16) is given by[26]

$$V_0 = \frac{2(a^2-\lambda^2)^2 a_s\{1-\kappa[(N-Z)/A]^2\}}{(3a^5-5a^3\lambda^2+2\lambda^5)\pi r_0{}^2}\,,$$

where a_s is the surface-energy constant, κ is the surface-asymmetry constant, λ is the range of the Yukawa effective two-nucleon interaction, a is the range of the Yukawa function that defines the nuclear density distribution, and r_0 is the nuclear-radius constant. This result is derived by evaluating Eq. (4.26) for a sphere, expanding the result in powers of $A^{-1/3}$, and recognizing that the $A^{2/3}$ term is the surface energy. [See our later Eqs. (4.36) and (4.37).]

As in Sec. IV A, we use Eq. (4.3) to obtain

$$E_N = -\frac{V_0}{2}\int_V\int_V d^3r_1 d^3r_2 \times \int_\infty d^3k\frac{g^2(k)}{(1+\lambda^2k^2)}e^{i\vec{k}\cdot(\vec{r}_2-\vec{r}_2)}\,. \qquad (4.27a)$$

This then becomes

$$E_N = -2\pi V_0\int_V\int_V \frac{d^3r_1\,d^3r_2}{|\vec{r}_1-\vec{r}_2|} \times \int_0^\infty dk\frac{kg^2(k)}{(1+\lambda^2k^2)}\sin(k|\vec{r}_1-\vec{r}_2|)\,, \qquad (4.27b)$$

which is a *general* result that is valid for an arbitrary folding function. For reasonably simple folding functions the integral over k can be performed, which yields an equation involving a double volume integral. Then, by use of the method outlined in Appendix B, Eq. (4.27b) can be transformed into a double surface integral. For axially symmetric shapes this integral can be evaluated by Gaussian-Legendre quadrature.[23]

Upon substituting Eq. (3.6) into Eq. (4.27b) and performing complex contour integration, we find that

$$E_N = -\frac{V_0}{8\pi(a^2-\lambda^2)^2}\int_V\int_V d^3r_1\,d^3r_2\left[\frac{\lambda^2}{|\vec{r}_1-\vec{r}_2|}\left(e^{-|\vec{r}_1-\vec{r}_2|/\lambda}-e^{-|\vec{r}_1-\vec{r}_2|/a}\right)+\left(\frac{a^2-\lambda^2}{2a}\right)e^{-|\vec{r}_1-\vec{r}_2|/a}\right]. \qquad (4.28)$$

This can be rewritten as

$$E_N = E_N(\text{sharp}) + \Delta E_N\,, \tag{4.29}$$

where

$$E_N(\text{sharp}) = -\frac{V_0}{8\pi\lambda^3}\int_V\int_V d^3r_1\,d^3r_2\,\frac{e^{-|\vec{r}_1-\vec{r}_2|/\lambda}}{|\vec{r}_1-\vec{r}_2|/\lambda} \tag{4.30}$$

and

$$\Delta E_N = -\frac{a^2(a^2-2\lambda^2)}{(a^2-\lambda^2)^2}E_N(\text{sharp}) + \frac{V_0}{8\pi(a^2-\lambda^2)^2}\int_V\int_V d^3r_1\,d^3r_2\left[\frac{\lambda^2}{|\vec{r}_1-\vec{r}_2|} - \frac{(a^2-\lambda^2)}{2a}\right]e^{-|\vec{r}_1-\vec{r}_2|/a}\,. \tag{4.31}$$

Equations (4.28)–(4.31) are valid for Yukawa folding functions.

By use of the double divergence relations[23,24] discussed in Appendix B, we convert Eqs. (4.30) and (4.31) into the surface integrals

$$E_N(\text{sharp}) = \frac{V_0}{8\pi\lambda^3}\oint_S\oint_S \frac{[d\vec{S}_1\cdot(\vec{r}_1-\vec{r}_2)][d\vec{S}_2\cdot(\vec{r}_1-\vec{r}_2)]}{(|\vec{r}_1-\vec{r}_2|/\lambda)^4}\left[\frac{|\vec{r}_1-\vec{r}_2|}{\lambda} - 2 + \left(2 + \frac{|\vec{r}_1-\vec{r}_2|}{\lambda}\right)e^{-|\vec{r}_1-\vec{r}_2|/\lambda}\right] \tag{4.32}$$

and

$$\Delta E_N = -a^2\frac{(a^2-2\lambda^2)}{(a^2-\lambda^2)^2}E_N(\text{sharp}) - \frac{V_0}{8\pi a(a^2-\lambda^2)^2}\oint_S\oint_S \frac{[d\vec{S}_1\cdot(\vec{r}_1-\vec{r}_2)][d\vec{S}_2\cdot(\vec{r}_1-\vec{r}_2)]}{(|\vec{r}_1-\vec{r}_2|/a)^4}$$
$$\times\left\{(3a^2-5\lambda^2) + (2\lambda^2-a^2)\frac{|\vec{r}_1-\vec{r}_2|}{a} + \left[(5\lambda^2-3a^2) + (3\lambda^2-2a^2)\frac{|\vec{r}_1-\vec{r}_2|}{a} - \tfrac{1}{2}(a^2-\lambda^2)\frac{|\vec{r}_1-\vec{r}_2|^2}{a^2}\right]e^{-|\vec{r}_1-\vec{r}_2|/a}\right\}. \tag{4.33}$$

As was true in Sec. III B, it is of interest to derive an expression for E_N for the special case in which $\lambda = a$. We substitute Eq. (3.6) into Eq. (4.27b) and evaluate the residue of a triple pole in the contour integral. We then obtain for this special case of $\lambda = a$ the result

$$E_N = -\frac{V_0}{64\pi\lambda^3}\int_V\int_V d^3r_1\,d^3r_2\left(1 + \frac{|\vec{r}_1-\vec{r}_2|}{\lambda}\right)e^{-|\vec{r}_1-\vec{r}_2|/\lambda}\,. \tag{4.34}$$

By use of the method of Appendix B, we can transform this result into

$$E_N = -\frac{V_0}{64\pi\lambda^3}\oint_S\oint_S \frac{[d\vec{S}_1\cdot(\vec{r}_1-\vec{r}_2)][d\vec{S}_2\cdot(\vec{r}_1-\vec{r}_2)]}{(|\vec{r}_1-\vec{r}_2|/\lambda)^4}$$
$$\times\left[30 - 8\frac{|\vec{r}_1-\vec{r}_2|}{\lambda} - e^{-|\vec{r}_1-\vec{r}_2|/\lambda}\left(30 + 22\frac{|\vec{r}_1-\vec{r}_2|}{\lambda} + 7\frac{|\vec{r}_1-\vec{r}_2|^2}{\lambda^2} + \frac{|\vec{r}_1-\vec{r}_2|^3}{\lambda^3}\right)\right]. \tag{4.35}$$

For this special case in which $\lambda = a$, the previous result for V_0 reduces to

$$V_0 = \frac{8}{15}\,\frac{a_s\{1-\kappa[(N-Z)/A]^2\}}{\pi r_0^{\,2}\lambda}\,.$$

For a sphere of radius R_0, Eq. (4.30) becomes[24,25]

$$E_N(\text{sharp}) = -\frac{2\pi}{3}V_0R_0^{\,3}\left[1 - \frac{3}{2}\left(\frac{\lambda}{R_0}\right) + \frac{3}{2}\left(\frac{\lambda}{R_0}\right)^3 - \frac{3}{2}\left(\frac{\lambda}{R_0}\right)\left(1 + \frac{\lambda}{R_0}\right)^2 e^{-2R_0/\lambda}\right] \tag{4.36}$$

and Eq. (4.31) becomes

$$\Delta E_N = -\frac{a^2(a^2-2\lambda^2)}{(a^2-\lambda^2)^2}E_N(\text{sharp})$$
$$+\frac{2\pi}{3}\frac{V_0R_0^{\,3}a^2}{(a^2-\lambda^2)^2}\left\{\lambda^2\left[1 - \frac{3}{2}\left(\frac{a}{R_0}\right) + \frac{3}{2}\left(\frac{a}{R_0}\right)^3 - \frac{3}{2}\left(\frac{a}{R_0}\right)\left(1 + \frac{a}{R_0}\right)^2 e^{-2R_0/a}\right] + (\lambda^2-a^2)\left[1 - \frac{9}{4}\left(\frac{a}{R_0}\right) + \frac{15}{4}\left(\frac{a}{R_0}\right)^3\right]\right.$$
$$\left. + (a^2-\lambda^2)\left[\frac{3}{2} + \frac{21}{4}\left(\frac{a}{R_0}\right) + \frac{15}{2}\left(\frac{a}{R_0}\right)^2 + \frac{15}{4}\left(\frac{a}{R_0}\right)^3\right]e^{-2R_0/a}\right\}. \tag{4.37}$$

Similarly, for the special case in which $\lambda = a$, Eq. (4.34) simplifies for a sphere to

$$E_N = -\frac{V_0\pi R_0^{\,3}}{12}\left\{8 - \frac{45}{2}\left(\frac{\lambda}{R_0}\right) + \frac{105}{2}\left(\frac{\lambda}{R_0}\right)^3 - 3\left[2\left(\frac{R_0}{\lambda}\right) + 11 + \frac{55}{2}\left(\frac{\lambda}{R_0}\right) + 35\left(\frac{\lambda}{R_0}\right)^2 + \frac{35}{2}\left(\frac{\lambda}{R_0}\right)^3\right]e^{-2R_0/\lambda}\right\} . \qquad (4.38)$$

As was true for the Coulomb energy, it is convenient to separate ΔE_N in Eq. (4.31) into two parts which are first order and second order in the density deviation defined in Eq. (4.13). The two components are given by

$$\Delta E_N^{(1)} = -\frac{2a^2}{(a^2-\lambda^2)}\,E_N(\text{sharp}) - \frac{V_0 a^2}{\rho_0(a^2-\lambda^2)}\int_V d^3r_1\,\rho(\vec{r}_1) \qquad (4.39)$$

and

$$\Delta E_N^{(2)} = \frac{a^4}{(a^2-\lambda^2)^2}\,E_N(\text{sharp}) + \frac{V_0}{8\pi(a^2-\lambda^2)^2}\int_V\int_V d^3r_1\,d^3r_2\left[\frac{(2a^2-\lambda^2)}{|\vec{r}_1-\vec{r}_2|} - \frac{(a^2-\lambda^2)}{2a}\right]e^{-|\vec{r}_1-\vec{r}_2|/a} , \qquad (4.40)$$

respectively.

As was done in Sec. IV A, we next derive a result that is valid when the range a is small compared to the nuclear radius. For this case the important contributions to Eqs. (4.39) and (4.40) come from the regions where $|\vec{r}_1 - \vec{r}_2| \lesssim a$. As before, we approximate these expressions by extending the region of integration in Eq. (4.39) and *one* of the regions of integration in Eq. (4.40) over all space. We then find that

$$\Delta E_N^{(1)} \approx -\frac{2a^2}{(a^2-\lambda^2)}\,E_N(\text{sharp}) - \frac{4\pi V_0 a^2 R_0^{\,3}}{3(a^2-\lambda^2)} ,$$

$$\Delta E_N^{(2)} \approx \frac{a^4}{(a^2-\lambda^2)^2}\,E_N(\text{sharp}) + \frac{2\pi}{3}\,\frac{V_0 a^4 R_0^{\,3}}{(a^2-\lambda^2)^2} ,$$

and

$$\Delta E_N \approx -a^2\,\frac{(a^2-2\lambda^2)}{(a^2-\lambda^2)^2}\,E_N(\text{sharp}) + \frac{2\pi V_0 a^2 R_0^{\,3}}{3(a^2-\lambda^2)^2}\,(2\lambda^2 - a^2) . \qquad (4.41)$$

V. SUMMARY AND CONCLUSION

We have seen that the calculation of various quantities for an arbitrarily shaped diffuse-surface density distribution becomes especially simple when the diffuse surface is generated by folding a short-range function over a uniform sharp-surface distribution of appropriate shape. For example, the rigid-body moment of inertia for rotation about an arbitrary axis is equal to the corresponding moment of inertia for the sharp surface plus a constant that depends only on the mass of the system and the width of the diffuse surface. An even simpler result is that the (ordinary) multipole moments of the diffuse-surface distribution are identically equal to the corresponding multipole moments for the sharp surface. By way of contrast, the analogous results for a diffuse-surface distribution obtained by generalizing a Fermi function are complicated expressions that must be evaluated numerically.

Our result for the rigid-body moment of inertia was seen to be of practical importance in connection with such questions as the production of compound nuclei in heavy-ion reactions, especially for light nuclear systems. The increase in the moment of inertia increases the critical angular momentum above which compound nuclei are no longer produced. This effect was seen to be possibly responsible for the recent production experimentally of compound nuclei with a higher cross section than was predicted by the Bass model on the basis of sharp-surface moments of inertia.

We also calculated the diffuse-surface corrections to the Coulomb and nuclear potentials and to the Coulomb and nuclear energies. These expressions were specialized to the case of a Yukawa folding function, although some of the results are more general. The diffuseness correction to the Coulomb potential is proportional to the square of the surface thickness and to the nuclear density. The second-order diffuseness correction to the Coulomb energy is independent of shape, but the third-order correction is proportional to the surface area. This increases slightly the effective nuclear surface tension. The effect of the diffuse nuclear surface on the nuclear potential and on the nuclear energy can be partially absorbed by calculating these quantities for a sharp surface but with a two-nucleon effective potential whose range is appropriately increased. However, for certain purposes, such as describing elastic and quasielastic scattering, where the tail of the ion-ion potential is relevant, the diffuseness corrections to the nuclear potential and to the nuclear energy are important.

In summary, there are many phenomena in nuclear physics where the diffuseness of the nuclear surface must be taken into account. The logical way to generate this diffuseness is by folding a short-range function over a uniform sharp-surface distribution of appropriate geometrical shape. We hope that the results presented here will prove useful in future studies that take into account the diffuseness of the nuclear surface.

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APPENDIX A: CONVERSION OF A VOLUME INTEGRAL INTO A SURFACE INTEGRAL BY USE OF A SINGLE DIVERGENCE RELATION

1. General method

Consider a volume integral of the form

$$I(\vec{r}_1)=\int_V d^3r_2 f(\vec{r}_{12}), \tag{A1}$$

where the integration extends over a volume enclosed by a *sharp* surface and where

$$\vec{r}_{12}=\vec{r}_1-\vec{r}_2. \tag{A2}$$

The problem is, for an *arbitrary* function $f(\vec{r}_{12})$, to find a function $F(\vec{r}_{12})$ that satisfies the divergence relation

$$f(\vec{r}_{12})=\nabla_2\cdot[\vec{r}_{12}F(\vec{r}_{12})]. \tag{A3}$$

Then, by virtue of Gauss's divergence theorem Eq. (A1) becomes

$$I(\vec{r}_1)=\oint_S (d\vec{S}_2\cdot\vec{r}_{12})F(\vec{r}_{12}), \tag{A4}$$

where the integration is over the surface of the sharp shape.

Relations of the form (A3) are already known to exist for the delta function

$$\delta(\vec{r}_{12})=-\frac{1}{4\pi}\nabla_2\cdot\left(\frac{\vec{r}_{12}}{r_{12}^{\,3}}\right), \tag{A5}$$

for the Coulomb potential[5]

$$\frac{1}{r_{12}}=-\frac{1}{2}\nabla_2\cdot\left(\frac{\vec{r}_{12}}{r_{12}}\right), \tag{A6}$$

and for the Yukawa potential[5,6]

$$\frac{e^{-r_{12}/a}}{r_{12}/a}=-\nabla_2\cdot\left\{\vec{r}_{12}\left(\frac{r_{12}}{a}\right)^{-3}\left[1-\left(1+\frac{r_{12}}{a}\right)e^{-r_{12}/a}\right]\right\}. \tag{A7}$$

The corresponding surface functions appearing in Eq. (A4) are therefore

$$F(r_{12})=-\frac{1}{4\pi}r_{12}^{\,-3}, \tag{A8}$$

$$F(r_{12})=-\tfrac{1}{2}r_{12}^{\,-1}, \tag{A9}$$

and

$$F(r_{12})=-\left(\frac{r_{12}}{a}\right)^{-3}\left[1-\left(1+\frac{r_{12}}{a}\right)e^{-r_{12}/a}\right] \tag{A10}$$

for a delta function, Coulomb potential, and Yukawa potential, respectively.

We note that by making the substitution $-1/a\to\pm ik$ in Eq. (A7) we obtain

$$\frac{e^{\pm ikr_{12}}}{ir_{12}}=-\frac{i}{k^2}\nabla_2\cdot\left\{\frac{\vec{r}_{12}}{r_{12}^{\,3}}\left[1-(1\mp ikr_{12})e^{\pm ikr_{12}}\right]\right\}. \tag{A11}$$

Before proceeding further, we need to make two assumptions regarding the behavior of $f(\vec{r}_{12})$ and its Fourier transform $f(\vec{k})$:

(i) First, we assume that

$$f(\vec{r}_{12})=f(r_{12}), \tag{A12a}$$

which implies that

$$f(\vec{k})=f(k). \tag{A12b}$$

In other words, both f and its Fourier transform depend only on the magnitudes of their arguments.

(ii) Next, we assume that the Fourier transform of $f(r_{12})$ *exists*. This implies that $f(r_{12})\to 0$ as $r_{12}\to\infty$ and that $f(k)\to 0$ as $k\to\infty$. In addition, $f(k)$ must satisfy the condition

$$\lim_{k\to 0}k^2 f(k)=K, \tag{A13}$$

where K is a *finite* constant whose value is zero unless $f(k)\sim k^{-2}$ as $k\to 0$. Equation (A13) states that at the origin in k space $f(k)$ is no more singular than k^{-2}. Thus, this assumption insures that all integrals are finite.

The above two assumptions are easily satisfied for most functions of physical interest.

We now Fourier transform $f(r_{12})$ to obtain

$$f(r_{12})=\frac{1}{(2\pi)^{3/2}}\int_\infty d^3k\, e^{i\vec{k}\cdot\vec{r}_{12}}f(k)=\left(\frac{2}{\pi}\right)^{1/2}\int_0^\infty dk\,\frac{\sin(kr_{12})}{r_{12}}kf(k), \tag{A14}$$

which by virtue of Eq. (A11) becomes

$$f(r_{12})=-\left(\frac{2}{\pi}\right)^{1/2}\nabla_2\cdot\left\{\frac{\vec{r}_{12}}{r_{12}^{\,3}}\int_0^\infty\frac{dk}{k}f(k)\times[\sin(kr_{12})-kr_{12}\cos(kr_{12})]\right\}. \tag{A15}$$

Upon comparing this result with Eq. (A3), we see that

$$F(r_{12}) = -\left(\frac{2}{\pi}\right)^{1/2} r_{12}^{-3} \times \int_0^\infty \frac{dk}{k} f(k)[\sin(kr_{12}) - kr_{12}\cos(kr_{12})], \tag{A16}$$

a *general* expression to be used in the surface integral of Eq. (A4).

If $f(k)$ is an even function of k, i.e., if

$$f(-k) = f(k), \tag{A17}$$

then Eqs. (A15) and (A16) become

$$f(r_{12}) = -\frac{i}{\sqrt{2\pi}} \nabla_2 \cdot \left\{ \frac{\vec{r}_{12}}{r_{12}^3} \int_{-\infty}^{\infty} \frac{dk}{k} f(k)[1-(1-ikr_{12})e^{ikr_{12}}] \right\} \tag{A18}$$

and

$$F(r_{12}) = -\frac{i}{\sqrt{2\pi}} r_{12}^{-3} \int_{-\infty}^{\infty} \frac{dk}{k} f(k)[1-(1-ikr_{12})e^{ikr_{12}}], \tag{A19}$$

respectively. Equation (A19) is especially useful for evaluating the surface function by complex contour integration. Note that the first term in Eq. (A19) identically vanishes. We retain this form in order that the integrand be explicitly well behaved at $k=0$.

An examination of the behavior of the integrands of Eqs. (A16) and (A19) for small values of k reveals again the necessity for the condition (A13). In Eq. (A16), we obtain the limit

$$k^{-1}[\sin(kr_{12}) - kr_{12}\cos(kr_{12})] \xrightarrow[k\to 0]{} k^2 \frac{r_{12}^3}{3}.$$

This k^2 term would cancel the k^{-2} singularity in $f(k)$ for the limiting case, which would make the integrand well behaved at $k=0$. Similarly, in Eq. (A19) we have the limit

$$k^{-1}[1-(1-ikr_{12})e^{ikr_{12}}] \xrightarrow[k\to 0]{} -k\frac{r_{12}^2}{2}.$$

This means that the integral would have a simple pole at $k=0$ if $f(k) \sim k^{-2}$. However, such an integral can easily be evaluated by use of complex contour integration because we need only evaluate the (principal-value) residue contribution from a pole situated *on* the contour.[27] Therefore, if $f(k)$ is more singular than k^{-2} at $k=0$, the integral is not finite.

2. Application to specific functions

In Eqs. (A8)–(A10) we have already listed the surface functions $F(r_{12})$ corresponding to a delta function, Coulomb potential, and Yukawa potential, respectively. In Table I we present some additional functions derived by use of Eq. (A16) or (A19).

These functions have been checked with Eq. (A3) by taking divergences with respect to $\vec{r}_2$. In addition, the exponential and $r_{12}e^{-r_{12}/a}$ functions have been checked using the formulas

$$e^{-r_{12}/a} = -\frac{\partial}{\partial(1/a)}\left(\frac{e^{-r_{12}/a}}{r_{12}}\right) \tag{A20a}$$

and

$$r_{12}e^{-r_{12}/a} = -\frac{\partial}{\partial(1/a)}(e^{-r_{12}/a}). \tag{A20b}$$

The error function appearing in Table I is defined as

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt. \tag{A21}$$

This is a standard library function on most modern computers and is thus easily computed.

3. Other methods

We now consider two special functions of physical interest whose Fourier transforms do not exist

TABLE I. Single divergence functions.

Volume function $f(r_{12})$	Fourier transform $f(k)$	Surface function $F(r_{12})$
r_{12}^{-2}	$\sqrt{\frac{\pi}{2}}\frac{1}{k}$	$-r_{12}^{-2}$
$e^{-r_{12}/a}$	$\frac{4}{\sqrt{2\pi}}\frac{1}{a}\frac{1}{(k^2+1/a^2)^2}$	$-\left(\frac{r_{12}}{a}\right)^{-3}\left[2-e^{-r_{12}/a}\left(2+2\frac{r_{12}}{a}+\frac{r_{12}^2}{a^2}\right)\right]$
$r_{12}e^{-r_{12}/a}$	$2\left(\frac{2}{\pi}\right)^{1/2}\frac{(3/a^2-k^2)}{(k^2+1/a^2)^3}$	$-a\left(\frac{r_{12}}{a}\right)^{-3}\left[-6+e^{-r_{12}/a}\left(6+6\frac{r_{12}}{a}+3\frac{r_{12}^2}{a^2}+\frac{r_{12}^3}{a^3}\right)\right]$
$e^{-r_{12}^2/a^2}$	$\frac{a^3}{2\sqrt{2}}e^{-a^2k^2/4}$	$-\frac{1}{2}\left(\frac{r_{12}}{a}\right)^{-3}\left[-\frac{r_{12}}{a}e^{-r_{12}^2/a^2}+\frac{\sqrt{\pi}}{2}\operatorname{erf}\left(\frac{r_{12}}{a}\right)\right]$

and for which the method described in Appendix A 1 is therefore not applicable.

The first example is the sharp-surface momenta of inertia given by Eq. (2.9). We note that

$$x^2 + y^2 = \nabla \cdot \vec{A}\,, \tag{A22}$$

where

$$\vec{A} = \tfrac{1}{3}(x^3\vec{e}_x + y^3\vec{e}_y) \tag{A23}$$

and where $\vec{e}_x$ and $\vec{e}_y$ are unit vectors in the x and y directions, respectively. From the divergence theorem it follows that

$$I_z(\text{sharp}) = \rho_0 \int_V d^3r(x^2+y^2) = \tfrac{1}{3}\rho_0 \oint_S d\vec{S}\cdot(x^3\vec{e}_x + y^3\vec{e}_y)\,. \tag{A24}$$

The second example is the sharp-surface generalized multipole moment defined in Eq. (2.24). The integrand of this expression satisfies the divergence relation[28]

$$r^{L+k}Y_{LM}(\theta,\phi) = \nabla\cdot\vec{N}(\vec{r})\,, \tag{A25}$$

where $\vec{N}$ has the two *equivalent* forms

$$\vec{N}(\vec{r}) = (k+2)^{-1}\left(\frac{2L+1}{L}\right)^{1/2} r^{L+k+1}\vec{\mathcal{Y}}_{LM}^{(L-1)}(\theta,\phi) \tag{A26a}$$

and

$$\vec{N}(\vec{r}) = -(2L+k+3)^{-1}\left(\frac{2L+1}{L+1}\right)^{1/2} r^{L+k+1}\vec{\mathcal{Y}}_{LM}^{(L+1)}(\theta,\phi)\,. \tag{A26b}$$

The function $\vec{\mathcal{Y}}_{LM}^{(J)}(\theta,\phi)$ is a *vector* spherical harmonic[20] defined by

$$\vec{\mathcal{Y}}_{LM}^{(J)}(\theta,\phi) \equiv \sum_{mq}\langle J,1,m,q\,|\,LM\rangle Y_{Jm}(\theta,\phi)\vec{e}_q\,, \tag{A27}$$

where $\langle ab\alpha\beta\,|\,c\gamma\rangle$ is a Clebsch-Gordan coefficient, $Y_{Jm}(\theta,\phi)$ is a spherical harmonic, and $\vec{e}_q$ is a spherical unit vector defined by

$$\vec{e}_{+1} = -\frac{1}{\sqrt{2}}(\vec{e}_x + i\vec{e}_y)\,,\qquad \vec{e}_0 = \vec{e}_z\,, \tag{A28}$$

and

$$\vec{e}_{-1} = \frac{1}{\sqrt{2}}(\vec{e}_x - i\vec{e}_y)\,.$$

Because Eq. (A26a) contains lower-order spherical harmonics than does Eq. (A26b), it is convenient for most applications to use the former expression. However, for $L=0$ one must use Eq. (A26b). Upon substituting Eqs. (A25) and (A26) into Eq. (2.24) and using the divergence theorem, we obtain Eqs. (2.25).

APPENDIX B: CONVERSION OF A DOUBLE VOLUME INTEGRAL INTO A DOUBLE SURFACE INTEGRAL BY USE OF A DOUBLE DIVERGENCE RELATION

1. General method

Consider a double volume integral of the form

$$I = \int_V\int_V d^3r_1 d^3r_2 f(\vec{r}_{12})\,, \tag{B1}$$

where $\vec{r}_{12}$ is defined by Eq. (A2). The problem is, for an *arbitrary* function $f(\vec{r}_{12})$, to find a function $F(\vec{r}_{12})$ that satisfies the double divergence relation

$$f(\vec{r}_{12}) = \sum_{i,j=1}^{3}\frac{\partial}{\partial(r_1)_i}\frac{\partial}{\partial(r_2)_j}(r_{12})_i(r_{12})_j F(\vec{r}_{12})\,, \tag{B2}$$

where $(r_1)_i$ is the ith component of the vector $\vec{r}_1$, $(r_{12})_i$ is the ith component of the vector $\vec{r}_{12}$, etc. Then, a double application of Gauss's divergence theorem transforms Eq. (B1) into

$$I = \oint_S\oint_S (d\vec{S}_1\cdot\vec{r}_{12})(d\vec{S}_2\cdot\vec{r}_{12})F(\vec{r}_{12})\,, \tag{B3}$$

which is a double surface integral.

Relations of the form (B2) are already known to exist for the delta function

$$\delta(\vec{r}_{12}) = -\frac{1}{4\pi}\sum_{i,j=1}^{3}\frac{\partial}{\partial(r_1)_i}\frac{\partial}{\partial(r_2)_j}\left[\frac{(r_{12})_i(r_{12})_j}{(r_{12})^3}\right]\,, \tag{B4}$$

for the Coulomb[23] potential

$$\frac{1}{r_{12}} = -\frac{1}{6}\sum_{i,j=1}^{3}\frac{\partial}{\partial(r_1)_i}\frac{\partial}{\partial(r_2)_j}\left[\frac{(r_{12})_i(r_{12})_j}{r_{12}}\right]\,, \tag{B5}$$

and for the Yukawa potential[24]

$$\frac{e^{-r_{12}/a}}{r_{12}/a} = -\sum_{i,j=1}^{3}\frac{\partial}{\partial(r_1)_i}\frac{\partial}{\partial(r_2)_j}(r_{12})_i(r_{12})_j\left[\frac{r_{12}}{a} - 2 + \left(\frac{r_{12}}{a}+2\right)e^{-r_{12}/a}\right]\left(\frac{r_{12}}{a}\right)^{-4}. \tag{B6}$$

The corresponding surface functions appearing in Eq. (B3) are therefore

$$F(r_{12}) = -\frac{1}{4\pi}r_{12}^{-3}\,, \tag{B7}$$

$$F(r_{12}) = -\tfrac{1}{6} r_{12}^{-1}, \tag{B8}$$

and

$$F(r_{12}) = -\left[\frac{r_{12}}{a} - 2 + \left(\frac{r_{12}}{a} + 2\right) e^{-r_{12}/a}\right] \left(\frac{r_{12}}{a}\right)^{-4}, \tag{B9}$$

for a delta function, Coulomb potential, and Yukawa potential, respectively.

We note that by making the substitution $-1/a \to \pm ik$ in Eq. (B6), we obtain

$$\pm\frac{e^{\pm ikr_{12}}}{ir_{12}} = \frac{1}{k^3} \sum_{i,j=1}^{3} \frac{\partial}{\partial (r_1)_i} \frac{\partial}{\partial (r_2)_j} \left\{ \frac{(r_{12})_i (r_{12})_j}{r_{12}^4} [\mp ikr_{12} - 2 + (\mp ikr_{12} + 2) e^{\pm ikr_{12}}] \right\}. \tag{B10}$$

We make the same two assumptions for $f(r_{12})$ and its Fourier transform $f(k)$ that we made in Appendix A. From Eqs. (A14), (B10), and (B2), it follows that

$$F(r_{12}) = \left(\frac{2}{\pi}\right)^{1/2} r_{12}^{-4} \int_0^\infty \frac{dk}{k^2} f(k)[-2 + kr_{12}\sin(kr_{12}) + 2\cos(kr_{12})], \tag{B11}$$

which is a completely *general* expression for the surface function $F(r_{12})$.

If $f(k)$ is an *even* function of k, then Eq. (B11) becomes

$$F(r_{12}) = \frac{1}{(2\pi)^{1/2}} r_{12}^{-4} \int_{-\infty}^{\infty} \frac{dk}{k^2} f(k)[-ikr_{12} - 2 + (-ikr_{12} + 2) e^{ikr_{12}}], \tag{B12}$$

which is especially useful for evaluating $F(r_{12})$ by complex contour integration. The first term in Eq. (B12) identically vanishes. This form is retained in order to have a well-behaved integrand at $k = 0$.

As was true in Appendix A, an analysis of the integrands of Eqs. (B11) and (B12) indicates that Eq. (A13) must be satisfied in order to obtain a finite integral. Thus, $f(k)$ must be no more singular than k^{-2} at $k = 0$.

If $f(k)$ is very complicated, then the integration over k in Eq. (B11) or (B12) might be difficult or impossible to perform in closed form. Evaluation of this integral numerically (e.g., by means of Gaussian-Laguerre or Gaussian-Hermite quadrature) means that the original sixfold integral (B1) is reduced to a fivefold integral, namely the fourfold integral in Eq. (B3) and the extra numerical integration over k.

2. Application to specific functions

In Eqs. (B7)–(B9) we have already listed the surface functions $F(r_{12})$ corresponding to a delta function, Coulomb potential, and Yukawa potential, respectively. In Table II we present some additional functions derived by use of Eq. (B11) or (B12). These functions have been checked with Eq. (B2) by taking derivates with respect to $(r_1)_i$ and $(r_2)_j$ and summing over i and j. In addition, the exponential and $r_{12}e^{-r_{12}/a}$ functions have been checked using Eqs. (A20).

APPENDIX C: DERIVATION OF THE EXPRESSION FOR THE COULOMB ENERGY BY TRANSFORMING THE INTEGRATION VARIABLES

Throughout Secs. III and IV of this paper we derived all of our results by taking Fourier trans-

TABLE II. Double divergence functions.

Volume function $f(r_{12})$	Surface function $F(r_{12})$
r_{12}^{-2}	$-\tfrac{1}{2} r_{12}^{-2}$
$e^{-r_{12}/a}$	$\left(\frac{r_{12}}{a}\right)^{-4}\left[6 - 2\frac{r_{12}}{a} - e^{-r_{12}/a}\left(6 + 4\frac{r_{12}}{a} + \frac{r_{12}^2}{a^2}\right)\right]$
$r_{12}e^{-r_{12}/a}$	$a\left(\frac{r_{12}}{a}\right)^{-4}\left[24 - 6\frac{r_{12}}{a} - e^{-r_{12}/a}\left(24 + 18\frac{r_{12}}{a} + 6\frac{r_{12}^2}{a^2} + \frac{r_{12}^3}{a^3}\right)\right]$
$e^{-r_{12}^2/a^2}$	$\frac{1}{2}\left(\frac{r_{12}}{a}\right)^{-4}\left[1 - e^{-r_{12}^2/a^2} - \frac{r_{12}}{a}\sqrt{\frac{\pi}{2}}\,\mathrm{erf}\left(\frac{r_{12}}{a}\right)\right]$

forms of various functions. However, this method cannot be used for all quantities of physical interest. For example, in Sec. II we did not use this method to derive the diffuse-surface corrections to the moment of inertia and generalized multipole moments because the Fourier transforms of such functions as (x^2+y^2) do not exist. Instead, we simply interchanged the order of integration and transformed the variable of integration to obtain Eqs. (2.10), (2.14), and (2.21). This latter method is also very powerful and could have been used in Secs. III and IV instead of the Fourier-transform method. As an example, we derive Eqs. (4.6)–(4.8) for the Coulomb energy of a diffuse-surface distribution by means of this alternate technique.

Upon substituting Eq. (2.4) into Eq. (4.2) and reversing the order of integrations, we obtain

$$E_C = \frac{1}{2}\left(\frac{\rho_0}{4\pi a^3}\right)^2 \int_V \int_V d^3r_3 d^3r_4 \times \int_\infty d^3r_2 \frac{e^{-|\vec{r}_2-\vec{r}_4|/a}}{|\vec{r}_2-\vec{r}_4|/a} J(\vec{r}_2,\vec{r}_3), \tag{C1}$$

where

$$J(\vec{r}_2,\vec{r}_3) \equiv \int_\infty d^3r_1 \frac{1}{|\vec{r}_1-\vec{r}_2|} \frac{e^{-|\vec{r}_1-\vec{r}_3|/a}}{|\vec{r}_1-\vec{r}_3|/a}. \tag{C2}$$

By making the substitution

$$\vec{u} = \frac{\vec{r}_1-\vec{r}_3}{a}$$

and performing the angular integrations, we obtain

$$J(\vec{r}_2,\vec{r}_3) = \frac{2\pi a^2}{|\vec{r}_2-\vec{r}_3|}\left\{\int_0^\infty (au+|\vec{r}_3-\vec{r}_2|)e^{-u}du - \int_0^{|\vec{r}_3-\vec{r}_2|/a}(|\vec{r}_3-\vec{r}_2|-au)e^{-u}du - \int_{|\vec{r}_3-\vec{r}_2|/a}^\infty (au-|\vec{r}_3-\vec{r}_2|)e^{-u}du\right\}. \tag{C3}$$

The integrals in Eq. (C3) can be performed easily, which leads to

$$J(\vec{r}_2,\vec{r}_3) = \frac{4\pi a^3}{|\vec{r}_2-\vec{r}_3|}(1-e^{-|\vec{r}_2-\vec{r}_3|/a}). \tag{C4}$$

Substitution of this result into Eq. (C1) gives

$$E_C = \frac{1}{2}\frac{\rho_0^{\,2}}{4\pi a^3}\int_V\int_V d^3r_3 d^3r_4 K(\vec{r}_3,\vec{r}_4), \tag{C5}$$

where

$$K(\vec{r}_3,\vec{r}_4) \equiv \int_\infty \frac{d^3r_2}{|\vec{r}_2-\vec{r}_3|}(1-e^{-|\vec{r}_2-\vec{r}_3|/a})\frac{e^{-|\vec{r}_2-\vec{r}_4|/a}}{|\vec{r}_2-\vec{r}_4|/a}. \tag{C6}$$

This time we redefine variables by making the substitution

$$\vec{u}' = \frac{\vec{r}_2-\vec{r}_4}{a}.$$

After some manipulation, Eq. (C6) becomes

$$K(\vec{r}_3,\vec{r}_4) = \frac{4\pi a^3}{|\vec{r}_3-\vec{r}_4|}\left\{1-e^{-|\vec{r}_3-\vec{r}_4|/a}+\tfrac{1}{2}e^{-|\vec{r}_3-\vec{r}_4|/a}\left[\int_0^\infty e^{-2u'}du' - \int_0^{|\vec{r}_3-\vec{r}_4|/a}du'\right] - \tfrac{1}{2}e^{+|\vec{r}_3-\vec{r}_4|/a}\int_{|\vec{r}_3-\vec{r}_4|/a}^\infty e^{-2u'}du'\right\}. \tag{C7}$$

The integrals in Eq. (C7) can be performed easily, which leads to

$$K(\vec{r}_3,\vec{r}_4) = \frac{4\pi a^3}{|\vec{r}_3-\vec{r}_4|}\left(1-e^{-|\vec{r}_3-\vec{r}_4|/a} - \frac{1}{2}\frac{|\vec{r}_3-\vec{r}_4|}{a}e^{-|\vec{r}_3-\vec{r}_4|/a}\right).$$

Substitution of this result into Eq. (C5) gives Eqs. (4.6)–(4.8), which were originally derived by means of the Fourier-transform method.

This method of transforming the integration variables could have been used for deriving all quantities obtained in this paper for the Yukawa folding function. However, when it can be applied, the Fourier-transform method is somewhat more powerful and the derivations using it are somewhat simpler than for the alternate method. Also, the Fourier-transform method was used in Secs. III and IV to derive *general* expressions for arbitrary folding functions. These expressions are usually handled fairly easily by means of complex-variable integration or some related technique.

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