JOURNAL OF COMPUTATIONAL PHYSICS 18, 311–325 (1975)

Calculation of Coulomb Energies for Uniform Charge Distributions of Arbitrary Shape*

K. T. R. DAVIES†

Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87544, and Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

AND

A. J. SIERK‡

Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87544

Received January 27, 1975

Three distinct surface-integral formulas are derived for calculating the Coulomb energies of uniform charge distributions of arbitrary shape. Of particular interest is an equation obtained by applying Gauss'divergence theorem twice. It is shown that this equation can be simply transformed to another expression which has been widely used for calculating Coulomb energies, with this derivation implying a third formula. The three formulas are also expressed in cylindrical coordinates for charge distributions possessing axial symmetry. For such shapes, numerical studies are presented showing the computational times and errors involved in calculating the Coulomb energies and generalized forces using Gaussian–Legendre quadrature formulas. We show that the double-divergence-derived formula is faster and more accurate than the other two surface-integral formulas and other formulas used in the literature.

I. INTRODUCTION

In the study of fission and heavy-ion reactions an important part of the total shape-dependent macroscopic energy of a nucleus is the Coulomb energy [1]. It is of interest to study various methods of calculating this energy, with particular emphasis on exploiting those methods which are fastest and most accurate. In this

* Research sponsored by the U. S. Atomic Energy Commission under contracts with the University of California and Union Carbide Corporation.

† Present address: Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830.

‡ Present address: Department of Physics, California Institute of Technology, Pasadena, California 91109.

paper we derive three surface-integral formulas for the Coulomb energy of uniform charge distributions, show how they are related to each other, and compare the speeds and accuracies of the formulas in numerical calculations of shapes with axial symmetry.

The general expression for the Coulomb energy of an arbitrary charge distribution is a double-volume integral. If this integral is transformed into a double-surface integral, the number of integrations is reduced from six to four. A general formula of this type can be obtained by combining a derivation by Frankel and Metropolis [2] with one given by Hill and Wheeler [3]. Frankel and Metropolis [2] used scaling properties to obtain a surface integral for the Coulomb energy involving the potential at the surface of the shape. Hill and Wheeler [3] showed how to evaluate this potential for axially symmetric shapes, and the resulting formula for the Coulomb energy has been extensively used in liquid-drop-model fission calculations [1, 4–7]. We derive another surface-integral formula by applying the divergence theorem twice to the original volume integral. We then show that the earlier formula can be obtained from the relation derived from the double-divergence -theorem and deduce a third surface-integral formula.

In practical applications, an important special case is that of axial symmetry. The formula of Frankel and Metropolis [2] reduces to a two-dimensional integral whose integrand contains complete elliptic integrals of the first and second kinds [3, 7]. Similarly, the other two surface-integral formulas can be expressed as double integrals containing complete elliptic integrals. For axially symmetric shapes, additional formulas for the Coulomb energy have been obtained in the literature [8, 9]. Beringer derives an approximate expression for the Coulomb energy by dividing the body into small slices and summing the interactions and self-energies of the slices in an approximate way. The accuracy of this method, which is rather poor, slowly improves as the number of slices is increased [8]. Another expression was derived by Lawrence [9], who slices the volume into infinitesimal disks. By a series of mathematical manipulations involving Bessel and hypergeometric functions, he obtains an exact equation for the Coulomb energy expressed as a three-dimensional integral with a relatively simple integrand. Lawrence's method has been used in the fission studies of Hasse [10].

For each of the three surface-integral formulas, we study the numerical accuracy resulting from calculating the Coulomb energy of axially symmetric shapes using Gaussian–Legendre quadrature. We find that the double-divergence formula is more accurate than either of the other two surface-integral formulas, and it is also the fastest of the three methods because of the symmetry of the integrand. All three of these formulas are much more accurate in a given time than the methods of Beringer [8] or Lawrence [9].

It should be mentioned that our studies are applicable to the calculation of any energy arising from a two-body potential proportional to the inverse distance

between the bodies. For example, the gravitational potential energy of a uniform mass distribution is trivially obtained from the Coulomb energy formula by a change of constant.

In Section II we derive the three surface-integral formulas and study the relations among them, and in Section III we specialize these equations to axially symmetric shapes. In Section IV we discuss the results of numerical studies using the various formulas.

II. General Surface Integrals for Calculating the Coulomb Energy

The general expression for the Coulomb energy is

$$E_c = \tfrac{1}{2}\rho_e^2 g, \tag{2.1}$$

where the factor of $\frac{1}{2}$ is used to avoid double counting and ρ_e is the constant charge density

$$\rho_e = Ze(4\pi R_0^3/3)^{-1}. \tag{2.2}$$

R_0 is the radius of a sphere having the same volume as the shape being considered, and Z is the total charge of the body in units of the proton charge, e. The function g is defined as

$$g = \iint \frac{d^3r\, d^3r'}{\rho}, \tag{2.3}$$

where ρ is the magnitude of

$$\boldsymbol{\rho} = \mathbf{r}' - \mathbf{r}, \tag{2.4}$$

and each three-dimensional integration is over the entire volume of the shape. (The vector $\boldsymbol{\rho}$ and its magnitude ρ should not be confused with the charge density ρ_e.) We next present various ways of converting this double-volume integral into a double-surface integral.

We may write

$$\rho^{-1} = -\frac{1}{6}\sum_{i,j=1}^{3} \frac{\partial}{\partial r_i}\frac{\partial}{\partial r_j'}\left(\frac{\rho_i\rho_j}{\rho}\right). \tag{2.5}$$

An analogous relation has been determined for the Yukawa potential [11]. The appropriate expression in Ref. [11] is misleading and is better written in the form

$$\frac{-\exp(-\rho/a)}{(\rho/a)} = \sum_{i,j=1}^{3} \frac{\partial}{\partial r_i}\frac{\partial}{\partial r_j'}\rho_i\rho_j[(\rho/a) - 2 + (\rho/a + 2)\exp(-\rho/a)](\rho/a)^{-4}. \tag{2.6}$$

If one takes the appropriate limit ($a \to \infty$) which transforms the Yukawa into the Coulomb potential, Eq. (2.6) reduces to Eq. (2.5). Substituting Eq. (2.5) into Eq. (2.3) and applying Gauss' divergence theorem twice, we obtain

$$g = -\frac{1}{6} \oint\oint \frac{(\mathbf{dS} \cdot \boldsymbol{\rho})(\mathbf{dS}' \cdot \boldsymbol{\rho})}{\rho}, \tag{2.7}$$

which from Eq. (2.1) gives us our first double-surface-integral expression for the Coulomb energy. (see also Ref. [12].)

A commonly used expression for the Coulomb energy was first obtained by Frankel and Metropolis using a suggestion of Hurwicz [2]. If the surface described by the radius vector from the origin $\mathbf{r}$ is changed by an infinitesimal amount $r(\Omega) \to r(\Omega)(1 + \epsilon)$, then the change in the Coulomb energy is

$$\delta E_c = \rho_e \int V_c(\mathbf{r})\, r^2(\Omega)\, dr\, d\Omega = \rho_e \epsilon \int V_c(\mathbf{r})\, r^3(\Omega)\, d\Omega, \tag{2.8}$$

where $V_c(\mathbf{r})$ is the potential at the surface of the distribution

$$V_c(\mathbf{r}) = \rho_e \int \frac{d^3r'}{\rho}. \tag{2.9}$$

We next observe that E_c depends on Z^2/r or, by the uniformity of the charge distribution on r^6/r or r^5, so that to first order in ϵ,

$$\delta E_c = 5\epsilon E_c. \tag{2.10}$$

Combining Eqs. (2.8) and (2.10) and noting that $r^3\, d\Omega = \mathbf{dS} \cdot \mathbf{r}$, we obtain

$$E_c = (\rho_e/5) \oint V_c(\mathbf{r})\, \mathbf{dS} \cdot \mathbf{r}. \tag{2.11}$$

Equation (2.9) can be transformed by the divergence theorem into the surface integral [3, 13]

$$V_c(\mathbf{r}) = (\rho_e/2) \oint \frac{\mathbf{dS}' \cdot \boldsymbol{\rho}}{\rho}, \tag{2.12}$$

so Eq. (2.11) becomes

$$E_c = (\rho_e{}^2/10) f, \tag{2.13}$$

where

$$f = \oint\oint (\mathbf{dS} \cdot \mathbf{r})(\mathbf{dS}' \cdot \boldsymbol{\rho})/\rho. \tag{2.14}$$

This formula is derived using the following two properties of the charge distribution: (1) the $1/r$ dependence of the two-body potential, and (2) the uniformity of the charge distribution, which implies that Z is proportional to the volume of the distribution.

We now show a relation between the g and f functions. First define

$$f' = \oint\oint (\mathbf{dS} \cdot \mathbf{r}')(\mathbf{dS}' \cdot \boldsymbol{\rho})/\rho, \tag{2.15}$$

and apply the divergence theorem twice to Eqs. (2.14) and (2.15), obtaining

$$f = \iint d^3r\, d^3r' \,(6/\rho + 2\mathbf{r} \cdot \boldsymbol{\rho}/\rho^3), \tag{2.16}$$

and

$$f' = 2 \iint d^3r\, d^3r' \,(\mathbf{r} \cdot \boldsymbol{\rho})/\rho^3. \tag{2.17}$$

Substituting Eq. (2.4) into Eq. (2.16), we find that

$$f = 2 \iint d^3r\, d^3r' \,(2/\rho + \mathbf{r}' \cdot \boldsymbol{\rho}/\rho^3). \tag{2.18}$$

Interchanging $\mathbf{r}$ and $\mathbf{r}'$ in Eq. (2.18) results in

$$f = 2 \iint d^3r\, d^3r' \,(2/\rho - \mathbf{r} \cdot \boldsymbol{\rho}/\rho^3). \tag{2.19}$$

We have shown that there are two ways of expressing f, Eqs. (2.16) and (2.19), which can be written using Eqs. (2.3) and (2.17) as

$$f = 6g + f' = 4g - f', \tag{2.20}$$

which implies

$$g = -f' = f/5. \tag{2.21}$$

From Eqs. (2.1) and (2.21) we are able to write a third formula for the Coulomb energy:

$$E_c = -\tfrac{1}{2}\rho_e^2 f'. \tag{2.22}$$

It should be emphasized that there is nothing special about the function f'. It is natural to introduce f' by replacing the factor $(\mathbf{dS} \cdot \mathbf{r})$ in Eq. (2.14) by $(\mathbf{dS} \cdot \mathbf{r}')$. For calculating the Coulomb energy, any one of the functions f, f', or g may be used

since they are all related through Eq. (2.21). In fact, any number of equations is possible since we may express E_c as

$$E_c = \tfrac{1}{2}\rho_e^2(xg + \tfrac{1}{5}yf - zf'), \tag{2.23}$$

where

$$x + y + z = 1.$$

To summarize, we have derived three expressions for the Coulomb energy of a uniform charge distribution:

$$E_c = -(\rho_e^2/12) \oint\oint (\mathbf{dS} \cdot \boldsymbol{\rho})(\mathbf{dS}' \cdot \boldsymbol{\rho})/\rho, \tag{2.24}$$

$$E_c = (\rho_e^2/10) \oint\oint (\mathbf{dS} \cdot \mathbf{r})(\mathbf{dS}' \cdot \boldsymbol{\rho})/\rho, \tag{2.25}$$

and

$$E_c = -(\rho_e^2/2) \oint\oint (\mathbf{dS} \cdot \mathbf{r}')(\mathbf{dS}' \cdot \boldsymbol{\rho})/\rho. \tag{2.26}$$

These equations are completely general and apply to distributions of charge of any shape. Equation (2.24) is invariant under the interchange of $\mathbf{r}$ and $\mathbf{r}'$, while Eqs. (2.25) and (2.26) are not, and as we demonstrate in Section IV by exploiting this symmetry for Eq. (2.24) the computing time can be reduced. The two examples considered there are axially symmetric but they are typical of the kinds of shapes encountered in fission and heavy-ion reactions. However, it is clear that the symmetry of Eq. (2.24) makes this formula faster than Eqs. (2.25) and (2.26) for calculating Coulomb energies for bodies of *arbitrary* shape, e.g., axially asymmetric or multiply connected shapes. Of course, any symmetry present in the shape allows one to further reduce the computational time, a property we also demonstrate in Section IV for a reflection-symmetric test body.

In studies of fission and other dynamical processes [1, 4–7] it is also of interest to calculate the generalized forces acting on the body studied. We then wish to evaluate the generalized Coulomb force

$$F_i^{(c)} = -\frac{\partial E_c}{\partial q_i}, \tag{2.27}$$

where q_i is any of the generalized coordinates describing the shape. Equations (2.24)–(2.26) are of the form

$$E_c(\mathbf{q}) = \int_{z_{\min}(\mathbf{q})}^{z_{\max}(\mathbf{q})} dz \int_{z_{\min}(\mathbf{q})}^{z_{\max}(\mathbf{q})} dz' \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi'\, I(z, z', \phi, \phi'; \mathbf{q}), \tag{2.28}$$

where $\mathbf{q} = (q_1, q_2, \ldots, q_n)$, and z and ϕ are cylindrical coordinates of points on the surface of the shape. Differentiating Eq. (2.28), we find that

$$F_i^{(c)}(\mathbf{q}) = -\left\{\int_{z_{\min}}^{z_{\max}} dz \int_{z_{\min}}^{z_{\max}} dz' \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi' \frac{\partial I(z, z', \phi, \phi'; \mathbf{q})}{\partial q_i}\right.$$

$$+ \frac{\partial z_{\max}(\mathbf{q})}{\partial q_i} \int_{z_{\min}}^{z_{\max}} dz \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi'$$

$$\times [I(z, z_{\max}, \phi, \phi'; \mathbf{q}) + I(z_{\max}, z, \phi, \phi'; \mathbf{q})]$$

$$- \frac{\partial z_{\min}(\mathbf{q})}{\partial q_i} \int_{z_{\min}}^{z_{\max}} dz \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi'$$

$$\left.\times [I(z, z_{\min}, \phi, \phi'; \mathbf{q}) + I(z_{\min}, z, \phi, \phi'; \mathbf{q})]\right\}. \tag{2.29}$$

This equation may be numerically integrated to obtain the generalized Coulomb forces. Since numerical integration is, in general, more accurate than numerical differentiation, using Eq. (2.29) is more efficient than performing a numerical differentiation, even though the integrand in Eq. (2.29) is substantially more complicated than those in any of the energy expressions.

An alternative method of calculating Coulomb forces is to consider the change in energy caused by an addition of an infinitesimal layer of charge on the surface distributed so that the change in the body's shape corresponds to an infinitesimal variation of one of the generalized coordinates q_i. For an arbitrary shape, the change in energy is given by [using the notation of Eq. (2.8)]

$$\delta E_c = \rho_e \oint_S V_c(\mathbf{r}; \mathbf{q})\, \delta[r^3(\Omega)]\, d\Omega, \tag{2.30}$$

with V_c being evaluated by means of Eq. (2.12).

III. Specialization to Axial Symmetry

We now express Eqs. (2.24)–(2.26) in cylindrical coordinates ($\mathbf{r} = [\rho, \phi, z]$) for axially symmetric shapes. For this case, one may integrate over one of the angles ϕ to get a factor of 2π. The remaining angular integration is over the angle between the projections of $\mathbf{r}$ and $\mathbf{r}'$ on the plane perpendicular to the axis of symmetry. This integration may also be performed yielding for E_c a two-dimensional integral in z

and z' whose integrand contains complete elliptic integrals. In Ref. [7], Eq. (2.25) was expressed as

$$E_c = (4\pi\rho_e^2/5)\int_{z_{\min}}^{z_{\max}} dz \int_{z_{\min}}^{z_{\max}} dz'\, P(z)\, P(z') \left[P(z) - z\,\frac{\partial P(z)}{\partial z}\right] \times \left(\frac{K(k)[P(z') + P(z) + (z - z')(\partial P(z')/\partial z')] - 2P(z)\, D(k)}{\{[P(z) + P(z')]^2 + (z - z')^2\}^{1/2}}\right), \quad (3.1)$$

where $P(z)$ is the ρ coordinate evaluated on the surface of the charge distribution,

$$k^2 = 4P(z)\, P(z')/\{[P(z) + P(z')]^2 + (z - z')^2\}, \quad (3.2)$$

$$D(k) = [K(k) - E(k)]/k^2, \quad (3.3)$$

and $K(k)$ and $E(k)$ are complete elliptic integrals of the first and second kinds. Similarly, we express Eqs. (2.24) and (2.26), respectively, as

$$E_c = (2\pi\rho_e^2/3)\int_{z_{\min}}^{z_{\max}} dz \int_{z_{\min}}^{z_{\max}} dz'\, P(z)\, P(z')\{[P(z) + P(z')]^2 + (z - z')^2\}^{-1/2} \times \left(\left[\frac{K(k) - 2D(k)}{3}\right]\left\{2[P^2(z) + P^2(z')] - (z - z')^2 + 3(z - z') \times \left[P(z')\,\frac{\partial P(z')}{\partial z'} - P(z)\,\frac{\partial P(z)}{\partial z}\right]\right\} + K(k)\left\{P(z)\, P(z')/3 + \left[P(z) - (z - z')\,\frac{\partial P(z)}{\partial z}\right]\left[P(z') + (z - z')\,\frac{\partial P(z')}{\partial z'}\right]\right\}\right), \quad (3.4)$$

and

$$E_c = 4\pi\rho_e^2 \int_{z_{\min}}^{z_{\max}} dz \int_{z_{\min}}^{z_{\max}} dz'\, P(z)\, P(z')\{[P(z) + P(z')]^2 + (z - z')^2\}^{-1/2} \times \left\{[K(k) - 2D(k)]\left[P^2(z') + (2/3)P(z)\, P(z') - (4/3)P(z)\, P(z')/k^2 + (z - z')\, P(z')\,\frac{\partial P(z')}{\partial z'} + z'P(z)\,\frac{\partial P(z)}{\partial z}\right] + K(k)\left[P(z)\, P(z')/3 + z'P(z')\,\frac{\partial P(z)}{\partial z} + z'(z - z')\,\frac{\partial P(z')}{\partial z'}\,\frac{\partial P(z)}{\partial z}\right]\right\}. \quad (3.5)$$

Notice that Eq. (3.4) is invariant under the interchange of z and z', while Eqs. (3.1) and (3.5) are not. The integrands in Eqs. (3.1), (3.4), and (3.5) must be replaced by

the appropriate limit when $z \to z'$, since $k^2 \to 1$ and $K(k) \to \infty$. The integrands in this limit for the three equations are, respectively,

$$P^3(z) - zP^2(z)\frac{\partial P(z)}{\partial z}, \tag{3.6}$$

$$4P^3(z)/3, \tag{3.7}$$

$$\frac{P^3(z)}{3} + zP^2(z)\frac{\partial P(z)}{\partial z}. \tag{3.8}$$

Lawrence [9] derives the following three-dimensional integral for axially symmetric shapes.

$$E_c = 2\pi\rho_e^2 \int_{z_{\min}}^{z_{\max}} dz \int_{z_{\min}}^{z_{\max}} dz'\, P^2(z)\, P^2(z') \int_0^{\pi} d\Psi \times \left\{ \frac{\sin^2 \Psi}{[(z-z')^2]^{1/2} + [P^2(z) + P^2(z') + (z-z')^2 - 2P(z)\,P(z')\cos\Psi]^{1/2}} \right\}, \tag{3.9}$$

which has been used by Hasse [10] and others. There does not seem to be any simple way of relating Eqs. (3.1), (3.4), and (3.5) to Lawrence's expression (3.9). The former formulas are derived from surface integral expressions and therefore contain factors $\partial P(z)/\partial z$ and $\partial P(z')/\partial z'$ arising from the surface elements $\mathbf{dS}$ and $\mathbf{dS}'$, whereas Eq. (3.9) is obtained from the original volume integral, Eq. (2.3). Also, while the three surface-integral formulas have been reduced to two-dimensional integrals containing complete elliptic integrals, Lawrence's formula involves a three-dimensional integral with the angular integration not expressible in terms of complete elliptic integrals. With a reliable method for evaluating the elliptic integrals [14], Eqs. (3.1), (3.4), and (3.5) should be faster to calculate than Eq. (3.9), which involves an extra numerical integration.

For axially symmetric shapes, Eq. (2.29) reduces to

$$F_i^{(c)}(\mathbf{q}) = -\left\{ \int dz \int dz' \frac{\partial I(z, z'; \mathbf{q})}{\partial q_i} + \frac{\partial z_{\max}(\mathbf{q})}{\partial q_i} \int dz\, [I(z, z_{\max}; \mathbf{q}) + I(z_{\max}, z; \mathbf{q})] - \frac{\partial z_{\min}(\mathbf{q})}{\partial q_i} \int dz\, [I(z, z_{\min}; \mathbf{q}) + I(z_{\min}, z; \mathbf{q})] \right\}. \tag{3.10}$$

The function I contains complete elliptic integrals, if one is using the integrands of Eqs. (3.1), (3.4), or (3.5), or a single integral over Ψ if one uses that of Eq. (3.9).

The symmetry of I in z and z' for Eq. (3.4) makes Eq. (3.10) faster to evaluate in this case.

For axial symmetry, Eq. (2.30) implies [7]

$$F_i^{(c)}(\mathbf{q}) = -2\pi\rho_c \int dz\, V_c(z)\, P(z)\, \frac{\partial P(z)}{\partial q_i}. \tag{3.11}$$

This equation is quite efficient, since one evaluates $V_c(z)$ [3, 7] once when computing E_c, and only needs to do a single integral for each force component.

IV. Numerical Results

We have calculated the Coulomb energy and generalized forces for a variety of shapes by numerically evaluating the integrals in Eqs. (3.1), (3.4), (3.5), and (3.9)–(3.11) using Gaussian–Legendre quadrature formulas. The axially symmetric shapes considered are described by three smoothly joined quadratic surfaces of revolution [6, 7]. Because of discontinuities in high-order derivatives of $P(z)$ at the points where the surfaces join, the shapes are divided into four parts, (at these joining points and at the center), with the integration in each part being performed by means of a Gaussian quadrature formula of a given order N. (The total number of integration points on the body is thus $4N$). Both reflection-symmetric and asymmetric shapes have been considered.

The Coulomb energies of symmetric and asymmetric shapes have about the same accuracy for a given formula and value of N. The numerical comparisons we make here are for the liquid-drop-model saddle-point shape for fissility $x = 0.86$ [6, 7], a relatively compact reflection-symmetric shape. The observed errors increase by about a factor of 10 when one considers very distorted or elongated shapes such as those encountered in a fissioning nucleus or in a fusion of heavy ions.

Table I presents the time required to compute the Coulomb energy of the test shape on a CDC 6600 computer, and the accuracy relative to the result computed using Eq. (3.4) with $N = 64$, for Eqs. (3.1), (3.4), and (3.5). The error presented is in the quantity B_c, defined so that $E_c = E_c^{(0)} B_c$, where $E_c^{(0)}$ is the Coulomb energy of a sphere.

The elliptic integrals appearing in the integrands of the three formulas are evaluated to 13 significant figures using the method of Ref. [14]. This method approximates the elliptic integrals in about the same time as a Gaussian quadrature of order 8, which has an accuracy of roughly 7–8 significant figures. Landen's transformation, used in Ref. [2] to evaluate elliptic integrals, is much less efficient than the method used here. The preference of Hasse [10] and others for the triple integral formula of Lawrence [9] over the double integral of Eq. (3.1) [6, 7] may be due to this type of inefficient method of evaluating elliptic integrals.

TABLE I

Errors in Coulomb Energy B_c for the $x = 0.86$ liquid-drop-model saddle-point shape relative to the result using Eq. (3.4) with $N = 64$.

Equation	N	Error	Time (sec) Symmetric	Time (sec) Asymmetric
(3.1)				
	4	-5×10^{-5}	0.04	0.08
	8	-8×10^{-6}	0.16	0.31
	16	-1×10^{-6}	0.61	1.21
	32	-1×10^{-7}	2.42	4.84
	64	-2×10^{-8}	9.66	19.33
(3.4)				
	4	$+7 \times 10^{-7}$	0.03	0.05
	8	$+3 \times 10^{-8}$	0.12	0.20
	16	$+9 \times 10^{-10}$	0.46	0.76
	32	$+3 \times 10^{-11}$	1.82	3.02
	64	$\sim 1 \times 10^{-12}$	7.27	12.05
(3.5)				
	4	$+3 \times 10^{-4}$	0.04	0.08
	8	$+4 \times 10^{-5}$	0.16	0.32
	16	$+5 \times 10^{-6}$	0.62	1.24
	32	$+7 \times 10^{-7}$	2.47	4.94
	64	$+9 \times 10^{-8}$	9.85	19.70

Note. The times are the computation times in seconds needed to compute the energy for arbitrary symmetric and asymmetric shapes on a *CDC* 6600 computer. Results are presented for Eqs. (3.1), (3.4), and (3.5).

Table II shows the time required to compute B_c for the test body using Lawrence's formula, Eq. (3.9), and the errors involved. The quantity N' is the order of the Gaussian quadrature formula used to evaluate the Ψ integral in Eq. (3.9).

The most striking result shown in Tables I and II is that the Lawrence formula, which is derived from the volume integral [Eq. (2.3)] is much less accurate than any of the three surface-integral formulas. When using Eq. (3.9), we find that doubling the number of integration points N improves the convergence by about a factor of 4. (Doubling the number of slices in Beringer's formula [8] also decreases its relatively high error by about a factor of 4.) The angular integration in Eq. (3.9) has converged to the accuracy of the z integration for $N' = 8$. Of the three remaining formulas, Eq. (3.4) is the most rapidly converging, by far the most accurate for a given value of N, and, because of the symmetry of the integrand, also the fastest to

TABLE II

Errors in Coulomb Energy B_c for the $x = 0.86$ liquid-drop-model saddle-point shape calculated from Eq. (3.9).

			Time (sec)	
N	N'	Error	Symmetric	Asymmetric
4	4	$+7 \times 10^{-3}$	0.03	0.04
8	4	$+1 \times 10^{-3}$	0.10	0.16
16	4	-2×10^{-4}	0.38	0.63
32	4	-6×10^{-4}	1.50	2.48
8	8	$+2 \times 10^{-3}$	0.17	0.29
16	8	$+5 \times 10^{-4}$	0.68	1.13
32	8	$+1 \times 10^{-4}$	2.71	4.50
64	8	$+3 \times 10^{-5}$	10.8	18.0
16	16	$+5 \times 10^{-4}$	1.28	2.14
32	16	$+1 \times 10^{-4}$	5.12	8.55
64	16	$+3 \times 10^{-5}$	20.0	34.1
32	32	$+1 \times 10^{-4}$	9.96	16.6
64	32	$+3 \times 10^{-5}$	39.8	66.3

Note. The times are the computation times in seconds needed to compute the energy for arbitrary symmetric and asymmetric shapes on a CDC 6600 computer. The errors are relative to the result using Eq. (3.4) with $N = 64$.

compute. Using Eq. (3.4), one finds that the convergence improves by about a factor of 30 when doubling N, while it improves by about a factor of 8 when one uses Eqs. (3.1) and (3.5). We present in Fig. 1 some of the data of Tables I and II plotted as the error in B_c as a function of computing time.

We have not exhaustively studied the calculation of the Coulomb forces by all possible equations, but compare the results using Eq. (3.11) with those obtained from Eq. (3.10) with the integrand of Eq. (3.4) Table III shows the computational times and fractional errors involved in using the alternative formulas for the $x = 0.86$ saddle-point shape mentioned above. Since the absolute errors for each component $F_i^{(c)} = -\partial B_c/\partial q_i$ are found to be proportional to the value of that component, we show fractional errors $\Delta F_i^{(c)}/F_i^{(c)}$. The fractional errors are the same (within a fractor of 2) for all components with a given shape and value of N.

Because of the simpler integrands involved, the computation time required when Eq. (3.11) is used for a given value of N is about one-half to two-thirds what it is when Eqs. (3.10) and (3.4) are used, but the calculation is at least a factor of 20 less accurate for $N \geqslant 8$. We have also calculated the generalized forces using Lawrence's

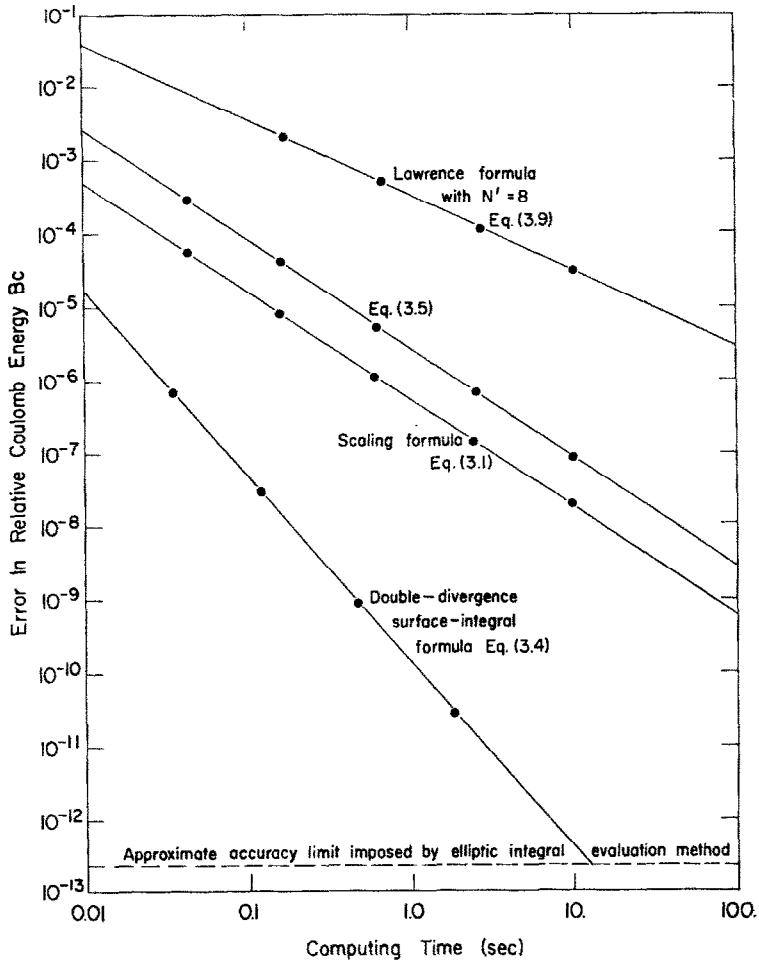

FIG. 1. The errors involved in computing the Coulomb energy for the reflection-symmetric test shape as a function of computing time on a CDC 6600 computer for the four formulas (3.1), (3.4), (3.5), and (3.9) with $N' = 8$. The points are the observed times; the lines are straight lines drawn approximately through the points. The accuracy limit indicated is for the particular elliptic integral evaluation technique used, which is also near the limit of machine accuracy for the CDC 6600 computer. Evaluation methods with greater or lesser accuracy are available.

TABLE III

Fractional Errors in the Coulomb Forces $\Delta F_i^{(c)}/F_i^{(c)}$ for the Same Test Shape as in Table I

Equation	N	Fractional error	Time (sec)	
			Symmetric	Asymmetric
(3.10) and (3.4)				
	4	$+2 \times 10^{-4}$	0.05	0.10
	8	$+1 \times 10^{-5}$	0.19	0.37
	16	$+6 \times 10^{-7}$	0.75	1.40
	32	$+2 \times 10^{-8}$	3.05	5.50
	64	$\sim 1 \times 10^{-9}$	14.0	26.0
(3.11)				
	4	$+1 + 10^{-3}$	0.03	0.05
	8	$+2 \times 10^{-4}$	0.13	0.20
	16	$+3 \times 10^{-5}$	0.51	0.75
	32	$+4 \times 10^{-6}$	2.00	2.90
	64	$+5 \times 10^{-7}$	8.00	11.0

Note. The times are the computation times for all the force components (three for symmetric shapes, six for asymmetric shapes), and the results are shown for Eqs. (3.10) and (3.4) compared to Eq. (3.11).

method [Eqs. (3.9) and (3.10)], and find the same relatively poor accuracy seen in the energy calculation using Eq. (3.9).

In our numerical calculations of Coulomb energies and derivatives, we find that Eq. (3.4) gives the most accurate method of calculating Coulomb energies in a given time, and in conjunction with Eq. (3.10) gives the most efficient method (of those considered) for computing generalized forces. The Lawrence method of calculating energy and forces, which has frequently been used in the past [10] is very inefficient by comparison. As remarked in Section II, it is clear that the symmetric formula Eq. (2.24) will be *faster* than Eqs. (2.25) and (2.26) for bodies of arbitrary shape. Our present results for axially symmetric shapes suggest that the symmetric formula would also be more *accurate*. However, since we have not actually performed calculations for more general shapes, we can only conclude that the symmetric formula is always faster, but not necessarily more accurate.

ACKNOWLEDGMENT

It is a pleasure to thank J. R. Nix for several stimulating conversations, and also for reading the original draft of this manuscript and for making a number of constructive suggestions.

REFERENCES

1. J. R. NIX, *Ann. Rev. Nucl. Sci.* **22** (1972), 65.
2. S. FRANKEL AND N. METROPOLIS, *Phys. Rev.* **72** (1947), 914.
3. D. L. HILL AND J. A. WHEELER, *Phys. Rev.* **89** (1953), 1102.
4. J. R. NIX AND W. J. SWIATECKI, *Nucl. Phys.* **71** (1965), 1; J. R. NIX, Ph.D. Thesis, University of California Report UCRL-11338, April 1, 1964.
5. S. COHEN AND W. J. SWIATECKI, *Ann. Phys.* **22** (1963), 406.
6. J. R. NIX, *Nucl. Phys.* **A130** (1969), 241.
7. J. R. NIX, University of California Report UCRL-17958, July 1, 1968.
8. R. BERINGER, *Phys. Rev.* **131** (1963), 1402.
9. J. N. P. LAWRENCE, *Phys. Rev.* **139** (1965), B1227; J. N. P. LAWRENCE, Ph.D. Thesis, Los Alamos Scientific Laboratory Report LA-3774, August 1967.
10. R. W. HASSE, *Nucl. Phys.* **A118** (1968), 577.
11. H. J. KRAPPE AND J. R. NIX, in Proceedings of the Third IAEA Symposium on the Physics and Chemistry of Fission" (Rochester, New York, August 13–17, 1973), Paper IAEA-SM-174/12, p. 159.
12. S. E. LARSSON AND G. LEANDER, in "Proceedings of the Third IAEA Symposium on the Physics and Chemistry of Fission" (Rochester, New York, August 13–17, 1973), Paper IAEA-SM-174/6, p. 177; G. LEANDER, *Nucl. Phys.* **A219** (1974), 245.
13. M. BOLSTERLI, E. O. FISET, J. R. NIX, AND J. L. NORTON, *Phys. Rev.* **C 5** (1972), 1050.
14. W. J. CODY, *Math. Comp.* **19** (1965), 105.