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THE LIQUID-DROP MODEL OF FISSION: EQUILIBRIUM CONFIGURATIONS AND ENERGETICS OF UNIFORM ROTATING CHARGED DROPS

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ABSTRACT

The problem of finding the equilibrium configurations of uniform rotating charged liquid drops is considered. An analytic treatment is given based on a parametric expansion for small ellipsoidal distortions about a sphere. This treatment is applied to finding the ground-state configurations and the saddle-shaped configurations leading to fission as functions of charge and angular momentum of the drop. A variation-iteration method for generating the configurations of equilibrium is described. The method is applied to finding the configurations of equilibrium of axially symmetric drops over the range $0 \leq x \leq 1$ and $0 \leq y \leq 0.5$, where x is the ratio of the coulomb energy to twice the surface energy for a sphere, and y is the ratio of the rotational energy to the surface energy for a sphere. The energetics of these configurations are calculated; the fission thresholds are calculated in the range of applicability of the parametric expansions.

I. INTRODUCTION

The introduction of heavy-ion accelerators in nuclear research makes possible exploration of nuclear reaction phenomena in which very large orbital angular momenta are involved. The neon beams available from the Berkeley and Yale heavy-ion accelerators are capable of inducing nuclear reactions on heavy nuclei in which orbital angular momenta in excess of 100 units of $\hbar$ are encountered. There is an increasing amount of experimental evidence to suggest that a large fraction of the total cross section is due to reactions in which the incident heavy ion fuses with the target nucleus to form a compound system. One would hope that the existence of such compound systems carrying large amounts of angular momenta would provide a means for studying the inertial properties and the stability of large rotating masses of nuclear matter.

An important mode of de-excitation of these compound systems is the fission process. For targets near the upper end of the periodic table, the fission mode overwhelms all other de-excitation mechanisms; for lower-Z targets, neutron emission becomes competitive, but fission induced by heavy-ion bombardment has been observed with targets as low as Ho_{67}^{165}.[1] One might suspect that existence of rotational forces in the compound system would significantly affect the fissionability of the system. These rotational forces should become particularly important for low-mass targets where the centrifugal forces may become large enough to prevent the formation of the compound system. Flerov and collaborators have shown that in the bombardment of gold by nitrogen ions the fissionability of the compound system is strongly enhanced relative to neutron emission as the energy of the incident ion and hence the orbital angular momentum of the compound system is increased.[2,3]

In this paper we shall consider the energetics and forms of equilibrium of uniform rotating charged liquid drops as a starting point for a liquid-drop model study of the effects of rotation on fission. Specifically, we shall be concerned here with finding the lowest-energy stable configurations of a rotating charged drop subject to a surface tension, and the lowest-energy saddle-shape configurations leading to the fission of the system. The energy difference between these two configurations is defined as the fission barrier. We should emphasize that a complete study of the configurations of equilibrium would involve discussion of the configurations of higher energy and the various linear series of these shapes and their points of bifurcation. Appel has outlined such a survey for the analogous problem of rotating gravitating masses.[4] The conventional liquid-drop model, containing a term in the coulomb energy and a term in the surface energy, is here extended to include in addition a rotational-energy term. In this work we are concerned with configurations of gyrostatic equilibrium, in which the drop, in its equilibrium configuration, is rotating as a rigid body.[5]

There are many articles in the literature on the problem of the configurations of equilibrium of rotating liquid masses as a consequence of the work on rotating gravitating liquid masses by Darwin, Jeans, Poincaré, Liapunoff and others.[6-12] More recently, Lyttleton has reconsidered these problems, primarily from the point of view of astrophysical interest.[13] Appel has discussed in addition the problem of a rotating mass subject to a surface tension, both with and without the gravitation term. The first to consider the problem of the configurations of equilibrium of a rotating charged liquid drop was Pik-Pichak, whose interest in the problem was also inspired by considerations of heavy-ion-induced fission.[14]

In the next section we shall follow this earlier work of Pik-Pichak and consider small ellipsoidal distortions about the spherical shape. We shall derive expressions for the distortion parameters which determine the shapes of the ground states and saddle shapes in the limit where these shapes deviate only slightly from spherical configurations. Also, we shall derive expressions for the energy barrier against fission.

In the succeeding section we shall describe a variation-iteration method for generating configurations of equilibrium as a step toward the general solution of the problem of finding the configurations of equilibrium of uniform rotating charged liquid drops. This method is applied to the axially symmetric configurations covering the entire range of charge states of interest and covering a wide range of rotational states. These equilibrium shapes and their energetics are illustrated in the enclosed graphs and tables.

II. QUANTITATIVE DISCUSSION

A. Kinematics

To illustrate the orders of magnitude of the orbital angular momenta and rotational energies the compound nucleus can assume, we shall begin the discussion with a few elementary kinematic considerations. For a quantitative estimate of the maximum angular momentum of the compound system we shall assume the incident heavy ion follows a trajectory which gives it a glancing contact with the target nucleus. There is considerable uncertainty however, regarding the shape of the incident projectile and of the target nucleus immediately prior to the collision. In addition, if we have estimated a value for the angular momentum of the system, the rotational energy of the compound system is not determined until a moment of inertia and hence a shape for the compound system is also specified. The solution of these problems would require a detailed dynamical study of the collision process and subsequent motions of the compound system, a study which is beyond the scope of this paper. For the purposes of these estimates we shall disregard these dynamical processes and take the projectile, target, and compound system to have spherical symmetry.

Let eZ_1, eZ_2, and A_1, A_2 be the charges and mass numbers of the incident ion and target nucleus, respectively. Assuming the two nuclei to be spherical at time of contact, their respective radii are $R_1 = r_0 A_1^{1/3}$, and $R_2 = r_0 A_2^{1/3}$. If $E_{c.m.} = \left[A_2/(A_1+A_2)\right] E_{lab}$, and $\mu = m A_1 A_2/(A_1+A_2)$ are the energy in the center of mass and reduced mass, respectively, the orbital angular momentum contained in the system is

$$L = R\left[2\mu\left(E_{c.m.} - \frac{e^2 Z_1 Z_2}{R}\right)\right]^{1/2} \qquad \text{(II.1)}$$

where $R = r_0 (A_1^{1/3} + A_2^{1/3})$. As an illustration of the values L can assume, consider the bombardment of U^{238} with C^{12}, Ne^{22}, and A^{40}, respectively. If we use $E_{lab} = 10$ Mev/nucleon and $r_0 = 1.2 \times 10^{-13}$ cm, and set $\ell \simeq \frac{L}{\hbar}$, Eq. (II.1) yields ℓ values of 48, 99, and 158, respectively; if we choose $r_0 = 1.5 \times 10^{-13}$ cm, we have $\ell = 71$, 133, and 238.

For an estimate of the upper limit of rotational energy carried by the compound system, assume the compound system to be carrying an amount of orbital angular momentum given by Eq. (II.1). Such an estimate of the rotational energy for the ground-state configuration must be an overestimate since as we shall see in later paragraphs the lowest configuration of equilibrium will have an approximately oblate shape; i.e. a higher moment of inertia.

Pik-Pichak has defined the parameter

$$y = \frac{\text{Rotational energy of spherical drop}}{\text{Surface energy of spherical drop}} = \frac{L^2}{2I_C} / 4\pi R_C^2 \sigma_0 ,$$

where I_C and R_C are the moment of inertia and radius of the compound system, and σ_0 is the surface energy parameter. It is easily shown that y has the value

$$y = \frac{5}{2} \frac{A_1 \left[1 + \left(\frac{A_1}{A_2}\right)^{1/3}\right]^2}{A_2^{5/3} \left[1 + \left(\frac{A_1}{A_2}\right)\right]^{10/3}} \left(E_{c.m.} - \frac{e^2 Z_1 Z_2}{R_C} \right) \frac{1}{4\pi r_0^2 \sigma_0} . \qquad \text{(II.2)}$$

In Fig. 1 this function is plotted against A_2 for several values of A_1. The values for Z_2 have been chosen to correspond to values lying close to the line of stability of the periodic table. For these calculations we have taken $4\pi r_0^2 \sigma_0 = 17.81$ Mev and $r_0 = 1.5 \times 10^{-13}$ cm.

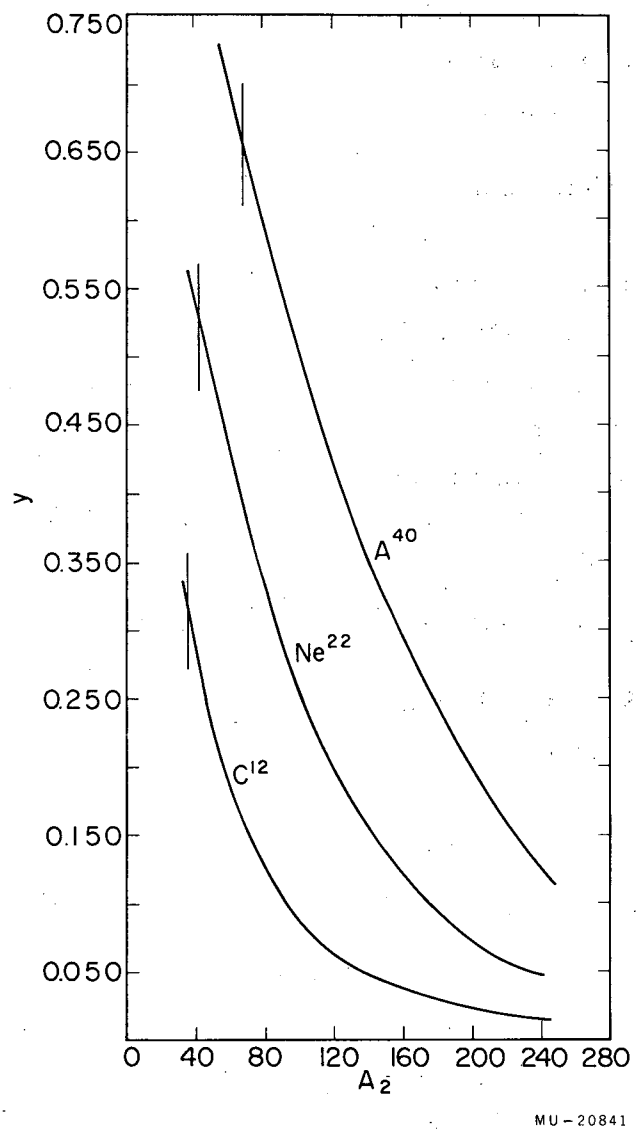

Fig. 1. Values for the rotational parameter, $y = E_R^{(0)}/E_s^{(0)}$, for a spherical compound nucleus formed by a glancing collision of either C^{12}, Ne^{22}, or A^{40} with targets of mass number A_2.

Below a certain value of A_2 this curve will actually exceed the upper limit of energy available in the center of mass.[15] For the ratio of rotational energy to center-of-mass energy one finds (again for idealized spherical nuclei)

$$\omega = \frac{E_{rot}}{E_{c.m.}} = \frac{5}{2} \frac{A_1 A_2}{(A_1 + A_2)^2} \left(1 - \frac{e^2 Z_1 Z_2}{E_{c.m.} R_C}\right) \frac{(A_1^{1/3} + A_2^{1/3})^2}{(A_1 + A_2)^{2/3}} .$$

In Fig. 1 the point at which ω is equal to one is indicated by the short vertical lines. We emphasize again that because of the simplification of assumed spherical symmetry this value of A_2 may have no particular significance. Indeed, in the spirit of the approximations at hand one would expect the condition $\omega = 1$ to occur at a lower value of A_2 than calculated here due to the oblateness of the ground state.

B. Analytical Calculations for Equilibrium Configurations

1. Parametrization

In this section we shall consider the shapes of equilibrium and energetics of a uniform rotating charged liquid drop. In a first approximation to this problem we proceed in the conventional way and describe the shape of the drop with a radius vector whose angular dependence is introduced parametrically.[16-24] In most treatments of the liquid-drop model the different configurations of the drop which are to be studied are limited to axial symmetry. However, with the introduction of rotation into the problem, intuitive considerations suggest that configurations that are not axially symmetric will also be of considerable importance. After the fission of a rapidly rotating liquid drop, one would expect the fragments to separate from each other in a plane which is oriented approximately at right angles to the angular-momentum axis of the compound system. One would not expect therefore that the saddle-shaped configuration that leads to fission would be axially symmetric about the angular-momentum axis.

For the nonrotating problem and in the limit that $1-x << 1$, the primary features of fission can be described by considering only an $\alpha_{20} P_{20}(\cos\theta)$ distortion. This suggests that in the same limit but with rotation we consider an equation for the surface of the drop which has the form

$$R = \frac{R_0}{\lambda} \left[1 + \alpha_{20} P_{20}(\cos\theta) + \alpha_{22} P_{22}(\cos\theta) \cos 2\phi \right], \tag{II.3}$$

with

$$P_{20} = \frac{1}{2} (3\mu^2 - 1)$$

and

$$P_{22} = 3(1 - \mu^2).$$

The z axis, $\theta = 0$, will be taken as the axis of rotation. Equation (II.3) describes a drop with an approximately ellipsoidal shape, i.e. with three unequal axes, and with the principal axes of the ellipsoid oriented along the coordinate axis. A term in $a_{21} P_{21} (\cos \theta) \cos \phi$ which might also have been included has been suppressed since such a term, for small a_{21}, has the effect only of tipping the ellipsoid with respect to the principal axes. Here we are concerned with the configurations of equilibrium which have minimum energy. The surface and coulomb energies are independent of the orientation of a particular shape, but the rotational energy of the lowest ellipsoidal saddle-shaped configuration will be a minimum when the principal axes are oriented along the coordinate axes.

For the calculation of saddle-shaped configurations and energetics, we shall require terms up to third order in a_{20}, a_{22}. The normalization factor λ in Eq. (II.3) is determined from the condition

$$\frac{4}{3} \pi R_0^3 = \int_0^{2\pi} \int_{-1}^{+1} \int_0^{R} r^2 \, dr \, d\mu d\phi, \tag{II.4a}$$

and has the value

$$\lambda^3 = 1 + \frac{3}{5} a_{20}^2 + \frac{36}{5} a_{22}^2 + \frac{2}{35} a_{20}^3 - \frac{72}{35} a_{20} a_{22}^2 . \tag{II.4b}$$

The moment of inertia is given by

$$I_C = \int_0^{2\pi} \int_{-1}^{+1} \int_0^{R} \rho_m r^4 (1 - \mu^2) \, dr \, d\mu \, d\phi$$

$$= \frac{8\pi}{15} \rho_m R_0^5 \left(1 - a_{20} + \frac{3}{7} a_{20} + \frac{3}{7} a_{20}^2 + \frac{132}{7} a_{22}^2\right) \tag{II.5}$$

The rotational energy, measured in units of the surface energy of a sphere, is then

$$E_R = \frac{L^2}{2I_C} / 4\pi R_0^2 \sigma_0 = y\left(1 + \alpha_{20} + \frac{4}{7}\alpha_{20}^2 - \frac{132}{7}\alpha_{22}^2\right). \tag{II.6}$$

The rotational energy is given only up to terms of order α_{20}^2, α_{22}^2, since the factor y is already a first-order quantity. In Appendix A the surface energy, coulomb potential, and coulomb energy are evaluated. The surface energy, measured in units of the surface energy of a sphere, is given by the integral

$$E_S = \frac{1}{4\pi R_0^2} \int_0^{2\pi} \int_{-1}^{+1} R\left[\frac{1}{1-\mu^2}\left(\frac{\partial R}{\partial \phi}\right)^2 + R^2 + (1-\mu^2)\left(\frac{\partial R}{\partial \mu}\right)^2\right]^{1/2} d\mu d\phi \tag{II.7a}$$

and has the value

$$E_S = \left(1 + \frac{2}{5}\alpha_{20}^2 + \frac{24}{5}\alpha_{22}^2 - \frac{4}{105}\alpha_{20}^3 + \frac{48}{35}\alpha_{20}\alpha_{22}^2\right). \tag{II.7b}$$

The coulomb energy

$$E_C = \frac{1}{8\pi R_0^2 \sigma_0} \int_0^{2\pi} \int_{-1}^{+1} \int_0^R \rho r^2 \, dr \, d\mu d\phi \int_0^{2\pi} \int_{-1}^{+1} \int_0^R \frac{\rho}{|\vec{r} - \vec{r}'|} r'^2 dr' \, d\mu' d\phi' \tag{II.8a}$$

becomes

$$E_C = \frac{3}{5}\frac{Q^2}{R_0}\frac{1}{4\pi R_0^2 \sigma_0}\left(1 - \frac{1}{5}\alpha_{20}^2 - \frac{12}{5}\alpha_{22}^2 - \frac{4}{105}\alpha_{20}^3 + \frac{48}{35}\alpha_{20}\alpha_{22}^2\right). \tag{II.8b}$$

Expressed in units of the fission parameter $x = E_C^{(0)}/2E_S^{(0)}$ Eq. (II.8b) becomes

$$E_C = 2x\left(1 - \frac{1}{5}\alpha_{20}^2 - \frac{12}{5}\alpha_{22}^2 - \frac{4}{105}\alpha_{20}^3 + \frac{48}{35}\alpha_{20}\alpha_{22}^2\right). \tag{II.8c}$$

The total energy, to third order, of the rotating liquid drop is then

$$E = 1 + 2x + \frac{2}{5}\,a_{20}^{\,2}(1 - x) + \frac{24}{5}\,a_{22}^{\,2}(1 - x) - \frac{4}{35}\,a_{20}^{\,3} + \frac{144}{35}\,a_{20}a_{22}^{\,2}$$

$$+ y\left(1 + a_{20} + \frac{4}{7}\,a_{20}^{\,2} - \frac{132}{7}\,a_{22}^{\,2}\right). \qquad \text{(II.9)}$$

Comparing our result in Eq. (II.9) with a similar result given by Pik-Pichak, we see that there is a consistent factor-of-six difference in the $a_{22}^{\,2}$ terms. Pik-Pichak has chosen to define the a_{22} in conjunction with the $D(\alpha, \beta, 0)$ functions[25] rather than with the P_{22} polynomial as is done here. His equivalent to our Eq. (II.3) is written

$$R = \frac{R_0}{\lambda}\left[1 + a_{20}D_{20} + a_{22}\,D_{22} + a_{2,-2}D_{2,-2}\right]$$

$$R = \frac{R_0}{\lambda}\left[1 + a_{20}\,P_{20} + \frac{1}{\sqrt{6}}\,a_{22}P_{22}\cos 2\phi\right]$$

with $a_{2,-2} = a_{2,2}$. Because of the different normalization of the D's, his a_{22} differs by a factor of $\sqrt{6}$ from the choice of a_{22} used in this paper.

Those distorted shapes that are equilibrium configurations are determined by the conditions

$$\frac{\partial E}{\partial a_{20}} = 0\,,$$

and

$$\frac{\partial E}{\partial a_{22}} = 0\,, \qquad \text{(II.10)}$$

with yield the two equations

$$\frac{4}{5}\,a_{20}\,z - \frac{12}{35}\,a_{20}^{\,2} + \frac{144}{35}\,a_{22}^{\,2} + y\left(1 + \frac{8}{7}\,a_{20}\right) = 0\,, \qquad \text{(II.11a)}$$

and

$$\frac{48}{5}\, a_{22}\, z + \frac{288}{35}\, a_{20}\, a_{22} - \frac{264}{7}\, a_{22}\, y = 0 . \qquad \text{(II.11b)}$$

Here we have set $z = 1 - x$. With $a_{22} = 0$ the first of these equations gives an axially symmetric equilibrium configuration; the value of the distortion parameter is given by

$$a_{20} = \frac{7}{6}\, z + \frac{5}{3}\, y \mp \left[\left(\frac{7}{6}\, z + \frac{5}{3}\, y \right)^2 + \frac{35}{12}\, y \right]^{1/2} . \qquad \text{(II.12a)}$$

The negative sign corresponds to an oblate spheroid, the positive sign gives a prolate spheroid. The prolate spheroid is a saddle-shaped, leading to fission along the angular-momentum axis. This saddle has a higher energy than one discussed in succeeding paragraphs and is therefore not of interest here. Expanding the radical in Eq. (II.12a), we have

$$a_{20} = -\frac{5}{4}\, y/z \qquad \text{(II.12b)}$$

For $a_{22} \neq 0$, the Eq. (II.11b) gives

$$a_{20} = \frac{15}{12}\, y - \frac{7}{6}\, z .$$

Inserting this value for a_{20} in Eq. (II.11a), we have

$$a_{22}^{\,2} = \frac{1}{4} \left(\frac{7}{6}\right)^2 \left(z^2 - \frac{5}{7} y\right) - \frac{35}{24}\, yz - \frac{275}{576}\, y^2 . \qquad \text{(II.13a)}$$

Corresponding to this nonzero value for a_{22}, we have for a_{20},

$$a_{20} = \frac{7}{6} z + \frac{5}{3}\, y - \left[\left(\frac{7}{6}\, z + \frac{5}{3} y \right)^2 + \frac{35}{12}\, y + 12\, a_{22}^{\,2} \right]^{1/2} . \qquad \text{(II.13b)}$$

Equations (II.13a) and (II.13b) represent an ellipsoidal equilibrium configuration which is the lowest-energy saddle shape the drop can assume. Equation (II.12) is the lowest-energy stable configuration of the drop; as y goes to 0, a_{20} goes to 0, and this axially symmetric ground state tends to a sphere.

One would suspect that for a fixed value of x, increasing the rotational energy of the drop would ultimately lead to an instability of the axially symmetric ground-state configuration. Stated in another way, one expects that as the rotation increases, the saddle-shaped configuration tends toward the ground-state configuration, and for that value of rotational energy at which these two configurations coalesce the drop has neutral stability. This is expressed by setting

$$\frac{\partial^2 E}{\partial a_{22}^2} = \frac{48}{5} z + \frac{288}{35} a_{20} - \frac{264}{7} y = 0 ,$$

and combining this result with Eq. (II.12) to give the critical relation between y and z. This critical value for y for which the drop has neutral stability is then

$$y = \frac{2}{7}(1 + 6z) - \left[\left(\frac{2}{7}\right)^2 (1 + 6z)^2 - \frac{4}{5} z^2 \right]^{1/2} . \qquad \text{(II.14a)}$$

Expanding the radical and retaining the first few terms gives

$$y = \frac{7}{5} z^2 (1 - 6z) , \qquad \text{(II.14b)}$$

in agreement with the result of Pik-Pichak.

For y less than this critical value, there is an energy barrier against fission. The fission threshold is defined as the energy difference between the saddle configuration given by Eq. (II.13) and the ground-state configuration given by Eq. (II.12). If we insert the expression for a_{20} given in Eq. (II.12a) into Eq. (II.9a) and set $a_{22} = 0$, the energy of the ground-state stable configuration, E_g, is then

$$E_g = 1 + 2x + y + \frac{7}{6} yz + \frac{49}{135} z^3 - \left(\frac{2}{3} y + \frac{14}{45} z^2 \right) \left[\left(\frac{7}{6} z\right)^2 + \frac{35}{12} y \right]^{1/2} , \qquad \text{(II.15)}$$

where we have retained terms up to order z^3. The energy at the saddle is given by inserting Eq. (II.13) in the energy expression. One finds

$$E_S = 1 + 2x + y + \frac{98}{135} z^3 - \frac{7}{6} zy. \qquad \text{(II.16)}$$

The fission barrier, E_B, is the difference of Eqs. (II.16) and (II.15), and has the value

$$E_B = \frac{49}{135} z^3 - \frac{7}{3} zy + \left(\frac{2}{3} y + \frac{14}{45} z^2\right) \left[\left(\frac{7}{6} z\right)^2 + \frac{35}{12} y\right]^{1/2} . \qquad \text{(II.17)}$$

Our expression for the barrier differs from that of Pik-Pichak who has given an expression for the energy difference between the saddle shape and the spherical shape. Figure 2 is a plot of E_B *vs* y for several values of z. Note that Pik-Pichak's equivalent of Fig. 2 gives a negative value for E_B at large y as a consequence of his expression for the threshold.

In Fig. 3 is illustrated the configuration of stable equilibrium and the saddle-shaped configuration for the values $y = 0.01$ and $x = 0.85$. These shapes have been determined by using Eqs. (II.12) and (II.13).

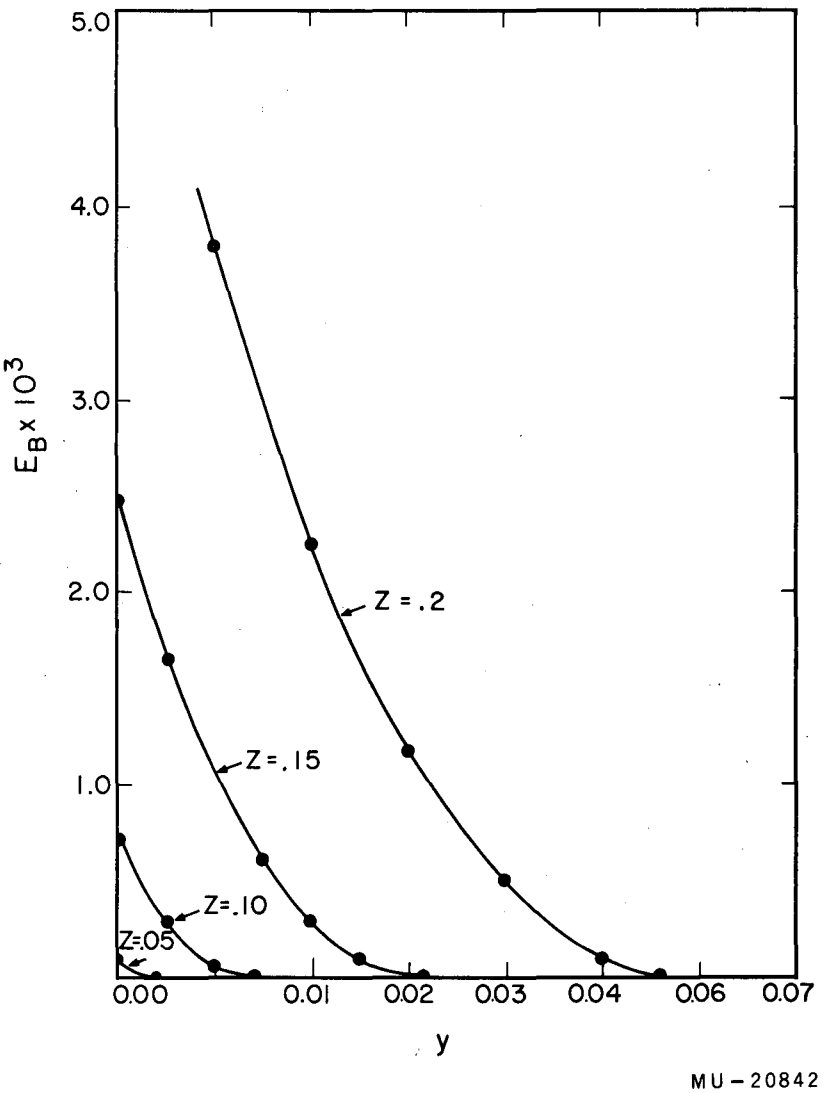

Fig. 2. Fission barriers E_B, versus $y = E_R^{(0)}/E_s^{(0)}$, for several values of the parameter $z = 1-x$. These curves are calculated by using Eq. (II. 17).

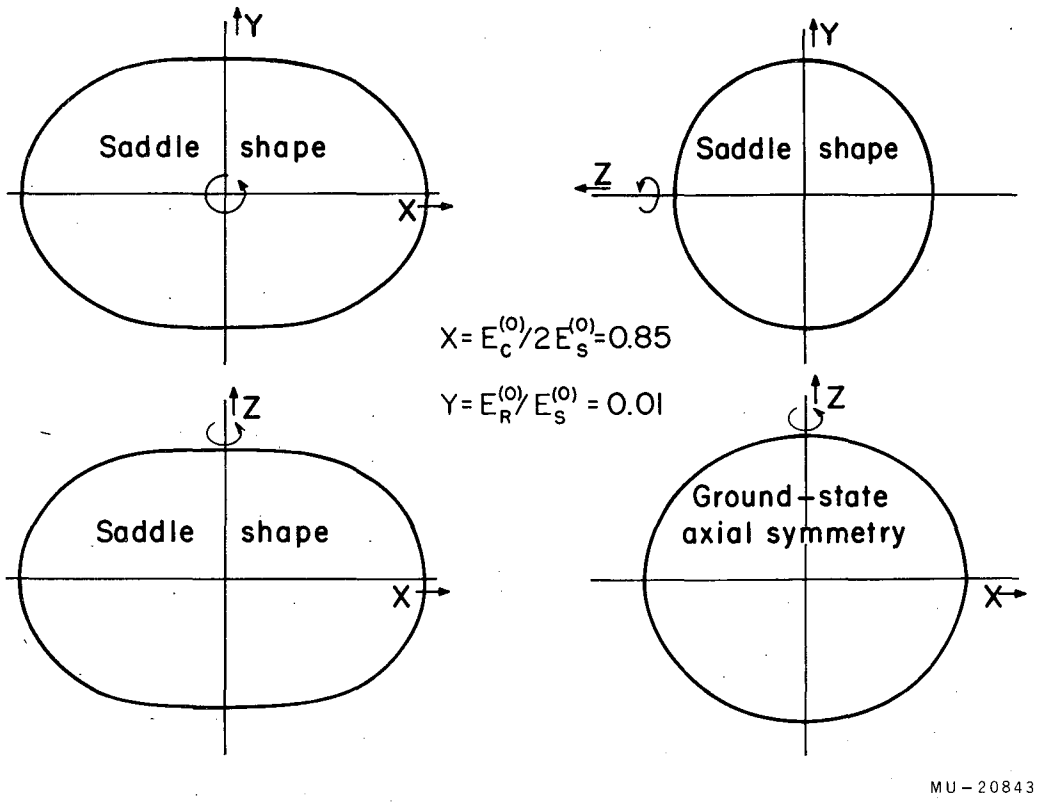

Fig. 3. The axially symmetric ground state and nonaxially symmetric saddle-shape configurations at x = 0.85 and y = 0.01. These shapes have been calculated by using Eqs. (II. 12a), (II. 13a), and (II. 13b).

2. A Variation-Iteration Method

A systematic study of the configurations of equilibrium of rotating charged liquid drops requires a means for calculating the energetics of such drops over the range $0 \leq x \leq 1$, and for y values ranging from zero up to that value for which the drop has only neutral stability. In principle, the parametric method used in the previous section could be extended to handle the more general problem simply by introducing a sufficient number of $a_{\ell m}$'s, and working with expansions of sufficiently high order. This approach has been adopted in many studies of the conventional axially symmetric liquid-drop problem in which the effects of rotation are not included. Such a procedure here would involve considerably more labor, since many important features of the problem including rotation require the inclusion of nonaxially-symmetric distortions. One recognizes that the parametric method could be facilitated for certain ranges of values of x and y by using a parametric expression in a more suitable coordinate system, as for example in spheroidal or ellipsoidal coordinates. Several authors have employed prolate spheroidal expansions intreating the axially symmetric problem.[16, 24] An expansion in ellipsoidal coordinates has been introduced by Poincaré to treat the stable configurations of rotating gravitating liquid masses. At the present state of our understanding of the current problem, however, we can suspect that such parametric expansions will each have its own limited scope of practical application.

In this section we shall develop a method for treating equilibrium configurations which is independent of parametrization. The starting point for this method is a variational condition, relating the coulomb surface potential, surface curvature, and a rotational term, such that the sum of these terms at any point on the surface has the same value if the surface is to be a surface of equilibrium. This variational principle has already been employed in the liquid-drop problem by Swiatecki as

a starting point for a parametric study in prolate spheroidal coordinates.[23, 24] If the surface in question is not an equilibrium configuration, the sum of terms will vary from point to point on the surface. This deviation of the sum from a constant value is treated as a trial function which is added to the radius vector to generate a new surface and hence a new trial function. These two trial functions are in turn used as a basis for extrapolating to a third trial function chosen in such a way as minimize the mean square deviations of the sum over the surface. Successive applications of this procedure are used to reduce the mean square deviation to an arbitrary minimum. Once this minimum has been reached, the equilibrium configuration has been determined and its energetics are then computed.

The variational condition is determined by considering the most general normal displacement, $\vec{\delta n}$, of the surface of the drop subject to the condition that the volume of the drop be conserved during this normal displacement. If the drop is initially in a configuration of equilibrium under the combined action of surface tension, coulomb forces, and rotational forces, we know, from the principle of virtual work, that the first-order changes in the total energy of the system must be zero. This is expressed by writing

$$\delta E = \delta E_C + \delta E_S + \delta E_R = 0 , \tag{II.17a}$$

with

$$\delta V = \int_{\text{surface}} \vec{\delta n} \cdot \vec{dA} = 0$$

as the statement of conservation of volume. If V'_s is the surface coulomb potential and κ' the total curvature of the surface, then to first order we have

$$\delta E_C = \int_{\text{surface}} \rho V'_S \, \vec{\delta n} \cdot \vec{dA},$$

$$\delta E_S = 0 \int_{\text{surface}} \kappa' \, \vec{\delta n} \cdot \vec{dA},$$

and

$$\delta E_R = \delta\left(\frac{L^2}{2I}\right) = -\frac{L^2}{2I^2}\,\delta I = -\frac{L^2\rho_m}{2I^2}\int_{\text{surface}} r'_S{}^2\,\vec{\delta n}\cdot\vec{dA},$$

where $r'_S{}^2$ is the square of the distance from the angular momentum axis to a point on the surface. Combining these expressions, we have, at equilibrium,

$$\delta E = \int_{\text{surface}}\left[\rho V'_S + 0\,\kappa' - \frac{L^2\rho_m}{2I^2}\,r'_S{}^2\right]\vec{\delta n}\cdot\vec{dA} = 0\,. \tag{II.17b}$$

If we choose the quantity in the brackets to be a constant, Γ', the constancy-of-volume condition insures that Eq. (II.17) is satisfied, since

$$\delta E = \int_{\text{surface}} \Gamma'\,\vec{\delta n}\cdot\vec{dA} = \Gamma'\,\delta V = 0.$$

Therefore, the condition that a certain configuration be a configuration of equilibrium can be stated as

$$\rho V'_S + 0\,\kappa' - \frac{L^2\rho_m}{2I^2}\,r'_S{}^2 = \Gamma'. \tag{II.18a}$$

Written in terms of x and y, Eq. (II.18a) becomes

$$5x\,V_S + \kappa - y\,r_S{}^2 = \Gamma\,. \tag{II.18b}$$

Here V_S, κ, $r_S{}^2$ are expressed in units of their values for a sphere of unit radius and unit charge. Specifically, for a sphere we have $V_S = \frac{4}{3}\pi$ and $\quad = 2$, and $r_S{}^2$ varies in magnitude from zero to one.

We are now prepared to describe the iterative procedure for generating configurations of equilibrium of the drop for various values of the two parameters x and y. The equation for the surface of the drop can be described in terms of two variables; for this work it was found useful to work with a spherical-coordinate system and to describe the surface in terms of the two spherical coordinates, θ and ϕ.

Having chosen values for x and y, we specify an equation for an initial surface

$$(a)\quad R = R'_0\,(\theta, \phi),$$

and the volume of this configuration is normalized to the volume of a sphere of unit radius,

$$(b)\quad R = R_0\,(\theta, \phi).$$

With this equation for the surface, the Eq. (II.18b) is calculated at every point on the surface:

$$(c)\quad 5x\,V_S + \kappa - y\,r_S^2 = \Gamma_0\,(\theta, \phi)\,.$$

Here we have written Γ as a function of θ and ϕ since in general our initial surface will not be a surface of equilibrium.

The average value of $\Gamma_0\,(\theta, \phi)$ is calculated from

$$(d)\quad \overline{\Gamma} \int_{\text{surface}} \Gamma_0\,(\theta, \phi)\,dA \Big/ \int_{\text{surface}} dA\,.$$

We then calculate the difference of $\Gamma_0\,(\theta, \phi)$ from the average value at each point on the surface:

$$(e)\quad \Delta\,\Gamma_0\,(\theta, \phi) = \Gamma_0\,(\theta, \phi) - \overline{\Gamma}\,.$$

The root-mean-square value of $\Delta\,\Gamma_0(\theta, \phi)$ over the surface is then calculated:

$$\text{(f)}\quad \sqrt{\overline{\Delta\Gamma_0}^2} = \left\{ \int_{\text{surface}} \left[\Delta\Gamma_0(\theta,\phi)\right]^2 dA \Big/ \int_{\text{surface}} dA \right\}^{1/2} .$$

The ratio $\sqrt{\overline{\Delta\Gamma_0}^2}/\overline{\Gamma}$ is chosen as the criterion for judging whether the shape is an equilibrium configuration. The ratio $\sqrt{\overline{\Delta\Gamma}^2}/\overline{\Gamma}$ is a measure of the fractional rate of change per unit displacement from equilibrium. Near a configuration of equilibrium the energy varies quadratically with distortion and consequently $\sqrt{\overline{\Delta\Gamma}^2}/\overline{\Gamma}$ is of order $\left|\frac{\delta n}{R}\right|$, the order of magnitude of the distortion. Examination of some of the numerical results confirmed this conclusion, e.g. $\left|\frac{\delta n}{R}\right| \simeq \frac{\sqrt{\overline{\Delta\Gamma}^2}}{\Gamma}$. It follows then that $\frac{\Delta E}{E} \sim \left(\sqrt{\overline{\Delta\Gamma}^2}/\overline{\Gamma}\right)^2$. Rigorously, the shape is not an equilibrium configuration unless this ratio is zero. In practice the shape is considered to be an equilibrium configuration provided this ratio is less than an arbitrarily chosen upper limit. If the ratio is less than this specified upper limit, the calculation is halted and the energetics of the drop are computed. Usually, however, the ratio is not sufficiently small at this point and the iterative procedure is continued.

In continuing the cycle we desire a means for varying the surface in such a way that our convergence criterion discussed in the previous paragraph can be made a minimum. To achieve this we use $\Delta\Gamma_0(\theta,\phi)$ as a trial function to be added to $R_0(\theta,\phi)$ to give the new surface. The contributions to $\Delta\Gamma(\theta,\phi)$ at any particular point on the surface are due to local variations in κ, the rotational term, and to a certain extent to local variations in V_s. To correct for this variation in Γ at the point in question we displace the surface along its normal an amount proportional to the magnitude of $\Delta\Gamma$ at that point. Such a procedure is primarily intuitive; its justification depends on the success of the convergence. Specifically, we write

$$\text{(g)}\quad R_1'(\theta,\phi) = R_0(\theta,\phi) + k_1 \Delta\Gamma_0(\theta,\phi)/\hat{r}\cdot\hat{n} ,$$

where k_1 is a suitably chosen constant, $\hat{r}$ is the unit vector along the radius vector from the origin to a point in question on the surface, and $\hat{n}$ is the unit vector along the normal to the surface at the point in question.

The volume of the shape given by operation (g) is normalized:

(h) $R = R_1 (\theta, \phi)$.

Operations (c) through (b) are repeated, yielding $\sqrt{\overline{\Delta\Gamma}_1^2}$. Using the values $\sqrt{\overline{\Delta\Gamma}_0^2}$ and $\sqrt{\overline{\Delta\Gamma}_1^2}$ and assuming that the relation between $\sqrt{\overline{\Delta\Gamma}^2}$ and k is linear, we extrapolate to determine a new k_2 chosen to give zero for $\sqrt{\overline{\Delta\Gamma}^2}$. One has

(i) $$k_2 = - k_1 \frac{\sqrt{\overline{\Delta\Gamma}_0^2}}{\sqrt{\overline{\Delta\Gamma}_1^2} - \sqrt{\overline{\Delta\Gamma}_0^2}} ,$$

which is used to give a new R_2 ,

(j) $$R_2^1 (\theta, \phi) = R_0 (\theta, \phi) + k_2 \frac{\Delta\Gamma_0 (\theta, \phi)}{\hat{r} \cdot \hat{n}} .$$

The operations are then returned to operation (b) and the cycle is repeated. When the convergence is satisfactory, as indicated by the value for $\sqrt{\overline{\Delta\Gamma}_0^2} / \overline{\Gamma}_0$, the cycle is halted and the energetics of the drop computed.

This iterative cycle has been coded for the IBM 704 using the FORTRAN symbolic coding system. The cycle has been coded to handle axially symmetric and nonaxially symmetric configurations with octant symmetry. To facilitate the convergence and to allow for greater accuracy in computing the energetics, we have left the mesh size in the numerical integration formula, $\Delta\theta = \Delta\phi = \frac{\pi}{2} \frac{1}{T}$, as an adjustable parameter by choosing different values for T. The details of these integrations and the expressions used for V_s, κ , and I are discussed in Appendix B.

III. DISCUSSION OF THE RESULTS

The iterative cycle described in the previous section has been applied to finding the configurations of equilibrium of axially symmetric drops for the range $0 \leq x \leq 1$, and $0 \leq y \leq 0.5$. These equilibrium configurations are plotted in Figs. 4 through 10. The energetics and moments of intertia for these solutions are tabulated in Table I.

In carrying out these calculations a compromise had to be made between the accuracy desired in the solutions, as determined by the mesh size, and the time available for computation. It was felt that in order for these results to beuseful in interpreting fission phenomena, the energetics should be more accurate than one part in a thousand. Most of these solutions were obtained with a mesh size $T = 6$. For this mesh the time required to complete a cycle was 72 sec, of which 20 sec was used for tape writing in recording the running result. These calculations were continued until the convergence criterion, $\sqrt{\Delta\Gamma^2}/\bar{\Gamma}$, was less than 10^{-3}. For most of the results listed in Table I the convergence criterion is appreciably less than 10^{-3}.

The iterative cycles were started in either one of two ways: for $y \leq 0.1$ the cycle was initiated by reading in an a_2P_2 distortion with $a_2 = -0.05$; for $y > 0.1$, the cycle was initiated by reading in the previous solution at the same x value. For $y < 0.1$, typical starting values of $\sqrt{\Delta\Gamma^2}/\bar{\Gamma}$ were about 0.025. The number of cycles required for convergence depended on the x value but typically were 10 to 15 cycles. The solutions for the largest values of y, those at $x = 0.6$, required 20 to 30 cycles. In most cases the iterations converged immediately, the largest fractional change occurring in $\sqrt{\Delta\Gamma^2}/\bar{\Gamma}$ during the first few cycles. In a few cases for large y values, the result diverged. Starting with the solution at $x = 0.6$, $y = 0.3$, the iterative procedure for $x = 0.6$, $y = 0.5$ would not converge, but did so for $x = 0.6$, $y = 0.4$. The result for $x = 0.6$, $y = 0.5$ would not converge starting with $x = 0.6$, $y = 0.4$; convergence for this case

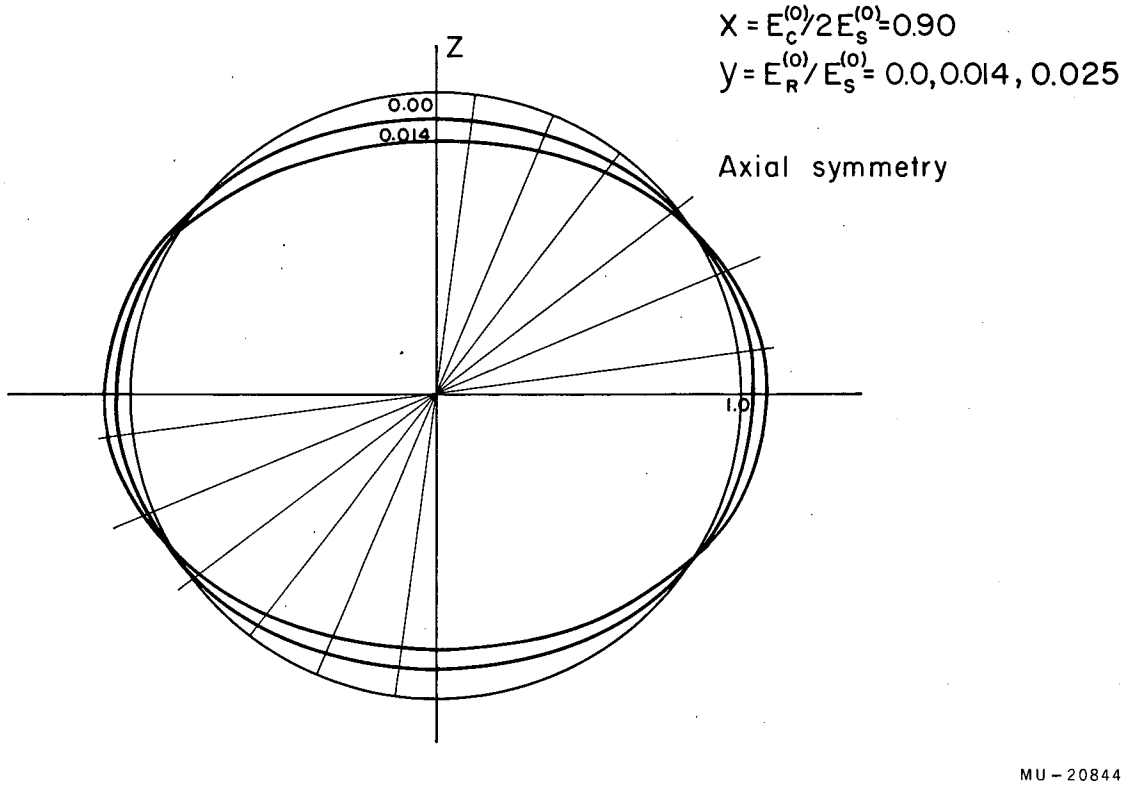

Fig. 4. The axially symmetric equilibrium configurations for x = 0.90 and for various values of y. These configurations and those illustrated in Figs. 5–10 have been calculated by using the variation-iteration method discussed in the text.

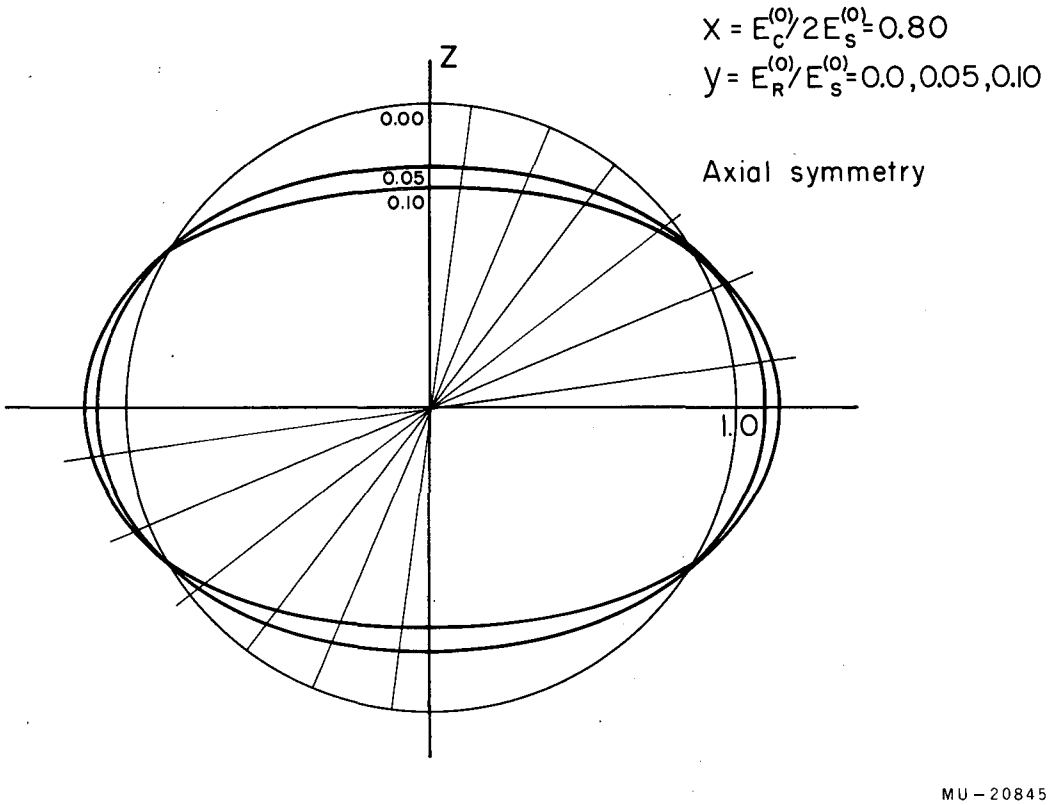

Fig. 5. Axially symmetric equilibrium configurations for x = 0.80 and for various values of the rotation parameter y.

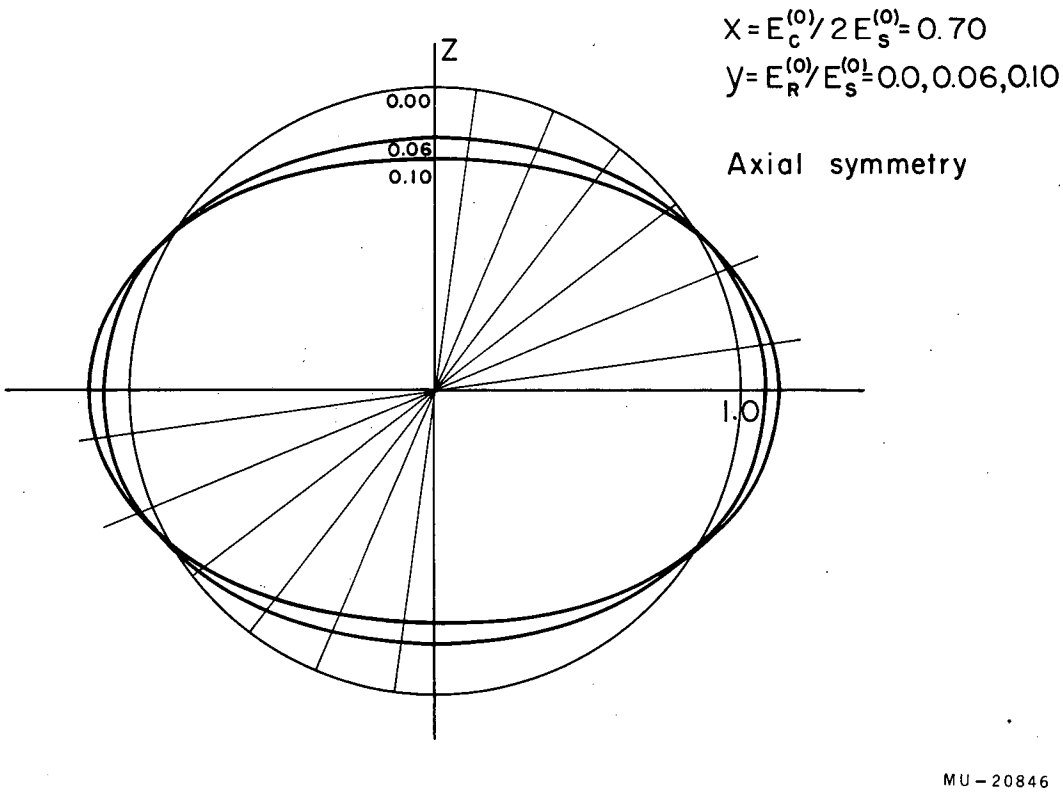

Fig. 6. Axially symmetric equilibrium configurations for x = 0.70 and for various values of the rotation parameter y.

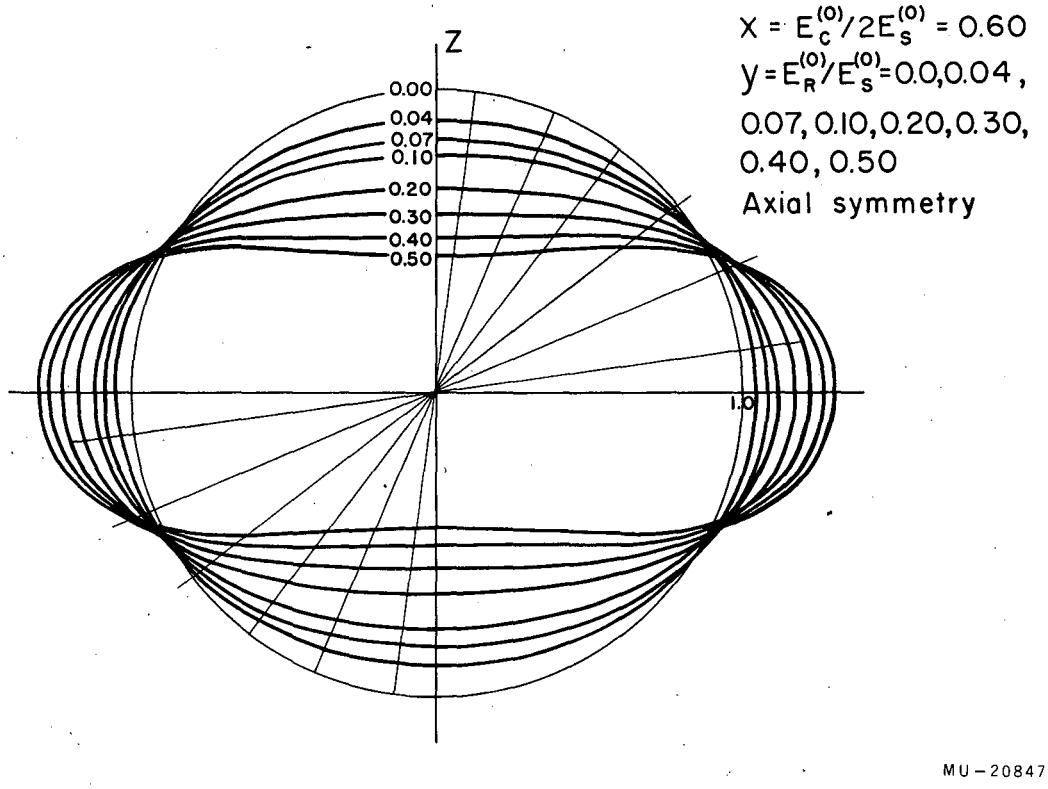

Fig. 7. Axially symmetric equilibrium configurations for x = 0.60 and for various values of the rotation parameter y.

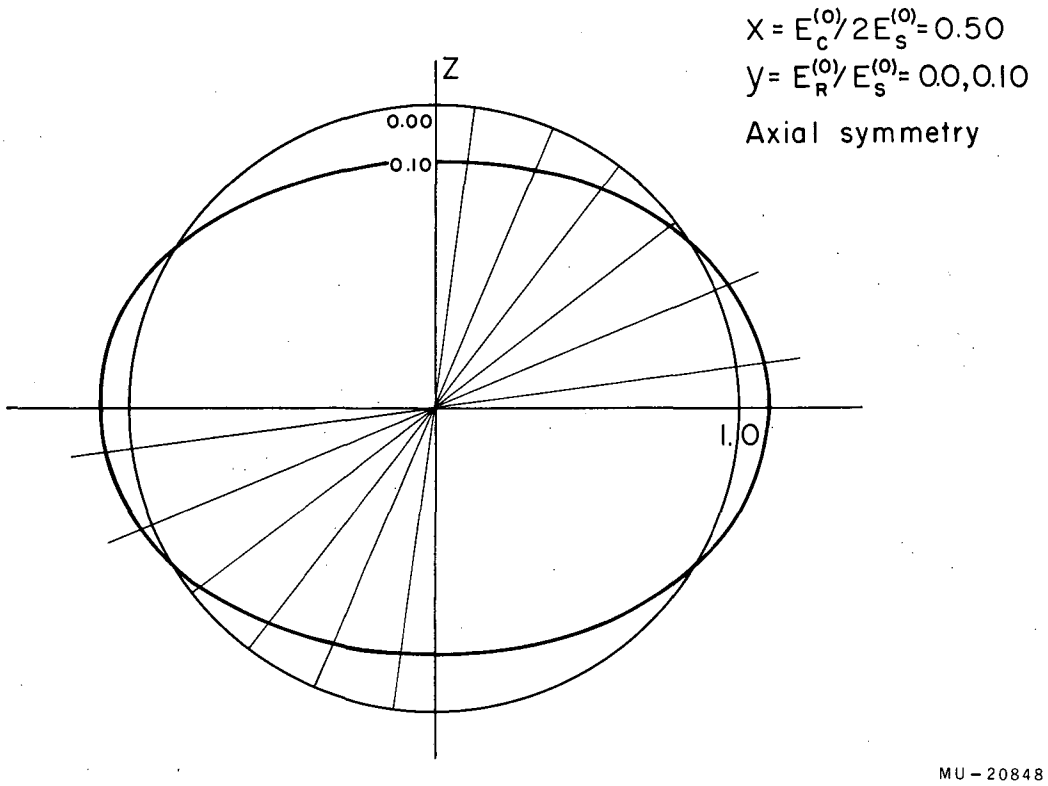

Fig. 8. Axially symmetric equilibrium configurations for x = 0.50 and for various values of the rotation parameter y.

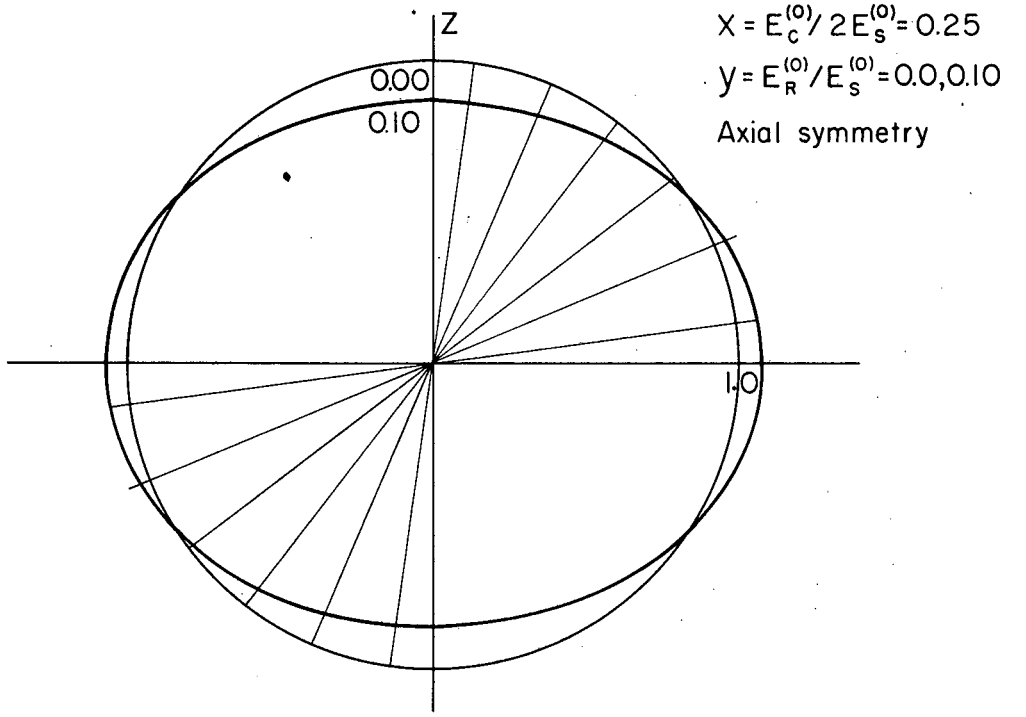

Fig. 9. Axially symmetric equilibrium configurations for x = 0.25 and for various values of the rotation parameter y.

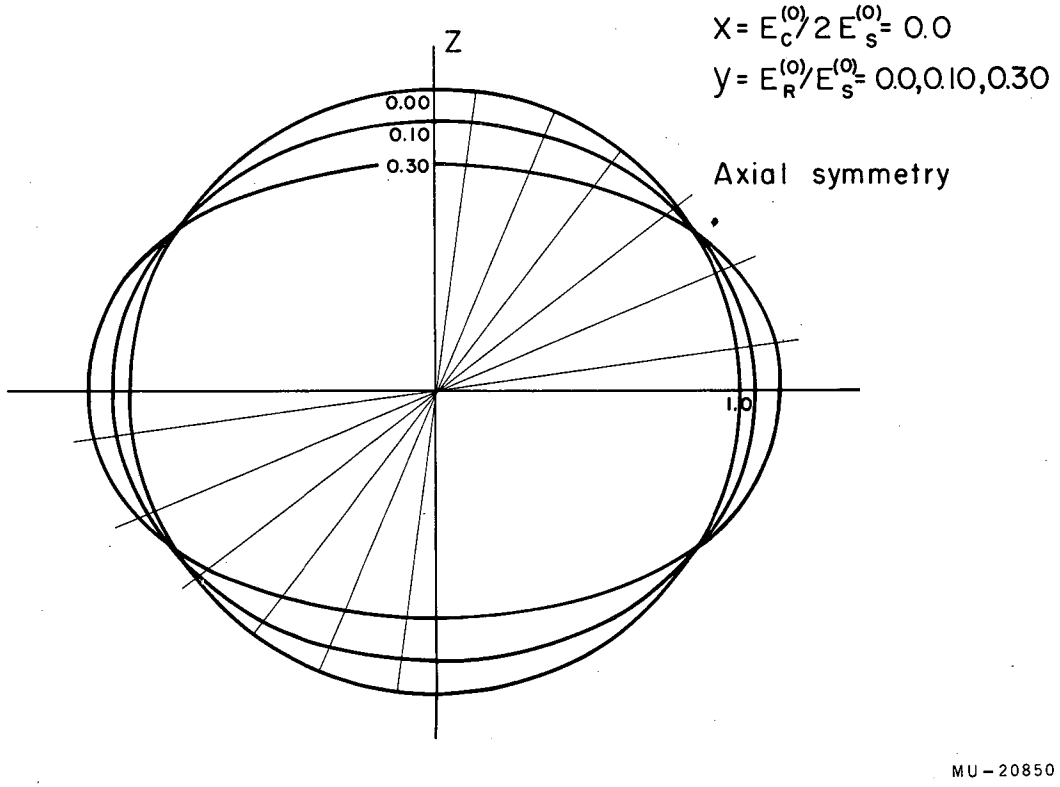

Fig. 10. Axially symmetric equilibrium configurations for x = 0.00 and for various values of the rotation parameter y.

was accomplished by starting with the solution at $x = 0.6$, $y = 0.4$ but with the values $x = 0.6$, $y = 0.45$. After five cycles this tentative result was restarted with $x = 0.6$, $y = 0.5$, and the convergence was accomplished.

As a measure of the effects of grid size on the convergence cycle the case $x = 0.5$, $y = 0.1$ was done a second time for $T = 9$. The initial values for $\sqrt{\overline{\Delta\Gamma^2}}/\overline{\Gamma}$ were identical in either case but convergence to the same final value required about 40% more cycles for the $T = 9$ mesh. Since the time required for calculating the surface potential varies as T^3 for these axially symmetric cases, the overall time required for convergence with $T = 9$ was appreciably longer than for $T = 6$. Both results are tabulated in Table I.

The moment of inertia and the energetics of the final configurations are shown in Table I. The results listed in Table I are given in double entry. The first row corresponds to the result obtained directly from the energetics calculation. This result contains the inherent error due to the finite mesh size used in these calculations. These absolute errors are indicated explicitly for those cases marked (sphere), in which case the energetics were computed but the configuration was constrained to a sphere. One would suspect that the variation in absolute error from one shape to the next would vary less rapidly than the magnitude of the absolute error, at least for those shapes which do not differ markedly from a sphere. Therefore, we have listed in the second row the values for the energetics normalized by that same factor which gives zero error for the spherical solution.

The error in the radius vector for these solutions has been determined by asking the convergence routine to converge on a sphere starting with an initial P_2 distortion and comparing the final calculated shape with a sphere. If $\sqrt{\overline{\Delta R^2}}$ is the root-mean-square deviation of the radius vector from the correct value, we find $\sqrt{\overline{\Delta R^2}}/R < 2 \times 10^{-3}$ for $\sqrt{\overline{\Delta\Gamma^2}}/\overline{\Gamma} \simeq 10^{-3}$.

Table I

Energetics for rotating liquid drops

T	$x=E_C^{(0)}/2E_s^{(0)}$ x	$y=E_R^{(0)}/E_S^{(0)}$ y	E_C	E_S	E_R	E_T	I	$\sqrt{\Delta T^2}/T$
6.00	0.00	0.10	0.00	1.00708	0.089737		1.867144	0.00056
			0.00	1.00417	0.089721	1.093891	1.867474	
	0.00	0.30	0.00	1.03155	0.229670		2.188576	
			0.00	1.02857	0.229628	1.258198	2.188963	
6.00	0.250	0.10	0.250016	1.00993	0.087140		1.922800	0.00066
			0.248617	1.00701	0.087124	1.591368	1.923140	
9.00	0.50	1.00 (sphere)	0.501251	1.001277	1.000034		1.675458	
			0.500000	1.000000	1.000000	3.000000	1.675512	
9.00	0.50	0.10	0.497301	1.015458	0.0829069		2.020960	0.00083
			0.496060	1.014163	0.0829041	2.089187	2.021024	
6.00	0.50	0.10	0.498199	1.016388	0.082958		2.019720	0.00083
			0.495411	1.013454	0.082943	2.087219	2.020077	
6.00	0.60	0.04	0.601331	1.006465	0.036165		1.853200	0.00023
			0.597966	1.003560	0.036158	2.235650	1.853528	
	0.60	1.00 (sphere)	0.603377	1.002895	1.000181		1.675216	
			0.600000	1.000000	1.000000	2.200000	1.675512	
	0.60	0.07	0.598892	1.01321	0.059372		1.975456	0.00056
			0.595540	1.010129	0.059361	2.260572	1.975805	
	0.60	0.08	0.598437	1.014574	0.067188		1.995016	0.00079
			0.595089	1.011645	0.067176	2.268999	1.995369	
6.00	0.60	0.10	0.596314	1.021155	0.080607		2.078616	0.00075
			0.592977	1.018207	0.080592	2.284753	2.078984	
	0.60	0.20	0.587144	1.052442	0.141312		2.371376	0.00065
			0.583858	1.049404	0.141286	2.358442	2.371796	
	0.60	0.30	0.577927	1.08635	0.191790		2.620848	0.00061
			0.574693	1.08321	0.191755	2.424351	2.621312	
	0.60	0.40	0.568243	1.123846	0.233682		2.868024	0.00055
			0.565063	1.120602	0.233640	2.484368	2.868532	
	0.60	0.50	0.559050	1.161362	0.269846		3.104584	0.0012
			0.555921	1.158010	0.269797	2.539649	3.105134	
6.00	0.70	0.0 (sphere)	0.703939	1.002895	0.0		1.675216	
			0.700000	1.000000		2.400000	1.675512	
	0.70	0.06	0.698569	1.013558	0.050760		1.980504	0.00061
			0.694660	1.010632	0.050751	2.450703	1.980854	
	0.70	0.10	0.693761	1.02655	0.078368		2.138000	0.00077
			0.689879	1.02358	0.078354	2.481692	2.138378	
6.00	0.80	0.05	0.796096	1.01877	0.040867		2.049920	0.0010
			0.791641	1.01583	0.040860	2.639972	2.050282	
	0.80	0.10	0.789104	1.03598	0.075111		2.230464	0.0015
			0.784689	1.03299	0.075097	2.677465	2.230858	
6.00	0.90	0.014	0.902661	1.0054	0.012847		1.825832	0.00087
			0.897610	1.002498	0.012844	2.810562	1.826155	
6.00	0.90	0.025	0.898304	1.01325	0.021199		1.985968	0.00081
			0.893278	1.01032	0.021150	2.818026	1.986318	

It is interesting to compare the solutions in Figs. 4 through 10 with the calculated distortion given by Eq. (II.12a). Over the entire x range, $0 \leq x \leq 1$, and for $y \leq 0.1$, the analytic result for the radius vector agrees with the calculated result to within a few percent. For $x = 0.6$, $y = 0.5$, the Eq. (II.12a) gives a radius which differs by 16% from the solution of Fig. seven. The analytic result Eq. (II.12a) is useful over the entire range of x provided the distortions are small.

VI. CONCLUSIONS

The problem of determining the configurations of equilibrium of rotating charged drops has been considered. The effects of the rotational forces in influencing the fissionability of these systems is illustrated in Fig. 2. From this figure one concludes that the effects of rotation are quite effective in reducing the fission barrier. Taking as an example the bombardment of Pu^{240} by Ne^{22} to form a compound nucleus with an $x \simeq 0.83$, we have from Fig. 1 possible values for y ranging from zero to 0.05. For this case even a relatively moderate impact parameter, giving a value $y = 0.02$, has the effect of reducing the fission barrier to one-third its value for the nonrotating system. For the largest impact parameters with a Ne^{22} projectile and over most of the range of impact parameters for A^{40}, the bombardment of targets near the upper end of the periodic table would result in compound systems which contain rotational energies in excess of that value necessary to give the system only neutral stability. We conclude, therefore, that in this range of targets and projectiles these large rotational forces will inhibit the formation of the compound systems.

The variation-iteration method described in the previous sections has been demonstrated to be useful in generating the configurations of equilibrium of axially symmetric drops in the ranges $0 \leq x \leq 1$, and $0 \leq y \leq 0.05$. This iterative procedure is adequate therefore to generate axially symmetric configurations over the entire range of values of x and y induced by heavy-ion bombardments with projectiles as heavy as A^{40} and for energies up to 10 Mev/nucleon. It is planned to extend these calculations by using this method to calculate the corresponding saddle-shaped configurations.

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APPENDICES

Appendix A

In this appendix we shall derive the expressions for the moment of inertia, rotational energy, surface energy, Coulomb potential, and Coulomb energy for small ellipsoidal distortions of a rotating liquid drop.

Expressed in spherical coordinates $\mu = \cos\theta, \phi$, the surface of the drop is specified by

$$R = \frac{R_0}{\lambda}\left[1 + \alpha_{20} P_{20}(\mu) + \alpha_{22} P_{22}(\mu) \cos 2\phi\right],$$

with

$$P_{20} = \frac{1}{2}(3\mu^2 - 1)$$

and

$$P_{22} = 3(1 - \mu^2).$$

Volume Normalization

The factor λ^{-1} is introduced in the expression for R to insure constancy of volume and is determined by the condition

$$\frac{4}{3}\pi R_0^3 = \int_0^{2\pi}\int_{-1}^{+1}\int_0^R r^2\, dr d\mu d\phi .$$

This expression yields, to third order in α_{20}, α_{22}, the value

$$\lambda^3 = 1 + \frac{3}{5}\alpha_{20}^2 + \frac{36}{5}\alpha_{22}^2 + \frac{2}{35}\alpha_{20}^3 - \frac{72}{35}\alpha_{20}\alpha_{22}^2 .$$

Moment of Inertia and Rotational Energy

The moment of inertia about the z-axis is given by

$$I = \rho_m \int_0^{2\pi} \int_{-1}^{+1} \int_0^R r^4 (1 - \mu^2)\, dr\, d\mu d\phi,$$

where ρ_m is the mass density. To second order in a_{20}, a_{22}, we have

$$I = \frac{8\pi\rho_m}{15} \left(\frac{R_0}{\lambda}\right)^5 \left(1 - a_{20} + \frac{10}{7} a_{20}^2 + \frac{216}{7} a_{22}^2\right).$$

Introducing into I the value for λ^{-5} determined from the previous paragraph gives

$$I = I_s \left(1 - a_{20} + \frac{3}{7} a_{20}^2 + \frac{132}{7} a_{22}^2\right),$$

where $I_s = (8\pi\rho_m R_0^5)/15$, the moment of inertia of a sphere.

The rotational energy, expressed in units of the surface energy of the drop, is then

$$E_R = \frac{L^2}{2I} \quad \frac{1}{4\pi R_0^2 0} = y \left(1 + a_{20} + \frac{4}{7} a_{20}^2 - \frac{132}{7} a_{22}^2\right)$$

where

$$y = E_R^{(0)}/E_s^{(0)} = \frac{L^2}{2I_s} \quad /4\pi R_0^2 0 .$$

Surface Energy

The surface of the drop is given by the integral

$$E_s^1 = 0 \int_0^{2\pi} \int_{-1}^{+1} D(\mu, \phi)\, d\mu d\phi,$$

where 0 is a measure of the surface tension and is expressed in units of energy/unit area. For the integrand $D(\mu, \phi)$ we have recourse to

differential geometry[26] to obtain

$$D(\mu, \phi) = \left[\left(\frac{\partial y}{\partial \mu}\frac{\partial z}{\partial \phi} - \frac{\partial z}{\partial \mu}\frac{\partial y}{\partial \phi}\right)^2 + \left(\frac{\partial z}{\partial \mu}\frac{\partial x}{\partial \phi} - \frac{\partial x}{\partial \mu}\frac{\partial z}{\partial \phi}\right)^2 + \left(\frac{\partial x}{\partial \mu}\frac{\partial y}{\partial \phi} - \frac{\partial y}{\partial \mu}\frac{\partial x}{\partial \phi}\right)^2\right]^{1/2} .$$

Using the relations

$$x = R\sqrt{1 - \mu^2}\cos\phi ,$$

$$y = R\sqrt{1 - \mu^2}\sin\phi ,$$

and

$$z = R\mu ,$$

we can show that the expression for $D(\mu, \phi)$ reduces to

$$D(\mu, \phi) = R\left[\frac{1}{1 - \mu^2}\left(\frac{\partial R}{\partial \phi}\right)^2 + R^2 + (1 - \mu^2)\left(\frac{\partial R}{\partial \mu}\right)^2\right]^{1/2} .$$

Inserting the value for R, expanding the bracket using the binomial theorem, and carrying out the integrations over μ and ϕ, we obtain

$$E_s = 1 + \frac{2}{5}\alpha_{20}^2 + \frac{24}{5}\alpha_{22}^2 - \frac{4}{105}\alpha_{20}^3 + \frac{48}{35}\alpha_{20}\alpha_{22}^2$$

for the surface energy expressed in units of the surface energy of the sphere.

Coulomb Potential and Energy

The Coulomb energy of the drop is given by the six-fold integral

$$E_c^1 = \frac{\rho}{2}\int_0^{2\pi}\int_{-1}^{+1}\int_0^R V(r_i, \mu, \phi)\, r^2\, dr_i\, d\mu_i\, d\phi_i ,$$

with

$$V(r_i, \mu_i, \phi_i) = \rho\int_0^{2\pi}\int_{-1}^{+1}\int_0^R \frac{1}{|r_i - r_j|}\, r_j^2\, dr_j\, d\mu_j\, d\phi_j ,$$

where ρ is the charge density of the drop.

The first integral can be reduced to a two-fold integral over the surface by employing a device used by Frankel and Metropolis following a suggestion of H. Hurwitz.[18] If $V_s(R,\mu,\phi)$ is the potential on the surface of the drop, we have

$$E_c^{\,1} = \frac{\rho}{5} \int_0^{2\pi} \int_{-1}^{+1} V_s(R,\mu,\phi)\,(x\lambda + y\,\bar{\mu} + z\,\bar{\nu})\,D\,d\mu d\phi\,.$$

The $\lambda, \bar{\mu}$, and $\bar{\nu}$ are the direction cosines of the normal to the surface and are given by

$$\lambda = \frac{1}{D}\left(\frac{\partial y}{\partial \mu}\frac{\partial z}{\partial \phi} - \frac{\partial z}{\partial \mu}\frac{\partial y}{\partial \phi}\right),$$

$$\bar{\mu} = \frac{1}{D}\left(\frac{\partial z}{\partial \mu}\frac{\partial x}{\partial \phi} - \frac{\partial x}{\partial \mu}\frac{\partial z}{\partial \phi}\right),$$

and

$$\bar{\nu} = \frac{1}{D}\left(\frac{\partial x}{\partial \mu}\frac{\partial y}{\partial \phi} - \frac{\partial y}{\partial \mu}\frac{\partial x}{\partial \phi}\right).$$

Inserting the expression for x, y, z given in the section on the surface energy one can readily show that the expression for $E_c^{\,1}$ reduces to

$$E_c^{\,1} = \frac{\rho}{5} \int_0^{2\pi} \int_{-1}^{+1} V_s(R,\mu,\phi)\,R^3(\mu,\phi)\,d\mu d\phi\,.$$

For the evaluation of the potential we shall use a method due to Mudd.[27] The method begins by dividing the deformed drop into an interior region defined by a surface (referred to as the standard surface) plus an outer deformed shell. The potential at a point inside the standard surface due to the charge within the standard surface and the charge in the outer shell is given by Mudd's expansion. The calculation is facilitated if we choose as the standard surface a sphere with a radius such that the surface of the deformed drop always lies outside the standard surface. It is essential to note, however, that the choice of the standard surface is arbitrary. The potential inside the standard surface due to the charge lying between the standard surface

and the surface of the deformed drop is given by a series expansion in $\delta R\ (\mu, \phi)$, the thickness of the outer shell.

If a is the radius of the standard surface, Mudd's expansion is written

$$V(r_i, \mu_i, \phi_i) = \rho \int_0^{2\pi} \int_{-1}^{+1} \int_0^{R} \frac{r_j^2}{r_{ij}}\, dr_j\, d\mu_j\, d\phi_j = V^{(a)} + V^{(b)} + V^{(c)} + \cdots\cdots$$

where

$$V^{(a)} = 2\pi\rho A^2 \left[1 - \frac{1}{3}\left(\frac{r_i}{a}\right)^2\right]$$

$$V^{(b)} = \rho \int_0^{2\pi} \int_{-1}^{+1} \left.\frac{r_j^2}{r_{ij}}\right|_{r_j = a} \delta R\, d\mu d\phi$$

$$V^{(c)} = \rho \int_0^{2\pi} \int_{-1}^{+1} \left.\frac{1}{2!}\,\frac{\partial}{\partial a}\,\frac{r_j^2}{r_{ij}}\right|_{r_j = a} (\delta R)^2\, d\mu d\phi$$

and

$$V^{(d)} = \rho \int_0^{2\pi} \int_{-1}^{+1} \left.\frac{1}{3!}\,\frac{\partial^2}{\partial a^2}\,\frac{r_j^2}{r_{ij}}\right|_{r_j = a} (\delta R)^3\, d\mu d\phi$$

with $\delta R = R - a$.

This series expression for V gives the potential at any point inside the standard surface. But since the choice of the standard surface is arbitrary, the result cannot depend on the standard surface. Therefore the potential expression must be valid up to the surface of the deformed drop. The surface potential for the deformed drop is then obtained by setting $r_i = R$.

For the radius, a, of the standard surface we take

$$a = \frac{R_0}{\lambda}\left(1 - \left|\alpha_{20}\right| - \left|\alpha_{22}\right|\right) = \frac{R_0}{\lambda}\left(1 - \alpha\right), \text{ with } \alpha = \left|\alpha_{20}\right| + \left|\alpha_{22}\right|.$$

Then we can write

$$\delta R = R - a = \frac{R_0}{\lambda} \left[a_{20} P_{20}(\mu) + a_{22} P_{22}(\mu) \cos 2\phi + a \right].$$

We shall now evaluate the four leading terms in the potential. For $r_i = R$, the $V^{(a)}$ term becomes

$$V^{(a)}(R) = \frac{4\pi\rho}{3} \left(\frac{R_0}{\lambda}\right)^2 \left(1 - 3a + \frac{3}{2} a^2 - a_{20} P_{20} - a_{22} P_{22} \cos 2\phi \right.$$

$$\left. - \frac{1}{2} a_{20}^2 P_{20}^2 - a_{20} a_{22} P_{20} P_{22} \cos 2\phi - \frac{1}{2} a_{22}^2 P_{22}^2 \cos^2 2\phi \right).$$

In the evaluation of the $V^{(b)}$, $V^{(c)}$, $V^{(d)}$, terms we shall have occasion to use

$$\frac{1}{r_{ij}} = \frac{1}{a} \sum_{n=0}^{\infty} \left(\frac{r_i}{a}\right)^n P_n(\mu_{ij}),$$

and

$$P_n(\mu_{ij}) = \sum_{m=0}^{n} (2 - \delta_{m0}) \frac{(n-m)!}{(n+m)!} P_{nm}(\mu_i) P_{nm}(\mu_j) \cos m(\phi_i - \phi_j).$$

Inserting these expressions in $V^{(b)}$ gives

$$V^{(b)} = \frac{4\pi\rho}{3} \frac{R_0 a}{\lambda} \left\{ 3a + \left(\frac{r_i}{a}\right)^2 \left[\frac{3}{5} a_{20} P_{20}(\mu_i) + \frac{3}{5} a_{22} P_{22}(\mu_i) \cos 2\phi_i \right] \right\}.$$

If we set $r_i = R$, and expand to third order in a_{20}, a_{22}, and a, $V^{(b)}$ is written

$$V^{(b)} = \frac{4\pi\rho}{3} \left(\frac{R_0}{\lambda}\right)^2 \left(3a - 3a^2 + \frac{3}{5} a_{20} P_{20} + \frac{3}{5} a_{22} P_{22} \cos 2\phi \right.$$

$$\left. + \frac{3}{5} a\, a_{20} P_{20} \right.$$

$$+ \frac{3}{5} a a_{22} P_{22} \cos 2\phi + \frac{3}{5} a^2 a_{20} P_{20} + \frac{3}{5} a^2 a_{22} P_{22} \cos 2\phi$$

$$+ \frac{6}{5} a_{20}^2 P_{20}^2 + \frac{6}{5} a_{22}^2 P_{22}^2 \cos^2 2\phi + \frac{12}{5} a_{22} a_{20} P_{20} P_{22} \cos 2\phi$$

$$+ \frac{6}{5} a a_{20}^2 P_{20}^2 + \frac{6}{5} a a_{22}^2 P_{22}^2 \cos^2 2\phi$$

$$+ \frac{12}{5} a a_{20} a_{22} P_{20} P_{22} \cos 2\phi$$

$$+ \frac{9}{5} a_{20}^2 a_{22} P_{20}^2 P_{22} \cos 2\phi + \frac{9}{5} a_{20} a_{22}^2 P_{20} P_{22}^2 \cos^2 2\phi$$

$$+ \frac{3}{5} a_{20}^3 P_{20}^3 + \frac{3}{5} a_{22}^3 P_{22}^3 \cos^3 2\phi) .$$

For the evaluation of $V^{(c)}$ there appears in the integrand the factor

$$\frac{1}{2!} \frac{\partial}{\partial a} \frac{r_j^2}{r_{ij}} \Bigg|_{r_j=a} = \frac{1}{2} \sum_{n=0}^{\infty} (1-n) \left(\frac{r_i}{a} \right)^n P_n (\mu_{ij}) .$$

The term $V^{(c)}$ becomes

$$V^{(c)} = \frac{4\pi\rho}{3} \left(\frac{R_0}{\lambda} \right)^2 \left\{ \frac{3}{10} a_{20}^2 + \frac{36}{10} a_{22}^2 + \frac{3}{2} a^2 \right.$$

$$- 3 \left(\frac{r_i}{a} \right)^2 \left[\left(\frac{1}{35} a_{20}^2 + \frac{1}{5} a a_{20} - \frac{12}{35} a_{22}^2 \right) P_{20} \right.$$

$$\left. \left. + \left(\frac{1}{5} a a_{22} - \frac{2}{35} a_{20} a_{22} \right) P_{22} \cos 2\phi \right] \right.$$

$$- 3 \left(\frac{r_i}{a}\right)^4 \left[\left(\frac{3}{35} a_{20}^2 + \frac{6}{35} a_{22}^2\right) P_{40} + \frac{1}{35} a_{20} a_{22} P_{42} \cos 2\phi + \frac{9}{1120} a_{22}^2 P_{44} \cos 4\phi\right]\Bigg\}.$$

The terms in P_{40}, P_{42}, P_{44} will not contribute to the energy integral and will not be carried further.

At $r_i = R$, $V^{(c)}$ becomes

$$V^{(c)} = \frac{4\pi\rho}{3} \left(\frac{R_0}{\lambda}\right)^2 \Bigg[\frac{3}{10} a_{20}^2 + \frac{36}{10} a_{22}^2 + \frac{3}{2} a^2$$

$$- 3 \left(\frac{1}{35} a_{20}^2 P_{20} + \frac{1}{5} a\, a_{20} P_{20} - \frac{12}{35} a_{22}^2 P_{20} + \frac{2}{35} a a_{20}^2 P_{20}\right.$$

$$+ \frac{2}{5} a^2 a_{20} P_{20} - \frac{24}{35} a\, a_{22}^2 P_{20} + \frac{2}{35} a_{20}^3 P_{20}^2$$

$$+ \frac{2}{5} a\, a_{20}^2 P_{20}^2 - \frac{24}{35} a_{20} a_{22}^2 P_{20}^2 + \frac{2}{35} a_{20}^2 a_{22} P_{20} P_{22} \cos 2\phi$$

$$+ \frac{4}{5} a\, a_{20} a_{22} P_{20} P_{22} \cos 2\phi - \frac{24}{35} a_{22}^3 P_{20} P_{22} \cos 2\phi$$

$$- \frac{2}{35} a_{20} a_{22} P_{22} \cos 2\phi + \frac{1}{5} a\, a_{22} P_{22} \cos 2\phi$$

$$\left. - \frac{4}{35} a\, a_{20} a_{22} P_{22} + \frac{2}{5} a^2 a_{22} P_{22} \cos 2\phi \right)$$

$$-\frac{4}{35}\ a_{20}{}^2\, a_{22} P_{20} P_{22} \cos 2\phi - \frac{4}{35}\ a_{20} a_{22}{}^2 P_{22}{}^2 \cos^2 2\phi$$

$$+\ \frac{2}{5}\ a\, a_{22}{}^2 P_{22}{}^2 \cos^2 2\phi\Big)\Big] .$$

In the integrand of $V^{(d)}$ there appears the factor

$$\frac{1}{3!}\ \frac{\partial^2}{\partial a^2}\ \frac{r_j^{\,2}}{r_{ij}}\Bigg|_{r_j=a} = \frac{1}{3a} \sum_{n=0}^{\infty} n\,(n-1)\,\Big(\frac{r_i}{a}\Big)^n P_n(\mu_{ij}) .$$

There is no contribution for $n = 0$ and $n = 1$, therefore the leading term in $V^{(d)}$ will be a term in P_{20}. In calculating the coulomb energy to third order in the a's, this P_{20} and other terms in $V^{(d)}$ will vanish under the μ, ϕ integration; since this $V^{(d)}$ term does not contribute to the energy integral, we need not write out its expansion.

Examining the sum $V^{(a)} + V^{(b)} + V^{(c)}$, we see that all terms up to second order which contain an a or a^2 combine to give a zero result. One can show that had we included the $V^{(d)}$ all terms in a up to third order would cancel. This cancellation is an expression of the fact that the potential on the surface of the drop is independent of our choice for the standard surface.

The Coulomb energy is given by the integrals

$$E_c{}^1 = E_c{}^{1(a)} + E_c{}^{1(b)} + E_c{}^{1(c)} + E_c{}^{1(d)} ,$$

where

$$E_c{}^{(a)} = \frac{\rho}{5} \int_{\mu,\phi} V^{(a)} R^3\, d\mu d\phi$$

$$= \frac{3}{5}\left(\frac{4\pi\rho}{3}\right)^2 \frac{1}{R_0} \frac{1}{\lambda^5}\left(1 - \frac{1}{10}a_{20}^2 - \frac{6}{5}a_{22}^2 - \frac{7}{35}a_{20}^3 + \frac{36}{35}a_{20}a_{22}^2\right),$$

$$E_c^{(b)} = \frac{\rho}{5}\int_{\mu,\phi} V^{(b)} R^3 \, d\mu d\phi = \frac{3}{5}\frac{Q^2}{R_0}\frac{1}{\lambda^5}\left(\frac{3}{5}a_{20}^2 + \frac{36}{5}a_{22}^2 + \frac{12}{35}a_{20}^3 - \frac{432}{35}a_{20}a_{22}^2\right),$$

$$E_c^{(c)} = \frac{\rho}{5}\int_{\mu,\phi} V^{(c)} R^3 \, d\mu d\phi = \frac{3}{5}\frac{Q^2}{R_0}\frac{1}{\lambda^5}\left(\frac{3}{10}a_{20}^2 + \frac{18}{5}a_{22}^2 - \frac{3}{35}a_{20}^3 + \frac{108}{35}a_{20}a_{22}^2\right),$$

and

$$E_c^{(d)} = \frac{\rho}{5}\int_{\mu,\phi} V^{(d)} R^3 \, d\mu d\phi = 0,$$

Here we have set $\left(\frac{4\pi\rho}{3}\right) = Q$, the total charge on the drop. Combining the above terms, inserting the value for λ^{-5}, and expressing the Coulomb energy in units of the fission parameter $x = E_c^{(0)}/2E_s^{(0)}$, we obtain for the Coulomb energy

$$E_c = 2x\left(1 - \frac{1}{5}a_{20}^2 - \frac{12}{5}a_{22}^2 - \frac{4}{105}a_{20}^3 + \frac{48}{35}a_{20}a_{22}^2\right).$$

Appendix B

Here we consider some of the details associated with evaluating the various integrals appearing in the iterative cycle and with the integrals necessary for the energetics calculations.

The surface of the drop is specified by points distributed over a θ, ϕ grid in a spherical-coordinate system. The numerical integrations here have been limited to shapes with octant symmetry, that is,

$$0 \leq \theta \leq \frac{\pi}{2}$$

and

$$0 \leq \phi \leq \frac{\pi}{2} .$$

There is no difficulty in extending the codes to quadrant symmetry. The mesh size, T, which determines the interval between successive points in θ and ϕ on the mesh is defined by

$$\Delta\theta = \Delta\phi = \frac{1}{T} \quad \frac{\pi}{2} .$$

For these calculations T has ranged from five to seventeen. The coordinates of the points on the surface are recorded in rectangular coordinates $x(\theta, \phi)$, $y(\theta, \phi)$, and $z(\theta, \phi)$ expressed in terms of the two primary variables θ and ϕ .

All volume integrals are written as surface integrals.

$$\text{Volume:} \int_{\text{volume}} dx\, dy\, dz = \int_{\text{surface}} y\bar{\mu} D\, d\theta d\phi$$

$$\text{Moment of Inertia:} \int_{\text{volume}} (x^2 + y^2)\, dx\, dy\, dz = \int_{\text{surface}} (x^2 + y^2)\, z\bar{\nu}\, D\, d\theta d\phi .$$

The direction cosines of the normal to the surface are $\lambda, \bar{\mu}, \bar{\nu}$. These are written explicitly[26]

$$\lambda = \frac{1}{D}\left(\frac{\partial y}{\partial \theta}\frac{\partial z}{\partial \phi} - \frac{\partial z}{\partial \theta}\frac{\partial y}{\partial \phi}\right),$$

$$\bar{\mu} = \frac{1}{D}\left(\frac{\partial z}{\partial \theta}\frac{\partial x}{\partial \phi} - \frac{\partial x}{\partial \theta}\frac{\partial z}{\partial \phi}\right),$$

and

$$\bar{\nu} = \frac{1}{D}\left(\frac{\partial z}{\partial \theta}\frac{\partial y}{\partial \phi} - \frac{\partial y}{\partial \theta}\frac{\partial x}{\partial \phi}\right),$$

with

$$D^2 = \left(\frac{\partial y}{\partial \theta}\frac{\partial z}{\partial \phi} - \frac{\partial z}{\partial \theta}\frac{\partial y}{\partial \phi}\right)^2 + \left(\frac{\partial z}{\partial \theta}\frac{\partial x}{\partial \phi} - \frac{\partial x}{\partial \theta}\frac{\partial z}{\partial \phi}\right)^2 + \left(\frac{\partial x}{\partial \theta}\frac{\partial y}{\partial \phi} - \frac{\partial y}{\partial \theta}\frac{\partial x}{\partial \phi}\right)^2 .$$

The derivatives are evaluated by using seven-point difference formulae given by Scarborough.[28] The surface integrals are evaluated using the seven-point cubature formula (double integration formula) given by Irwin.[29]

The expression for the curvature, κ, is given by a formula from differential geometry,[26]

$$\kappa = \frac{1}{R_1} + \frac{1}{R_2} = \frac{EN - 2FM + GL}{D^2},$$

where R_1 and R_2 are the two principal radii of curvature of the surface. The other quantities are given by

$$E = \left(\frac{\partial x}{\partial \theta}\right)^2 + \left(\frac{\partial y}{\partial \theta}\right)^2 + \left(\frac{\partial z}{\partial \theta}\right)^2 ,$$

$$F = \frac{\partial x}{\partial \theta}\frac{\partial x}{\partial \phi} + \frac{\partial y}{\partial \theta}\frac{\partial y}{\partial \phi} + \frac{\partial z}{\partial \theta}\frac{\partial z}{\partial \phi} ,$$

$$G = \left(\frac{\partial x}{\partial \phi}\right)^2 + \left(\frac{\partial y}{\partial \phi}\right)^2 + \left(\frac{\partial z}{\partial \phi}\right)^2 ,$$

$$L = \lambda \frac{\partial^2 x}{\partial \theta^2} + \bar{\mu} \frac{\partial^2 y}{\partial \theta^2} + \bar{\nu} \frac{\partial^2 z}{\partial \theta^2} ,$$

$$M = \lambda \frac{\partial^2 x}{\partial \theta \partial \phi} + \bar{\mu} \frac{\partial^2 y}{\partial \theta \partial \phi} + \bar{\nu} \frac{\partial^2 z}{\partial \theta \partial \phi} ,$$

and

$$N = \lambda \frac{\partial^2 x}{\partial \phi^2} + \bar{\mu} \frac{\partial^2 y}{\partial \phi^2} + \bar{\nu} \frac{\partial^2 z}{\partial \phi^2} .$$

The second derivatives are evaluated by using Scarborough's seven-point difference formulae. The second-order mixed partial derivatives are evaluated by using a difference expression obtained by differentiating a mid-panel central-difference double interpolation formula given by Irwin.[29]

The fractional errors of these integrals and curvature when evaluated for a sphere are illustrated in Fig. 11 for various values of the mesh size, T.

The expression for the surface potential is also written as a surface integral,[30]

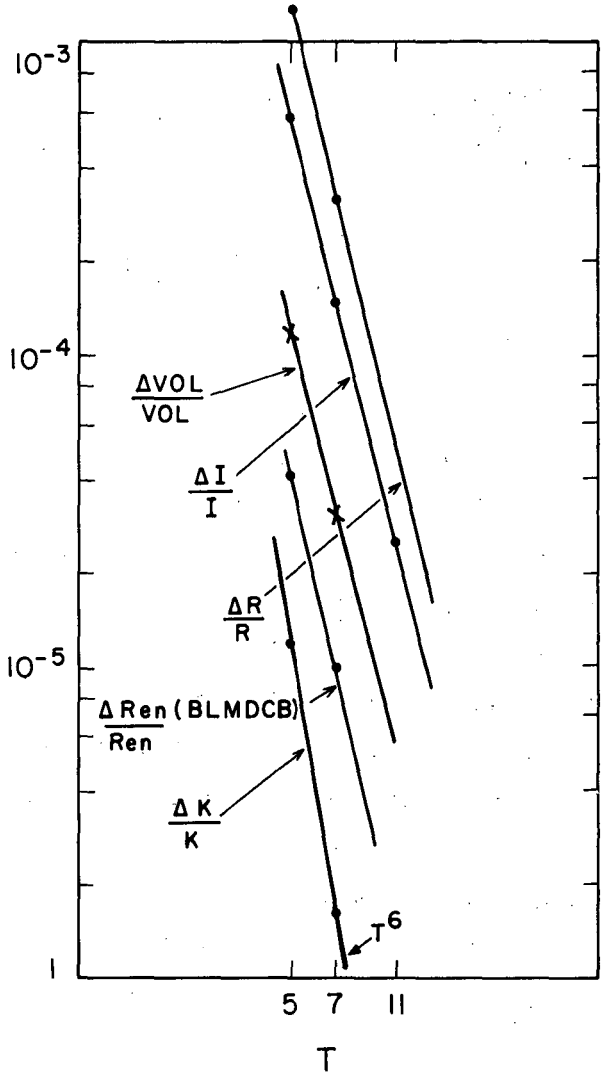

Fig. 11. Fractional errors in the numerical formulae used in the variation-iteration method plotted versus the mesh parameter T for spherical shapes. Here Δ Vol/Vol = error in volume; $\Delta I/I$ = error in moment of inertia; $\Delta R/R$ = error in the rotational term; Δ Ren/Ren = error in the volume renormalization; $\Delta K/K$ = error in the curvature.

$$V_s(r) = \int_{\text{volume}} \frac{dx'\, dy'\, dz'}{\left|\vec{r} - \vec{r}'\right|} = -\frac{1}{2} \int_{\text{surface}} \frac{(\vec{r} - \vec{r}')}{\left(\left|\vec{r} - \vec{r}'\right|\right)^{1/2}} \cdot \vec{d}\, A'$$

$$V_s(r) = -\frac{1}{2} \int_{\text{surface}} \frac{(x - x')\lambda + (y - y')\bar{\mu} + (z - z')\nu}{\left[(x - x')^2 + (y - y')^2 + (z - z')^2\right]^{1/2}} D\, d\theta'\, d\phi'.$$

The fractional error in the potential when evaluated for a sphere is illustrated in Fig. 12 for the cases of a one-point and a three-point cubature formula. The error near the poles is the same for either case, but the error near the equator is less for the three-point formula than for the one-point formula.

In carrying out the numerical integrations for the cycle, the evaluation of the surface potential requires more than half the total time. The evaluation of the potential using the three-point cubature formula requires approximately 25% more time than does the one-point formula. Although the three-point formula gives a better relative error over the surface, it does not improve the absolute error. Consequently, for these calculations it was decided to use the one-point cubature formula in the iterative cycle and to rely on varying the mesh size to improve the accuracy.

The coulomb energy is evaluated using the same integral discussed in Appendix A, that is

$$\frac{1}{5} \int_{\text{surface}} V_s\, (x\lambda + y\bar{\mu} + z\,\bar{\nu})\, D\, d\,\theta\, d\phi,$$

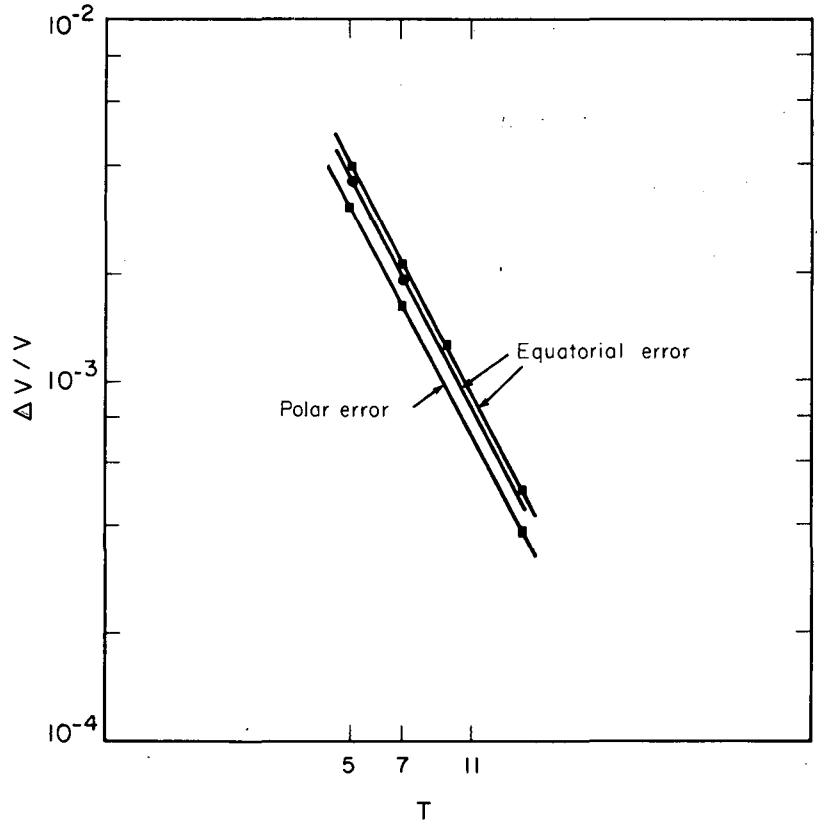

Fig. 12. Fractional error in the Coulomb surface potential as a function of the mesh parameter T for a sphere and using a one-point or a three-point cubature formula.

again using a seven-point cubature formula. The rotational energy is determined once the moment of inertia is calculated. The surface energy is given by the integral

$$0 \int_{\text{surface}} D \, d\theta \, d\phi \, .$$

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