Appendix B2
The Coulomb Potential Energy of a Uniform Ellipsoidal Charge Density

1. Introduction

The Coulomb energy associated with a uniform ellipsoidal charge density is required in the theory of nuclear stability against symmetrical fission. We derive an expression for this energy here, assuming small distortions from a sphere. For a prolate ellipsoid the Coulomb energy is reduced with respect to that of a sphere by,

$$\Delta P_{prolate} = -\frac{\varepsilon^2}{5} P_{sphere} \tag{1.1}$$

where ε measured the distortion from the spherical. Specifically, the semi-major and semi-minor axes are,

(prolate) $$c = R(1+\varepsilon) \quad \text{and} \quad b = R\left(1 - \frac{1}{2}\varepsilon + \frac{3}{8}\varepsilon^2\right) \tag{1.2}$$

These expressions correspond to a distortion at constant volume to within an accuracy of order ε^3. That is,

(prolate) $$V = \frac{4\pi}{3} R^3 = \frac{4\pi}{3} b^2 c + O(\varepsilon^3) \tag{1.3}$$

In (1.1) the Coulomb energy of the uniform spherical charge density is,

$$P_{sphere} = \frac{3}{5} \cdot \frac{Q^2}{4\pi\varepsilon_0 R} \tag{1.4}$$

where Q is the total charge. This is proved below (Section 2).

A uniform spherical shell with the same charge as a uniform *surface* charge density has Coulomb energy,

$$P_{sphere}^{shell} = \frac{1}{2} \cdot \frac{Q^2}{4\pi\varepsilon_0 R} \tag{1.5}$$

So, the uniform spherical charge density has an energy which is a factor 6/5 times *larger* than the same charge distributed uniformly over a spherical surface. We stress this because the factor of 3/5 in (1.4) may give the opposite impression. Note that (1.5) follows from the potential by considering a small charge δQ to be added to the surface, the increment of energy being,

$$\delta P = \Phi_{sphere}^{shell}\Big|_{r=R} \delta Q = \frac{Q \cdot \delta Q}{4\pi\varepsilon_0 R} \tag{1.6}$$

and integrating over Q from 0 to Q produces (1.5). We emphasise this because it is tempting to just multiply the surface potential by Q to get the Coulomb energy, but this omits the required factor of ½. Falsely thinking that the shell energy has no factor of ½ gave me the incorrect impression for a long time that the uniform volumetric distribution has a *lower* energy by a factor of 3/5. Completely wrong!

2. The Sphere

It is worth going through the derivation for the spherical case. It is not as trivial as you might imagine. There is an interesting blunder which is easy to make – and which, by fluke, seems to yield the correct Coulomb energy. Gauss's theorem readily gives the (purely radial) electric field to be,

$$(r > R) \quad E = \frac{Q}{4\pi\varepsilon_0 r^2}; \qquad (r < R) \quad E = \frac{Qr}{4\pi\varepsilon_0 R^3} \tag{2.1}$$

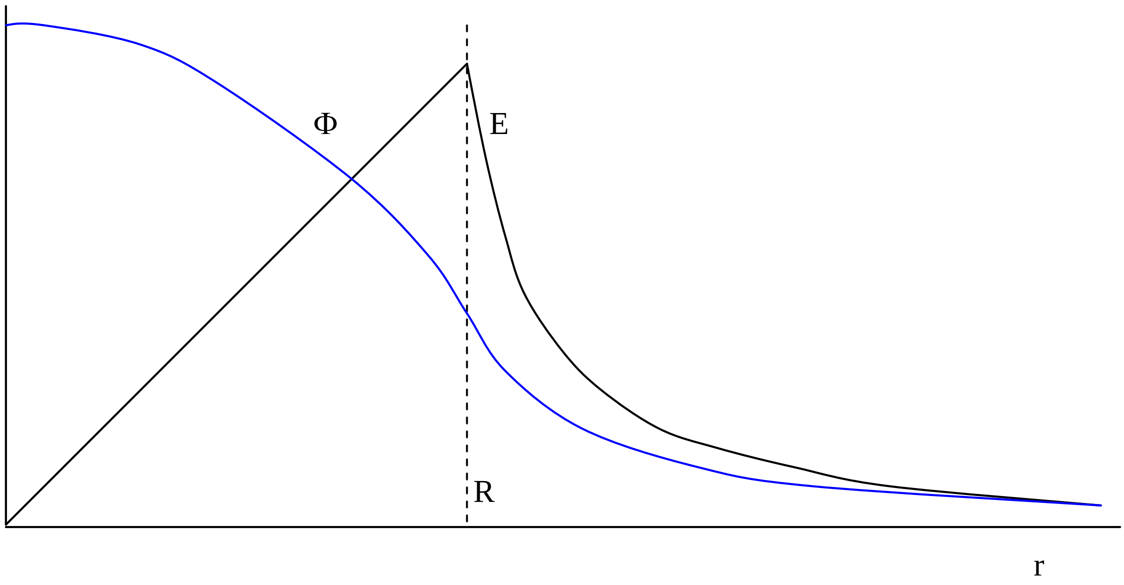
The corresponding electric potentials are,

$$(r > R) \quad \Phi = \frac{Q}{4\pi\varepsilon_0 r}; \qquad (r < R) \quad \Phi = \frac{Q}{4\pi\varepsilon_0 R}\left[\frac{3}{2} - \frac{r^2}{2R^2}\right] \tag{2.2}$$

We see that (2.1) and (2.2) are consistent with $E = -\partial_r \Phi$ in both regimes (paying attention to the signs!). The constant term in the interior solution for the potential is chosen so that the potential is continuous at r = R. This implies that the potential at the centre of the sphere is,

$$\Phi_{centre} = \frac{3}{2} \cdot \frac{Q}{4\pi\varepsilon_0 R} \tag{2.3}$$

Graphically we have,



The Coulomb energy of the sphere can be obtained in two ways: either from the field of from the potential. We consider both in turn:-

From the field

The energy density and hence the total energy are given by,

$$\xi = \frac{\varepsilon_0}{2} E^2 \qquad \text{hence,} \quad P = \int_0^\infty \frac{\varepsilon_0}{2} E^2 4\pi r^2 dr \qquad (2.4)$$

Substituting from (2.1), we find that the exterior region contributes to the energy an amount equal to that for a spherical surface distribution of charge, i.e. $P_{sphere}^{shell} = \frac{1}{2} \cdot \frac{Q^2}{4\pi\varepsilon_0 R}$. It is obvious that this must be the case because the fields in the exterior region are identical in the two cases (but carrying out the field-based integral confirms the result). However, the interior region contributes another 1/5 of this amount, this factor resulting from $\int_0^R r^4 dr$ in comparison with $\int_R^\infty \frac{dr}{r^2}$. Hence we get (1.4). Note that it is physically obvious that the volumetric distribution must give a larger Coulomb energy than the spherical surface distribution because they have the same exterior solution, but the former has a non-zero interior field whereas the latter does not.

From the Potential

Consider the charge to be increased by δQ, but retaining its spherically symmetrical volumetric distribution. The increase in energy is,

$$\delta P = \int_0^R \Phi \delta\rho dV = \int_o^R \frac{Q}{4\pi\varepsilon_0 R}\left[\frac{3}{2} - \frac{r^2}{2R^2}\right] \cdot \frac{\delta Q}{(4\pi/3)R^3} \cdot 4\pi r^2 dr \qquad (2.5)$$

Note that only the interior solution for the potential contributes to this integral (since it is only where the charge is that the potential matters). (2.5) gives,

$$\delta P = \frac{6}{5} \cdot \frac{Q \cdot \delta Q}{4\pi\varepsilon_0 R} \qquad (2.6)$$

and finally integrating over the increment of charge from Q = 0 to Q gives the same result as the previous method, i.e.,

$$P_{sphere} = \frac{3}{5} \cdot \frac{Q^2}{4\pi\varepsilon_0 R} \qquad (1.4)$$

A blunder that is easy to make is to use Gauss's theorem incorrectly to conclude that the potential inside the sphere at any radius r is given by $\frac{(4\pi/3)r^3\rho}{4\pi\varepsilon_0 r}$. This is completely wrong. It implies that the potential at the centre is zero, and that the electric field is pointing radially *inwards* for a positive charge! The latter can be fixed by changing the sign, but this implies that the potential energy is negative (like charges attract?) and the potential is discontinuous at r = R – where the potential becomes positive again. In can't be fixed. It's just wrong. Oddly, though, the correct expression for the Coulomb energy results from this spurious potential if the error is compounded by forgetting about the need to integrate over the charge. Thus,

$$\int \frac{(4\pi/3)r^3\rho}{4\pi\varepsilon_0 r}\rho\cdot 4\pi r^2 dr = \frac{3}{5}\cdot\frac{Q^2}{4\pi\varepsilon_0 R} \qquad \text{where } \rho = \frac{Q}{(4\pi/3)R^3}$$

Which demonstrates that is possible to get the right answer by completely spurious reasoning.

3. The Prolate Ellipsoid – The Quadrupole Method Does Not Work!

The distortion of the spherical distribution of charge into an ellipse gives rise to a quadrupole moment. Duffin, problem 5.5, gives this quadrupole moment for a prolate ellipsoid to be,

$$q = \frac{2}{5}Q\left(c^2 - b^2\right) \tag{3.1}$$

Using (1.2) this becomes,

$$q = \frac{6}{5}\varepsilon Q R^2 + O(\varepsilon^2) \tag{3.2}$$

(This is the quadrupole moment about the axis of symmetry, taken to be the spherical polar z-axis, or θ = 0). Duffin, Equ.(5.15), gives the electric potential due to such a quadrupole as,

$$\Phi_{quad} = \frac{q}{4\pi\varepsilon_0 r^3}\cdot\frac{3\cos^2\theta - 1}{4} \tag{3.3}$$

From this we can work out the electric field components, noting that there is a radial and an azimuthal (theta) component. The radial component of the field due to the spherically symmetric part must be added to this. The energy density can then be evaluated in the outside region (r > R), namely, after multiplying out and simplifying,

$$\xi = \frac{\varepsilon_0}{2}\cdot\frac{1}{(4\pi\varepsilon_0)^2}\cdot\left\{\frac{Q^2}{r^4} + \frac{3qQ}{2r^6}\left(3\cos^2\theta - 1\right) + \left(\frac{3q}{4r^4}\right)^2\left[\left(3\cos^2\theta - 1\right)^2 + 4\sin^2\theta\cos^2\theta\right]\right\} \tag{3.4}$$

On performing the volume integral of (3.4), the qQ cross-term cancels (orthogonal Legendre polynomials). The first term in (3.4) is just the energy for the undistorted sphere. Hence, the third term in (3.4) gives the energy change due to being ditorted to an ellipsoid. Evaluation is easy and gives,

$$\Delta P_{quad} = \frac{9}{10}\cdot\frac{1}{5}\cdot\frac{3}{5}\cdot\frac{Q^2\varepsilon^2}{4\pi\varepsilon_0 R} \tag{3.5}$$

Hence, at first sight it appears that (3.5) is just a factor of 9/10 away from being the sought answer, namely that in distorting a sphere to a prolate ellipsoid the Coulomb energy changes by an amount equal to 1/5 of the sphere's Coulomb energy. However, this derivation is actually totally spurious. This is clear because the energy change is positive, rather than negative as it should be. This results from (3.4) where it can be seen that the quadrupole inevitably contributes a positive definite energy density everywhere.

Thus, the mistake is in using the quadrupole field at all. Such fields only apply at large distance from the source. Thus, the expressions above are only valid for $r \gg R$. We are not justified in integrating the quadrupole-based energy density down to $r = R$. It must be that the true fields depart markedly from the simple quadrupole form near the ellipsoid. This must lead top energy densities near the ellipsoid being reduced compared with the shperical case, contrary to (3.4).

4. The Prolate Ellipsoid Solution

The method we shall use is applicable only for small distortions from the spherical (i.e. for $\varepsilon \ll 1$). It is based on considering the (thin) region which stands proud of (or within) the original sphere. We will call this the 'excess charge', noting that it is an excess only near the ends of the semi-major axes of the ellipsoid. Near the ends of the semi-minor axes it is a deficit of charge. The change in the Coulomb energy can be considered as arising due to the sum of two terms,

- the potential energy of the 'excess charge' due to the bulk of the sphere;
- the self-energy of the excess charge.

The second of these must be a positive energy. If the overall energy change is negative it must be that the first of these is negative, and larger in magnitude than the second. Before turning to the details it is worth looking at a crude estimate which illustrates that this first term is indeed negative, and, moreover, is of quadratic magnitude in ε (as is the second term, of course).

We orient the z-axis ($\theta = 0$) of a spherical polar co-ordinate system such that it coincides with the axis of rotation of the ellipsoid, i.e. z is the major axis. The bulge of the excess on z extends by a maximum amount $c - R = \varepsilon R$ proud of the sphere. At the ends of the semi-minor axes the ellipsoid is inside the sphere by $R - b \approx \varepsilon R / 2$. The volumes of the positive and negative regions of the excess are equal. The excess charge in each (equal and opposite) is of order ε. Now the distortion may be thought of as removing the charge that was originally near the ends of the semi-minor axes and replacing it at the ends of the semi-major axes. Thus, it is removed from a location whose centroid is, crudely, at a distance of $R(1 - \varepsilon / 4)$ from the centre of the sphere. It is replaced at a location whose centroid is, equally crudely, at a distance of $R(1 + \varepsilon / 2)$ from the centre of the sphere. Recalling that the amount of charge being thus moved is proportional to ε, the change in energy is roughly proportional to,

$$\propto Q^2 \varepsilon \left[-\frac{1}{R(1-\varepsilon/4)} + \frac{1}{R(1+\varepsilon/2)} \right] = \frac{Q^2 \varepsilon}{R} \left[-\left(1 + \frac{\varepsilon}{4}\right) + \left(1 - \frac{\varepsilon}{2}\right) \right] = -\frac{3}{4} \cdot \frac{Q^2 \varepsilon^2}{R} \qquad (3.6)$$

The magnitude of this crude estimate should not be taken literally. However it serves to demonstrate that *both* parts of the excess represent a *reduction* in Coulomb energy as regards their energy with respect to the bulk of the sphere, i.e. the first term above.

We now calculate this first term more accurately. The radial 'thickness' of the excess can be found as follows. The ellipsoid is given by,

$$z = c\cos\theta \qquad \text{and} \qquad y = \left(c^2 - a^2\right)^{1/2}\sin\theta \tag{3.7}$$

where, for sake of argument, we consider the section with x = 0, and where,

$$a^2 \equiv c^2 - b^2 = 3\varepsilon\left(1 - 3\varepsilon^2\right)R^2 \tag{3.8}$$

Strictly this θ is not the polar angle, but the 'angular' co-ordinate of an elliptical-hyperbolic system. The two differ by a term of order ε. We can ignore it since it would give rise to a correction to the energy change of order ε^3. The points (or, rather, the circles) at which the ellipsoid and the sphere coincide are given by $z^2 + y^2 = R^2$. Using (3.7) this becomes $c^2 - a^2\sin^2\theta = R^2$. Using $c = R(1+\varepsilon)$ and (3.8) this becomes, retaining only lowest order,

$$\sin\theta_0 = \sqrt{\frac{2}{3}} \tag{3.9}$$

Thus, ignoring corrections of order ε, the sphere and ellipsoid meet at the circles defined by θ_o equal to 54.7° and 125.3°. For $\theta_o < 54.7^o$ or $\theta_o > 125.3^o$ the excess charge is positive, whereas for $54.7^o < \theta_o < 125.3^o$ the excess charge is negative.

At other polar angles $r^2 = c^2 - a^2\sin^2\theta$ defines the radial distance of the ellipsoid surface from the centre of the sphere. The thickness of the excess is t = r – R, i.e.,

$$t = \sqrt{c^2 - a^2\sin^2\theta} - R = R\left\{\left[(1+\varepsilon)^2 - 3\varepsilon\sin^2\theta\right]^{1/2} - 1\right\} \approx \varepsilon R\left[1 - \frac{3}{2}\sin^2\theta\right] \tag{3.10}$$

Thus, the thickness of the excess is of order ε. It varies from εR at θ = 0 to -εR/2 at θ = π/2, as it must since these values correspond correctly to c and b as given by Equs.(1.2).

If $\rho = \dfrac{3Q}{4\pi R^3}$ is the charge density, the excess charge at any angle is simply ρt. The first term, above, i.e. the energy of the excess with respect to the bulk charge of the sphere is thus,

$$\Delta P_1 = \frac{Q}{4\pi\varepsilon_0}\int_0^\pi \frac{\rho t\cdot dS}{R + t/2} = \frac{3Q^2}{(4\pi)^2\varepsilon_0 R^3}\int_0^\pi \frac{\varepsilon R\left(1 - 1.5\sin^2\theta\right)\cdot 2\pi R^2 d(\cos\theta)}{R + \varepsilon R\left(1 - 1.5\sin^2\theta\right)/2} \tag{3.11}$$

Note that the negative excess contributes negatively to this energy, as it should because it represents charge that had positive energy but which has been removed.

Note that the centroid of each element of the excess has been placed at R +t/2. This is crucial to the argument. The use of an effective radial distance of R would falsely imply a change in Coulomb energy of first order in ε. We replace the denominator in (3.11) by its first order Taylor expansion, thus,

$$\Delta P_1 = \frac{3Q^2}{8\pi\varepsilon_0 R}\int_0^\pi \varepsilon\left(1-1.5\sin^2\theta\right)\cdot d(\cos\theta)\left\{1-\varepsilon\left(1-1.5\sin^2\theta\right)/2\right\} \qquad (3.12)$$

The term linear in ε, arising from the 1 in {…}, is zero (i.e. the angular integral is zero). The second term in {…} comes from the displacement of the excess, i.e. the t/2 in the denominator of (3.11). Note the minus sign. Thus we have,

$$\Delta P_1 = \frac{3Q^2\varepsilon^2}{8\pi\varepsilon_0 R}\int_0^{\pi/2}\left(1-1.5\sin^2\theta\right)^2\cdot d(\cos\theta) \qquad (3.13)$$

where we have reduced the integration range to 0 to π/2 by symmetry. The integral is trivial to evaluate as 1/5. Hence,

$$\Delta P_1 = -\frac{3Q^2\varepsilon^2}{40\pi\varepsilon_0 R} = -\frac{3}{10}\cdot\varepsilon^2\cdot\frac{Q^2}{4\pi\varepsilon_0 R} = -\frac{1}{2}\cdot\varepsilon^2\cdot\frac{3}{5}\frac{Q^2}{4\pi\varepsilon_0 R} \qquad (3.14)$$

i.e. the first term is –0.5 times the Coulomb energy of the unperturbed sphere.

We must now evaluate the second term we alluded to above, i.e. the self-energy of the excess charge. For this purpose the excess is treated as a surface charge density of ρt on the original sphere. Firstly we evaluate the potential at some polar angle θ_f, where the subscript 'f' denotes the field point to distinguish it from the source points which will be integrated over to form the potential. Thus the source point is given by polar angles θ and ϕ. It is simple to show that the distance from the source point to the field point is,

$$r = \sqrt{2}\left[1-\sin\theta_f\sin\theta\cos\phi-\cos\theta_f\cos\theta\right]^{1/2}R \qquad (3.15)$$

Thus the potential at θ_f is,

$$\Phi(\theta_f) = \int\frac{\rho t(\theta)\cdot R^2 d(\cos\theta)d\phi}{4\pi\varepsilon_0 r}$$
$$= \frac{Q}{4\pi\varepsilon_0 R}\cdot\frac{3\varepsilon}{4\pi\sqrt{2}}\int_0^\pi\int_0^{2\pi}\frac{\left(1-1.5\sin^2\theta\right)d(\cos\theta)d\phi}{\left[1-\sin\theta_f\sin\theta\cos\phi-\cos\theta_f\cos\theta\right]^{1/2}} \qquad (3.16)$$

The Coulomb energy can be found by integrating the product of the potential with the charge element at each point. But remember that we should really use a small increment of charge element and then integrate over charge. This produces a factor of ½ which we include below,

$$\begin{aligned}\Delta P_2 &= \frac{1}{2}\int_0^{\pi} 2\pi R^2 d(\cos\theta_f)\rho t(\theta_f)\Phi(\theta_f) \\ &= \frac{Q^2\varepsilon^2}{4\pi\varepsilon_0 R}\cdot\frac{9}{16\pi\sqrt{2}}\int_0^{\pi}\int_0^{\pi}\int_0^{2\pi}\frac{(1-1.5\sin^2\theta_f)(1-1.5\sin^2\theta)d(\cos\theta_f)d(\cos\theta)d\phi}{[1-\sin\theta_f\sin\theta\cos\phi-\cos\theta_f\cos\theta]^{1/2}}\end{aligned} \tag{3.17}$$

We have resorted to numerical integration. It may be possible to integrate algebraically since a similar integral occurs for the case of uniform surface charge on a sphere, for which the potential is given by,

$$\Phi(\theta_f) = \frac{Q}{4\pi\varepsilon_0 R}\cdot\frac{1}{4\pi\sqrt{2}}\int_0^{\pi}\int_0^{2\pi}\frac{d(\cos\theta)d\phi}{[1-\sin\theta_f\sin\theta\cos\phi-\cos\theta_f\cos\theta]^{1/2}} \tag{3.18}$$

So it follows the integral in (3.18) must be $4\pi\sqrt{2}$. Numerical integration confirms this to an accuracy of 0.01%, and also provides a validation of the routine used to evaluate the integral in (3.17) – the same routine being used apart from the extra factors in the integrand being inserted. Thus we find,

$$\int_0^{\pi}\int_0^{\pi}\int_0^{2\pi}\frac{(1-1.5\sin^2\theta_f)(1-1.5\sin^2\theta)d(\cos\theta_f)d(\cos\theta)d\phi}{[1-\sin\theta_f\sin\theta\cos\phi-\cos\theta_f\cos\theta]^{1/2}} = 1.431... \tag{3.19}$$

where we believe the result to be accurate to the 4 decimal places quoted. Insertion in (3.17) thus gives,

$$\Delta P_2 = 0.1812\cdot\frac{Q^2\varepsilon^2}{4\pi\varepsilon_0 R} \tag{3.20}$$

Thus, adding this to the first term, (3.14), gives the total Coulomb energy change when the sphere of charge is distorted to an ellipsoid to be,

$$\Delta P_{TOT} = -0.1188\cdot\frac{Q^2\varepsilon^2}{4\pi\varepsilon_0 R} = -0.1980\cdot\frac{3}{5}\cdot\frac{Q^2\varepsilon^2}{4\pi\varepsilon_0 R} \tag{3.21}$$

Thus we have confirmed the result widely quoted in the literature that the energy is *reduced* by *about* $\varepsilon^2/5$ of the Coulomb energy of the sphere. If the numerical integration is as accurate as claimed, then this is not a precise factor of 1/5 but rather 0.1980.