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The Bohr–Wheeler spontaneous fission limit: an undergraduate-level derivation

B Cameron Reed

Department of Physics, Alma College, Alma, MI 48801, USA

E-mail: reed@alma.edu

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Abstract

An upper-undergraduate level derivation of the $Z^2/A \sim 50$ limit against spontaneous fission first published by Bohr and Wheeler (1939 *Phys. Rev.* **56** 426) is provided. The purpose in offering this derivation is that most textbooks give no details of it and sometimes fail to make clear key assumptions and mathematical manipulations underlying the Bohr and Wheeler model.

1. Introduction

September 2009 marks the 70th anniversary of the publication of Niels Bohr and John Wheeler's historic paper *The Mechanism of Nuclear Fission* in [1]. In that remarkable paper, Bohr and Wheeler analysed the energetics of nuclear fission based on the 'liquid-drop' model of nuclei that Gamow had advanced a few years earlier. Among a number of insights into the nature of the fission process, Bohr and Wheeler showed how calculation of the surface and Coulomb energies of a nucleus imagined to be distorted from an initially spherical shape revealed that there is a natural limit to the stability of nuclei against spontaneous fission (SF). This limit is expressible as $(Z^2/A) = 2(a_S/a_C)$, where Z and A are the atomic and nucleon numbers and a_S and a_C are surface and Coulomb energy parameters, which were known from fits to the semi-empirical mass formula to have values ~ 18 and 0.72 MeV, respectively. (a_C is related to the self-potential of a charged sphere and can be expressed analytically; see section 4.)

The significance of this SF limit is evidenced by the fact that discussions of it appear in numerous nuclear physics texts. However, few texts actually present a derivation of it. Some present partial treatments based on starting from 'it-can-be-shown-that' expressions for the area and self-energy of an ellipsoid of variable eccentricity [2], a derivation of which from first principles appears in [3]. However, the ellipsoidal model does not really reflect the approach taken by Bohr and Wheeler, who used a sum of Legendre polynomials to describe the shape of the surface of the nucleus as it distorts. To be sure, if the SF limit is a matter of instability against slight distortions then it should be completely irrelevant how the distortion is modelled,

but it seems unfortunate that pedagogical tendency has shifted away from the ‘true’ historical approach. Worse, however, is that some treatments fail to be fully clear about some of Bohr and Wheeler’s assumptions or make misleading statements concerning them. The result of all of this is that it is very difficult to find a treatment of the Bohr and Wheeler derivation that follows what they originally did.

This unfortunate situation is no doubt due to the fact that some of the mathematics of the Bohr and Wheeler analysis is tricky, even if one is facile with multivariable calculus and properties of Legendre polynomials. Bohr and Wheeler published virtually none of the algebraic details of their work; indeed, they called it a ‘straightforward calculation’. Present and Knipp [4, 5] pointed out that there is an internal inconsistency in Bohr and Wheeler and that they changed the definition of some of their surface-distortion parameters partway through their derivation. In a paper that now seems all but forgotten, Plesset [6] reconstructed the details of the Bohr and Wheeler derivation, but his work is difficult to follow in view of some tangled notation and the fact that he carries through his algebra to higher orders of perturbation than are necessary to understand the SF limit.

In view of the platinum anniversary of Bohr and Wheeler’s paper, it seems appropriate to present a derivation of the SF limit true to their original model but at a level accessible to upper-level undergraduates and non-expert professional physicists. This is the purpose of this paper. No treatment is given here of the much more complex question of the fission *barrier*, which requires carrying the algebra to higher orders of perturbation.

In reconstructing the Bohr and Wheeler derivation, one faces the question of what level of detail to present. To lay out every step of the algebra would result in a manuscript that is far too lengthy for sensible publication. Conversely, the danger of brevity is that subtle but important points can get overlooked. In this paper, I try to tread a middle path by setting down benchmark steps in the calculations between which most readers should be able fill in the intervening gaps. A supporting appendix of all algebraic details is freely available online¹.

The structure of this paper is as follows. In section 2 the Legendre-polynomial model of a distorted nucleus is described, and the calculation of the volume of nucleus is carried out. The surface area energy is calculated in section 3. Section 4 deals with the lengthy and somewhat tricky calculation of the Coulomb self-energy of the nucleus, which, when combined with the results of the preceding sections, leads to understanding how the SF limit arises. Some concluding remarks are presented in section 5.

2. Nuclear surface profile and volume

Bohr and Wheeler began by imagining an initially spherical nucleus of radius R_0 undergoing a distortion expressible as a sum of Legendre polynomials:

$$r(\theta) = R_0\{1 + \alpha_0 + \alpha_2 P_2(\cos \theta) + \dots\}, \quad (1)$$

where θ is the polar angle in the usual system of spherical coordinates. Such a perturbation, greatly exaggerated, is sketched schematically in figure 1, where the nucleus has been perturbed into a dumbbell shape along the polar axis. The perturbation coefficients α_0 and α_2 are presumed to be small; using only two coefficients is enough to derive the SF limit. Coefficient α_2 dictates the non-spherical shape of the nucleus; α_0 is necessary to be able to ensure volume conservation as the distortion occurs. It is conventional to consider α_2 as the ‘independent’ coefficient and ultimately express both the area and Coulomb energies as functions of it alone. The gist of the Bohr–Wheeler calculation is to compare the total energy of the deformed nucleus

¹ <http://othello.alma.edu/~reed/Bohr&Wheeler.pdf>.

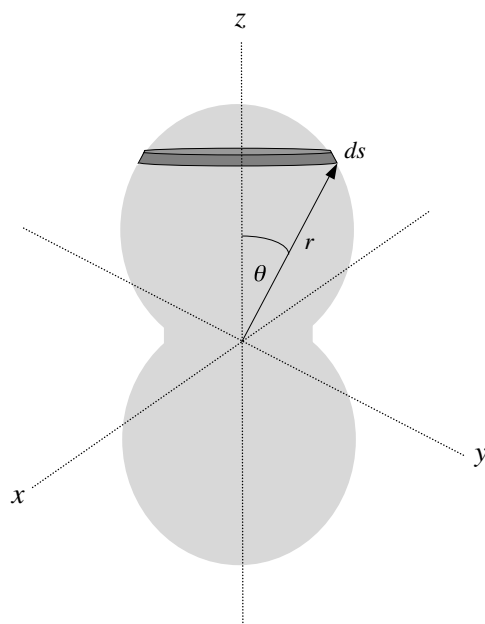


Figure 1. The surface of a distorted nucleus is described by the function $r(\theta)$ of equation (1). A ribbon of a surface of edge length ds and area $dA = 2\pi r \sin \theta ds$ at co-latitude θ is shown.

($\alpha_2 \neq 0$) to that which it had in its initial spherical condition ($\alpha_2 = 0$), and then determining what circumstance must hold so that *any* perturbation, no matter how slight, will lead to a lower energy configuration. The lowest order contributions to these energies both prove to be of order α_2^2 , so it is not necessary to carry through terms to any higher orders. Some texts do not emphasize that the volume of the nucleus is assumed to be conserved, that is, nuclei are considered to be incompressible.

Note that there is no ‘first-order’ term $\alpha_1 P_1$ in (1). The reason for this is sometimes given that such a term (or, indeed, any odd-parity perturbation) creates only a displacement of the centre of mass of the nucleus along the z -axis, but this is not quite true: Such a term would introduce a distortion of the shape of the nucleus, rendering it somewhat flattened at the ‘south pole’ ($\theta = \pi$). Incorporating only even-order Legendre polynomials simplifies the situation to having a nucleus whose centre of mass remains at the coordinate origin and which is symmetric about the xy plane. Because $r(\theta)$ contains no dependence on the azimuthal angle ϕ , the nucleus remains axially symmetric about the polar axis. The sign of α_2 dictates the nature of the distortion. If $\alpha_2 > 0$, the nucleus becomes squeezed at the equator and elongated at the poles, as suggested in figure 1; $\alpha_2 < 0$ produces the opposite effect, rendering the nucleus somewhat doughnut-shaped in the equatorial plane.

At this point, an inquisitive student might well ask: ‘Why Legendre polynomials?’ After all, the surface of the nucleus could presumably be described by any arbitrarily chosen function of the spherical coordinates (θ, ϕ) , subject only to the condition that it contains enough parameters to be able to ensure volume conservation. The value of Legendre polynomials, and particularly of the associated Legendre polynomials and spherical harmonics built up from them, is that they constitute an orthogonal set of functions over (θ, ϕ) with a particularly simple orthogonality relationship (see (4)). Consequently, they form a natural family of functions for describing perturbations from circularity or sphericity.

The first task is to ensure conservation of volume. The volume of the distorted nucleus is given by

$$V = \int_{\theta=0}^{\pi} \int_{r=0}^{r(\theta)} \int_{\phi=0}^{2\pi} r^2 \sin \theta \, d\theta \, dr \, d\phi. \quad (2)$$

Note carefully here the order of integrations over r and θ . Because the upper limit of r is a function of θ , the integral over r must be done first and then that over θ . The integral over ϕ gives 2π directly. Hence, we have

$$V = \frac{2\pi}{3} \int_{\theta=0}^{\pi} r^3(\theta) \sin \theta \, d\theta. \quad (3)$$

Be sure to understand the distinction between the integrands in (2) and (3): in the former, r is a variable whose limits are 0 and $r(\theta)$; $r^3(\theta)$ in (4) means a function of θ as given by the cube of (1).

The Bohr and Wheeler calculation involves numerous integrals of the form of (3), with different powers of $r(\theta)$ and sometimes other functions of θ in the integrand. In all such cases it is convenient to make a change of variable $x = \cos \theta$, which renders $\sin \theta \, d\theta$ as $-dx$, with limits $x = (1, -1)$. The limits can be flipped, with the result that the negative sign in $-dx$ can be dropped. The orthonormalization relation for Legendre polynomials,

$$\int_{-1}^1 P_i P_j \, dx = \frac{2 \delta_i^j}{i + j + 1}, \quad (4)$$

is also extremely valuable.

Keeping terms to order α_2^2 , the volume integral evaluates as

$$V = \left(\frac{4\pi R_0^3}{3} \right) \left\{ (1 + \alpha_0)^3 + \frac{3}{5} (1 + \alpha_0) \alpha_2^2 + \dots \right\}. \quad (5)$$

If the volume is to be conserved, then the contents of the brace bracket in (5) must equal unity. If α_0 and α_2 are presumed small, then the $\alpha_0 \alpha_2^2$ and α_0^3 terms can be dropped; what remains is a quadratic equation in α_0 whose solution is

$$\alpha_0 \sim -\frac{1}{5} \alpha_2^2. \quad (6)$$

This result will prove valuable in computing the area and Coulomb energies.

3. The area integral

Figure 1 shows a ‘ribbon’ of the surface area at co-latitude θ that goes all the way around the nucleus with angular width $d\theta$. The area of the ribbon will be its arc length times its circumference $r \sin \theta$. But the deformed nucleus does not have a spherical profile, so the arc length is not simply $r \, d\theta$. Rather, we have to compute it by using the general expression for the arc length in spherical coordinates for a trajectory running along a line of constant ‘longitude’ ϕ :

$$ds^2 = dr^2 + r^2 d\theta^2. \quad (7)$$

As r is a function of θ , we can write this as

$$ds^2 = dr^2 + r^2 d\theta^2 = r^2 d\theta^2 \left[1 + \frac{1}{r^2} \left(\frac{dr}{d\theta} \right)^2 \right]. \quad (8)$$

The area of the ribbon is then

$$dA = 2\pi r \sin \theta \, ds = 2\pi r^2 \sin \theta \sqrt{1 + \frac{1}{r^2} \left(\frac{dr}{d\theta} \right)^2} \, d\theta. \quad (9)$$

If the nucleus is not greatly distorted, then $dr/d\theta$ will be small. We can then invoke a binomial expansion

$$\sqrt{1 + \frac{1}{r^2} \left(\frac{dr}{d\theta}\right)^2} \sim 1 + \frac{1}{2} \frac{1}{r^2} \left(\frac{dr}{d\theta}\right)^2 - \frac{1}{8} \frac{1}{r^4} \left(\frac{dr}{d\theta}\right)^4 + \dots \quad (10)$$

From (1), $(dr/d\theta) = \alpha_2 R_0 (dP_2/d\theta)$, so, to retain terms to order α_2^2 , we need to only carry two terms in the expansion in (10):

$$dA = 2\pi \sin \theta \left\{ r^2 + \frac{1}{2} \left(\frac{dr}{d\theta}\right)^2 + \dots \right\} d\theta. \quad (11)$$

The surface area of the deformed nucleus, to this level of approximation, then comprises two contributions:

$$A = 2\pi \left\{ \int_0^\pi r^2 \sin \theta d\theta + \frac{1}{2} \int_0^\pi \left(\frac{dr}{d\theta}\right)^2 \sin \theta d\theta + \dots \right\}. \quad (12)$$

These integrals are fairly straightforward, and reduce to

$$A \sim 4\pi R_0^2 \left\{ (1 + \alpha_0)^2 + \frac{4}{5} \alpha_2^2 + \dots \right\}. \quad (13)$$

Substitute into this the result of volume conservation, $\alpha_0 \sim -\alpha_2^2/5$. Also invoke the usual nuclear radius approximation $R_0 \sim a_0 A^{1/3}$ ($a_0 \sim 1.2$ fm), and write the factor which converts the surface area to equivalent energy as Ω . U_S can then be written as

$$U_S \sim (a_S A^{2/3}) \left\{ 1 + \frac{2}{5} \alpha_2^2 + \dots \right\}, \quad (14)$$

where $a_S = 4\pi \Omega a_0^2 \sim 18$ MeV. The areal energy *increases* upon perturbation of the nucleus from its initially spherical shape; this is understandable in that a sphere is the surface of minimum area which encloses a given volume.

4. The Coulomb integral and the SF limit

Figure 2 illustrates the geometry of computing the Coulombic self-potential of the distorted nucleus. The nucleus is divided into elements of volume $d\tau$ throughout which the protons are assumed to be uniformly distributed. By considering pairs of volume elements labelled as '1' and '2', the electrostatic self-energy is computed from

$$U_C = \frac{1}{2} \frac{\rho^2}{4\pi \epsilon_0} \int_{(1)} \int_{(2)} \frac{d\tau_1 d\tau_2}{r_{12}}, \quad (15)$$

where ρ is the charge density and r_{12} is the distance between the two volume elements. Each volume element is three dimensional, so (15) is actually a *sextuple integral*. As in the computation of the surface area, integrals over r must be done before those over θ . Care must be taken to keep track of the '1' and '2' integrals and coordinates.

To treat the factor of r_{12} in the denominator, invoke the identity

$$\frac{1}{r_{12}} = \begin{cases} \sum_{k=0} \left(\frac{r_2^k}{r_1^{k+1}} \right) P_k(\cos \theta_{12}), & r_2 < r_1 \\ \sum_{k=0} \left(\frac{r_1^k}{r_2^{k+1}} \right) P_k(\cos \theta_{12}), & r_2 > r_1, \end{cases} \quad (16)$$

where θ_{12} is the angle between the directions from the origin to volume elements 1 and 2.

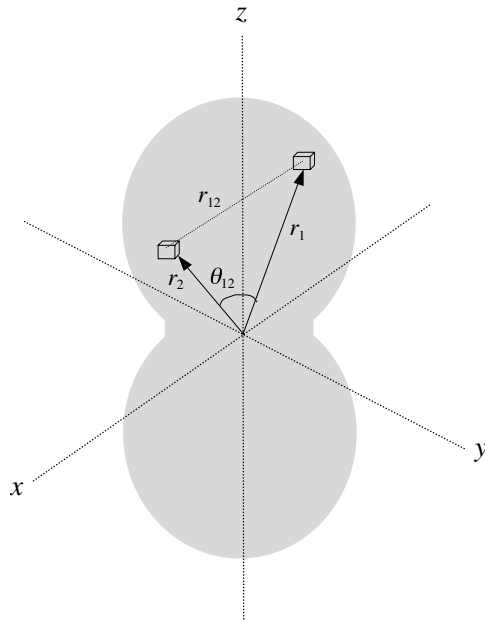


Figure 2. Geometry for computing the Coulomb self-energy of the nucleus. The two volume elements are located at distances r_1 and r_2 from the origin, separated by distance r_{12} . The angle between them as viewed from the origin is θ_{12} .

It is immaterial whether one integrates over the ‘1’ or ‘2’ coordinate first; I elect the latter and proceed by writing (15) as

$$U_C = \frac{\rho^2}{8\pi\epsilon_0} \int_{(1)} \left\{ \int_{(2)} \frac{d\tau_2}{r_{12}} \right\} d\tau_1. \quad (17)$$

Call the inner integral U_2 . To proceed, break it into two regimes, one for $r_2 = 0$ to r_1 (for which $r_2 < r_1$) and then from r_1 to $r_2(\theta_2)$ (for which $r_2 > r_1$), and use (16):

$$U_2 = \int_{(2)} \frac{d\tau_2}{r_{12}} = \int_0^{r_1} \sum_k \left(\frac{r_2^k}{r_1^{k+1}} \right) P_k d\tau_2 + \int_{r_1}^{r_2(\theta_2)} \sum_k \left(\frac{r_1^k}{r_2^{k+1}} \right) P_k d\tau_2. \quad (18)$$

Note carefully that P_k still means $P_k(\cos \theta_{12})$. As these integrals are over the ‘2’ coordinates, factors of r_1 can be extracted from within them but must remain within the sums. Writing the volume elements explicitly as $d\tau = r^2 dr d\Omega$ then gives

$$U_2 = \sum_k \frac{1}{r_1^{k+1}} \int_{\theta,\phi} \int_0^{r_1} r_2^{k+2} P_k dr_2 d\Omega_2 + \sum_k r_1^k \int_{\theta,\phi} \int_{r_1}^{r_2(\theta_2)} r_2^{1-k} P_k dr_2 d\Omega_2. \quad (19)$$

The first integral over r_2 is trivial and gives $r_1^{k+3}/(k+3)$; the second requires care in the case of $k=2$, where a logarithmic term arises:

$$U_2 = r_1^2 \sum_k \int_{\theta,\phi} \frac{P_k}{(k+3)} d\Omega_2 + \sum_{k \neq 2} \frac{r_1^k}{(2-k)} \int_{\theta,\phi} r_2^{2-k}(\theta) P_k d\Omega_2 \\ - r_1^2 \sum_{k \neq 2} \frac{1}{(2-k)} \int_{\theta,\phi} P_k d\Omega_2 + r_1^2 \int_{\theta,\phi} \ln \left(\frac{r_2(\theta)}{r_1} \right) P_2 d\Omega_2. \quad (20)$$

Now, from the addition theorem for spherical harmonics, $P_k(\cos \theta_{12})$ can be written in terms of products of associated Legendre polynomials whose arguments are the cosines of the *individual* direction angles of the volume elements:

$$P_k(\cos \theta_{12}) = \sum_{m=-k}^k \frac{(k-m)!}{(k+m)!} P_k^m(\cos \theta_1) P_k^m(\cos \theta_2) \exp[im(\phi_1 - \phi_2)]. \tag{21}$$

Imagine (21) substituted into (17). In integrating over ϕ_1 and ϕ_2 , only $m = 0$ will give non-zero contributions. The associated Legendre polynomials consequently reduce to regular Legendre polynomials, which I designate as $P_{k(1)}$ and $P_{k(2)}$ to keep track of which belongs to which volume elements. Thus, for example, $P_{k(1)}$ designates the k th-order Legendre polynomial for coordinate set '1'. Then we have

$$U_2 = r_1^2 \sum_k \frac{P_{k(1)}}{(k+3)} \int_{\theta,\phi} P_{k(2)} d\Omega_2 + \sum_{k \neq 2} \frac{r_1^k P_{k(1)}}{(2-k)} \int_{\theta,\phi} r_2^{2-k}(\theta) P_{k(2)} d\Omega_2 - r_1^2 \sum_{k \neq 2} \frac{P_{k(1)}}{(2-k)} \int_{\theta,\phi} P_{k(2)} d\Omega_2 + r_1^2 P_{2(1)} \int_{\theta,\phi} \ln\left(\frac{r_2(\theta)}{r_1}\right) P_{2(2)} d\Omega_2. \tag{22}$$

The first and third integrals in (22) vanish except when $k = 0$ in view of (4); they respectively give $4\pi r_1^2/3$ and $-2\pi r_1^2$ for a total of $-2\pi r_1^2/3$. The second and third integrals in (22) are a little more involved and involve further series expansions of the $r(\theta)$ terms; details are given in the online appendix. A crucial manipulation in carrying along expansions to correct orders in these two integrals is to factor terms of the form $r^p(\theta)$ as

$$\{1 + \alpha_0 + \alpha_2 P_{2(k)}\}^p = (1 + \alpha_0)^p \left\{ 1 + \frac{\alpha_2 P_{2(k)}}{(1 + \alpha_0)} \right\}^p, \tag{23}$$

and then undertake a binomial expansion of the brace bracket to order α_2^2 . The overall result for U_2 is

$$U_2 = -\frac{2\pi}{3} r_1^2 + 2\pi R_0^2 (1 + \alpha_0)^2 + \frac{4\pi}{5} P_{2(1)} \frac{r_1^2 \alpha_2}{(1 + \alpha_0)} + \pi \alpha_2^2 R_0^2 \sum_k P_{k(1)} \left(\frac{r_1}{R_0}\right)^k \frac{(1-k)}{(1 + \alpha_0)^k} \{k, 2, 2\}, \tag{24}$$

where $\{i, j, k\}$ designates the integral of the product of three Legendre polynomials over $x = \cos \theta$:

$$\{i, j, k\} = \int_{-1}^1 P_i P_j P_k dx. \tag{25}$$

At this point, (24) goes back into (17) to give the Coulomb energy as

$$U_C = \frac{\rho^2}{8\pi \epsilon_0} \left\{ -\frac{2\pi}{3} \int_{\theta,\phi} \int_0^{r_1(\theta)} r_1^4 dr_1 d\Omega_1 + 2\pi R_0^2 (1 + \alpha_0)^2 \int_{\theta,\phi} \int_0^{r_1(\theta)} r_1^2 dr_1 d\Omega_1 + \frac{4\pi}{5} \frac{\alpha_2}{(1 + \alpha_0)} \int_{\theta,\phi} \int_0^{r_1(\theta)} P_{2(1)} r_1^4 dr_1 d\Omega_1 + \pi \alpha_2^2 R_0^2 \sum_k \frac{(1-k)\{k, 2, 2\}}{R_0^k (1 + \alpha_0)^k} \int_{\theta,\phi} \int_0^{r_1(\theta)} r_1^{k+2} P_{k(1)} dr_1 d\Omega_1 \right\}. \tag{26}$$

Solutions for these integrals are detailed in the appendix; the result, again to order α_2^2 , is

$$U_C = \frac{\rho^2}{8\pi \epsilon_0} \pi^2 R_0^5 \left\{ \frac{32}{15} (1 + \alpha_0)^5 + \frac{128}{75} (1 + \alpha_0)^3 \alpha_2^2 \right\}. \tag{27}$$

On writing the charge density as $\rho = 3Ze/4\pi R_0^3$, again invoking $R_0 \sim a_0 A^{1/3}$ and substituting the volume-conservation condition $\alpha_0 \sim -\alpha_2^2/5$, U_C reduces to

$$U_C \sim a_C \left(\frac{Z^2}{A^{1/3}} \right) \left\{ 1 - \frac{1}{5} \alpha_2^2 + \dots \right\}. \quad (28)$$

where $a_C = (3e^2/20\pi\epsilon_0 a_0) \sim 0.72$ MeV is the Coulomb energy parameter. The Coulomb self-energy *decreases* upon perturbation of the nucleus from its initially spherical shape.

We can now determine the limiting condition for stability against spontaneous fission. If the nucleus becomes slightly distorted, that is, if $\alpha_2 \neq 0$, then fission will proceed spontaneously if the total energy of the deformed nucleus is less than what it was in its initial undeformed spherical shape ($\alpha_2 = 0$), that is, if $\Delta E = (U_S + U_C)_{\text{deformed}} - (U_S + U_C)_{\text{undeformed}} < 0$. On substituting (14) and (28), ΔE emerges as

$$\Delta E = \left(\frac{2}{5} a_S A^{2/3} \alpha_2^2 \right) \left\{ 1 - \frac{1}{2} \left(\frac{a_C}{a_S} \right) \left(\frac{Z^2}{A} \right) \right\}. \quad (29)$$

Clearly, whatever the value of α_2 , ΔE will be negative as long as

$$\frac{Z^2}{A} > 2 \left(\frac{a_S}{a_C} \right), \quad (30)$$

the Bohr and Wheeler SF condition. With $a_S \sim 18$ MeV and $a_C \sim 0.72$ MeV, the limiting Z^2/A evaluates to about 50. Readers seeking expressions for U_S and U_C to higher orders of perturbation are urged to consult [4–6].

With empirically known values for a_S and a_C , the Z^2/A limit provides an understanding of why nature stocks the periodic table with only about 100 elements: nuclei have $A \sim 2Z$, so $Z^2/A \sim 50$ corresponds to a limiting Z of about 100. In extending their analysis to higher orders of perturbation, Bohr and Wheeler also provided the first real understanding as to why only a very few isotopes at the heavy end of the periodic table are subject to fission by slow neutrons: yet heavier ones are too near the Z^2/A limit to remain stable for long against SF, while for lighter ones the fission barrier is too great to be overcome by the binding energy released upon neutron absorption. The theory of fission barriers later evolved into a computationally intense area involving factors such as shell effects and pairing corrections [7], but Bohr and Wheeler had set the stage.

5. Concluding remarks

It is always interesting to see how ‘classic’ results in the history of physics were obtained, and the Bohr–Wheeler calculation is no exception to this. On considering that Bohr arrived in America in early 1939 right after the discovery of fission and that their paper was submitted only 6 months later and covers extensive ground, they must have worked with great speed and agility in an area where experimental results were evolving rapidly. Their physical insight and command of the relevant mathematics was, and still is, nothing short of masterful.

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