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ANOMALIES IN NUCLEAR MASSES

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William D. Myers and Wladyslaw J. Swiatecki

August 10, 1966

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ABSTRACT

Recently gained insight into the nature of the shell correction to the mass of a nucleus, regarded as a function of nuclear deformation, enables one to understand some of the outstanding anomalous trends in nuclear masses, including the behavior of fission barriers.

In this talk I will describe recent work by William D. Myers and me.

When I started preparing this paper I was going to discuss five anomalies in nuclear masses, but, within the last month, two and a half of them have been explained. One of them is nothing less than the 15-year-old puzzle of the anomalous behavior of the fission barriers. We are rather excited about these developments, and I will spend most of my time describing the progress made and only briefly mention the remaining discrepancies.

First, let me list the five anomalies:

1. Heavy-Element Anomaly,
2. Rare-Earth Anomaly,
3. Fission-Barrier Anomaly,
4. Coulomb-Radius Discrepancy,
5. The "Wigner Term."

When I say "anomaly" I mean a pronounced trend that does not agree with the theory of nuclear masses and deformations that W. D. Myers and I have developed recently (Ref. 1). Since my "anomalies" are deviations from this theory, let me sketch it out for you in a few sentences.

Our theory gives a rough account of the wiggles in nuclear masses due to shell structure and of the accompanying nuclear deformations. The central idea in our treatment is that the energy of a nucleus is made up of a liquid-drop part and of a shell correction, the shell correction disappearing for a sufficiently large deformation of the nucleus. From

Fig. 1 you will see that if the shell correction for the sphere is negative, as is the case for a magic nucleus, there results a spherical equilibrium shape with unusual stability. On the other hand, if the shell correction is sufficiently positive (as in a region away from magic numbers), there results automatically a deformed nucleus. The amplitude of the bump goes up and down as one moves across the periodic table in a way indicated in Fig. 1. This is the result of assuming the single-particle levels in the spherical potential to be bunched into bands corresponding to the magic numbers. The shape of the bump was assumed to be a Gaussian function of deformation, and is supposed to represent the way in which the bunching disappears as the nucleus is distorted. Our choice of a Gaussian was just an admission of ignorance: we had no clear idea exactly how shells should disappear with deformation so we tried to be noncommittal and took a Gaussian. The new development that I will describe in a moment has to do precisely with an improved insight into this question.

Our original theory with a Gaussian bump whose amplitude goes up and down in arched humps as one goes from one magic number to another worked fairly well, but there were several remaining systemmatic discrepancies, which I listed at the beginning. The first two have to do with the behavior of masses in the region of deformed nuclei--the rare earths and the actinides ($N \gtrsim 88$ and $N \gtrsim 136$). Figure 2 shows the experimental and calculated shell effects, i.e., experimental and calculated deviations from a liquid drop formula, as functions of the

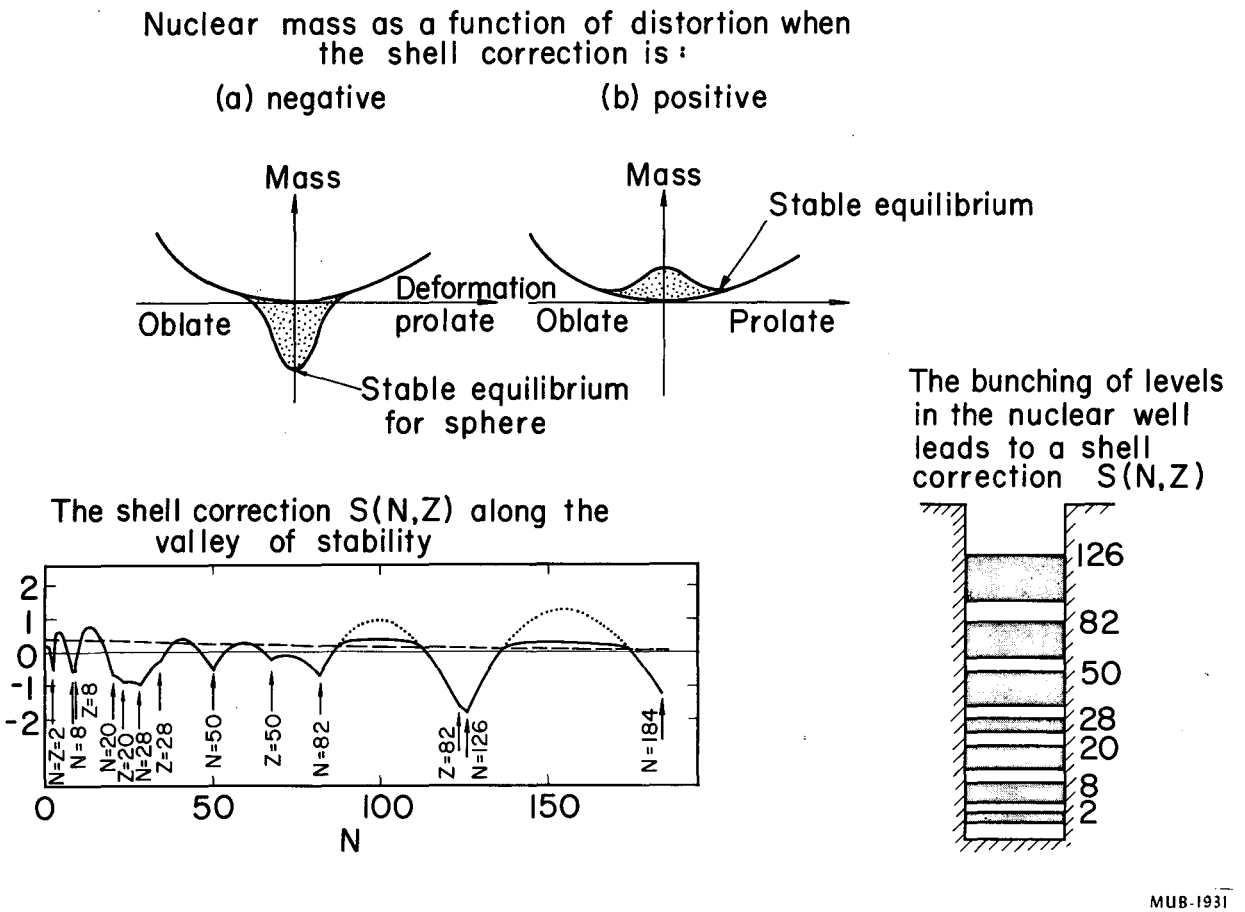


Fig. 1. The top part of the figure shows schematically how a negative shell correction leads to a spherical shape with special stability, whereas a positive shell correction leads to a deformed equilibrium shape. In the bottom left-hand part the amplitude of the shell-correction bump along the valley of stability is shown. (The plot is against neutron number.) When the amplitude exceeds a certain critical value, indicated by the dashed line, deformed equilibrium shapes appear. The shell correction is a consequence of the bunching of levels into bands corresponding to magic numbers, as shown schematically on the right. (This is an old figure--in our mass formula we preferred to leave out the magic number 20 and introduced 14 instead.)

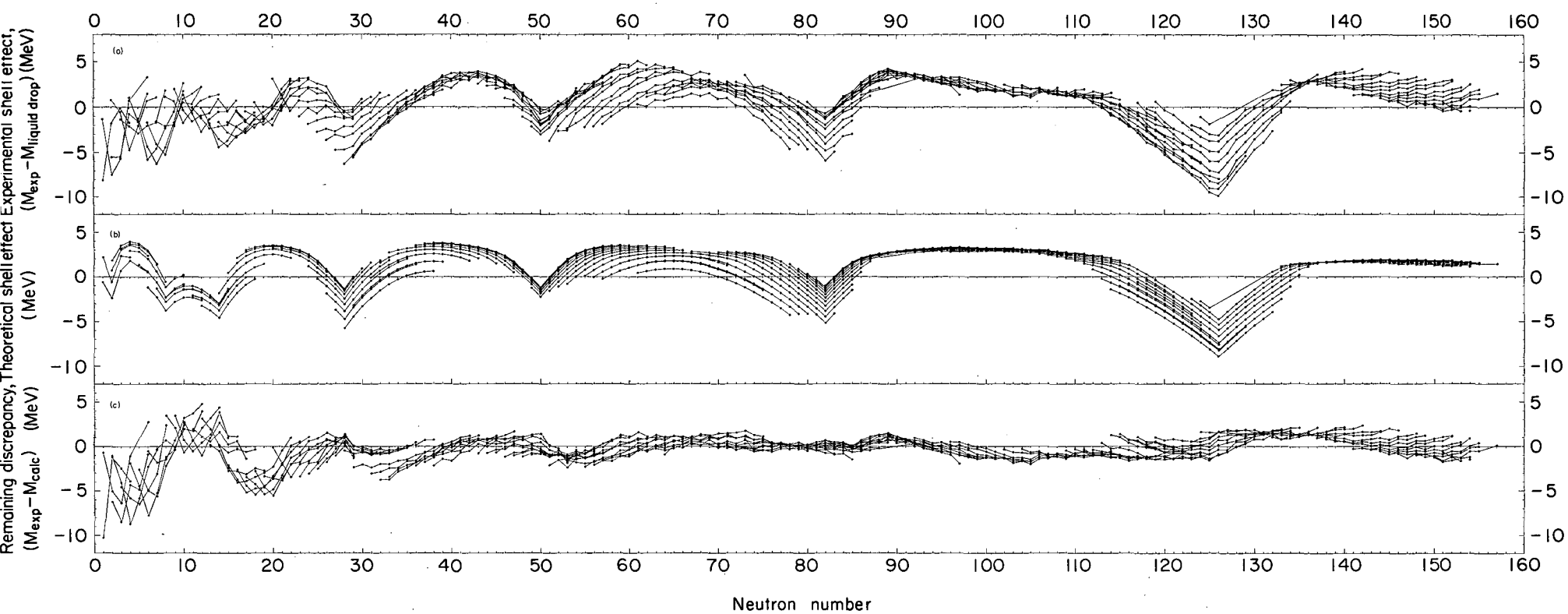


Fig. 2. The experimental and calculated shell effects and their difference are shown as functions of the neutron number. Isotopes of an element are connected by a line. This plot is based on our original mass formula and is to be compared with the revised version in Fig. 7.

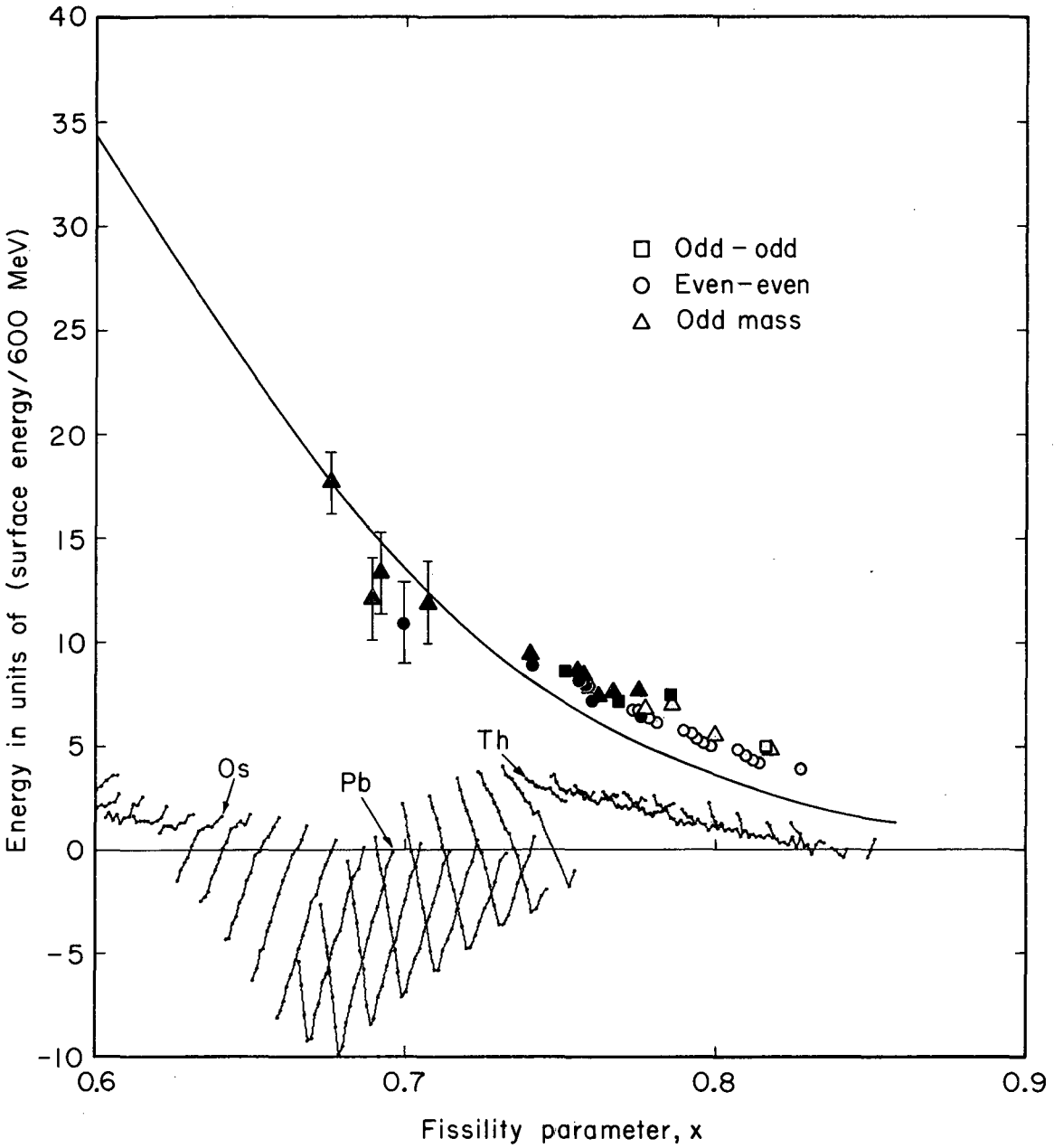
neutron number. Both experiment and theory show that with the onset of deformations there occurs an approximate flattening out of the otherwise arched mass deviations, but the experimental points tend to sag, whereas the calculated points remain somewhat arched. In the heavy elements the unexplained experimental sag is as much as 3 to 4 MeV between radium and fermium.

These are the rare-earth and heavy-element anomalies.

The fission-barrier anomaly is the old problem of why are the experimental barriers such slowly varying functions of Z^2/A? For example, the liquid-drop formula would predict fission barriers that decrease from 8.6 MeV for Th^{232} to 2.6 MeV for Fm^{254}, whereas experimentally these numbers are 5.2 MeV and 3.4 MeV. One way to illustrate the discrepancy is by comparing the calculated and experimental saddle-point masses (the masses of nuclei when at the top of the fission barrier). Figure 3 shows this comparison when our original mass formula is used. The smooth curve is the calculated saddle-point mass and, when normalized to pass through the point on the left (Tl^{201}), it misses the heavy elements by 1.5 to 2 MeV: the experimental fission barriers do not decrease fast enough.

The fission-barrier anomaly and the anomalous behavior of the masses of heavy nuclei in their ground states are closely related. After all, the ground-state mass of a nucleus defines one of the two extremities of a barrier, namely its bottom. We shall see how both anomalies, as well as half of the rare-earth anomaly, are explained by the same physical effect.

Fig. 3. This figure compares the calculated and experimental saddle-point masses. All masses are plotted with respect to a smooth reference surface, the mass of a liquid drop. The energies are in units of the surface energy of the drop. (The factor of 600 MeV, included in the units of the ordinate, is of the order of the surface energy of a heavy nucleus and makes a unit on the vertical scale approximately equal to 1 MeV.) The smooth curve is the calculated saddle-point mass. Closed symbols indicate measured barriers while open symbols are used for barriers inferred from spontaneous fission half-lives. Thallium-201, the normalizing point, is on the left. The lower part of the figure shows the behavior of the ground-state mass deviations for the heavy elements, with lines connecting isotopes. Compare this figure with Fig. 8.


Odd – odd
Even – even
Odd mass
Os
Pb
Th
Energy in units of (surface energy/600 MeV)
Fissility parameter, x
40
35
30
25
20
15
10
5
0
-5
-10
0.6
0.7
0.8
0.9

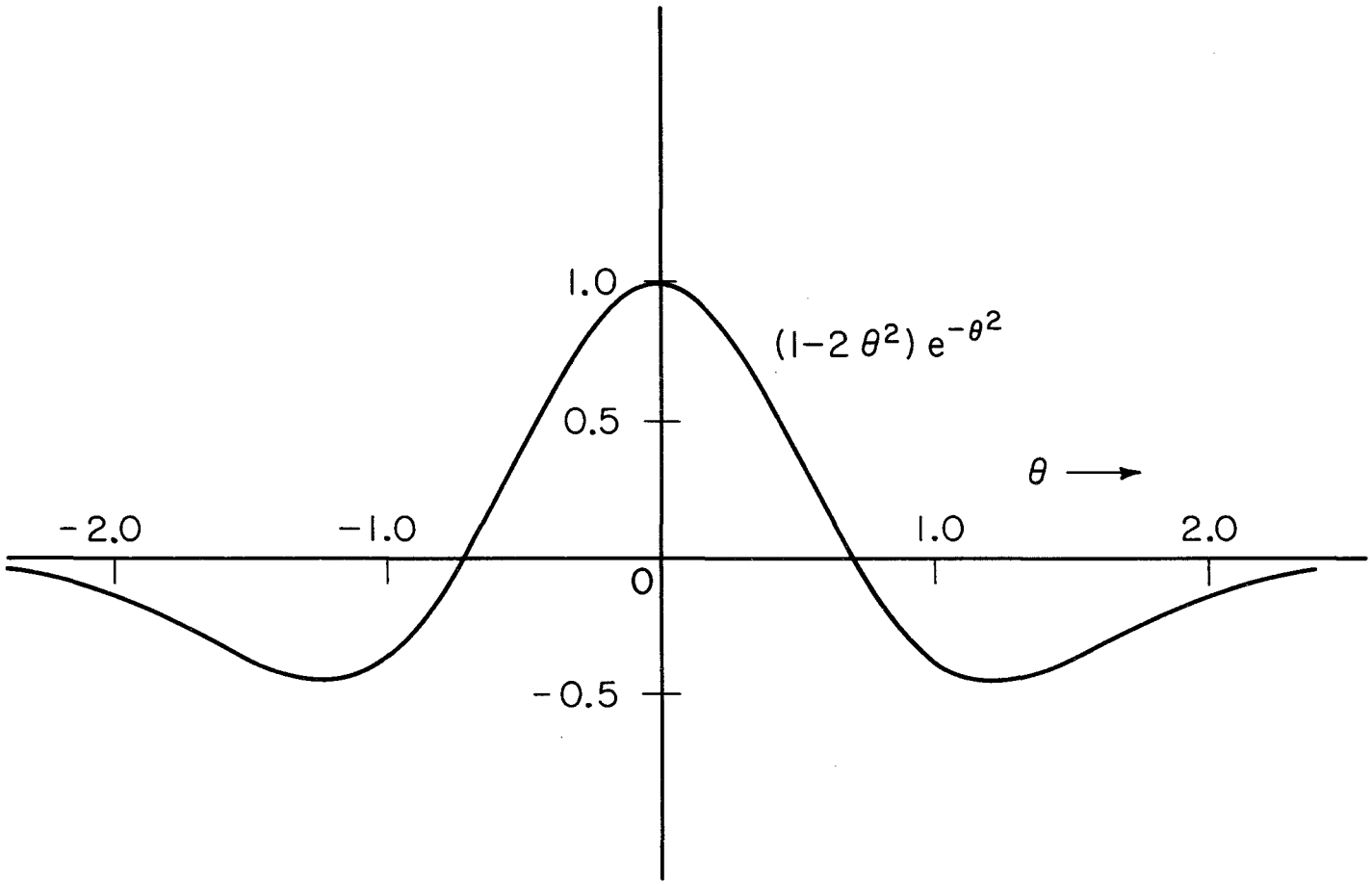


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Fig. 4. This is a plot of the revised shell damping function which replaces the Gaussian in our original mass formula. Its equation is $(1 - 2\theta^2)\exp(-\theta^2)$, where θ is a deformation variable.

What is this new physical effect?

It has to do with the nature of the shell damping function, which in our treatment was taken to be a Gaussian function of distortion. In what follows I shall present an argument why it is probably more like the function in Fig. 4 than a Gaussian. The difference is that there is one wiggle (or more) following the central bump.

The argument for the wiggles comes from looking more closely at the way that bands of bunched levels become debunched with deformation. Figure 5a shows a very schematic Nilsson level diagram, with levels fanning out from completely degenerate and equally spaced shells. We note that where the fans begin to overlap, regions of relatively higher level density replace the original gaps responsible for magic numbers. Thus, what used to be a closed shell (the end of a bunch of levels) is now, for a deformed nucleus, just the opposite, namely the middle of a bunched region. Thus special stability--an unusually low mass-- is replaced by special instability--a mass higher than normal. As the deformation increases further the shell effects keep getting reversed (though with decreased amplitude) and this gives rise to a wiggly approach towards the asymptotic (liquid-drop) situation.

The diagram in Fig. 5b is meant to indicate that with a more realistic level scheme the crossings between different fans are not likely to be all in phase, and that consequently the higher-order wiggles at larger deformations are less likely to survive. But the first shell reversal effect--the replacement of gaps by regions of increased density--seems an inescapable consequence of the basic features of the debunching of levels.

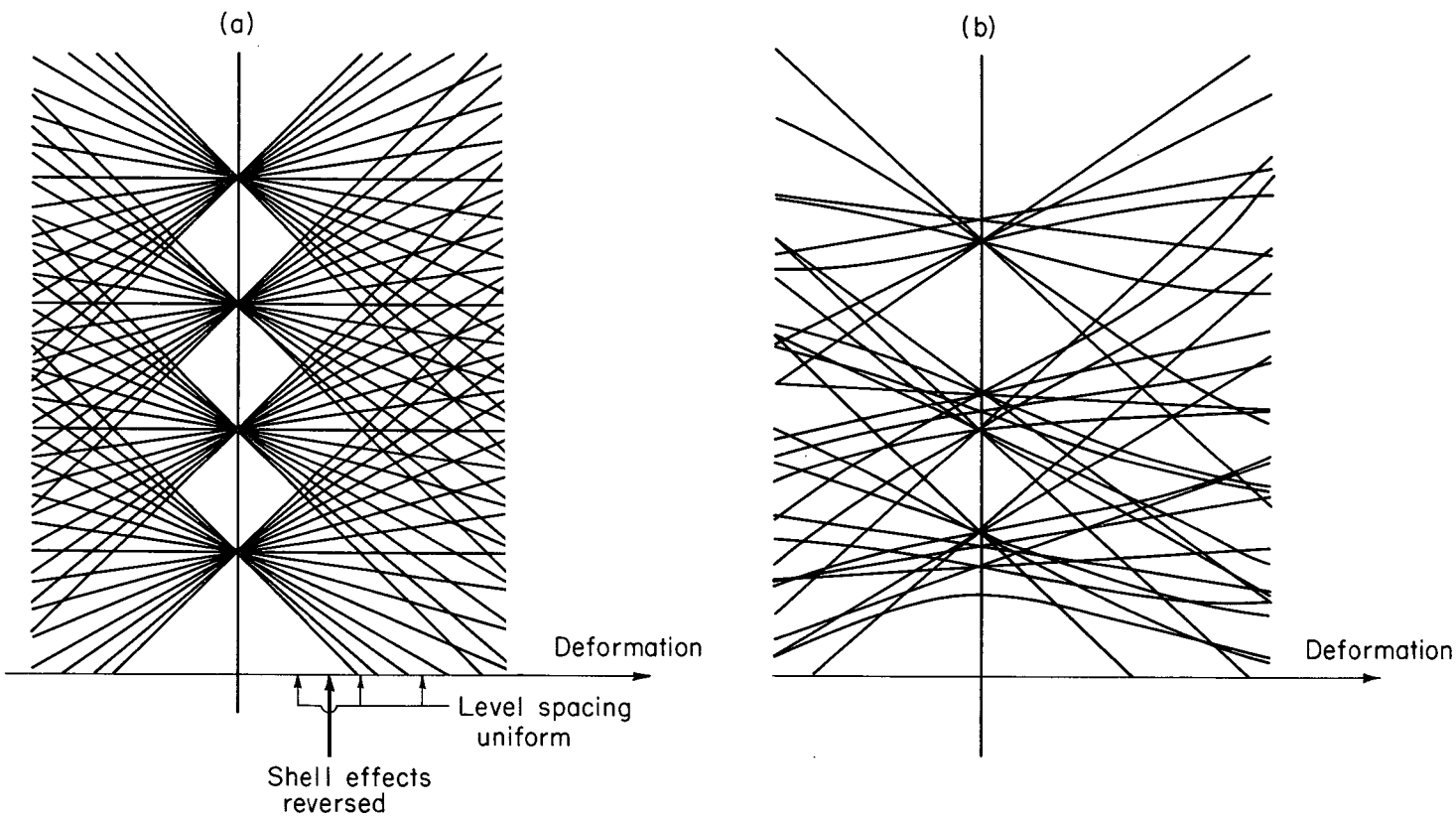

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Fig. 5. In (a) we show a highly schematic Nilsson level diagram with fans of levels radiating from equally spaced, completely degenerate bunches. The overlap of fans leads to regions of increased densities of levels. Every so often the level spacing becomes uniform, followed by a reversal of bunched and rarefied regions.
In (b) a more realistic, though still schematic, diagram illustrates the expectation that the higher-order reversals in (a) are less likely to survive.

Bearing all this in mind, we went ahead and invented a function that was like a Gaussian bump in being rapidly damped, but which possessed one extra wiggle. The function we like is essentially the second derivative of a Gaussian:

$$e^{-\theta^2} \quad \text{is replaced by} \quad -\frac{1}{2}\left[e^{-\theta^2}\right]'' = (1 - 2\theta^2)e^{-\theta^2} ,$$

where θ is a deformation variable, say a measure of the eccentricity of the spheroidal nuclear shape. (For a precise definition of θ consult Ref. 1, Section V.)

You can see at once the relevance of this change for the rare-earth and heavy-element anomalies. For a deformed nucleus the deformation energy now looks like Fig. 6a and the mass sags below the liquid-drop value--which is what we want.

Figure 7 shows the result of using the new shell function. We note that the heavy-element anomaly is reproduced quite well. The first half of the rare-earth region also looks very nice. The second half of the rare earths was poorly represented before and this has not improved (it is worse, if anything).

Figure 8 shows the new calculation of saddle-point masses. There is no longer any major or systematic discrepancy in the calculated fission barriers. The reason for the improvement, and the explanation of the notorious fission-barrier anomaly, is as follows. For the heavy deformed nuclei a fission barrier is a sum of two parts: the sag in the ground-state mass (a shell effect) and a liquid-drop part. The

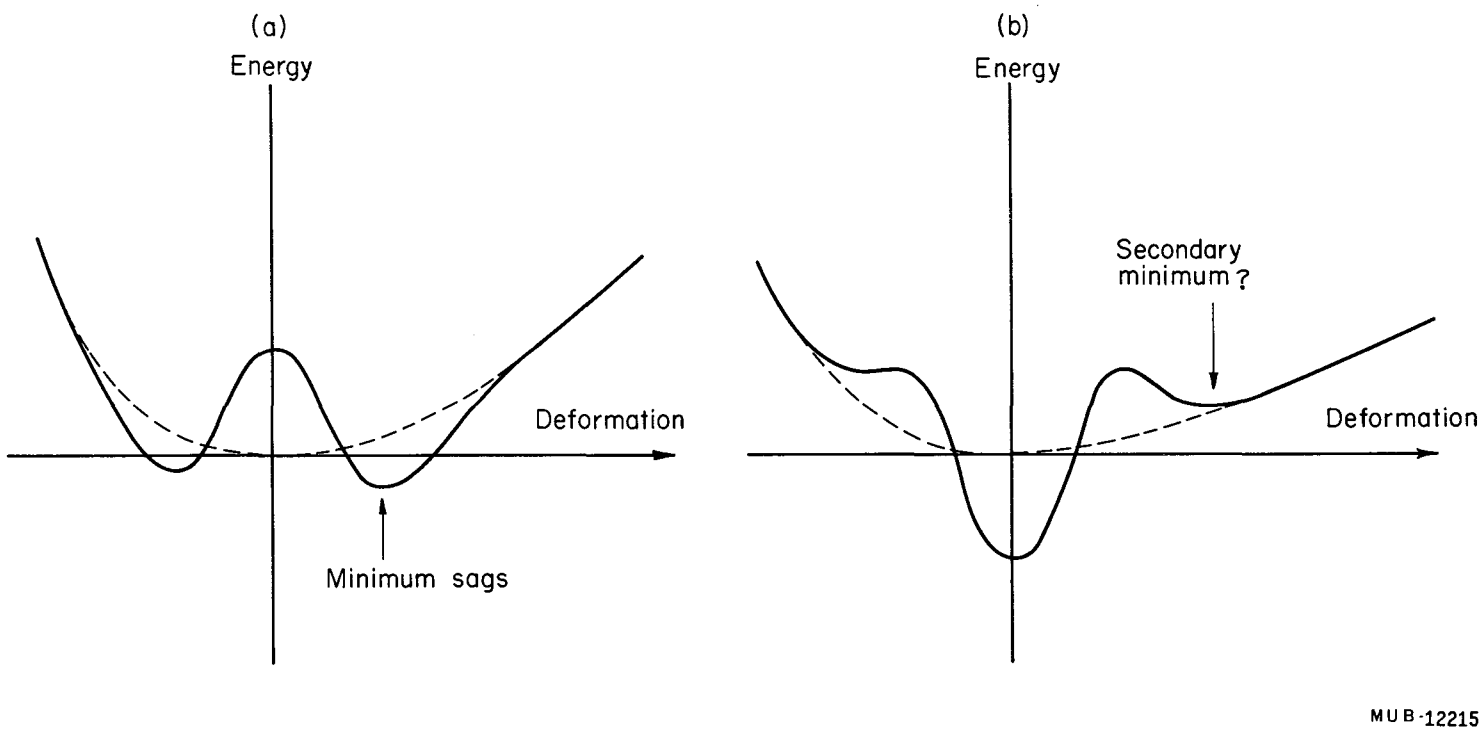


Fig. 6. Here we illustrate schematically the deformation energy when the new shell correction is included. In (a) the shell correction for the sphere is positive, and this leads to a deformed equilibrium shape whose mass sags below the liquid drop value. In (b) we illustrate the case of a magic nucleus, for which a secondary deformed equilibrium shape is predicted.

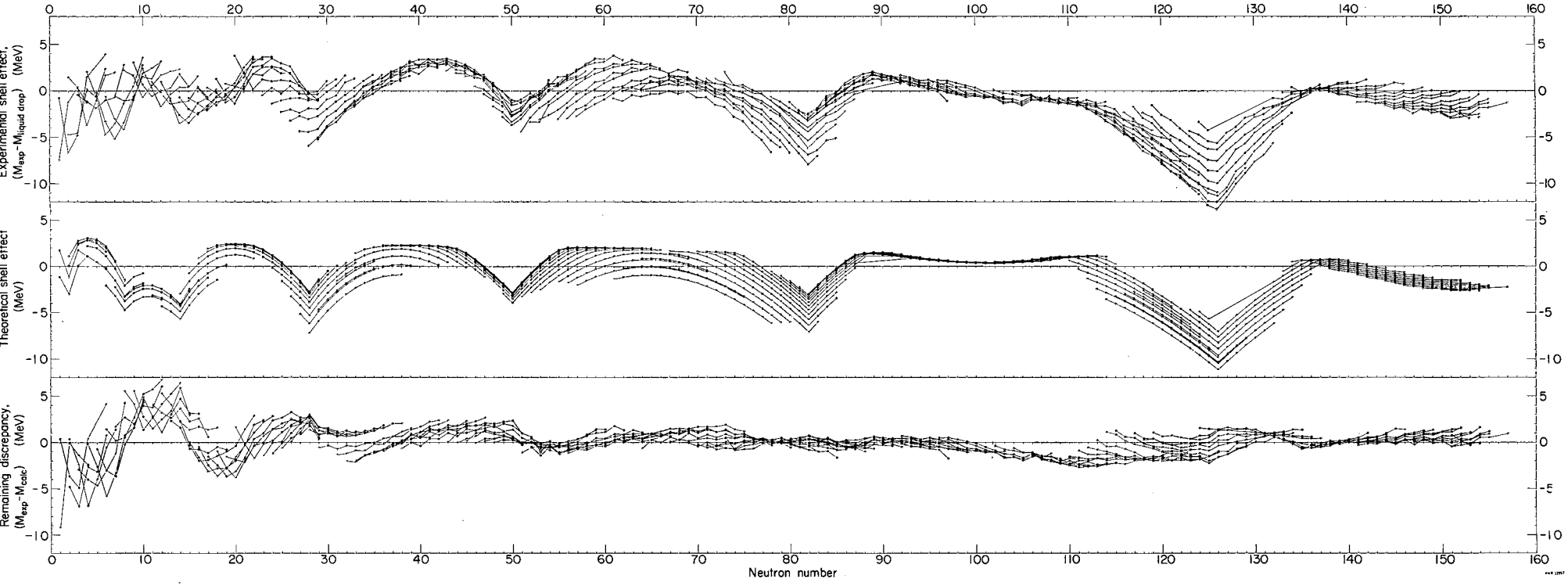
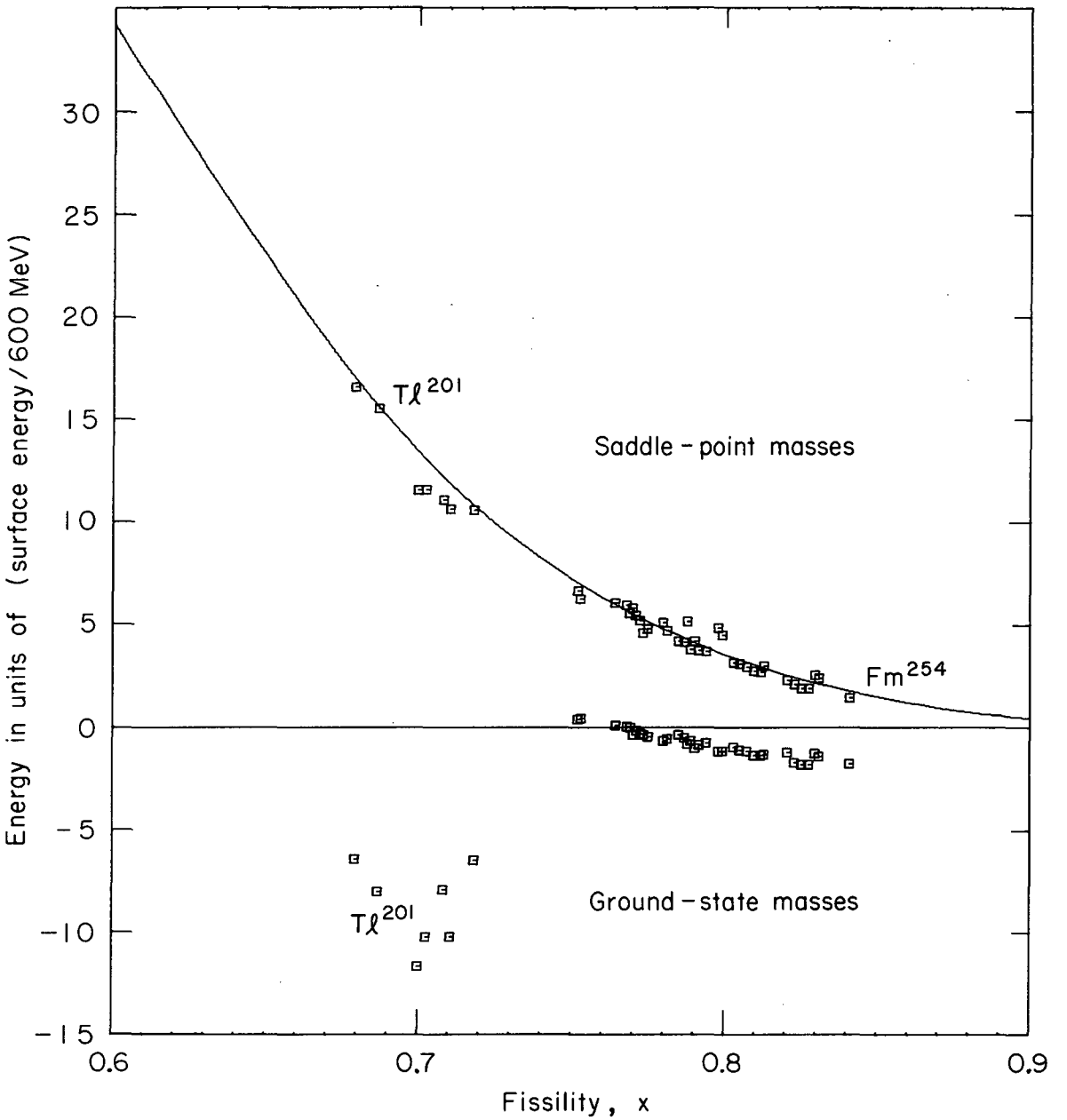


Fig. 7. This is like Fig. 2 but using our revised mass formula with a preliminary set of adjustable parameters. The "sagging" of the masses of the heaviest nuclei is now reproduced, as well as the trend in the first half of the rare-earth region. The representation of the second half of the rare-earth region has deteriorated.

Fig. 8. This is like Fig. 3 but using our revised mass formula. Six new barrier measurements due to Khodai (Ref. 6) have been included, and four less accurate determinations in the same region have been left out.


30
25
20
15
10
5
0
-5
-10
-15
Energy in units of (surface energy/600 MeV)
0.6
0.7
0.8
0.9
Fissility, x
Tℓ201
Saddle-point masses
Fm254
Ground-state masses
Tℓ201

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sagging itself increases as one goes towards the heavier elements (a result of the "mid-shell stability"), and this largely cancels the decrease in the liquid-drop part of the barrier, with the result that the barriers are almost constant between Th and Fm. So, at last, we are happy about the fission barrier problem and we will have somewhat more confidence in the future in predicting fission barriers and spontaneous fission half-lives.

While Bill Myers and I were working on these developments some weeks ago, a preprint from V. I. Strutinskii (Ref. 2) arrived which fitted in beautifully with what we were doing and gave us confidence that we were on the right track. Strutinskii gives a detailed analysis of nuclear masses and deformations by actually summing the energies of realistic Nilsson level diagrams. This is like older attempts along these lines by Mottleson and Nilsson,[3] Bés and Szymański,[4] and Marshalek et al.,[5] but Strutinskii is, I think, the first one to have made sure that the absolutely essential requirement of an asymptotic liquid-drop deformability is satisfied. Strutinskii's results exhibit explicitly the shell-reversal effect. (He refers to the mid-shell stabilities--our "sagging"--as "secondary shell effects."). In Fig. 9 you see an example of Strutinskii's wiggly shell correction functions, which in our theory are represented by the second derivative of a Gaussian. An interesting prediction pointed out by Strutinskii is the possible appearance of secondary minima in the deformation energy of magic nuclei (see Fig. 6b). Strutinskii's paper is also most relevant for predictions concerning superheavy elements.

In Ref. 2 Strutinskii also describes the effect of the shell

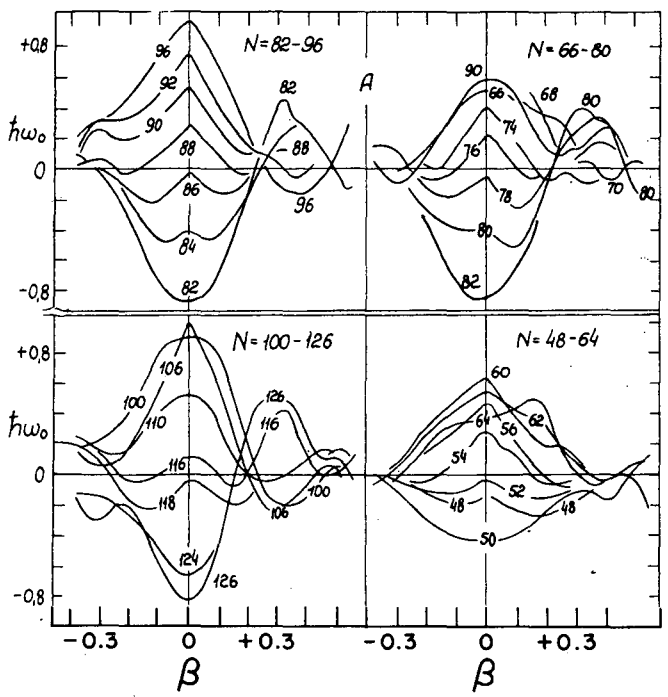

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Fig. 9. This is a reproduction of part of Fig. 4 from Strutinskii's paper (Ref. 2). It illustrates the dependence on deformation of the shell correction (in units of $\hbar\omega_0$) obtained by summing single-particle energies in a Nilsson oscillator potential. Note the shell reversal effect--a secondary wiggle following the primary bump.

correction on fission barriers. This, as well as an earlier paper by Strutinskii,[7] appears to be in at least qualitative agreement with our conclusions concerning fission barriers.

The relation between Strutinskii's work and ours is that his treatment is much more realistic, whereas ours is simpler. (The two treatments illustrate the complementary approaches corresponding to the dictums. "A theory need not be right, provided it is simple" and "a theory need not be simple, provided it is right.") The common feature of both treatments is the new insight gained into the nature of shell effects: the shell-reversal effect, or secondary shells, resulting from the overlap of the fans of Nilsson levels during the debunching of shells. It will be interesting to follow up this new insight and work out the consequence in other applications, for example, in discussions of fission-fragment deformabilities and in the problem of nuclear level densities.

Let me finally mention the discrepancies and anomalies that still remain. I have already pointed out the discrepancy in the heavy rare-earth region. This we are not particularly worried about--we presume it is a minor peculiarity of the single-particle level spacings. In fact it must be so, since Strutinskii seems to be able to account very well for the masses and deformations of nuclei in this region.

A more serious problem is the so-called "Wigner Term." The experimental evidence from the lighter part of the periodic table is quite clear that something like a "Wigner Term"--a contribution to the

masses proportional to $|N - Z|$ --is necessary. Chin-Fu Tsang in Berkeley has been studying this problem for some time. One difficulty is that in order to include such a term in our mass formula we have to know how it depends on the nuclear shape, and there is little guidance on this point from existing theory and none from experiment. Still, there are several reasonable suggestions as to the origin of a term in $|N - Z|$, and the problem is one of isolating the correct explanation and describing the effect in a simple and adequate manner.

The most puzzling discrepancy at this moment is perhaps the 5 to 10% difference in the Coulomb energies or Coulomb radii deduced from the nuclear masses and fission barriers on the one hand, and from the Stanford electron-scattering experiments on the other. We tend to take this discrepancy very seriously because the accuracy of the determination of the Coulomb energy term from nuclear masses, when fission barriers are taken into account, is very high, of the order of the accuracy of the Stanford measurements, which is about 1%. Thus we have a discrepancy which is 5 to 10 times any reasonable estimate of errors. We have no explanation to offer. We intend to look into the effect of including the exchange correction to the Coulomb energy (we already have a correction for the diffuseness of the change distribution). Could it be some indirect result of a curvature correction to the surface energy or of a Wigner Term in the symmetry energy?

To summarize, we seem to have the following situation. We have available today a fair overall understanding of nuclear masses and

deformations, including the effects of shell structure. The main features of masses, quadrupole moments, and fission barriers can be accounted for with an astonishingly simple mass formula (with seven parameters), and if one wants a more detailed description one can bring in Nilsson-type calculations and obtain a really quantitative understanding of many finer details.

Some of the outstanding problems are:

1. The Wigner Term, especially its shape dependence,
2. The Coulomb-radius discrepancy,
3. A comprehensive extension of Strutinskii's work to all nuclei and to more general deformations.

APPENDIX

We give here a preliminary set of parameters for our revised mass formula. The notation is exactly the same as in Ref. 1. The revised formula is obtained by replacing the Gaussian $\exp(-\theta^2)$ in Eq. (10) of Ref. 1 by $(1 - 2\theta^2)\exp(-\theta^2)$. The new parameters, which replace those given in Section VI of that reference, are then

$$a_1 = 15.4941 \text{ MeV},$$

$$a_2 = 17.9439 \text{ MeV},$$

$$c_3 = 0.7053 \text{ MeV} \quad (\text{hence } r_0 = 1.2249 \text{ fermi}),$$

$$\kappa = 1.7826,$$

$$C = 5.8 \text{ MeV},$$

$$c = 0.325,$$

$$\frac{a}{r_0} = 0.444.$$

These are preliminary values. We do not expect the final values to differ materially.

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FOOTNOTES AND REFERENCES

* Text of talk to be given by W. J. Swiatecki at the International Symposium on "Why and How Should We Investigate Nuclides Far Off the Stability Line?," Lysekil, Sweden, August 21-27, 1966.

† Work done under auspices of the U. S. Atomic Energy Commission.

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