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Unified Theory of Nuclear Structure, Fission and Alpha-decay and New Predictions for Superheavy Nuclei

Jednolita teoria struktury jądrowej, rozszczepienia i rozpadu α
oraz nowe przewidywania dla jąder superciężkich

Единая теория ядерной структуры, деления и альфа-распада,
и новые предположения в области сверхтяжелых ядер

I. INTRODUCTION

Before deciding on a particular approach to the rather complicated nuclear many-body problem, it is prudent to first consider the main ingredients which must necessarily be included in a general model of atomic nuclei.

In a recent and excellent review of nuclear models, Elliott [1] has identified a number of ingredients which are thought to be essential for an understanding of nuclear structure: (1) The central field (responsible for single-particle effects like magic numbers and shell effects). (2)

The freedom to deform this field in a quadrupole manner (so as to explain the collective effects like large quadrupole moments and moments of inertia). (3) The need for pairing correlations (so as to explain pairing effects like odd-even mass differences and the reduction of moments of inertia compared to the rigid-body values). (4) The use of deformation parameters as dynamical variables (so as to explain shape fluctuations leading to beta- and gamma- vibrational bands).

To these four, we would add a fifth ingredient: (5) Inclusion of pairing fluctuations, so as to explain the very low-lying $K\Pi = 0^+$ bands (for instance those in the spectra of Ge isotopes [2]), and so as to include important contributions to the mass parameter associated with time-dependent variations in the energy gap and in the Fermi energy [see Ref. [3], Eq. (7.15-7.35)].

Several models employed for a large range of nuclei include the first three of these ingredients, but neglect the last two. Aside from the Dynamic Deformation Model (DDM) [2-4] developed by the present author (with occasional help on the computational problems from some collaborators), there is only one other general model (one applied to nuclei of different shapes and of different mass regions) of nuclear structure which includes all five ingredients discussed above, namely the Interacting Boson Model (IBM) [1,5,6]. However, the IBM is not valid for the problems of nuclear fission and for superheavy nuclei.

One of the major arguments presented in this article is that inclusion of the last two ingredients (the dynamics of shape and pairing fluctuations) is essential not only for the theory of nuclear structure but also for that of nuclear fission. The two main reasons are: (1) Although one may in some cases estimate the fission life-time quite well by calculating the penetration through one-dimensional barriers, the zero-point energy due to various collective degrees of freedom should not be ignored. (2) One may neglect the dynamics of shape and pairing fluctuations and still fit many nuclear properties by adjusting model parameters (for example, spin-orbit strengths). However, this may lead to model parameters which are fine for fitting the available data but which are unreliable for making extrapolations to unknown regions.

Although a fully unified theory of nuclear structure, fission, and reactions has not been attained as yet, much progress has been made. The following partial unifications have been attained in the DDM: (i)Unified theory of spherical-transitional-deformed even nuclei [7]. (ii) Unified theory of light-medium- heavy even nuclei [3]. (iii) Unified theory of nuclear structure, fission, and α-decay [4]. Attempts are in progress towards the unification of (iv) structure and reaction theory [8], (v) structure of even and odd nuclei [9], and of (vi) low-energy and high-energy (giant quadrupole resonance) vibrations [10].

Some recent developments concerning the unification of the theories of nuclear structure, fission, and alpha-decay are summarized below. This work has been inspired first by the confidence in this approach exhibited by Dr. M. G. Mustafa of Lawrence Livermore Laboratory (who also provided invaluable help with some of the computations), and secondly by the constructive criticism of Professor Stan Szpikowski who provided the necessary impetus to further improve the theory. This led to the unexpected unification of the theories of fission and alpha-decay. Hopefully, this is also more acceptable to him as well as to other critics.

II. Summary of Previous Developments Of The DDM

The DDM employs the Adiabatic-Time-Dependent-Hartree-Fock (ATDHF) method. A nice review of several earlier versions of this method has been given in the textbook by Ring and Schuk [11]. The version used in the DDM is closest to that discussed by Baranger and Kumar [12]. Very briefly, the important differences are the following.

The quadrupole-quadrupole interaction part of the Pairing-Plus-Quadrupole (PPQ) model has been replaced by the Nilsson - Strutinsky method where the average field is deformed in general simply because the field vibrates with different frequencies in different directions [13] (The assumption of equal frequencies in all directions is dropped, but the nucleus has the freedom to choose such equality in special cases.), and where the problems associated with "double-counting" in the calculation of the deformation energy are removed by employing the shell-correction method [14]. This removes the problems associated with the long range behaviour of the quadrupole force which would make all nuclei completely unstable against fission if it were allowed to mix as many shells as needed for convergence and for the correct calculation of the inertial functions. Eleven major shells are allowed to mix completely in the latest version of the DDM [4,15] and no fudge factors are needed for the inertial functions. No effective charges are needed for the B(E2) values. No effective gyromagnetic ratios are needed for the magnetic moments.

Thus the DDM combines the best features of the Nilsson-Strutinsky method (handling of large configuration spaces, thus avoiding the need for adjustment of model parameters from nucleus to nucleus or from one nuclear region to another, at computation times reduced by many orders of magnitude compared to the full Hartree-Fock-Bogoliubov calculations) and of the PPQ model (inclusion of the full dynamics of the five-dimensional quadrupole motion and of the four-dimensional pairing fluctuations , thus providing a unified theory of spherical - transitional - deformed nuclei).

It has been shown that this model is capable of predicting the low energy properties of practically all even-even nuclei without any adjustment of parameters from nucleus to nucleus [3]. In fact the codes have been made available to graduate students in experimental nuclear physics at Sussex who have computed quite detailed spectroscopic properties of about 100 nuclides with Z = 36-88, A = 72-228 (Ref. [16], and to be published).

III. EXTENSION OF THE DDM TO FISSION AND TO ALPHA-DECAY

This extension has involved four different steps which are summarized below. Details will be presented in a book in preparation [4].

A. The configuration space was expanded from the $9\hbar\omega$ space used earlier [2,3,16] to a $11\hbar\omega$ space. While the $B(E2;0\rightarrow2)$ value of ^{240}Pu, calulated in the smaller space used previously, was too small by 40%, the correct value (within

1%) is obtained in the enlarged space calculations.

B. The quadrupole deformation, which plays such an important role in nuclear structure, is not sufficient for describing nuclear fission. Inclusion of the hexadecapole multipole would help, but it is not sufficient for a correct description of the asymptotic region near and beyond the scission point. Also, it woud not be enough for a unified description of fission and alpha-decay. Therefore, we have employed several unconventional steps.

(1) The structure associated with the ground state is determined by solving the nine-dimensional problem formulated in terms of eight conventional variables (neutron & proton energy gaps, neutron & proton Fermi energies, three Euler's angles, and the axial asymmetry angle γ), and one unconventional variable, the "eccentricity" variable defined by

$$\varepsilon = [(1 - R_1 R_2 / R_3^2)_{\gamma=0}]^{1/2} , \tag{1}$$

where R_k (k=1,2,3 for x,y,z) is a semi-axis length of the equivalent ellipsoid (which has the same $\langle r^2 \rangle$, $\langle Q_0 \rangle$, $\langle Q_2 + Q_{-2} \rangle$ as the nucleus). The three semi-axis lengths are related to the deformation variables (δ, γ) of Hill and Wheeler [17]:

$$R_k = R_0 \exp [\delta \cos (\gamma - 2 k \pi / 3)] . \tag{2}$$

On combining Eq. (1) and (2), one obtains

$$\delta = [- (2/3) \ln (1 - \varepsilon 2)]^{1/2} . \tag{3}$$

(2) A variable "r" is defined which represents in the asymptotic region the distance between the centers of mass of the two fission fragments, and which represents the distance

between the centers of mass of two halves of the parent nucleus (taken to be symmetric at small deformation where the eventual charge and mass asymmetry have no effect). This variable is thus related to the nuclear length along the fission axis (taken to be the 3-axis) via

$$r = (3/4)\ R_3 \ , \tag{4}$$

and consequently to the shape variables ($\epsilon\ \delta\ \gamma$).

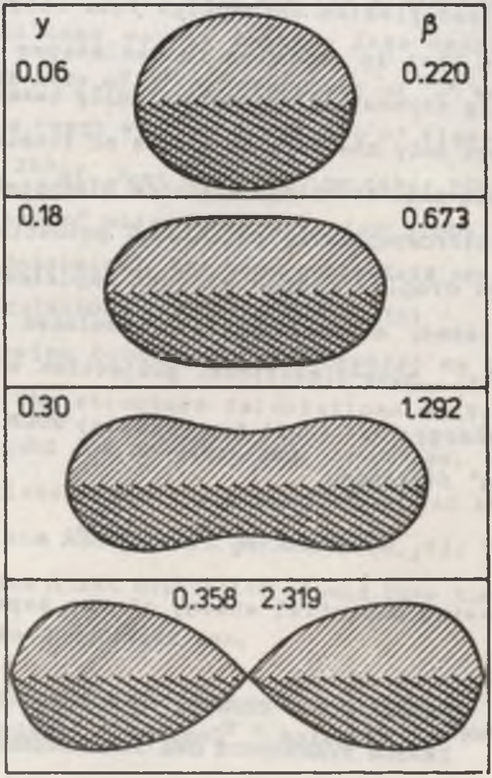


Fig. 1. Typical Nuclear Shapes in The Extended DDM

The eccentricity variable, defined via Eq.(1-4), allows us to include all even multipole deformations since as ε varies from 0 to 1, all even multipole deformations (of a multpolar expansion of the nuclear surface) vary from 0 to ∞. However, the shape remains ellipsoidal and necking is not formed. Hence, we match the shapes defined above to those of the y-family defined by Hill and Wheeler [17]. The matching is performed via the eccentricity variable defined by Eq. (1). The consequent shapes for some typical values of "y" and β are given in Fig. 1. Clearly, the present formulation allows us to describe nuclear fission upto quite late stages of nuclear fission. Note that in addition to the shapes shown in the figure, axially asymmetric shapes are fully taken into account but they affect only the earlier stages of fission, before the nucleus reaches the "touching" distance discussed below.

C. The microscopically calculated potential energy (the y-γ-dependent droplet energy without empirical shell-effect and pairing terms; microscopically calculated shell effect, pairing energy, nine-dimensional projection correction, and zero-point energy; see [2,3] for details) V^{DDM} is matched at the "touching" distance,

$$r_t = 1.4 \text{ fm } (A_1^{1/3} + A_2^{1/3}) , \tag{5}$$

to the following potential energy of two separated fission fragments,

$$V_{NN} = - Q_{fission} + V_{Coulomb} + V_{nuclear} , \tag{6}$$

where the first term is just the fragment mass energy relative to that of the parent nucleus, the second term is the Coulomb interaction between the two fragments,

$$V_{Coulomb} = Z_1 Z_2 e^2/r \ , \qquad (7)$$

and the third is the nuclear interaction,

$$V_{nuclear} = - V_0 r_{0n} A^2 (A_1 A_2)^{2/5} \exp[-r/r_{0n}] / r \ . \qquad (8)$$

The Yukawa form is chosen for the nuclear part of the nucleus-nucleus (or ion-ion) interaction. The corresponding range, r_{0n}, is assumed to arise from pion exchange and equals $\hbar / (m_\pi c) = 1.438$ fm. The strength parameter V_0 and the power of $(A_1 A_2)$ were determined by fitting two quantities, the spontaneous-fission half-life and the alpha-decay (which is treated in the same way as fission into nearly symmetric fragments) half-life of ^{240}Pu. The power of "A" was determined by fitting in a rough way the variation of fission half-life from ^{240}Pu to ^{260}Rf. Just like all the other DDM parameters, the three "fission" parameters are also global parameters. Once they are determined, the same parameters are used for all subsequent calculations for different nuclei.

The following conditions are imposed on the matching function: (1) The structure calculations of $E_{ZPM} = E_{g.s.} - V_{min}$, etc., should not be disturbed. Therefore, the potential minimum associated with the ground state and the curvature near the minimum should not be affected. (2) The modified potential and its first derivative should have the same values at $r = r_t$ as the unmodified one.

IV. DISCUSSION OF RESULTS FOR SELECTED TRANSURANIC AND SUPERHEAVY NUCLEI

Four examples of the effects of the two matchings (ε to "y" which affects the droplet energy, and the matching to the nucleus-nucleus potential) discussed above are given in Fig.2.

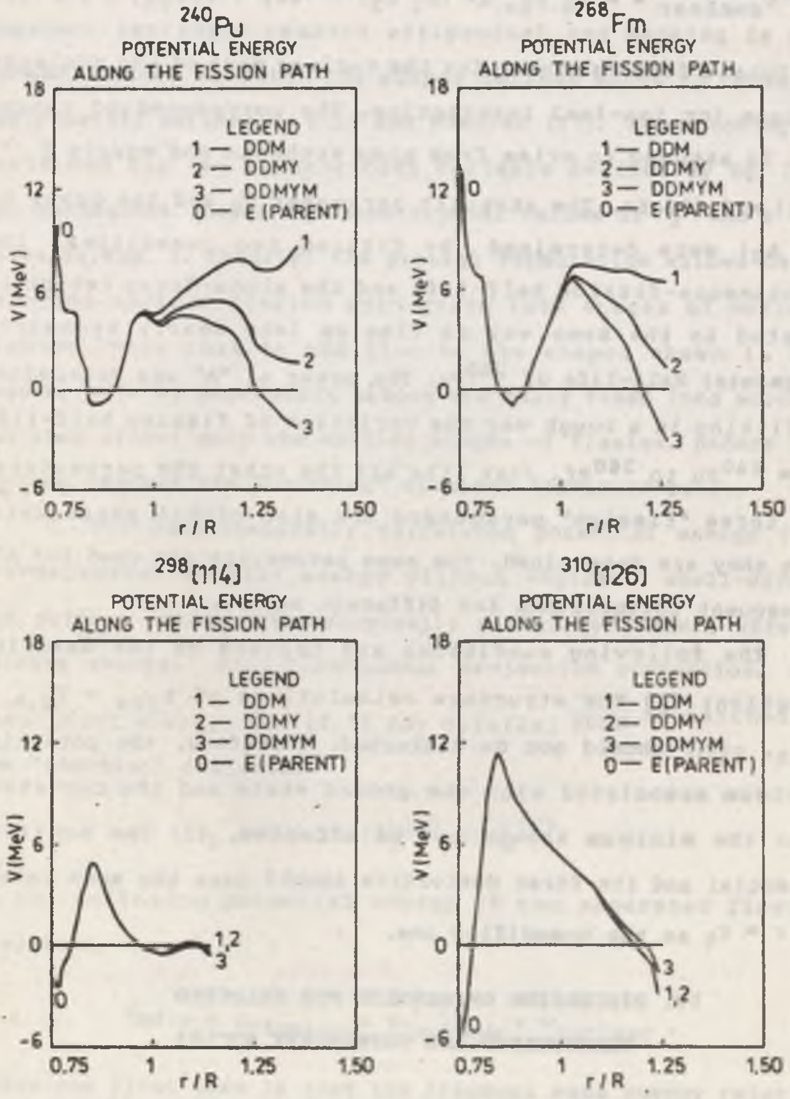


Fig. 2. Potential Energy Along The Fission Path.

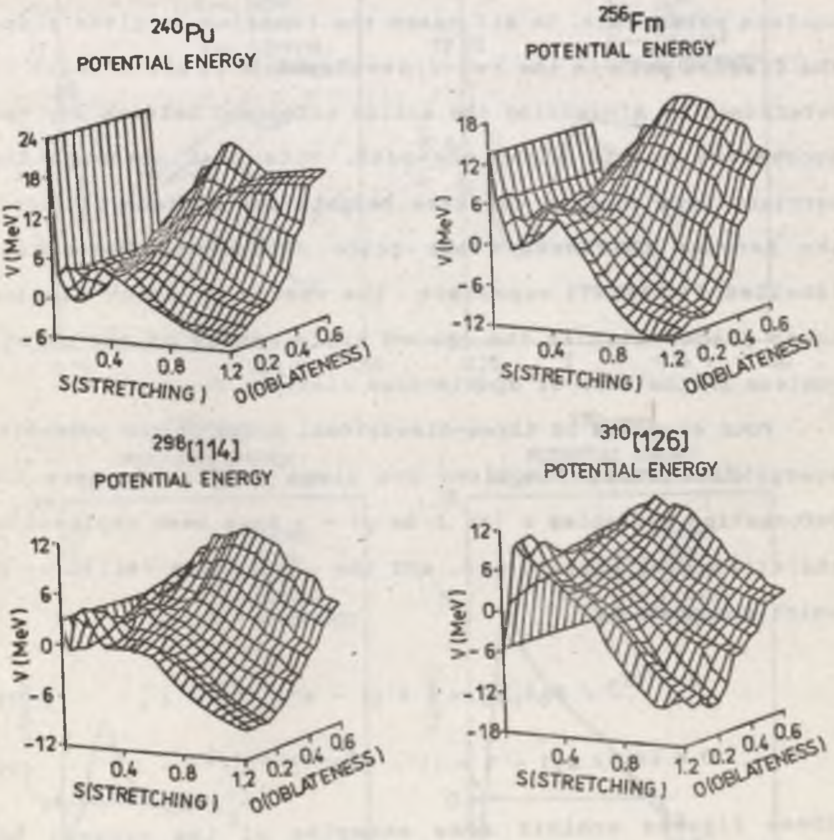
The abscissa are the dimensionless ratios r/R, where r is the separation distance (see Eq. 4) and R is the radius of the equivalent sphere. The ordinates are the three potential energy values: DDM (potential energy calculated microscopically in the DDM). DDMY (after inclusion of correction due to matching to the y-family of shapes). DDMYM (after inclusion of correction due to matching to the nucleus-nucleus potential). In all cases the function is given along the fission path in the two-dimensional ($\varepsilon\ \gamma$) plane which is determined by minimizing the action integrand between any two successive points along the path. Note that although the barriers have roughly the same heights for different nuclei, the barrier thicknesses are quite different. THe curves labelled E (PARENT) represent the energy at which fission takes place which is the ground state energy of the parent nucleus in the case of spontaneous fission.

Four examples of three-dimensional plots of the potential energy (the final function) are given in Fig. 3. Here the deformation variables ε (or δ or y) - γ have been replaced by the stretching variable, S, and the oblateness variable, O, which are given by

$$S = (R_3 / R_0)_{\gamma=0} - 1 = (1 - \varepsilon^2)^{-1/3} - 1 \, , \tag{9}$$

$$O = (R_1 / R_2) - 1 = (1 - \varepsilon^2)^{-(\sin\gamma)/\sqrt{3}} - 1 \, . \tag{10}$$

These figures exhibit some examples of the general DDM prediction that although the ground state potential minimum, associated with the parent nucleus, occurs in the case of most deformed nuclei for the axially symmetric shapes ($\gamma = 0 = O$), and the fission exit (or scission) also occurs for such shapes, the fission valley passes through non-axial shapes in all cases. Hence, aside from its effect on the zero-point-motion energy (the ground state energy, normalized to zero in the figures, minus the potential minimum energy), the γ degree of freedom is absolutely essential for an accurate description of nuclear fission.


^{240}Pu POTENTIAL ENERGY

^{256}Fm POTENTIAL ENERGY

^{298}[114] POTENTIAL ENERGY

^{310}[126] POTENTIAL ENERGY

Fig. 3. Three-Dimensional Plots Of The Potential Energy.

Fig. 4-5 give comparisons of some of the calculated (EXTENDED DDM) alpha-decay- and fission- related results with those of previous theoretical calculations of Fiset and Nix

[18] and of Randrup et al. [19]. Comparisons with experiment are also given there.

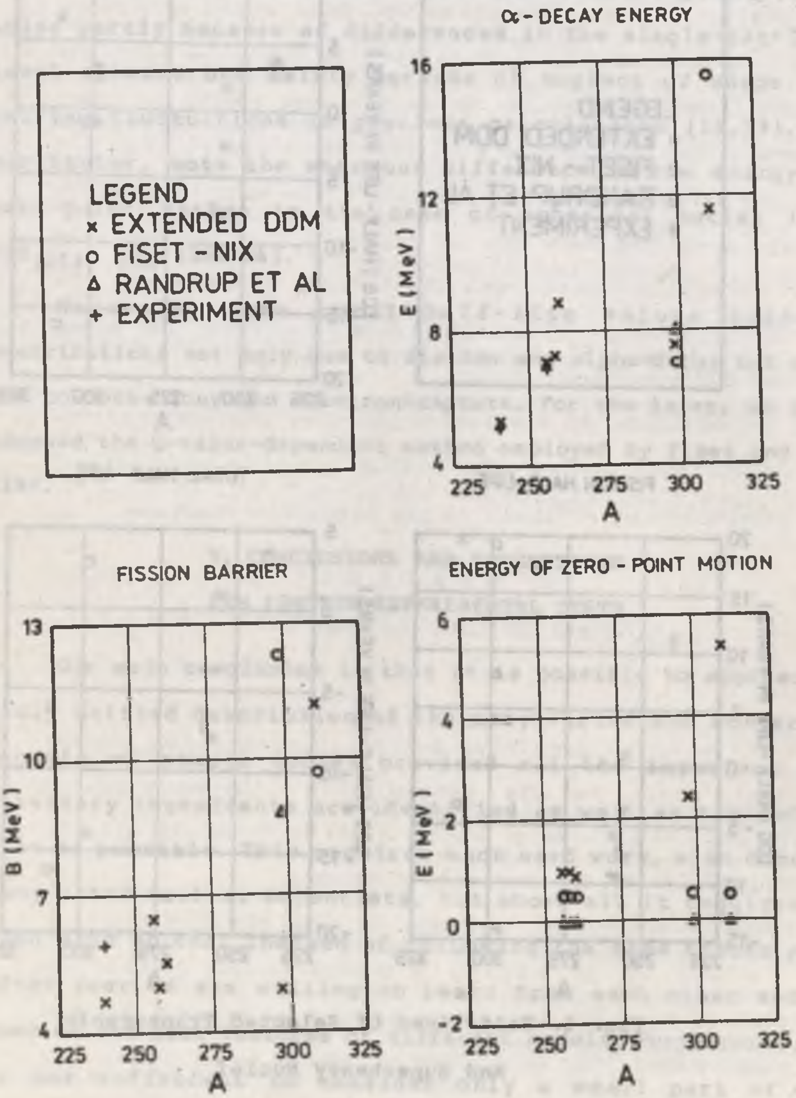


Fig. 4. Properties Of Selected Transuranic And Superheavy Nuclei

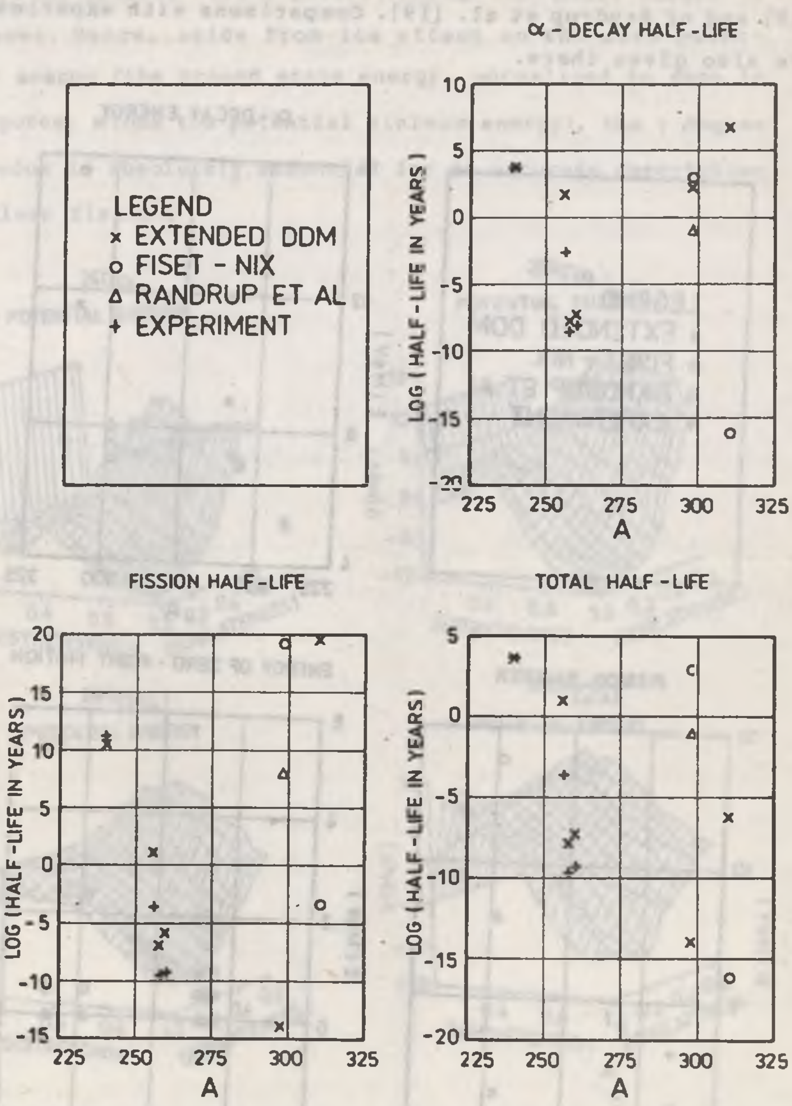


Fig. 5. Half-Lives Of Selected Transuranic And Superheavy Nuclei

Although agreement with experiment is not perfect, it is clear that the present theory can be employed for predicting the trends of fission as well as alpha-decay properties.

The large differences in the theoretical predictions arise partly because of differences in the single-particle level schemes but mainly because of neglect of shape and pairing fluctuations in previous calculations [18,19]. In particular, note the enormous difference in the energy of zero-point motion in the case of spherical nuclei like $^{298}[114]$ and $^{310}[126]$.

Note that the total half-life values include contributions not only due to fission and alpha-decay but also due to beta-decay and electron-capture. For the later, we have adopted the Q-value-dependent method employed by Fiset and Nix [18].

V. CONCLUSIONS AND SUGGESTIONS FOR FURTHER EXPERIMENTAL TESTS

Our main conclusion is that it is possible to approach a truly unified description of the many varied and wonderful aspects of atomic nuclei provided all the important and necessary ingredients are identified as well as treated as best as possible. This requires much hard work, also done by many other nuclear scientists, but above all it requires an open mind so that instead of following the same tracks year after year we are willing to learn from each other and to combine the best features of different models. Furthermore, it is not sufficient to consider only a small part of the landscape observed through a small window or through a tunnel. What good is calculating some nuclear property to the third decimal place if we have not considered some mode of decay which may change nuclear life-time by several orders of magnitude?

Hopefully, the results presented here would encourage theorists as well as experimentalists to continue with the "traditional" nuclear physics. We do not need quarks in order to understand the non-discovery of superheavy nuclei with Z = 110-114. The extended DDM explains this quite well. Naturally, the results presented here are not eough to convince everyone that this is really the correct theoretical track. Hence, we suggest the following two possibilities of testing the major predictions for superheavy nuclei.

Our calculations of the fusion barriers suggest that the best candidate (not taking into account neutron evaporation) for the production of $^{310}[126]$ is the heavy-ion reaction,

$$^{72}Se + {}^{238}U \longrightarrow {}^{310}[126]$$

at E_{CM} = 287 MeV. The predicted fusion cross-section, 20 μb, is admittedly small, but the rather large alpha-decay energy (11.6 MeV) and the beta-decay energy (3.85 MeV) should help in the identification of the superheavy nucleus.

Another possibility, perhaps in the not too distant future, would be to employ a space-based gamma-ray spectrograph to look for the siqnature of a superheavy created during a supernova. Our predicted values of some gamma-ray energies of $^{310}[126]$ are: 1.0 MeV ($2_1 \to 0_1$), 1.5 MeV ($0_2 \to 2_1$), and 2.2 MeV ($0_3 \to 2_1$).

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STRESZCZENIE

Rozszerzono model dynamicznych deformacji struktury jądrowej (DDM) uogólniając parametryzację kształtu jądra wprowadzoną przez Hilla i Wheelera. Liczona mikroskopowo kolektywna energia potencjalna uwzględnia oddziaływanie pomiędzy dwoma fragmentami rozszezepiającego się jądra. W rozszerzonym modelu DDM są wzięte pod uwagę efekty wynikające z asymetrii masy i ładunków fragmentów. Przedstawiono szereg porównań z danymi eksperymentalnymi. Rozpatrzono możliwość syntezy jąder superciężkich Z=114 i Z=126.

РЕЗЮМЕ

Расширена модель динамических деформаций ядерной структуры (DDM) путем обобщения параметризации формы ядра введенной Хилли и Уилером. Коллективная энергия, расчитана микроскопически, учитывает взаимодействие между двумя фрагментами делящегося ядра. В расширенной DDM-модели включены эффекты вытекающие из ассимметрии масс и зарядов фрагментов. Прилагается много сравнений с экспериментальными данными. Рассматривается возможность синтеза сверхтяжелых ядер с $Z = 114$ и $Z = 126$.

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STRESZCZENIE

Rozszerzono model dynamicznych deformacji struktury jądrowej (DDM) uogólniając parametryzację kształtu jądra [illegible] przez Hilla i Wheelera. [illegible] fragmentów. [illegible] DDM [illegible] pod uwagę [illegible] [illegible] fragmentów. [illegible] [illegible] [illegible].