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Stable and unstable deformed nuclei in terms of shell-structure in deformed mean-field approximation

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Abstract: The very basic and simplest description of nuclear many-body systems is the (self-consistent) mean-field approximation to the many-body problem. In particular, shape is the property of mean field. Thus, if some nuclei show the specific feature of axially-symmetric quadrupole deformation, it is most convenient to start with the mean field, which has the same symmetry. In order to obtain shape and size of deformation, on which Jahn-Teller effect (JTE) says nothing, shell-structure of one-particle spectra in deformed potentials must be studied. The study has been developed uniquely and extensively in nuclear physics.

For simplicity, taking phenomenological one-body potentials which are well applied to observed deformed nuclei, I try to explain the shell-structure and how to use those one-particle spectra as a function of deformation (so-called 'Nilsson diagram'), in the study of the shape (and other physics quantities) of particular nuclei with (N,Z) such as stable prolate nuclei, oblate nuclei, nuclei with weakly-bound neutrons etc.

Jahn-Teller effect (JTE)

In a molecule with many atoms where the spatial distribution of nuclei has a high symmetry, the energy levels of the electron system are often degenerate. In such cases, when the geometrical distribution of nuclei is changed to lower symmetry, some degeneracy of the electron states is removed and some of the resulting states may have lower energy.

Nuclear deformation (interpreted as a JTE) - (especially the ground-state deformations)

Nuclear system is a self-consistent system, and constituents are only nucleons.

Spherical (high symmetry) nuclei with partially-filled shell have a high degeneracy, when pair-correlation is neglected. When those nuclei are deformed (lower symmetry), a lower total energy may be obtained

JTE says nothing about the resulting shape and size of deformation. In order to obtain shape and size of deformation, shell-structure of deformed potentials must be studied. The study is developed uniquely and extensively in nuclear physics.

JTE has no direct relation to specific 2-body interactions in the system. Instead , JTE is directly related to the symmetry of the mean-field. Instability of high symmetry is expressed in terms of the fluctuation of the mean-field.



The very basic and simplest description of many-body systems is the (self-consistent) mean-field approximation to the many-body problem.

Note : Shape (= one-body operator) is the property of the mean-field.

If some nuclei show the specific feature of axially-symmetric quadrupole deformation, such as

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rotational spectra \propto I(I+1)
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it is most efficient to start with a mean-field, which has the same symmetry.

Effective interaction in the derivation of self-consistent potential is not yet fixed. Details of radial shape of self-consistent potential depends on N and Z. Radial dependence of phenomenological potential may be used semi-quantitatively.

phenomenological potential is used in the following.

A simple and convenient one-body potential is harmonic-oscillator potential, which has a radial dependence

$$\propto x^2$$
 , y^2 , z^2

though it cannot be used, for example, for weakly-bound neutrons.

Axially-deformed quadrupole deformation (Y20 deformation)

 $V(r,\theta) = V_0(r) + V_2(r)Y_{20}(\theta) + V_{\ell s}(r)(\vec{\ell} \cdot \vec{s}) \quad | \text{Woods-Saxon case; } V_2(r) = -\beta V_{WS}R_0 \frac{df(r)}{dr}$ deformation parameter β $R(\theta, \varphi) = R_0 (1 + \beta Y_{20}^*(\theta) + ...)$

Spherical Woods-Saxon with spin-orbit potential with standard parameters (Bohr & Mottelson, vol.I, p.239) ---an approximation to Hatree-Fock potential



$$V_{ls}(\mathbf{r}) = V_{ls}(\boldsymbol{\ell} \cdot \mathbf{s}) r_0^2 \frac{1}{r} \frac{d}{dr} f(r)$$

standard parametersBohr & Mottelson, Nuclear Structure, vol.I, p.239 $r_0 \approx 1.27 \text{ fm}$ $a \approx 0.67 \text{ fm}$ $V_{\ell s} \approx 17 \text{ MeV}$ $V_{WS} = \left(-51 \pm 33 \frac{N-Z}{A}\right)$ MeV for+ for neutrons
- for protons

1. Stable prolate nuclei ; ex. The N=13 th neutron orbits observed as low-lying excitations in ²⁵Mg₁₃

5.53 (11/2)

$$V(r,\theta) = V_0(r) + V_2(r)Y_{20}(\theta) + V_{\ell s}(r)(\vec{\ell} \cdot \vec{s})$$



5.012 7/2



4.712 9/2 4.277 1/2 7/2 3.971 3.908 5/23.413 3/2 3.405 9/2 $K \pi = 1/2$ -2.801 2.738 7/2 [330 1/2] ┥ - f_{7/2}, p_{3/2} 1/22.563 A = 0.113 $K \pi = 1/2 +$ 1.964 5/2 a = -3.54[200 1/2] 1.612 7/2 A = 0.1500.975 3/2 a = -0.47 0.585 1/2 $K \pi = 1/2 +$ 5/2[211 1/2] S(n) = 7.3 MeV $K \pi = 5/2 +$ ²⁵MG A = 0.163[202 5/2] a = -0.020 A = 0.231

- One-particle levels named with asymptotic quantumnumbers [N $n_z \wedge \Omega$] are doublely (± Ω) degenerate.
- Z=12 favors prolate deformation, while Z=14 favors oblate deformation.

 $\epsilon_{res}(f_{5/2}) = 10.4 \text{ MeV}$ $\epsilon_{res}(f_{7/2}) = 0.32 \text{ MeV}$ $\epsilon_{res}(p_{3/2}) = 0.31 \text{ MeV}$ Ω : angular momentum component along sym axis is a good quantum-number

> observed E2- and M1-intensity relations \rightarrow $g_s^{eff} = (0.7 - 0.9) g_s^{free}$

Prolate side of the Nilsson diagram for neutrons of stable 70 Yb-isotopes



Roughly speaking, one-particle levels for spherical shape with 82 < N < 126are degenerate. Thus, if pairing interaction is absent, systems with some neutrons above the N=82 energy-gap are deformed (JTE).

Stable rare-earth even-even nuclei with $90 \le N \le 112$ are known to be axiallysymmetric quadrupole-deformed. (text book examples)

Observed properties of deformed stable rare-earth nuclei are quantitatively understood in terms of one-particle motion in the Y20-deformed mean-field (B. & M., vol.II). Notion of one-particle motion in deformed mean-field works much better in deformed nuclei, compared with one-particle motion in spherical potential for spherical nuclei.

The wave functions of all one-particle levels, except those coming from high-j (here, $i_{13/2}$) orbits, approach the asymptotic (i.e. very large β) [$N n_z \wedge \Omega$] wave-functions, already at $\beta = 0.3 \sim 0.4$.

(The slope of asymptotic wave-functions, $d\epsilon_{\Omega}/d\beta$, is determined by *N* and n_z .)

2. Oblate nuclei

Overwhelming dominance of prolate shape in observed even-even deformed nuclei is not yet really clarified.

At least, one may say that shell-structure, which strongly favors oblate shape,

is needed for obtaining oblate nuclei.

Even-even nuclei in the range of $6 \le Z \le 40$, of which observed electric Q moment of the 2₁⁺ state shows clearly oblate shape (or a fluctuation towards oblate shape), are only the following five (six) nuclei;

 ${}^{12}{}_{6}C_{6}$, ${}^{28}{}_{14}Si_{14}$, ${}^{34}{}_{16}S_{18}$, ${}^{36}{}_{18}Ar_{18}$, ${}^{64}{}_{28}Ni_{36}$ (${}^{72}{}_{36}Kr_{36}$)

Z (or N) = 6, 14, 18, 28, 36, prefer oblate shape ?

Neutron numbers at large energy gaps on the oblate side ($\beta \sim -0.4$) of realistic potentials are indeed equal to 14, 18, 28, 36, 48, etc.

← Magic numbers for the ω_{\perp} : $\omega_{z} = 2:3$ deformation of harmonic-oscillator potential =..., 14,18,28,34,48,58, ...



β **≈** -0.43

Y₂₀ deformed harmonic-oscillator potential



$$V_{def.h.o.} = \frac{M}{2} \left(\omega_z^2 z^2 + \omega_\perp^2 (x^2 + y^2) \right)$$

One-particle energy
$$\varepsilon(N)$$
 at $\delta = 0$
 \rightarrow (N+1) levels for $\delta \neq 0$, $\varepsilon(n_{\perp}, n_{z})$
where $N = n_{x} + n_{y} + n_{z} = n_{\perp} + n_{z}$
 $\varepsilon(n_{\perp}, n_{z}) = \left(n_{z} + \frac{1}{2}\right)\hbar\omega_{z} + (n_{\perp} + 1)\hbar\omega_{\perp}$
 $= \hbar\omega\left(N + \frac{3}{2} - \frac{3}{3}(3n_{z} - N)\right)$
where $\delta \approx \frac{R_{z} - R_{\perp}}{2}$ and $\omega = \omega \approx R_{z} + R_{z}$

where
$$\delta \approx \frac{R_Z - R_\perp}{R_{av}}$$
 and $\omega_\perp : \omega_Z \approx R_Z : R_\perp$



Oblate side

Magic-numbers for $(\omega_{\perp}: \omega_z) = (1:2)$ = 6, 14, 26, 44, 68, ...

Magic-numbers for $(\omega_{\perp} : \omega_z) = (2 : 3)$ = 6, 8, 14, 18, 28, 34, 48, 58, ... Degeneracy of one-particle levels in axially-symmetric quadrupole-deformed pure harmonic-oscillator potential

ex. Harmonic-oscillator N=4 shell







 $N = \underline{n_x + n_y} + n_z$ $= \underline{n_\perp} + n_z$

In Nilsson diagrams (= one-particle energies as a function of deformation parameter β),

Shell-structure on the oblate side is simple and common to various realistic potentials. (can be almost simulated in terms of deformed pure harmonic-oscillator potential).
Shell-structure on the prolate side depends more sensitively on various parameters of realistic potential. Ex., the magic numbers of the pure h.o. (3:2) deformation (8,10,14,22,26,34, ...) have nothing to do with large energy gaps in realistic potentials. I.H., PRC 89, 057301 (2014)

Strong deviation of realistic one-particle spectra from harmonic-oscillator

← high-j orbits, such as $1d_{5/2}$, $1f_{7/2}$, $1h_{11/2}$, ..., which are pushed down by strong ($\ell \bullet s$) potential.



Splitting of high-j one-particle levels due to deformation is asymmetric between ptolate and oblate sides. On the oblate ($\beta < 0$) side the internal structure of one-particle levels with $\Lambda \le N-2$ has to change drastically soon after $|\beta|$ increases from zero, due to the interaction with above-lying one-particle levels with the same Ω^{π} . \rightarrow shell-structure gets similar to harmonic oscillator.

3. Nuclei with weakly-bound neutrons ; Unique behavior of weakly-bound neutrons with small



Spherical shape

When potential gets weaker, or when one-particle energy approaches zero,

- (a) halo-phenomena are observed associated with s1/2, p1/2 and p3/2 neutrons;
- (b) the shell-structure changes so that s1/2, p1/2 and p3/2 levels become energetically lower relative to levels with larger *l*.

Deformed shape Deformed halo

 $\Omega^{\pi} = \frac{1}{2}^{+}$ one-particle levels have $\ell_{\min} = 0$ component. The s-component increases to unity as $\epsilon_{\Omega} \to 0$. As $\epsilon_{\Omega} \to 0$, $\Omega^{\pi} = 1/2^{+}$ level becomes energetically lower relative to levels with larger Ω .

Similarly, $\Omega^{\pi} = \frac{1}{2}$ and $\frac{3}{2}$ one-particle levels have $\ell_{min} = 1$ component. The p-component increases as $\epsilon_{\Omega} \rightarrow 0$, with respect to levels with larger ℓ .

As ϵ_{Ω} (<0) \rightarrow 0, the structure of one-particle wave-functions may deviate from [N n_z $\wedge \Omega$], even for $|\beta| \rightarrow$ large. Nevertheless, one-particle levels are denoted by original [N n_z $\wedge \Omega$].

 $\Omega^{\pi} = 1/2^+$ one-particle level has $\ell_{\min} = 0$ component.

ex. Radial wave functions of the [200 1/2] level in Woods-Saxon potentials.

(The radius of potentials is adjusted to obtain respective eigenvalues ϵ_{Ω} .)



Bound state with $\varepsilon_{\Omega} = -8.0$ MeV.

Bound state with $\varepsilon_{\Omega} = -0.0001$ MeV.



Similar behavior to wave functions in harmonic osc. potentials.

Wave functions unique in finite-well potentials.

- For $\varepsilon \to 0$, the s-dominance will appear in all $\Omega^{\pi} = 1/2^+$ bound orbits. However, the energy, at which the dominance shows up, depends on both deformation and respective orbits.
- ex. Calculated $s_{1/2}$ probability in three $\Omega^{\pi} = 1/2^+$ Nilsson orbits in the *sd*-shell as a function of energy eigenvalue ϵ_{Ω} . I.H., PRC **69**, 041306 (2004).







Deformed shape (pf-shell)

ex. $\Omega^{\pi} = 1/2^{-1}$ and $3/2^{-1}$ one-particle levels have $\ell_{min} = 1$ component.

The *p*-components increase as $\varepsilon_0 \rightarrow 0$, but the probability at $\varepsilon_0 = 0$ depends on respective levels, deformations, and the diffuseness of potentials.

[321 3/2] orbit

Calculated probabilities of (l j) components of one-particle [N n₂ $\Lambda \Omega$] levels in the *pf* shell as a function of energy eigenvalue ε_0 .



One-particle neutron energies as a function of quadrupole deformation β

 Ω : angular-momentum component along the sym axis $[N n_{\tau} \Lambda \Omega]$



In the case of very weak binding N=28 is not a magic number ! At $\beta = 0$; $\epsilon(2p_{3/2}) - \epsilon(1f_{7/2})$ = 680 keV ³⁷Mg₂₅ S(n) = a fewhundreds keV? deformed halo? Mg-isotopes are most likely prolately-deformed up till ca N=28, $_{12}Mg_{28}$. IH, PRC 76, 054319 (2007)

All Mg- and Ne-isotopes with N = 21, 23 and 25 may show deformed p-wave halo?

$$I^{\pi} = \begin{cases} 5/2 - \text{ from } [312 5/2] & \text{for } 0 < \beta < 0.3 & \text{ no halo } (\overset{\cdots}{} \ell_{\min} = 3) \\ 1/2 - \text{ from } [321 1/2] & \text{for } 0.3 < \beta < 0.6 & p(\ell = 1) \text{ halo} \end{cases}$$

³⁷Mg is observed as deformed p-wave halo; N.Kobayashi, T.Nakamura, et al., PRL 112, 242501 (2014):

One-particle neutron energies as a function of quadrupole deformation β



Near degeneracy of $f_{7/2}$, $p_{3/2}$ and $p_{1/2}$ resonant levels can be the origin of deformed shape of those N \approx 20 nuclei.

N = 21 neutron $I^{\pi} = \begin{cases} 3/2 - \text{ from } [330 \ 1/2] & \text{for } 0.20 < \beta < 0.30 & \longleftarrow p(\ell = 1) \text{ halo } \\ 3/2 + \text{ from } [202 \ 3/2] & \text{for } 0.30 < \beta < 0.40 & \longleftarrow \text{ no halo } (\because)_{\ell_{\min}} = 2 \end{pmatrix} \times \\ 3/2 - \text{ from } [321 \ 3/2] & \text{for } 0.40 < \beta < 0.58 & \longleftarrow p(\ell = 1) \text{ halo } \\ 1/2 + \text{ from } [200 \ 1/2] & \text{for } \beta > 0.58 & \longleftarrow s(\ell = 0) \text{ halo } \end{cases}$

One-particle neutron energies as a function of quadrupole deformation β

 $N \sim 8$ region



¹¹Be can be deformed s-wave halo.

Computer programs, in which neutron one-particle (both bound and resonant) energies are calculated for given β and Ω^{π} , for a given Woods-Saxon potential, are available.

In order to solve the eigenvalue and eigenphase problems for neutron one-particle bound and resonant levels, respectively, as a function of axially symmetric quadrupole deformation, the coupled differential equations obtained from the Schrodinger equation are integrated in coordinate space with correct asymptotic behavior at $r = R_{max}$, where R_{max} is so large that the nuclear potential (including spin-orbit potential) is totally negligible. For $\beta \neq 0$ the resonant energy is defined as the energy, at which one of the eigenphases increases through $\pi/2$ as the energy increases. One-particle resonance is absent, if none of eigenphases increase through $\pi/2$ as the energy increases.

For one-particle resonance in deformed potentials and eigenphase etc. see, for example, I.H., PRC72, 024301 (2005); PRC73, 064308 (2006)

Those who want to have the programs should contact me.