

Nuclear mean field theories and collective phenomena

L. Próchniak

Maria Curie-Skłodowska University, Lublin

Outline

Introduction. Collective phenomena

Mean field theories

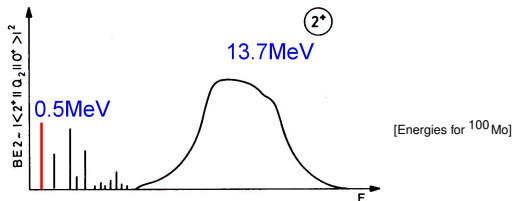
Microscopic theory of collective motion

Quadrupole excitations, Bohr Hamiltonian

Examples

Introduction. Collective phenomena

- ▶ Fission
- ▶ Giant resonances
- ▶ Low energy excitations (rotation-vibrational type)



Strength of an electromagnetic transition

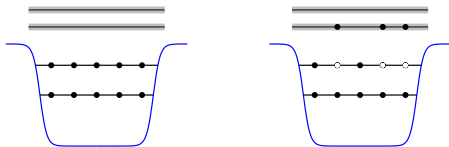
$$1/\tau_i \sim E_\gamma^{2L+1} B(EL; i, f)$$

$B(E2) = 30 - 200$ Weisskopf units (single particle estimates)

Collective phenomena cont.

Mean-field description

Giant resonances, Random Phase Approximation (RPA)



Low energy (large amplitude) excitations, ATDHFB or GCM+GOA



[often called the beyond mean field methods]

Experimental data on the 2_1^+ state

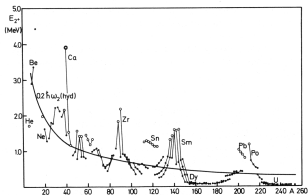
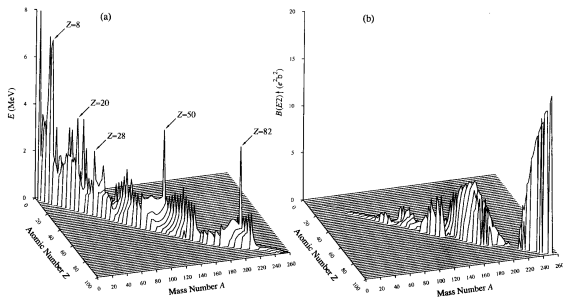
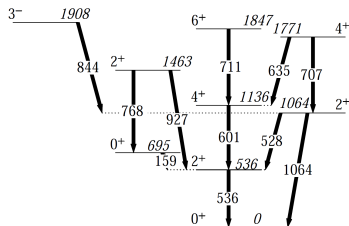
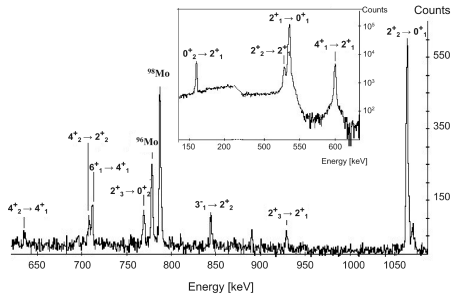


Figure 1.7. The energy of the first 2_1^+ state in even-even nuclei. The nuclei with closed neutron or proton shells are marked by open circles. (From [NN 65].)

Example of results from experiments at HIL

^{100}Mo , Coulomb excitation with ^{32}S beam



Hartree-Fock mean field

Phenomenological one-particle potentials: harmonic oscillator, square well, deformed HO (Nilsson potential), Woods-Saxon potential and others.

HF equations

$$T\phi_k(\mathbf{r}) + \left(\int d^3 r' V(\mathbf{r}, \mathbf{r}') \sum_k |\phi_j(\mathbf{r}')|^2 \right) \phi_k(\mathbf{r}) - \sum_j \phi_j(\mathbf{r}) \int d^3 r' V(\mathbf{r}', \mathbf{r}) \phi_j^*(\mathbf{r}') \phi_k(\mathbf{r}') = e_k \phi_k(\mathbf{r})$$

$$\Psi_{\text{HF}} = \prod_k c_k^+ |0\rangle$$

Effective nucleon-nucleon interactions V — not from NN scattering

Pairing and the BCS method

More general product states (BCS-type)

$$\Psi_{\text{BCS}} = \prod_{\mu>0} (u_{\mu} + s_{\mu} v_{\bar{\mu}} c_{\mu}^{\dagger} c_{\bar{\mu}}^{\dagger}) |0\rangle$$

Quasiparticles

$$\alpha_{\mu}^{\dagger} = u_{\mu} c_{\mu}^{\dagger} + s_{\mu}^* v_{\bar{\mu}} c_{\bar{\mu}}$$

$$\alpha_{\mu} \Psi_{\text{BCS}} = 0$$

Density matrix \mathcal{R}

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix} = \begin{pmatrix} \langle \Psi | c_v^{\dagger} c_{\mu} | \Psi \rangle & \langle \Psi | c_v c_{\mu} | \Psi \rangle \\ \langle \Psi | c_v^{\dagger} c_{\mu}^{\dagger} | \Psi \rangle & \langle \Psi | c_v c_{\mu}^{\dagger} | \Psi \rangle \end{pmatrix}$$

Canonical basis

$$\rho_{\mu\nu} = v_{\mu}^2 \delta_{\mu\nu} \quad \kappa_{\mu\nu} = s_{\bar{\mu}} u_{\mu} v_{\nu} \delta_{\bar{\mu}\nu}$$

Hartree-Fock-Bogolyubov theory

NN (microscopic) Hamiltonian

$$\hat{H}_{\text{micr}} = \sum_{\mu,\nu} T_{\mu\nu} c_{\mu}^{\dagger} c_{\nu} + \frac{1}{4} \sum_{\mu,\nu,\alpha,\beta} \tilde{V}_{\mu\nu\alpha\beta} c_{\mu}^{\dagger} c_{\nu}^{\dagger} c_{\beta} c_{\alpha}$$

Hartree-Fock-Bogolyubov equation

$$[\mathcal{W}(\mathcal{R}), \mathcal{R}] = 0$$

Mean field (induced by \mathcal{R}) Hamiltonian

$$\mathcal{W}(\mathcal{R}) = \begin{pmatrix} T + \Gamma - \lambda I & \Delta \\ -\Delta^* & -T^* - \Gamma^* + \lambda I \end{pmatrix} = \begin{pmatrix} h_0 - \lambda I & \Delta \\ -\Delta^* & -h_0 + \lambda I \end{pmatrix}$$

$$\Gamma_{\mu\nu} = \sum_{\mu',\nu'} \tilde{V}_{\mu\mu'\nu\nu'} \rho_{\nu'\mu'}$$

$$\Delta_{\mu\nu} = \frac{1}{2} \sum_{\mu',\nu'} \tilde{V}_{\mu\nu\mu'\nu'} \kappa_{\mu'\nu'}$$

The Skyrme interaction

Momentum space

$$\langle \mathbf{k} | V | \mathbf{k}' \rangle = \tilde{t}_0(1 + x_0 P_\sigma) + \frac{1}{2} \tilde{t}_1(k^2 + k'^2) + \tilde{t}_2 \mathbf{k} \mathbf{k}' + i \tilde{W}_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{k} \times \mathbf{k}') + v_{123}$$

Kernel of the integral operator $\langle f(1, 2) | V_S | g(1, 2) \rangle$

$$\begin{aligned} V_S = & t_0(1 + x_0 P_\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) + \frac{1}{2} t_1(k^2 \delta(\mathbf{r}_1 - \mathbf{r}_2) + \delta(\mathbf{r}_1 - \mathbf{r}_2) k'^2) + t_2 \mathbf{k} \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k}' + \\ & + i W_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{k} \times \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k}') + \\ & + \tilde{t}_3 \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_2 - \mathbf{r}_3) \longrightarrow \frac{1}{6} t_3 (1 + P_\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) \rho^\alpha((\mathbf{r}_1 + \mathbf{r}_2)/2) \end{aligned}$$

$$\mathbf{k}' = \frac{1}{2i} (\vec{\nabla}_1 - \vec{\nabla}_2), \quad \mathbf{k} = -\frac{1}{2i} (\vec{\nabla}_1 - \vec{\nabla}_2),$$

plus the Coulomb potential for protons

The Gogny interaction

$$\begin{aligned}
 V_G = & \sum_{j=1,2} \exp(|\mathbf{r}_1 - \mathbf{r}_2|^2/a_j^2) (W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau) + \\
 & + iW_{G0} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{k} \times \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k}') + \\
 & + t'_{G3} (1 + P_\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) \rho^\alpha ((\mathbf{r}_1 + \mathbf{r}_2)/2)
 \end{aligned}$$

$$a_1 = 0.7 \text{ fm}, \quad a_2 = 0.2 \text{ fm}, \quad \alpha = 1/3$$

plus Coulomb for protons

Relativistic Mean Field

One of numerous versions. Dirac equation with the self-consistent potential.
 NN interaction mediated by several types of mesons.

$$(\boldsymbol{\alpha} \cdot \mathbf{p} + V(\mathbf{r}) + \beta(M + S(\mathbf{r})))\psi_j(\mathbf{r}) = \epsilon_j\psi_j(\mathbf{r})$$

$$V(\mathbf{r}) = g_\omega\omega^0(\mathbf{r}) + g_\rho\tau_3\rho^0(\mathbf{r}) + e\frac{1-\tau_3}{2}A^0(\mathbf{r})$$

$$S(\mathbf{r}) = g_\sigma\sigma(\mathbf{r})$$

$$(-\Delta + m_\sigma^2)\sigma(\mathbf{r}) + g_2\sigma^2(\mathbf{r}) + g_3\sigma^3(\mathbf{r}) = -g_\sigma\rho_s(\mathbf{r})$$

$$(-\Delta + m_\omega^2)\omega^0(\mathbf{r}) = g_\omega\rho_v(\mathbf{r})$$

$$(-\Delta + m_\rho^2)\rho^0(\mathbf{r}) = g_\rho\rho_3(\mathbf{r})$$

$$-\Delta A^0(\mathbf{r}) = e\rho_c(\mathbf{r})$$

$$\rho_s(\mathbf{r}) = \sum_i \bar{\psi}_i(\mathbf{r})\psi_i(\mathbf{r}) \quad \rho_v(\mathbf{r}) = \sum_i \psi_i^\dagger(\mathbf{r})\psi_i(\mathbf{r})$$

$$\rho_3(\mathbf{r}) = \sum_i \psi_i^\dagger(\mathbf{r})\tau_3\psi_i(\mathbf{r}) \quad \rho_c(\mathbf{r}) = \sum_i \psi_i^\dagger(\mathbf{r})\frac{1-\tau_3}{2}\psi_i(\mathbf{r}).$$

Pairing interaction (p-p and n-n)

- ▶ Constant G (seniority force)

$$G \sum_k c_k^+ c_{\bar{k}}^+ c_k c_{\bar{k}}$$

- ▶ δ interaction:

$$V_0 \delta(\mathbf{r} - \mathbf{r}'),$$

$$V_0(\rho(\mathbf{r})) \delta(\mathbf{r} - \mathbf{r}'), \text{ e.g. } V_0(\rho) = 1 - \rho(\mathbf{r})/\rho_0$$

- ▶ Gogny type interaction (only the Gaussian part)

Applications of the mean field approach

Nuclear ground state properties (binding energies, radii, static deformation, fission barriers), giant resonances, nuclear matter properties

Recent review papers

M. Bender, P.-H. Heenen and P.-G. Reinhard, *Self-consistent mean-field models for nuclear structure*, Rev.Mod.Phys. **75** (2003) 121.

J.R. Stone and P.-G. Reinhard, *The Skyrme interaction in finite nuclei and nuclear matter*, Prog. Part. Nucl. Phys. **58** (2007) 587.

T. Nikšić, D. Vretenar and P. Ring, *Relativistic nuclear energy density functionals: Mean-field and beyond*, Prog. Part. Nucl. Phys. **66** (2011) 519.

Microscopic theory of collective states

Mean field is changing while occupation numbers are fixed

Main methods:

- ▶ Adiabatic Time Dependent Hartree-Fock-Boglyubov
- ▶ Generator Coordinate Method (plus Gaussian Overlap Approximation):

Set of product states parametrized by several collective variables



Schroedinger type equation in the collective space

Adiabatic approximation of the Time Dependent HFB theory

Time dependent HFB equation

$$i\hbar\dot{\mathcal{R}} = [\mathcal{W}(\mathcal{R}), \mathcal{R}]$$

Adiabatic approximation, $\mathcal{R} = \mathcal{R}_0 + \mathcal{R}_1 + \mathcal{R}_2 + \dots$

$$[\mathcal{W}_0, \mathcal{R}_0] \approx 0$$

Collective variables α , $\mathcal{R}(t) = \mathcal{R}(\alpha(t))$

$$\langle \Psi | H_{\text{micr}} | \Psi \rangle = T_{\text{cl}} + V_{\text{cl}} = H_{\text{cl}}$$

$$V_{\text{cl}} = \langle \Psi_0(\alpha) | H_{\text{micr}} | \Psi_0(\alpha) \rangle$$

$$T_{\text{cl}} = \frac{1}{2} \sum_{kj} B_{kj}(\alpha) \dot{\alpha}_k \dot{\alpha}_j$$

Mass parameters (inertial functions)

Kinetic energy determined by

$$B_{kj} = \frac{\hbar^2}{2} \sum_{\mu, \nu} \frac{f_{j, \mu \nu} f_{k, \mu \nu}^* + f_{j, \mu \nu}^* f_{k, \mu \nu}}{(E_{\mu} + E_{\nu})} .$$

$$f_{k, \mu \nu} = s_{\nu} (\partial_k \rho)_{\mu \bar{\nu}} (u_{\mu} v_{\nu} + v_{\mu} u_{\nu}) + (\partial_k \kappa)_{\mu \nu} (u_{\mu} u_{\nu} - v_{\mu} v_{\nu})$$

$$f_{k, \mu \nu} = \langle \Psi_0 | a_{\nu} a_{\mu} | \partial_k \Psi_0 \rangle, \quad a_{\mu} \text{ — quasiparticle operators}$$

$$f_{k, \mu \nu} = -\frac{1}{E_{\mu} + E_{\nu}} [s_{\nu} (\partial_k h_0)_{\mu \bar{\nu}} (u_{\mu} v_{\nu} + v_{\mu} u_{\nu}) + (\partial_k \Delta)_{\mu \nu} (u_{\mu} u_{\nu} - v_{\mu} v_{\nu})]$$

Requantization

Classical expression $T_{\text{cl}} + V_{\text{cl}} \rightarrow H_{\text{quant}}$

$$T_{\text{cl}} = \frac{1}{2} \sum_{k,j} B_{kj}(\alpha) \dot{\alpha}_k \dot{\alpha}_j$$

The Laplace-Beltrami operator

$$T_{\text{quant}} = -\frac{\hbar^2}{2} \frac{1}{\sqrt{\det B}} \sum_{k,j} \frac{\partial}{\partial \alpha_k} \sqrt{\det B} (B^{-1})_{kj} \frac{\partial}{\partial \alpha_j}$$

Volume element $\sqrt{\det B} d\alpha_1 \dots d\alpha_n$

Generator Coordinate Method +GOA

Variational principle with test functions $\int d\alpha f(\alpha)\Psi(\alpha)$

Gaussian Overlap Approximation

$$\langle \Psi(\alpha'') | \Psi(\alpha') \rangle = \exp\left(-\sum_{k,j} g_{kj}(\alpha)(\alpha''_k - \alpha'_k)(\alpha''_j - \alpha'_j)/2\right),$$

$$H_{\text{GCM}}\tilde{f}(\alpha) = E\tilde{f}(\alpha)$$

$$H_{\text{GCM}} = T_{\text{GCM}} + V_{\text{GCM}}$$

No need for requantization

$$T_{\text{GCM}} = -\frac{\hbar^2}{2} \frac{1}{\sqrt{\det g}} \sum_{k,j} \frac{\partial}{\partial \alpha_k} \sqrt{\det g} (B_{\text{GCM}}^{-1})^{kj} \frac{\partial}{\partial \alpha_j}.$$

Potential energy

$$V_{\text{GCM}} = V_{\text{cl}}(\alpha) + V_{\text{ZPE}}(\alpha)$$

Odd and odd-odd nuclei

- ▶ Core-particle coupling
- ▶ Particle in the deformed field

Quadrupole variables

1. Quadrupole mass tensor $Q_{2\mu} = \langle \Psi | \sum_i r_i^2 Y_{2\mu}(i) | \Psi \rangle$
2. Nuclear surface $r(\alpha) = r_0(1 + \sum_{\mu} \alpha_{\mu}^* Y_{2\mu})$
3. Ellipsoidal shape (e.g. of a nucleus or one-particle potential) $\sum_{k,j} w_{kj} x_k x_j = 1$
(...)

Principal axes system (intrinsic system)

Spherical tensors (α or Q)

$$\{\alpha_{\mu}\} \xrightarrow{R(\Omega)} \{\tilde{\alpha}_0, \tilde{\alpha}_1 = \tilde{\alpha}_{-1} = 0, \tilde{\alpha}_2 = \tilde{\alpha}_{-2}\}$$

Cartesian case (ellipsoid)

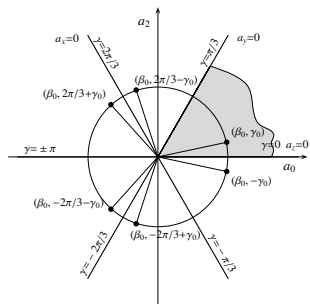
$$\sum_{k,j} w_{kj} x_k x_j = 1 \xrightarrow{R(\Omega)} \sum_k \tilde{w}_k x_k^2 = 1$$

Quadrupole variables, cont.

Deformation variables β, γ

$$\begin{aligned}\tilde{\alpha}_0 &= \beta \cos \gamma, \\ \tilde{\alpha}_2 = \tilde{\alpha}_{-2} &= \beta \sin \gamma / \sqrt{2}\end{aligned}$$

LAB \longleftrightarrow INT: $\alpha_\mu(Q_{2\mu}) \longleftrightarrow (\beta, \gamma, \text{Euler angles } \Omega)$



Quadrupole variables in the mean field approach

Deformation variables

$$\beta \cos \gamma = c q_0 = c \langle \Psi | Q_0 | \Psi \rangle = \langle \Psi | \sum_{i=1}^A (3z_i^2 - r_i^2) | \Psi \rangle$$

$$\beta \sin \gamma = c q_2 = c \langle \Psi | Q_2 | \Psi \rangle = \langle \Psi | \sum_{i=1}^A \sqrt{3}(x_i^2 - y_i^2) | \Psi \rangle; \quad c = \sqrt{\pi/5}/A\bar{r}^2$$

HFB with constraints

$$\delta \langle \Psi | H_{\text{micr}} - \lambda_0 Q_0 - \lambda_2 Q_2 | \Psi \rangle = 0$$

$$\langle \Psi | Q_0 | \Psi \rangle = q_0, \quad \langle \Psi | Q_2 | \Psi \rangle = q_2$$

Mass parameters

$$B_{q_i q_j} = \hbar^2 (S_{(1)}^{-1} S_{(3)} S_{(1)}^{-1})_{ij}$$

$$(S_{(n)})_{ij} = \sum_{\mu, \nu} \frac{\langle \mu | Q_i | \bar{\nu} \rangle \langle \bar{\nu} | Q_j | \mu \rangle}{(E_\mu + E_\nu)^n} (u_\mu v_\nu + u_\nu v_\mu)^2$$

Moments of inertia

$$J_k = \hbar^2 \sum_{\mu, \nu} \frac{|\langle \nu | j_k | \bar{\mu} \rangle|^2 (u_\mu v_\nu - u_\nu v_\mu)^2}{(E_\mu + E_\nu)}$$

Kinetic energy in the intrinsic frame

Five variables β, γ, Ω .

Mass parameters matrix (5×5)

$$B = \begin{pmatrix} B_{\text{vib}} & 0 \\ 0 & B_{\text{rot}} \end{pmatrix}$$

$$B_{\text{vib}} = \begin{pmatrix} B_{\beta\beta} & \beta B_{\beta\gamma} \\ \beta B_{\beta\gamma} & \beta^2 B_{\gamma\gamma} \end{pmatrix}$$

$$B_{\text{rot}} = \begin{pmatrix} J_x & 0 & 0 \\ 0 & J_y & 0 \\ 0 & 0 & J_z \end{pmatrix}$$

$$J_k = 4\beta^2 B_k(\beta, \gamma) \sin^2(\gamma - 2\pi k/3)$$

Quantum Hamiltonian in the intrinsic frame

General Bohr Hamiltonian

$$H_{\text{Bohr}} = T_{\text{vib}} + T_{\text{rot}} + V$$

$$T_{\text{vib}} = -\frac{1}{2\sqrt{wr}} \left\{ \frac{1}{\beta^4} \left[\partial_{\beta} \left(\beta^4 \sqrt{\frac{r}{w}} B_{\gamma\gamma} \right) \partial_{\beta} - \partial_{\beta} \left(\beta^3 \sqrt{\frac{r}{w}} B_{\beta\gamma} \right) \partial_{\gamma} \right] + \right. \\ \left. + \frac{1}{\beta \sin 3\gamma} \left[-\partial_{\gamma} \left(\sqrt{\frac{r}{w}} \sin 3\gamma B_{\beta\gamma} \right) \partial_{\beta} + \frac{1}{\beta} \partial_{\gamma} \left(\sqrt{\frac{r}{w}} \sin 3\gamma B_{\beta\beta} \right) \partial_{\gamma} \right] \right\}$$

$$T_{\text{rot}} = \frac{1}{2} \sum_{k=1}^3 I_k^2(\Omega) / J_k; \quad J_k = 4B_k(\beta, \gamma) \beta^2 \sin^2(\gamma - 2\pi k/3)$$

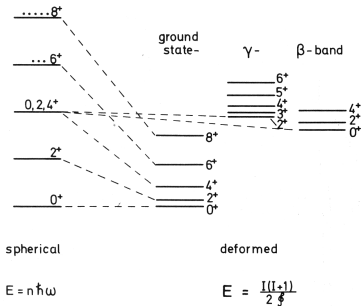
$$w = B_{\beta\beta} B_{\gamma\gamma} - B_{\beta\gamma}^2; \quad r = B_x B_y B_z$$

Energy levels, B(E2) transition probabilities

Special cases

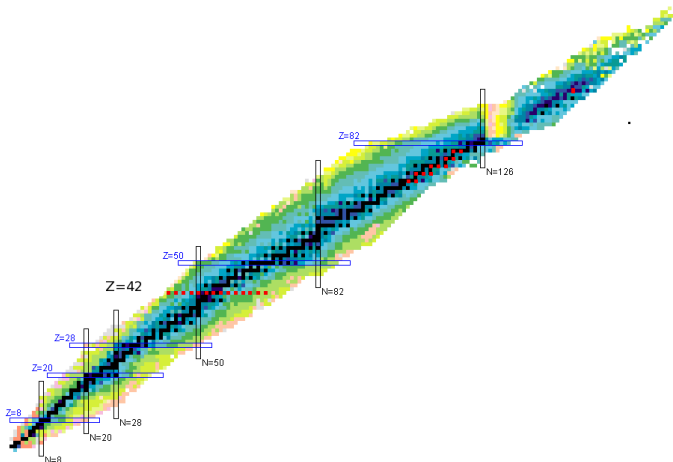
Simple kinetic energy: $B_{\beta\beta} = B_{\gamma\gamma} = B_k = B$, $B_{\beta\gamma} = 0$

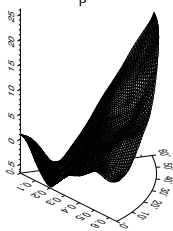
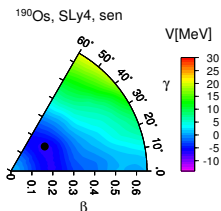
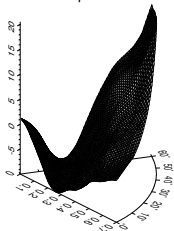
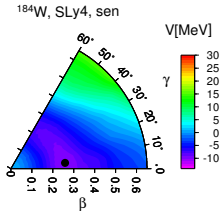
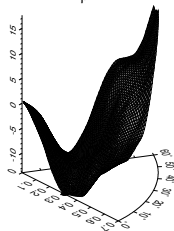
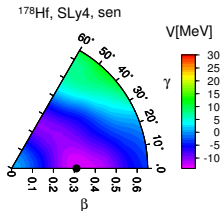
Harmonic oscillator: $V \sim \beta^2$

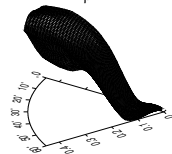
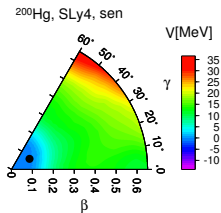
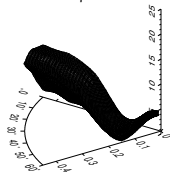
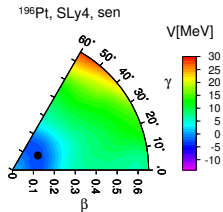


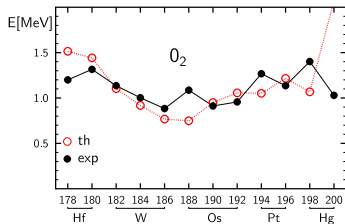
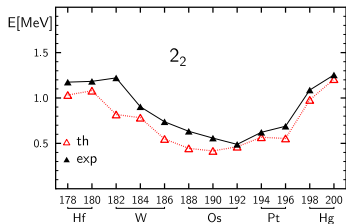
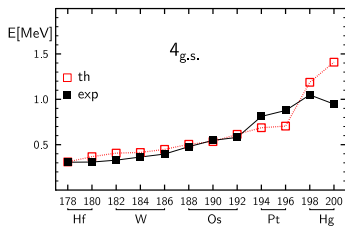
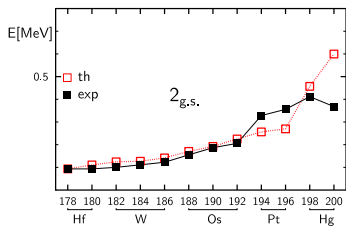
Examples

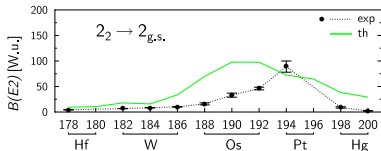
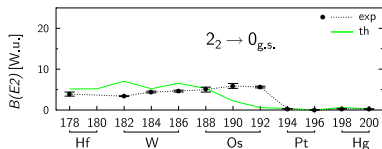
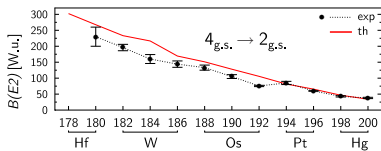
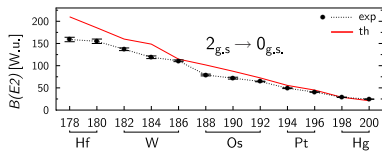
1. From well deformed Hf to almost spherical Hg: $^{178,180}_{72}\text{Hf}$, $^{182-186}_{74}\text{W}$, $^{188-192}_{76}\text{Os}$,
 $^{194,196}_{78}\text{Pt}$, $^{198,200}_{80}\text{Hg}$
2. Molybdenum isotopes, $^{84-110}\text{Mo}$
3. ^{240}Pu

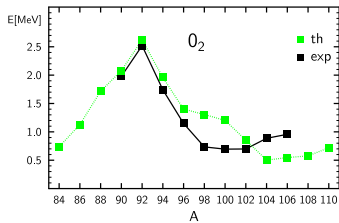
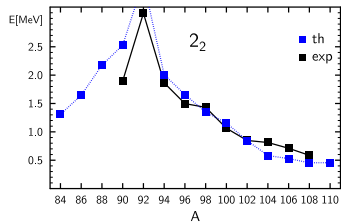
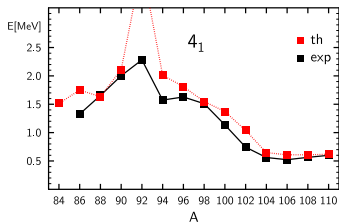
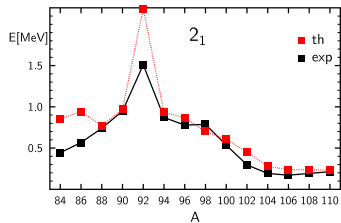


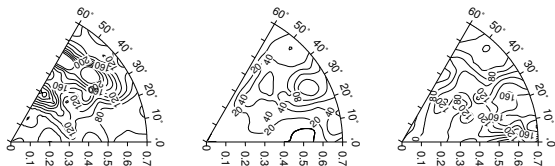
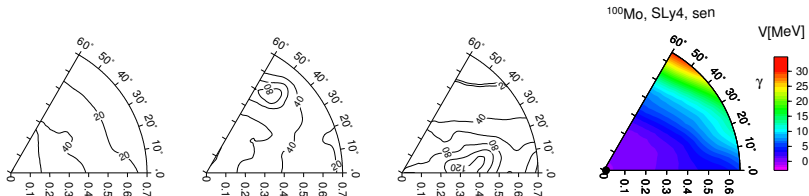
^{178}Hf — ^{200}Hg . Potential energy surfaces

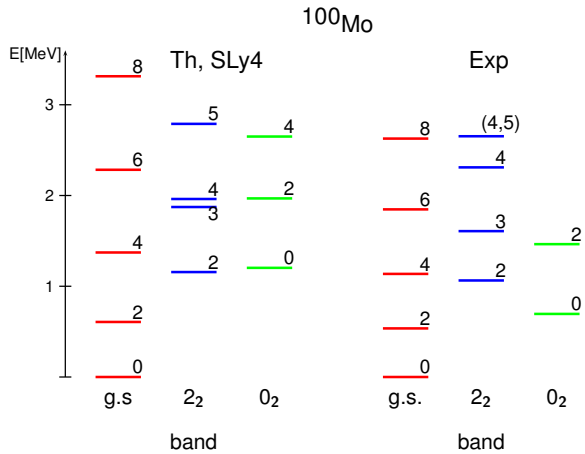
^{178}Hf — ^{200}Hg . Potential energy surfaces, cont.

$^{178}\text{Hf} - ^{200}\text{Hg}$. Energy levels

$^{178}\text{Hf} - ^{200}\text{Hg}$. $B(E2)$ transition probabilities

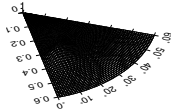
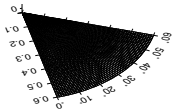
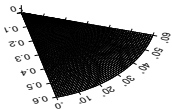
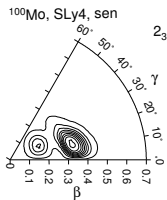
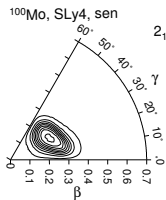
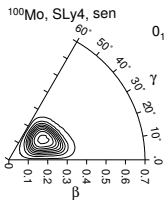
$84-110$ Mo isotopes. Energy levels

¹⁰⁰Mo. Potential energy, mass parametersMass parameters $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$ Parameters B_k , $k = x, y, z$, potential energy

^{100}Mo . Energy levels

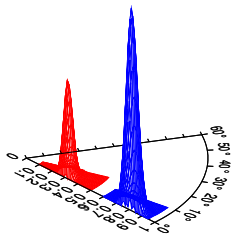
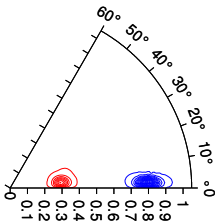
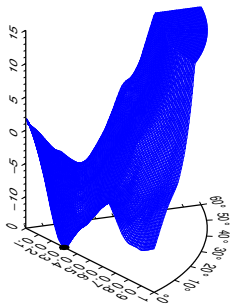
¹⁰⁰Mo. Collective wave functions

Probability density $|\Phi_{\text{coll}}|^2 d\tau = |\Phi_{\text{coll}}|^2 \beta^4 |\sin 3\gamma| \tilde{w}(\beta, \gamma)$



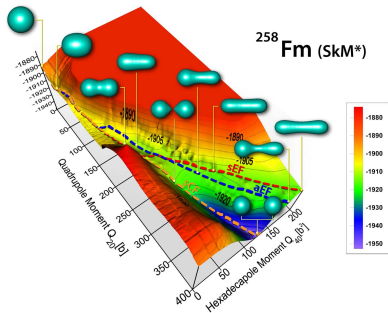
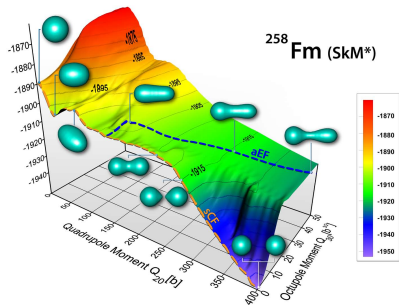
^{240}Pu . Collective states in the second minimum of the potential

Probability density for the normal and superdeformed ground state



Fission

WKB , fission paths, lifetimes
Different variables, axial shapes



A.Staszczak, A.Baran, J.Dobaczewski, W.Nazarewicz, Phys.Rev. C **80**, 014309 (2009)