Nuclear mean field theory and collective phenomena

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Outline

Introduction. Collective phenomena

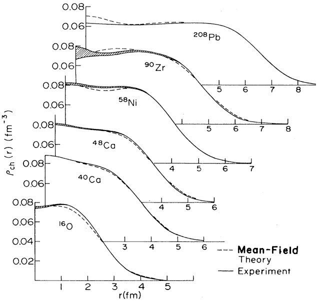
- Collective vs one-particle phenomena
- Translational motion, rotations, fission, giant resonances, changes of shape (deformation) of a nucleus
- Collective variables (not too many), collective Hamiltonian
- Other fields of physics (condensed matter, plasma etc)

Nuclear matter distribution, shape of a nucleus

Mass density distribution

$$\rho_{\mathrm{mass}}(\boldsymbol{r}) = \langle \Psi(\boldsymbol{r}_1, ..., \boldsymbol{r}_A)| \sum_i \delta(\boldsymbol{r} - \boldsymbol{r}_i) |\Psi(\boldsymbol{r}_1, ..., \boldsymbol{r}_A)\rangle$$

Sum over protons for the charge distribution



Closed shells, spherical nuclei

Multipole moments of density distribution. Quadrupole variables

Multipole moments

$$q_{lm} = \int \rho(\boldsymbol{r}) r^l Y_{lm}(\theta, \phi) d^3\boldsymbol{r} = \langle \Psi(\boldsymbol{r}_1, ..., \boldsymbol{r}_A) | \sum_i r_i^l Y_{lm}(\theta_i, \phi_i) | \Psi(\boldsymbol{r}_1, ..., \boldsymbol{r}_A) \rangle$$

- $q_{00} = A$
- only some l's are taken into account, e.g. $l = 2$ — quadrupole moments

$$q_{2m} = \langle \Psi | \sum_i r_i^2 Y_{2m}(\theta_i, \phi_i) | \Psi \rangle$$

- q_{lm} — complex numbers (but $q_{lm}^* = (-1)^m q_{l-m}$), depending on a reference frame, tensors of a rank l w.r.t. rotation group
- parity $\pi = (-1)^l$

Other types of quadrupole variables

1. Nuclear surface expansion

$$r(\theta,\phi,\alpha) = r_0(1 + \sum_{lm} a^*_{lm} Y_{lm}(\theta,\phi)) \longrightarrow r_0(1 + \sum_m a^*_{2m} Y_{2m}(\theta,\phi))$$

2. Ellipsoid (nuclear surface or one-particle potential), $x_i = x, y, z$

$$\sum_{k,j} w_{kj} x_k x_j = 1, \quad w_{kj} = w_{jk}$$

$$\xrightarrow{R(\Omega)} \frac{\tilde{x}^2}{v_x^2} + \frac{\tilde{y}^2}{v_y^2} + \frac{\tilde{z}^2}{v_z^2} = 1$$

Principal axes (intrinsic) frame of reference

- Normalization

$$\alpha_m = c q_{2m}, \quad c = \sqrt{\pi/5}/A\overline{r^2}, \quad \overline{r^2} = 3/5 r_0^2 A^{2/3}$$

- Intrinsic frame

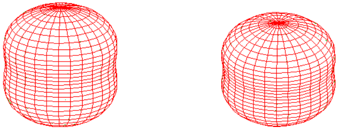
$$\{\alpha_m\} \xrightarrow{R(\Omega)} \{\tilde{\alpha}_0,\ \tilde{\alpha}_1 = \tilde{\alpha}_{-1} = 0,\ \tilde{\alpha}_2 = \tilde{\alpha}_{-2}\}$$

- Deformation variables β, γ

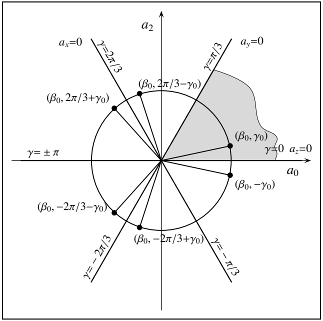
$$\beta \cos\gamma = \tilde{\alpha}_0$$
$$\beta \sin\gamma = \sqrt{2}\,\tilde{\alpha}_2$$

- Special case $\tilde{\alpha}_2 = 0$ – axial symmetry
  $\tilde{\alpha}_0 > 0$ — prolate (cigar-like) shape
  $\tilde{\alpha}_0 < 0$ — oblate (disk-like) shape

β, γ variables, cont.

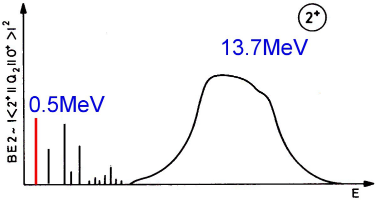


Symmetries on the $(\alpha_0, \alpha_2) \longrightarrow (\beta, \gamma)$ plane



Experimental hints

- For almost all even-even nuclei the first excited state is 2^+
- Schematic spectrum of 2^+ excitation in [100]Mo



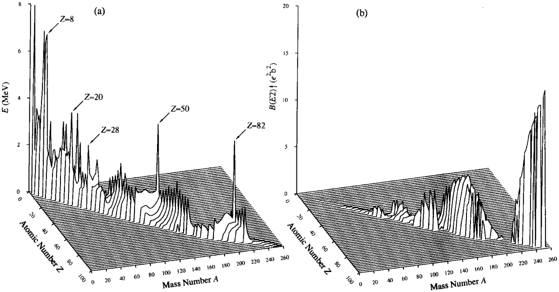
[Energies for [100]Mo]

- Strength (reduced probability) of an electromagnetic transition

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

For most nuclei $B(E2)$ for $2_1^+ \to$ g.s. is $30 - 200$ Weisskopf units (single particle estimates)

Experimental data on the 2_1^+ state



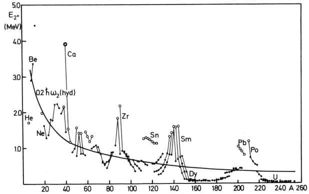
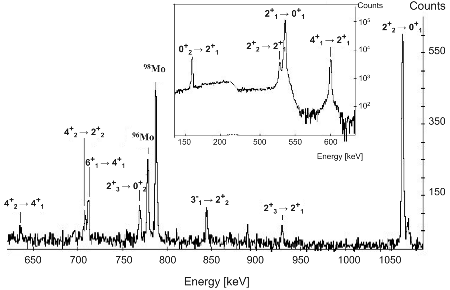
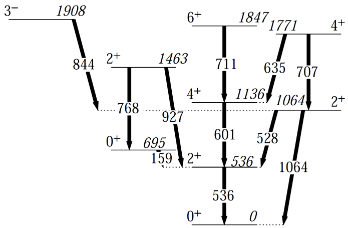


Figure 1.7. The energy of the first 2^+ state in even–even nuclei. The nuclei with closed neutron or proton shells are marked by open circles. (From [NN 65].)

Example of results from experiments at HIL

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





Collective Hamiltonian. Kinetic energy

Classical kinetic energy
Laboratory frame

$$E_{\rm kin} = \frac{1}{2}\sum_{mn} B_{mn}(\alpha)\dot{\alpha}_m\dot{\alpha}_n$$

Intrinsic frame

$$E_{\rm kin} = T_{\rm vib} + T_{\rm rot} = \frac{1}{2}(B_{\beta\beta}\dot{\beta}^2 + 2B_{\beta\gamma}\beta\dot{\beta}\dot{\gamma} + B_{\gamma\gamma}\beta^2\dot{\gamma}^2) + \sum_{k=1}^{3}\frac{I_k^2}{2J_k}$$

$$B_{\beta\beta}(\beta,\gamma),\quad B_{\beta\gamma}(\beta,\gamma),\quad B_{\gamma\gamma}(\beta,\gamma),\quad J_k = 4\beta^2 B_k(\beta,\gamma)\sin^2(\gamma - 2\pi k/3),\ k = 1,2,3$$

Quantization. Laplace-Beltrami operator

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

Volume element (for scalar product in the Hilbert space) $\sqrt{\det B}\, d\alpha_{-2}\ldots d\alpha_2$

Quantum Hamiltonian in the intrinsic frame

General Bohr Hamiltonian (Aage Bohr)

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

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

$$\left.+\frac{1}{\beta\sin 3\gamma}\left[-\partial_\gamma\left(\sqrt{\frac{r}{w}}\sin 3\gamma B_{\beta\gamma}\right)\partial_\beta + \frac{1}{\beta}\partial_\gamma\left(\sqrt{\frac{r}{w}}\sin 3\gamma B_{\beta\beta}\right)\partial_\gamma\right]\right\}$$

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

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

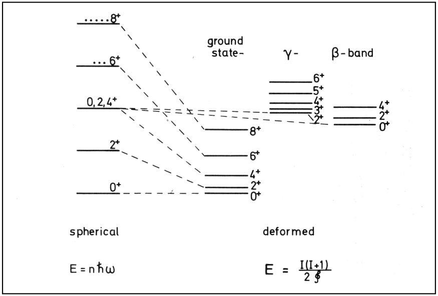
Special cases

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

$$T_{\rm vib} = -\frac{\hbar^2}{2B}\left[\frac{1}{\beta^4}\partial_\beta \beta^4 \partial_\beta + \frac{1}{\beta^2 \sin 3\gamma}\partial_\gamma \sin 3\gamma \partial_\gamma\right]$$

  Various potentials

- Harmonic oscillator: $V = C\beta^2/2,\ \ H_{\rm osc} = \frac{B}{2}|\dot{\alpha}|^2 + \frac{C}{2}|\alpha|^2,\ \ |\alpha|^2 = \sum_m \alpha_m \alpha_m^*$



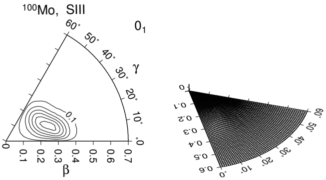
Quantum Hamiltonian, cont.

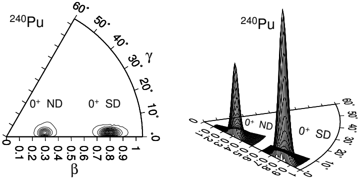
- Energy levels
- Matrix elements of the E2 transition operator — halflives of levels, quadrupole moments
- Wave functions

$$\Psi^{\text{(coll)}}_{IM\xi}(\beta,\gamma,\Omega) = \sum_{K=0(2),\text{even}}^{I \text{ or } I-1} F_{IK\xi}(\beta,\gamma)\phi^{I}_{MK}(\Omega)$$

- Probability distributions (of various shapes!)

$$p_{I\xi}(\beta,\gamma) = \sum_K |F_{IK\xi}(\beta,\gamma)|^2 \sqrt{wr}\beta^4 |\sin 3\gamma|$$





Mean field, Hartree-Fock method

- Free (quasi)particles in an average potential
- Product wave function, Slater determinant $\det|\phi_k(\boldsymbol{r}_k)|$.
- Phenomenological potentials: harmonic oscillator, square well, deformed (anisotropic) harmonic oscillator (Nilsson potential), Woods-Saxon potential,...
- Variational principle
- Hartree-Fock equations

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

- Effective nucleon-nucleon interactions
- Pairing correlations

Hartree-Fock method, second quantization

- Microscopic Hamiltonian for a system of nucleons

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

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

- Hartree-Fock equations

$$[H_{\text{mf}}(\rho), \rho] = 0$$

Mean field Hamiltonian

$$H_{\text{mf}} = \sum_{\mu,\nu} (T_{\mu\nu} + \Gamma_{\mu\nu}) c_\mu^+ c_\nu$$

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

$$\rho_{\mu\nu} = \langle \Psi_{\text{HF}} | c_\nu^+ c_\mu | \Psi_{\text{HF}} \rangle$$

Mean field, Hartree-Fock-Bogolyubov method

- Pairing correlations
- More general product state (BCS type), undetermined particle number (!)

$$\Psi_{\mathrm{BCS}} = \prod_{\mu>0}(u_\mu + s_\mu v_{\bar{\mu}} c^+_{\bar{\mu}} c^+_\mu) \left|0\right\rangle$$

Quasiparticles

$$\alpha^+_\mu = u_\mu c^+_\mu + s^*_\mu v_{\bar{\mu}} c_{\bar{\mu}}$$

- Density matrix $\mathcal{R}$

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} = \begin{pmatrix} \langle\Psi| c^+_\nu c_\mu |\Psi\rangle & \langle\Psi| c_\nu c_\mu |\Psi\rangle \\ \langle\Psi| c^+_\nu c^+_\mu |\Psi\rangle & \langle\Psi| c_\nu c^+_\mu |\Psi\rangle \end{pmatrix}$$

Canonical basis

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

Hartree-Fock-Bogolyubov theory, cont.

- Hartree-Fock-Bogolyubov equations

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

- Mean field Hamiltonian

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

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

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

Skyrme effective nucleon-nucleon interaction

- Momentum space representation

$$\langle \boldsymbol{k}|\, V\, |\boldsymbol{k}'\rangle = t_0(1 + x_0 P_\sigma) + \frac{1}{2} t_1(\boldsymbol{k}^2 + \boldsymbol{k}'^2) + t_2 \boldsymbol{k}\boldsymbol{k}' + iW_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\cdot(\boldsymbol{k}\times\boldsymbol{k}') + v_{123}$$

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

$$\begin{aligned} V_S \;=\;& t_0(1 + x_0 P_\sigma)\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) + \frac{1}{2} t_1(\boldsymbol{k}^2 \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) + \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\boldsymbol{k}'^2) + t_2 \boldsymbol{k}\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\boldsymbol{k}' + \\ & + iW_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\cdot(\boldsymbol{k}\times\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\boldsymbol{k}') + \\ & + \tilde{t}_3 \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\delta(\boldsymbol{r}_2 - \boldsymbol{r}_3) \longrightarrow \frac{1}{6} t_3(1 + P_\sigma)\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\rho^\alpha((\boldsymbol{r}_1 + \boldsymbol{r}_2)/2) \end{aligned}$$

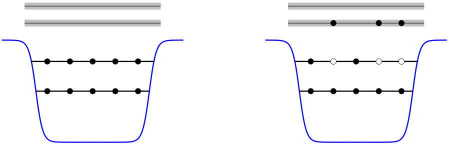
$$\boldsymbol{k}' = \frac{1}{2i}(\overrightarrow{\boldsymbol{\nabla}}_1 - \overrightarrow{\boldsymbol{\nabla}}_2), \quad \boldsymbol{k} = -\frac{1}{2i}(\overleftarrow{\boldsymbol{\nabla}}_1 - \overleftarrow{\boldsymbol{\nabla}}_2),$$

plus Coulomb interaction for protons

- Several variants $(t_0, t_1, t_2, t_3, x_0, W_0)$: SIII, SLy4-6, SkM*, UNEDF, ...
  Parameters fixed by fitting masses, radii, etc of some chosen nuclei

Mean field description of collective phenomena

Giant resonances, Random Phase Approximation (RPA)



Low energy collective excitations, Adiabatic Time Dependent Hartree-Fock-Bogolyubov

Mean field description of collective phenomena, cont.

- Set of product states depending on collective variables,
  HFB calculations with constraints
  $\delta \langle\Psi| |H_{\mathrm{micr}} |\Psi\rangle = 0, \quad \langle\Psi| Q_{20} |\Psi\rangle = q_{20}, \ \langle\Psi| Q_{22} |\Psi\rangle = q_{22}$

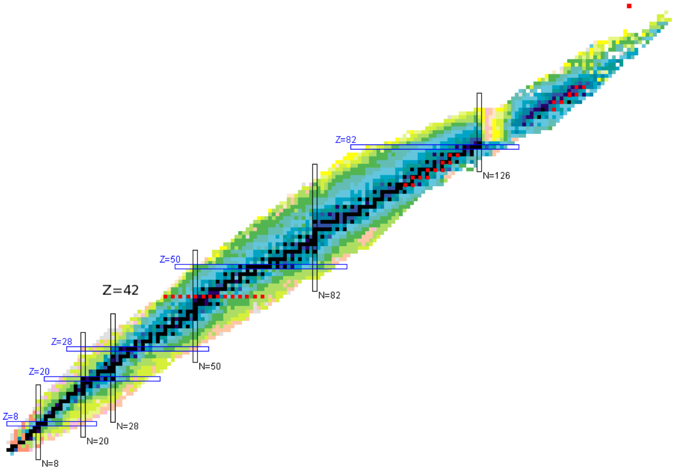
- Adiabatic Time Dependent Hartree-Fock-Bogolyubov

$$\downarrow$$

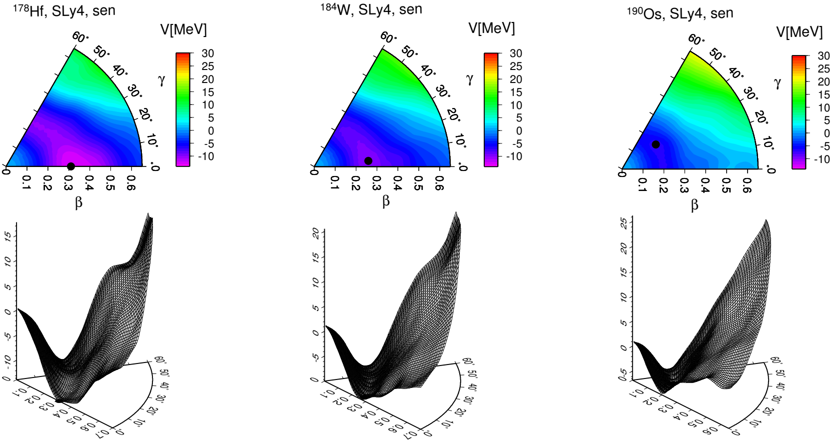
- Schrödinger-type equation in the collective space
  In our case Bohr Hamiltonian with $B_{\beta\beta}, B_{\beta\gamma}, B_{\gamma\gamma}, B_k, V$ calculated from the mean field theory

Some applications

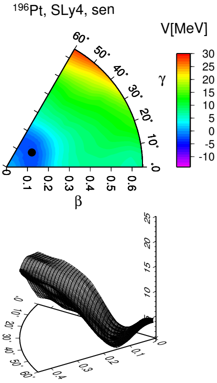
1. From strongly deformed Hf isotopes to almost spherical Hg
2. $^{84-110}$Mo isotopes
3. Actinides

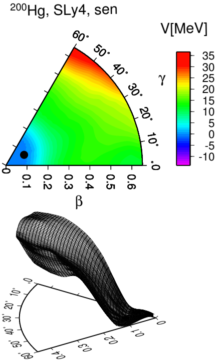


^{178}Hf — ^{200}Hg. Collective potential energy

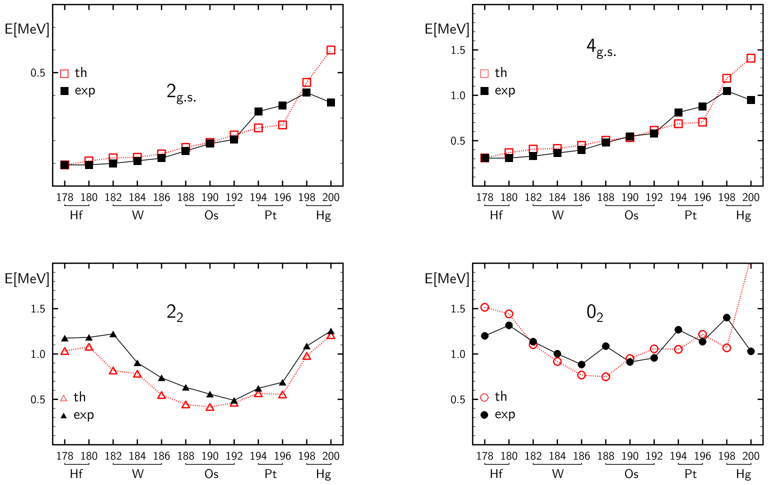


^{178}Hf — ^{200}Hg. Collective potential energy

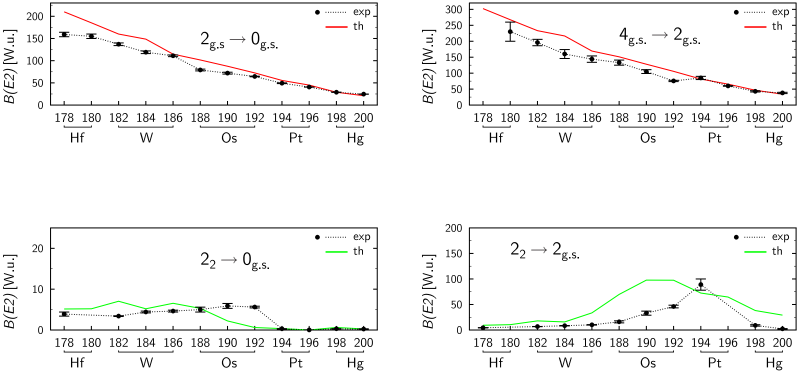




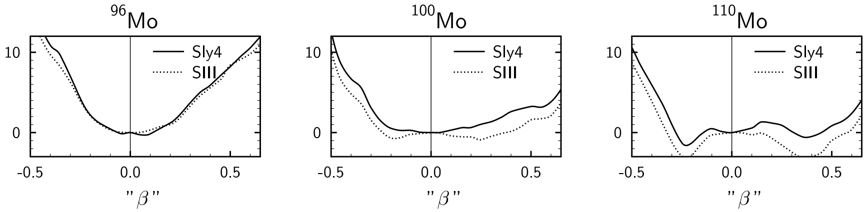
^{178}Hf — ^{200}Hg. Energy levels



^{178}Hf — ^{200}Hg. E2 transition probabilities

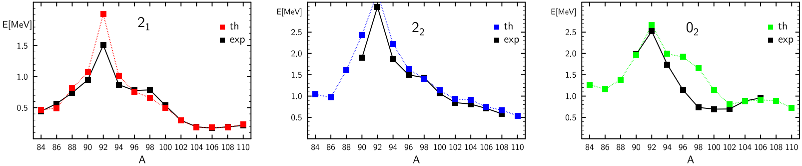


Mo isotopes. Potential energy

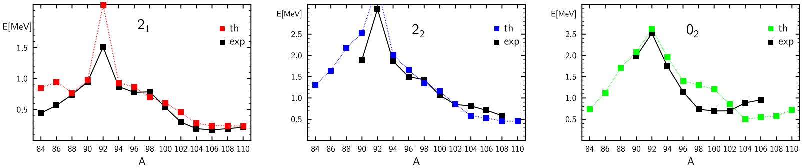


Mo isotopes. Energy levels

SIII

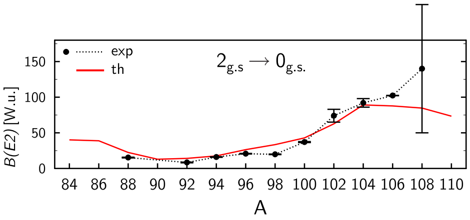


SLy4

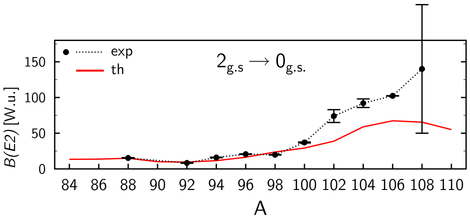


Mo isotopes. E2 transitions $2_1 \rightarrow 0_{g.s.}$

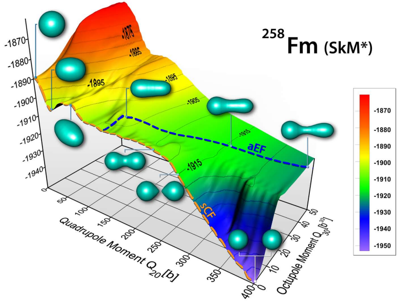
SIII

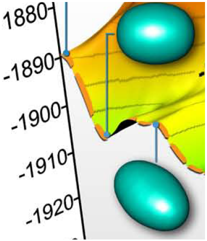


SLy4



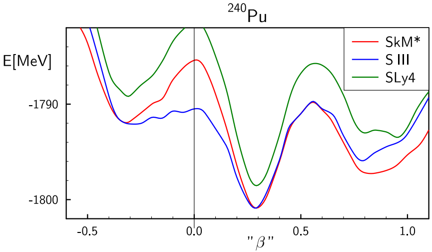
Actinides

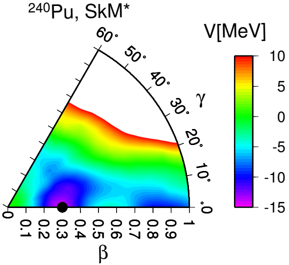


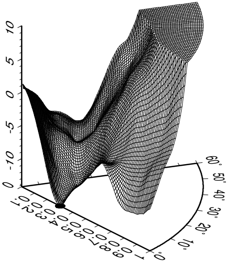


A. Staszczak, A. Baran, J. Dobaczewski, W. Nazarewicz, Phys.Rev. C **80**, 014309 (2009)

^{240}Pu potential energy







Some remarks

- Limitations of the theory
- Coupling collective and one-particle modes
- What about odd and odd-odd nuclei?