Nuclear structure: part 2

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- 1. Nuclear theory selection of starting point
- 2. What can be done 'exactly' (*ab-initio* calculations) and why we cannot do that systematically?
- 3. Effective interactions
- 4. Density functional theory
- 5. Shell structure and shell effects. Their consequences.
- 6. Nuclear landscape: what we know and how well we extrapolate
- 7. Superheavy nuclei
- 8. Going beyond mean field approximation: particle-vibration coupling in spherical nuclei
- 9. Rotation in nuclei

Reminder from previous lecture

Deformation dependence of the single-particle energies in a realistic Nilsson potential

- 1. removing of the 2j+1 degeneracy of single-particle state seen at spherical shape
- single-particle states at deformation ε₂ not equal 0 are only two-fold degenerate
- 3. creation of deformed shell gaps



Shell structure and shell correction energies $\delta E_{shell} = 2 \sum_{v} e_{v} - 2 \int e \widetilde{g}(e) de \quad \text{shell correction energy}$ $e_{v} \text{ - single-particle energies} \qquad \widetilde{g}(e) \text{ - smeared level density}$ $E_{tot} = E_{LD} + \delta E_{sh}(p) + \delta E_{sh}(n)$ $\varepsilon \quad \varepsilon \quad \varepsilon$



Superheavy nuclei



Stability of superheavy nuclei is determined exclusively by quantum (shell) effects

Competition of two processes after formation of superheavy nucleus: spontaneous fission and α -decay



 $\log_{10} T_{\alpha} = (a Z + b) Q_{\alpha}^{-1/2} + (c Z + d)$

1. Increase of stability on approaching deformed N=162 shell gap 2. Increase of stability on increase of N above 166



A Russian artist depicts the modern nuclear theory of the heaviest elements. At the upper far right is the island of stability, which was demonstrated by the production of long-lived element 114 in 1998 by a Russian–Livermore team.







Shell correction energy: difference between tin and SHE regions





What are the possible sources of different centers of the islands of SHE?

self-consistency effects [density profiles]

may explains mic+mac vs DFT

- **spin-orbit splittings** may explain CDFT versus Skyrme DFT Lesson from quantum mechanics: spherical harmonic oscillator



A: the radial wave function $R(\rho)$

B: effective radial potential, i.e. with the centrifugal term

 $\hbar^2 \ell(\ell+1)/(2Mr^2)$ added.



Densities of superheavy nuclei: spherical CDFT calculations with the NL3 force



Spin – orbit interaction – fully relativistic phenomenon

$$j = l \pm 1/2$$

$$V_{LS} = W(r)\vec{l}\vec{s}$$



Spin-orbit splittings



Need for accurate description of fission barriers since they strongly affect:

1. The probability for the **formation** of superheavy nuclei in heavy-ion-fussion reaction (the cross-section very sensitively depends on the fission barrier height).

2.survival probability of an excited nucleus in its cooling by emitting neutrons and γ-rays in competition with fission (the changes in fission barrier height by 1 MeV changes the calculated survival probability by about one order of magnitude or more)

3. spontaneous fission lifetimes





Fission barriers: theory versus experiment [state-of-the-art]



Mac+mic, LSD model A.Dobrowolski et al, PRC 75, 024613 (2007) Mac+mic, FRDM model P. Moller et al, PRC 79, 064304 (2009) Gogny DFT, J.-P. Delaroche et al, NPA 771, 103 (2006).

CDFT : actinides H. Abusara, AA and P. Ring, PRC 82, 044303 (2010) superheavies: H. Abusara, AA and P. Ring, PRC 85, 024314 (2012)







Inner fission barrier heights according to different models

Going beyond mean field approximation: particle-vibration coupling in spherical nuclei







3. energy corrections due to particle-vibration coupling (PVC)

Relativistic particle-vibration coupling (PVC) model

The equation of the one-nucleon motion has the form (in single-particle Green functions) $D = 2\pi i \left(\sum_{i=1}^{n} D_{i} \right) = 2\pi i \left(\sum_{i=1}^{n} D_{i} \right)$

$$\sum_{l} \{(\varepsilon - \varepsilon_{k})\delta_{kl} - \Sigma_{0}^{e}(\varepsilon)\}G(\varepsilon) = 1$$

$$\sum_{l} \{(\varepsilon - \varepsilon_{k})\delta_{kl} - \Sigma_{kl}^{e}(\varepsilon)\}G_{lk'}(\varepsilon) = \delta_{kk'}$$

particle-phonon coupling model:

energy-dependent part of the mass operator is a convolution of the particlephonon coupling amplitude Γ and the exact single-particle Green's function

$$\Sigma_{kl}^{e}(\varepsilon) = \sum_{k'l'} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi i} \Gamma_{kl'lk'}(\omega) G_{k'l'}(\varepsilon + \omega)$$

depends on phonon vertexes $\gamma_{kl}^{\mu} = \sum_{l'l'} V_{kl'lk'} \delta \rho_{k'l'}^{\mu}$

 $V_{kl'lk'}$ - the relativistic matrix element of the residual interaction and $\delta\rho$ is the transition density. We use the linearized version of the model which assumes that $\delta\rho$ is not influenced by the particle-phonon coupling and can be computed within relativistic RPA.

Cut-off of phonon basis in the RRPA calculations

Phonons of the multipolarities 2⁺, 3⁻, 4⁺, 5⁻, 6⁺ with energies below 15 MeV are included in the model space of the PVC calculations. The addition of phonon modes with energies above 15 MeV does not affect the results. The phonon energies and their coupling vertices have been computed within the self-consistent RRPA.





Spectroscopic factors

Nucleus	State	S_{th}	S_{exp}	S_{exp}
²⁰⁹ Bi	1hovo	0.88	1 17 [75]	0.80 [69]
Di	$2f_{7/2}$	0.78	0.78 [75]	0.76 [69]
	$1i_{13/2}$	0.63	0.56 75	0.74 [69]
	$2f_{5/2}$	0.61	0.88 [75]	0.57 [69]
	$3p_{3/2}$	0.62	0.67 [75]	0.44 [69]
	$3p_{1/2}$	0.37	0.49[75]	0.20 [69]
	Nucleus	State	S_{th}	S_{exp}
	133 Sn	$2f_{7/2}$	0.89 0	$.86 \pm 0.16$
		$3p_{3/2}$	0.91 0	$.92 \pm 0.18$
		$1 h_{9/2}$	0.88	
		$3p_{1/2}$	0.91	1.1 ± 0.3
		$2f_{5/2}$	0.89	1.1 ± 0.2

The absolute values of experimental spectroscopic factors are characterized by large ambiguities and depend strongly on the reaction employed in experiment and the reaction model used in the analysis



vibration coupling ("def+TO+PVC")] calculations in ⁵⁶Ni, ¹³²Sn and ²⁰⁸Pb, respectively.

The impact of particle-vibration coupling on pseudospin doublets.



is taken into account.

Exp (protons)

Dominant neutron states in Z = 120



Shell evolution in superheavy Z = 120 isotopes: Quasiparticle-vibration coupling (QVC) in a relativistic framework





Major features of rotation

1. The nucleus has to be deformed to rotate (most nuclei have a deformed axial shape in the ground state)

- 2. The nucleus rotates as a whole \rightarrow **collective** degrees of freedom
- 3. The nucleons move independently inside the deformed potential → intrinsic (single-particle) degrees of freedom

4. The nucleonic motion is much faster than the rotation \rightarrow adiabatic approximation





Maximum spin of the N=50 ground state is I=0



2p-2h excitation in the N=50 system \rightarrow induces deformation \rightarrow increases maximum spin in this configuration

$$(g_{9/2})_{4.5+3.5=8}^{-2} (g_{7/2}d_{5/2})_{3.5+2.5=6}^{2} \implies I_{\max} = 14$$





Physical observables in rotating nuclei



e

Kinematic moment of inertia $J^{(1)}$

$$J^{(1)}_{band} \;=\; \frac{2I-1}{E_{\gamma}(I \to (I-2))} \;\; MeV^{-1}$$

inverse of the slope of the curve of energy E versus I(I+1)
 requires the knowledge of the spin

Dynamic moment of inertia J⁽²⁾

$$J^{(2)}(I) = \frac{4}{E_{\gamma}((I+2) \to I) - E_{\gamma}(I \to (I-2))} \quad \text{MeV}^{-1}$$

 \succ curvature of the of energy curve E versus I(I+1))

Very useful for superdeformed bands which are not linked to the low-spin level scheme (spin I is not known)

Charge quadrupole moment

How to describe rotating nuclei?



Transformation to rotating frame \rightarrow CRANKING MODEL

$$\hat{H}^{\omega} = \hat{H} - \omega \hat{J}_{x}$$

Laboratory frame: potential V is time-dependent Rotating frame: potential V* is time-independent

The state |> is the stationary mean field solution in the frame that rotates uniformly with the angular velocity ω about the x axis.

In the laboratory frame it corresponds to a uniformly rotating mean field state.

$$\left\langle \begin{array}{c} |\hat{J}_{x}| \end{array} \right\rangle = \sum_{i} \left\langle |\hat{j}_{x}| \right\rangle_{i} \qquad \left\langle |\hat{J}_{x}| \right\rangle = \sqrt{I(I+1)} \\ \left(\begin{array}{c} h_{D} - \lambda - \Omega_{x} \hat{J}_{x} & \hat{\Delta} \\ -\hat{\Delta}^{*} & -h_{D}^{*} + \lambda + \Omega_{x} \hat{J}_{x} \end{array} \right) \begin{pmatrix} U_{k} \\ V_{k} \end{pmatrix} = E_{k} \begin{pmatrix} U_{k} \\ V_{k} \end{pmatrix}$$

 $-\Delta^{*}$









Paired band crossings: CRHB+LN versus CSM+PNP

CSM+PNP (Z.-H.Zhang et al, PRC 85, 014324 (2012)). Carefull fit of:

- Parameters of Nilsson
 potential to the energies of
 the single-particle states
- Different pairing strength in even-even and odd nuclei
- Experimental deformations



Nuclear structure: extras

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- 10. Rotating nuclei

What experimentalists see in experiment? α-decay chains



Can we obtain "bare" single-particle energies that can be used for comparison with plain DFT?





	Nucleus	State	S_{th}	S_{exp}	S_{exp}
Spectroscopic factors The absolute values of	²⁰⁹ Pb	$\begin{array}{c} 2g_{9/2} \\ 1i_{11/2} \\ 1j_{15/2} \\ 3d_{5/2} \\ 4s_{1/2} \\ 2g_{7/2} \\ 3d_{2/2} \end{array}$	$0.85 \\ 0.89 \\ 0.66 \\ 0.89 \\ 0.92 \\ 0.87 \\ 0.89$	0.78 ± 0.1 [76] 0.96 ± 0.2 [76] 0.53 ± 0.2 [76] 0.88 ± 0.1 [76] 0.88 ± 0.1 [76] 0.78 ± 0.1 [76] 0.88 ± 0.1 [76]	$\begin{array}{c} 0.94 \ [80] \\ 1.05 \ [80] \\ 0.57 \ [80] \end{array}$
experimental spectroscopic factors are characterized by large ambiguities and depend strongly on the reaction employed in experiment and the reaction model used in the analysis	²⁰⁹ Bi ²⁰⁷ Pb	$\begin{array}{c} 1h_{9/2} \\ 2f_{7/2} \\ 1i_{13/2} \\ 2f_{5/2} \\ 3p_{3/2} \\ 3p_{1/2} \\ 3p_{1/2} \\ 2f_{5/2} \end{array}$	$\begin{array}{c} 0.88\\ 0.78\\ 0.63\\ 0.61\\ 0.62\\ 0.37\\ 0.90\\ 0.87\\ 0.90\\ 0.87\\ \end{array}$	$\begin{array}{c} 1.17 \ [75] \\ 0.78 \ [75] \\ 0.56 \ [75] \\ 0.88 \ [75] \\ 0.67 \ [75] \\ 0.49 \ [75] \\ \end{array}$	$\begin{array}{c} 0.80 & [69] \\ 0.76 & [69] \\ 0.74 & [69] \\ 0.57 & [69] \\ 0.44 & [69] \\ 0.20 & [69] \\ 1.08 & [83] \\ 1.05 & [83] \\ 0.05 & [8$
used in the undrysis	²⁰⁷ Tl	$\begin{array}{c} 3p_{3/2} \\ 1i_{13/2} \\ 2f_{7/2} \\ 1h_{9/2} \\ \\ 3s_{1/2} \\ 2d_{3/2} \\ 1h_{11/2} \\ 2d_{5/2} \\ 1g_{7/2} \end{array}$	$\begin{array}{c} 0.86 \\ 0.82 \\ 0.64 \\ 0.38 \end{array}$ $\begin{array}{c} 0.84 \\ 0.86 \\ 0.80 \\ 0.68 \\ 0.22 \end{array}$	$\begin{array}{c} 1.00 \ [78] \\ 1.04 \ [78] \\ 0.89 \ [78] \end{array}$ $\begin{array}{c} 0.95 \ [77] \\ 1.15 \ [77] \\ 0.89 \ [77] \\ 0.62 \ [77] \\ 0.40 \ [77] \end{array}$	$\begin{array}{c} 0.95 & [83] \\ 0.61 & [83] \\ 0.64 & [83] \\ 0.85 & [68] \\ 0.90 & [68] \\ 0.88 & [68] \\ 0.63 & [68] \\ 0.27 & [68] \end{array}$

ucleus	State	S_{th}	S_{exp} [79]	S_{exp} [59]
⁵⁷ Ni	$2D_{2/2}$	0.83	0.95 ± 0.29	0.58 ± 0.11
	$1f_{5/2}$	0.79	1.40 ± 0.42	
	$2p_{1/2}$	0.76	1.00 ± 0.30	
	$1g_{9/2}$	0.79		
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1.030	Nucleus	State	S_{th}	S_{exp}
	100			
	133 Sn	$2f_{7/2}$	0.89	0.86 ± 0.16
08 00		$3p_{3/2}$	0.91	0.92 ± 0.18
Call		$1h_{9/2}$	0.88	0
A was		$3p_{1/2}$	0.91	1.1 ± 0.3
0.00		2f5/2	0.89	1.1 ± 0.2