Shell model Monte Carlo level density calculations in the rare-earth region

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Outline

- Introduction
- Shell-model Monte Carlo approach
- Level densities in the rare-earth region
- Crossover from vibrational to rotational collectivity
- Odd-even and odd-odd nuclei: Challenge to get E_{gs}
- Conclusions

Nuclear Level Density

Nuclear level density is the number of nuclear levels per excitation energy at a given excitation energy

$$\rho(E_x) = \sum_J \rho_J(E_x) \qquad \text{level density}$$

$$\rho(E_x) = \sum_J (2J+1)\rho_J(E_x) \qquad \text{state density or total level density}$$

- Fundamental quantity for nuclear structure at finite T
- Essential for Hauser-Feschbach theory of nuclear reaction rates (astrophysical nucleosynthesis)
- Important ingredient for nuclear transmutation calculations

Methods

Experimental

- Level counting (low energies)
- Charged particles, Oslo method (medium energies)
- Neutron resonances
- Ericson fluctuations (higher energies)

Phenomenological

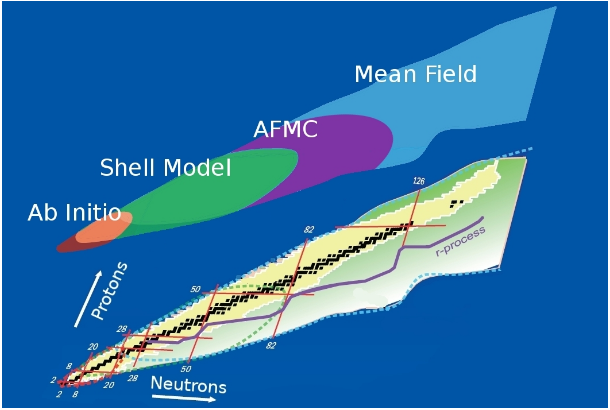
- Simple parametrizations (Back-shifted Bethe formula, composite formula etc.)
- Generalized supefluid model

Theoretical

- Microscopic combinatorial models (+ collective effects)
- Shell-model Monte Carlo (SMMC)

Level density calculations in the SMMC approach

Auxiliary-field Monte Carlo (AFMC) or **Shell-model Monte Carlo (SMMC)**:
A powerful technique to calculate finite temperature properties and (total) level densities of heavy nuclei.



AFMC in a nutshell

Auxiliary-field Monte Carlo method for nuclear shell model

AFMC describes the nucleus by a canonical ensemble at $\beta = \frac{1}{T}$.

$$\langle X \rangle = \frac{\mathrm{Tr}\ [e^{-\beta H} X]}{\mathrm{Tr}\ e^{-\beta H}}$$

Hubbard-Stratonovich transformation:

$$e^{-\beta H} \longrightarrow \int \mathfrak{D}[\sigma] G(\sigma) U_\sigma \quad \text{where} \quad U_\sigma = \prod_{n=1}^{N_t} e^{-\Delta\beta h(\sigma)}$$

SMMC Total level density:

$$E(\beta) = \frac{\mathrm{Tr}[He^{-\beta H}]}{\mathrm{Tr}[e^{-\beta H}]} = \frac{\int \mathrm{d}E\ e^{-\beta E} E \rho(E)}{Z(\beta)} \longrightarrow \rho(E)$$

Koonin, Dean, Langanke, Phys. Rep. **278**, 1, 1997 and references therein.

Effective Interactions without the Sign Problem

effective nuclear int. $\approx$ collective part $+$ non-collective part

collective part $\downarrow$ gives *good* sign
important for level densities

non-collective part $\downarrow$ gives *bad* sign
not so important for level density

In the SMMC level density calculations: pairing + multipole-multipole (quadrupole,octupole,hexadecupole) interactions are used.

Empirical Level Densities

Experimentally level density can be directly obtained only at sufficiently low E_x (level counting regime) and at neutron binding energy.

At other E_x, "level counting $+$ neutron resonance data" can be used to parametrize level densities using the ansatz:

Back-shifted Bethe Formula (BBF):

$$\rho(E_x) = \frac{\sqrt{\pi}}{12} a^{-1/4} (E_x - \Delta)^{-5/4} e^{2\sqrt{a(E_x - \Delta)}}$$

Composite Formula:

$$\rho(E) = \begin{cases} e^{(E-E_1)/T_1} & (E < E_M) \\ \frac{\sqrt{\pi}}{12} a^{-1/4} (E_x - \Delta)^{-5/4} e^{2\sqrt{a(E_x - \Delta)}} & (E > E_M). \end{cases}$$

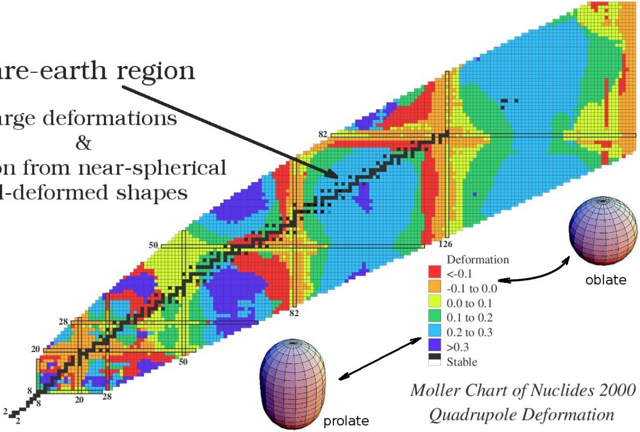
We have studied ≈ 300 nuclei across the chart of the nuclei

Özen and Alhassid, *in preparation*

A Challenging Region of the Nuclear Chart

Rare-earth region

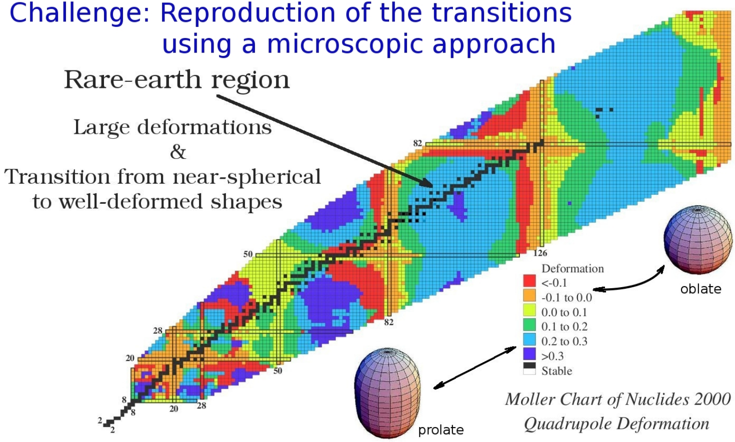
Large deformations
&
Transition from near-spherical
to well-deformed shapes



Moller Chart of Nuclides 2000
Quadrupole Deformation

A Challenging Region of the Nuclear Chart

Challenge: Reproduction of the transitions using a microscopic approach



Gearing up SMMC for heavy nuclei

- Protons and neutrons occupy different shells

  SMMC in the proton-neutron formalism

  Özen and Dean, Phys.Rev.C**73** 014302, (2006)

  Alhassid, Fang, Nakada, Phys. Rev. Lett. **101** , 082501 (2008)

- Gap between the ground state and the first excited state is typically much smaller than the one in the case of medium-mass nuclei

  Cooling down to lower temperatures is necessary

- Larger single-particle spaces and smaller temperatures (*i.e.* larger β)imply ill-conditioned matrices (propagator)

  Matrix operations require stabilization

  Alhassid, Fang, Nakada, Phys. Rev. Lett. **101** , 082501 (2008)

SMMC Calculations in the Rare-earth Region

^{170}Dy (Dean, Koonin, Lang, Ormand, and Radha, 1993)
(isospin formalism)

^{162}Dy (Alhassid, Fang, and Nakada, 2008)
(pn-formalism, even-even nucleus)

Our current work (Özen, Alhassid, and Nakada, *in progress*):

Even-even Sm and Nd isotope chains
Challenge: Transition from near-spherical to deformed structure.

Odd-even and odd-odd nuclei
Challenge: A sign problem caused by projections onto an odd number of nucleons.

Applications in the Rare-earth Region

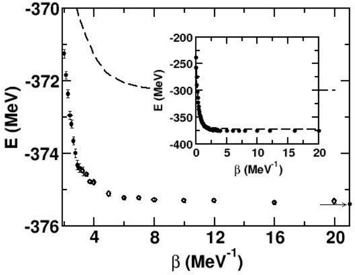
Protons:
50-82 shell plus $1f_{7/2}$
Neutrons:
82-126 shell plus $0h_{11/2}$ and $1g_{9/2}$

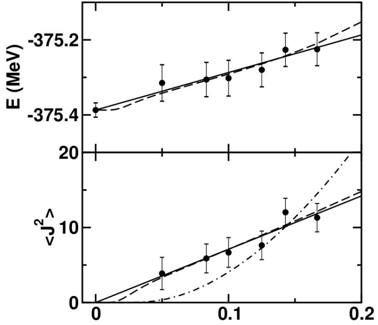
$\approx 10^{29}$ configurations

Single-particle energies: from Woods-Saxon plus spin-orbit
Interaction: Pairing plus multipole-multipole (quadrupole, octupole, and hexadecupole) interaction.
Pairing interaction is determined from odd-even mass differences.
Multipole-multipole interaction is determined self-consistently and renormalized.

Even-even case: ^{162}Dy

Alhassid, Fang, Nakada, 2008
Stabilized calculations achieved cooling up to $\beta = 20$ MeV^{-1}!

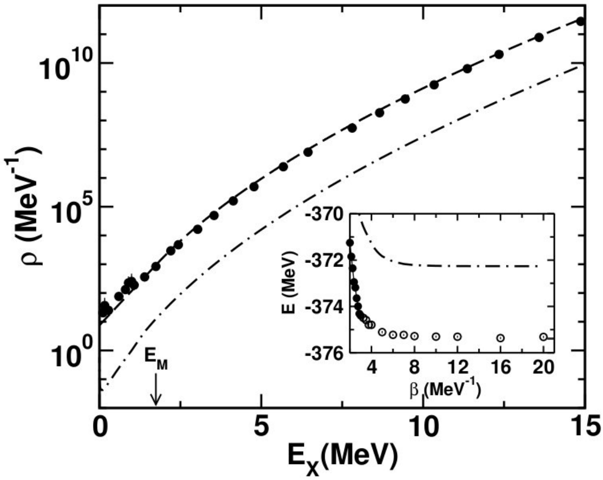




$E(T) \approx E_0 + T$ and $\langle J^2 \rangle \approx 2IT$

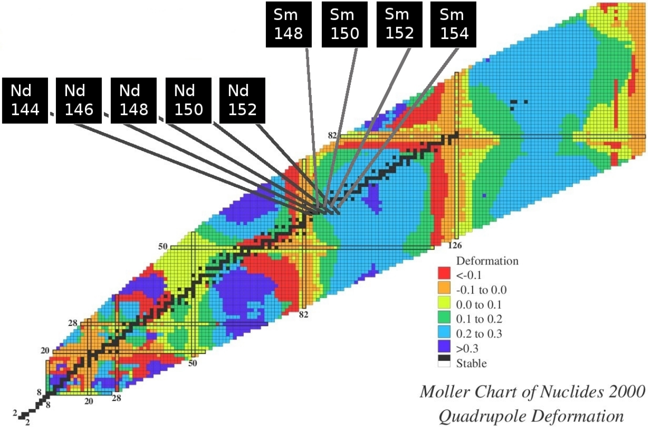
Even-even case: ^{162}Dy

Alhassid, Fang, Nakada, 2008



SMMC Calculations in the Rare-earth Region

Özen, Alhassid and Nakada, *in preparation*



Moller Chart of Nuclides 2000
Quadrupole Deformation

- SMMC stands out as a powerful method for fully microscopic calculation of level densities in large model spaces.
- SMMC calculations is extended to odd-odd and odd-even heavy deformed nuclei. Transitional character of Sm isotopes is reproduced. Results are in good agreement with the experimental data.
- SMMC approach has the prospect of more systematic study of level densities for heavy nuclei.

Acknowledgements

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