Nuclear shapes from self-consistent mean-field and beyond approaches: deformation of *A*=96 isobars

Tomás R. Rodríguez

INT Program 23-1a

Intersection of nuclear structure and high-energy nuclear collisions

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IPARCOS

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gfn UCM Grupo de Física Nuclear

Outline

1. Introduction

2. Self-consistent mean-field: HFB

3. Beyond self-consistent mean-field: symmetry restoration and configuration mixing

4. PGCM for 96Ru and 96Zr

   3.1. Triaxial quadrupole deformation

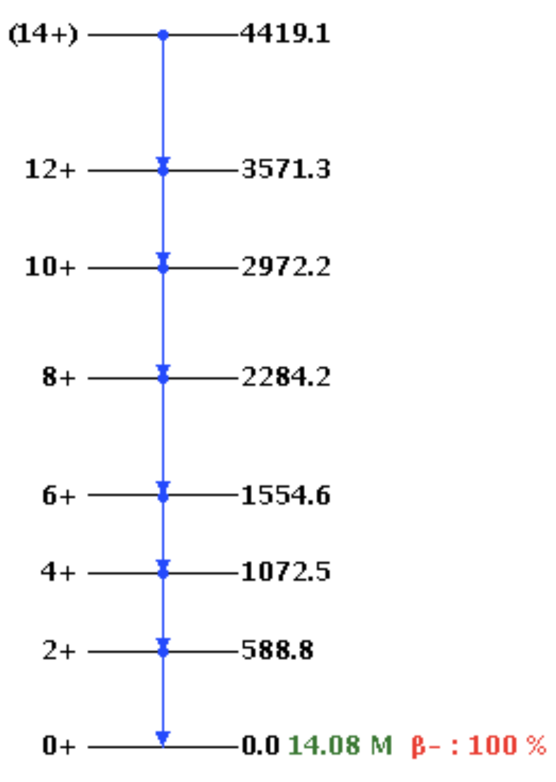
   3.2. Axial quadrupole-octupole deformation

   3.3. What is missing?

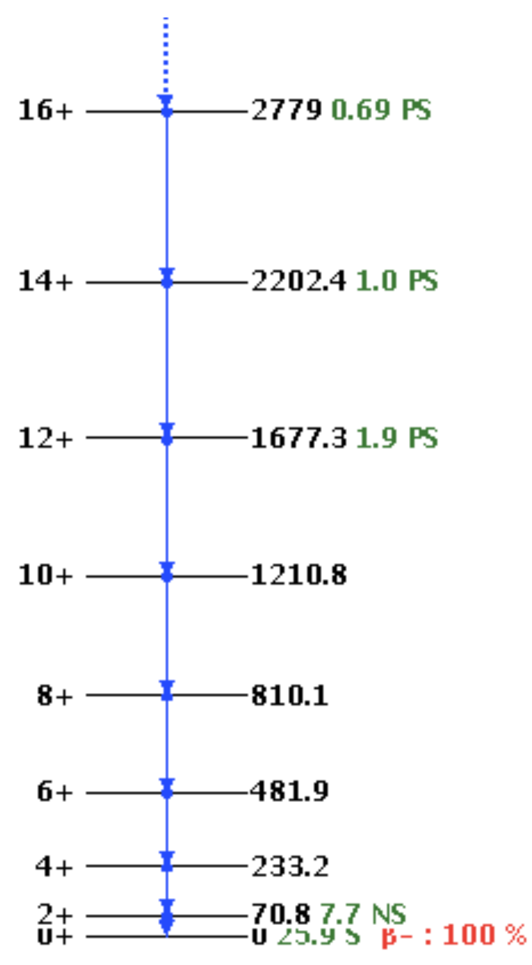
Introduction

• The **intrinsic shape** of the nuclear states is **not a direct observable**, but...

• Intrinsic nuclear shapes can be inferred from the experimental data (energies and electromagnetic moments and transitions) by comparison with the predictions given by geometrical (simple) models.



$^{138}_{54}Xe_{84}$



$^{154}_{60}Nd_{94}$

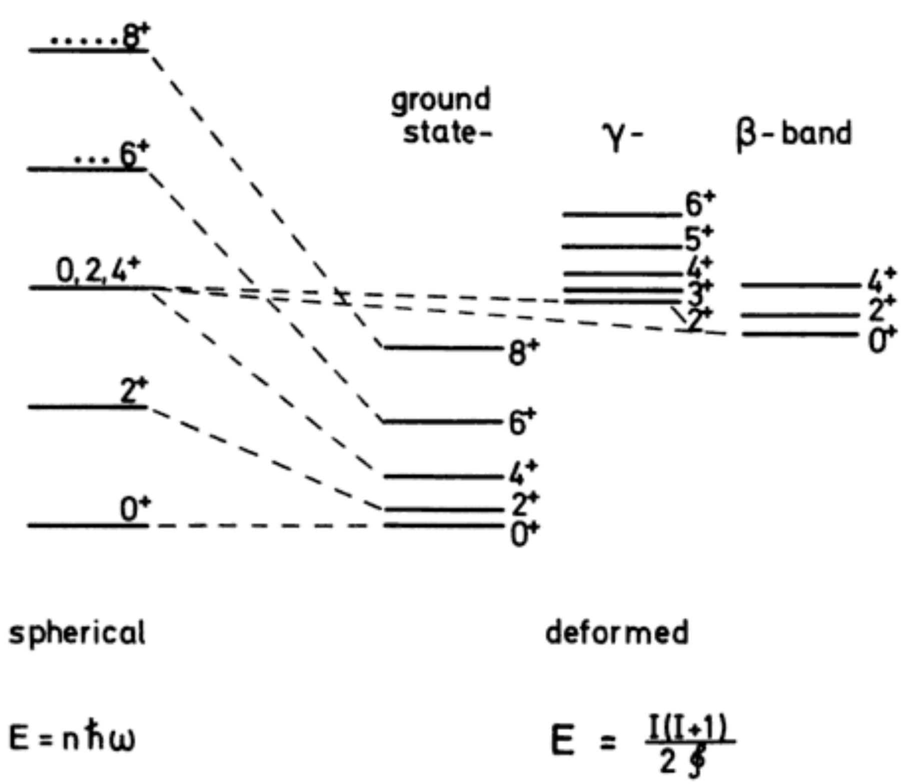


Figure 1.12. Schematic level schemes of spherical and deformed nuclei. (From [SDG 76].)

P. Ring and P. Schuck, *The Nuclear Many-Body Problem*

Introduction

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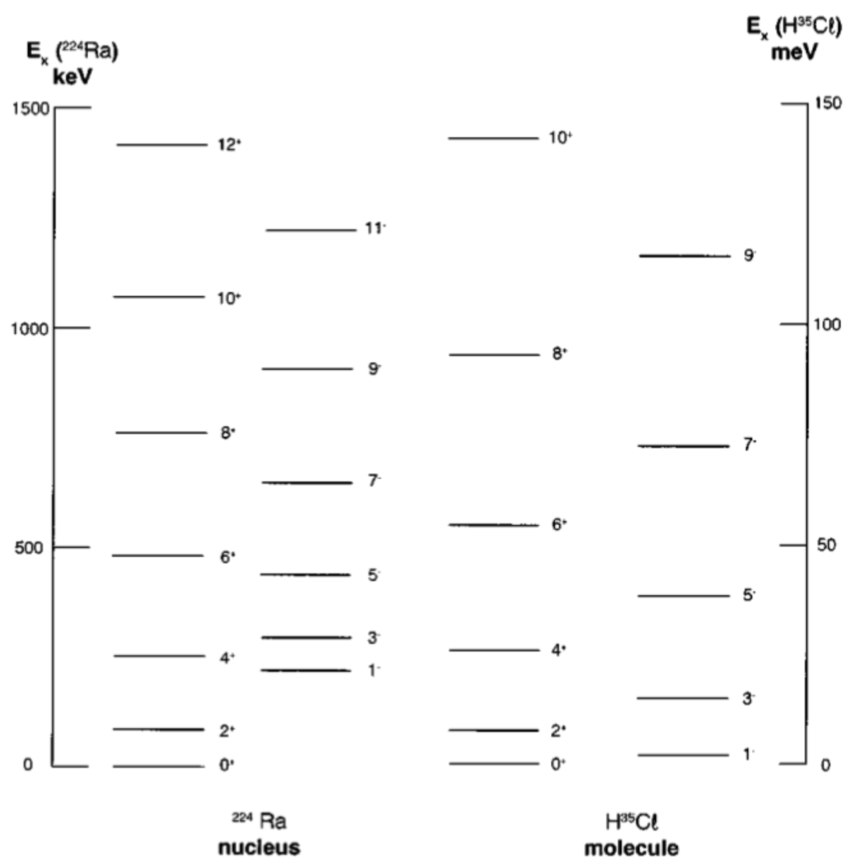
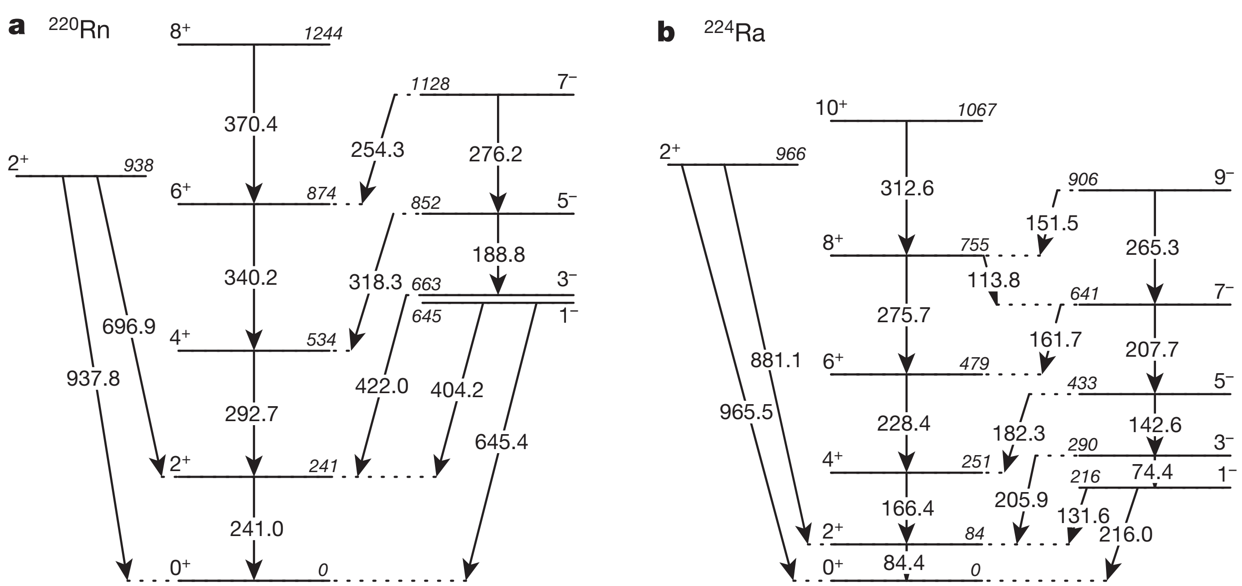


FIG. 1. The low-lying rotational spectra of ^{224}Ra, compared with that of the H^{35}Cl molecule. The spectrum of ^{224}Ra is taken from Poynter *et al.* (1989a). The rotational constants for the H^{35}Cl molecule are taken from Landolt-Börnstein (1974).

P. A. Butler, W. Nazarewicz, Rev. Mod. Phys. 68, 349 (1996)

Positive and negative parity interleaved bands as rotational states of octupole shapes

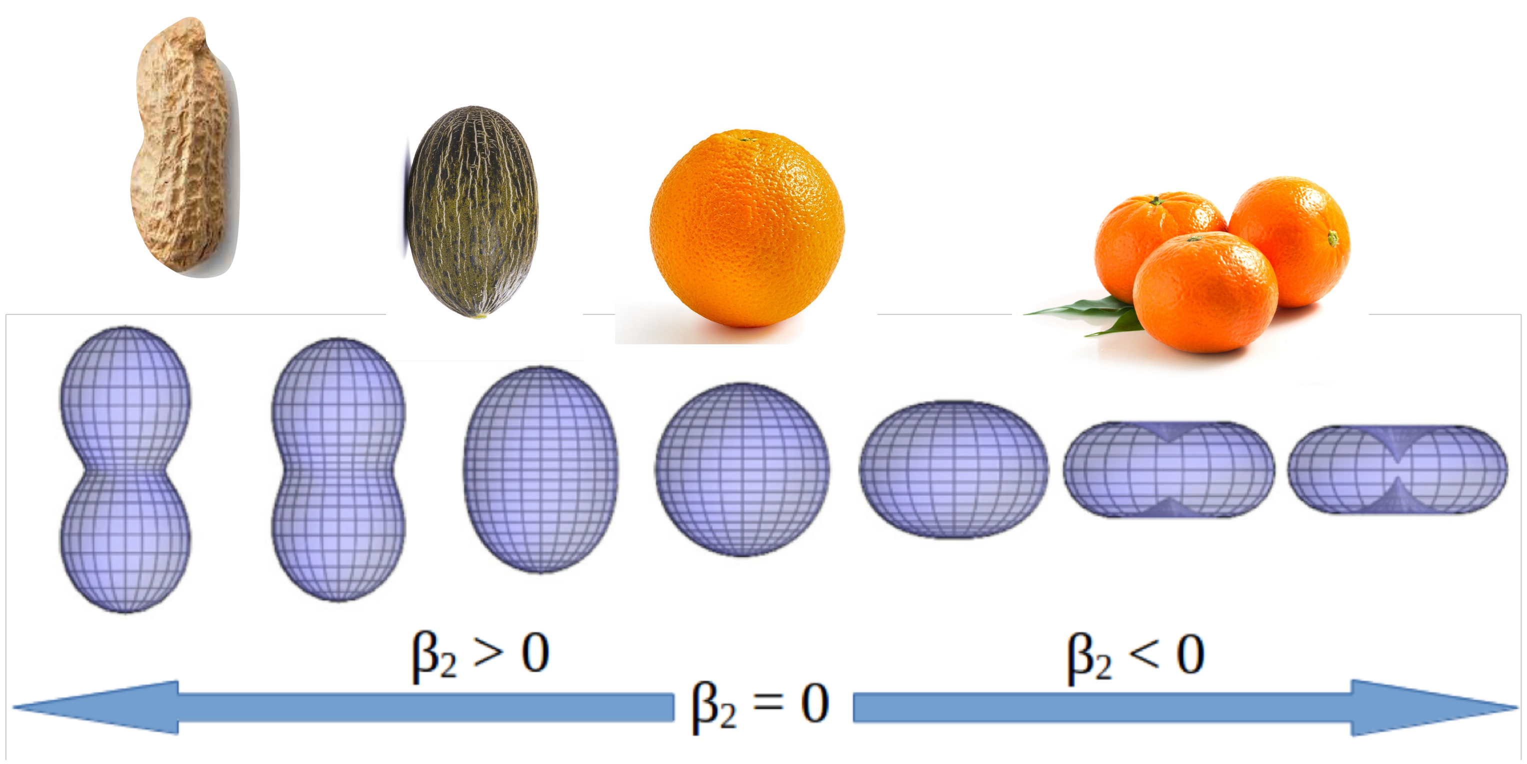


L.. P. Gaffney et al., Nature 497, 199 (2013)

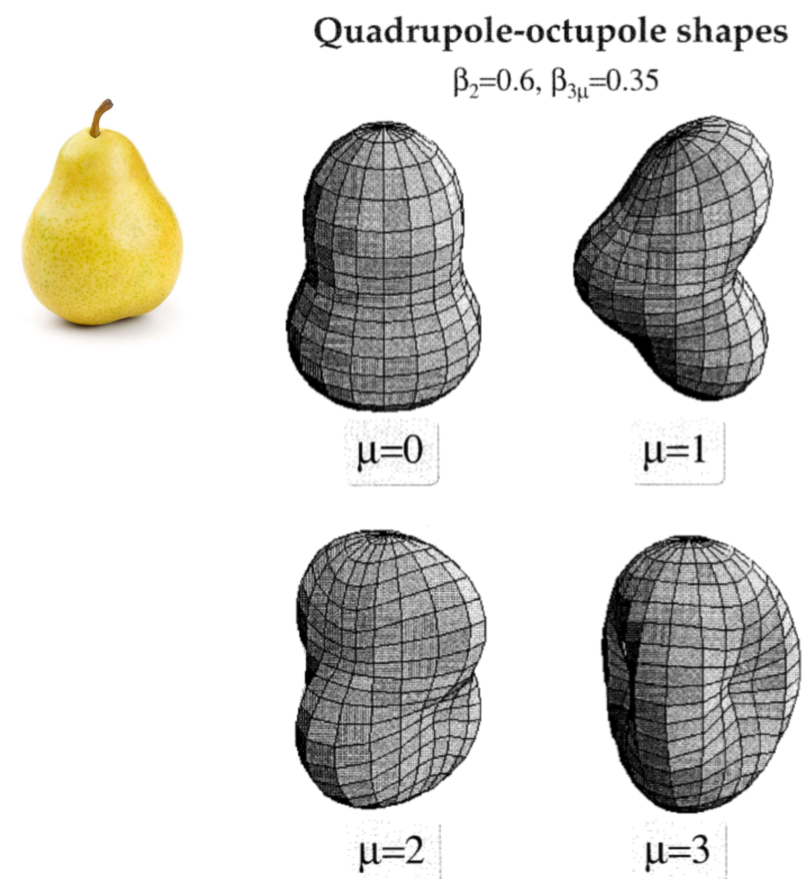
Introduction

- **Collective models** are based on the parametrization of the nuclear radius with a multipole expansion

$$R(\Omega) = c(\alpha) R_0 \left[1 + \sum_{\lambda=2}^{\lambda_{\max}} \sum_{\mu=-\lambda}^{+\lambda} \alpha_{\lambda\mu} Y^*_{\lambda\mu}(\Omega) \right]$$



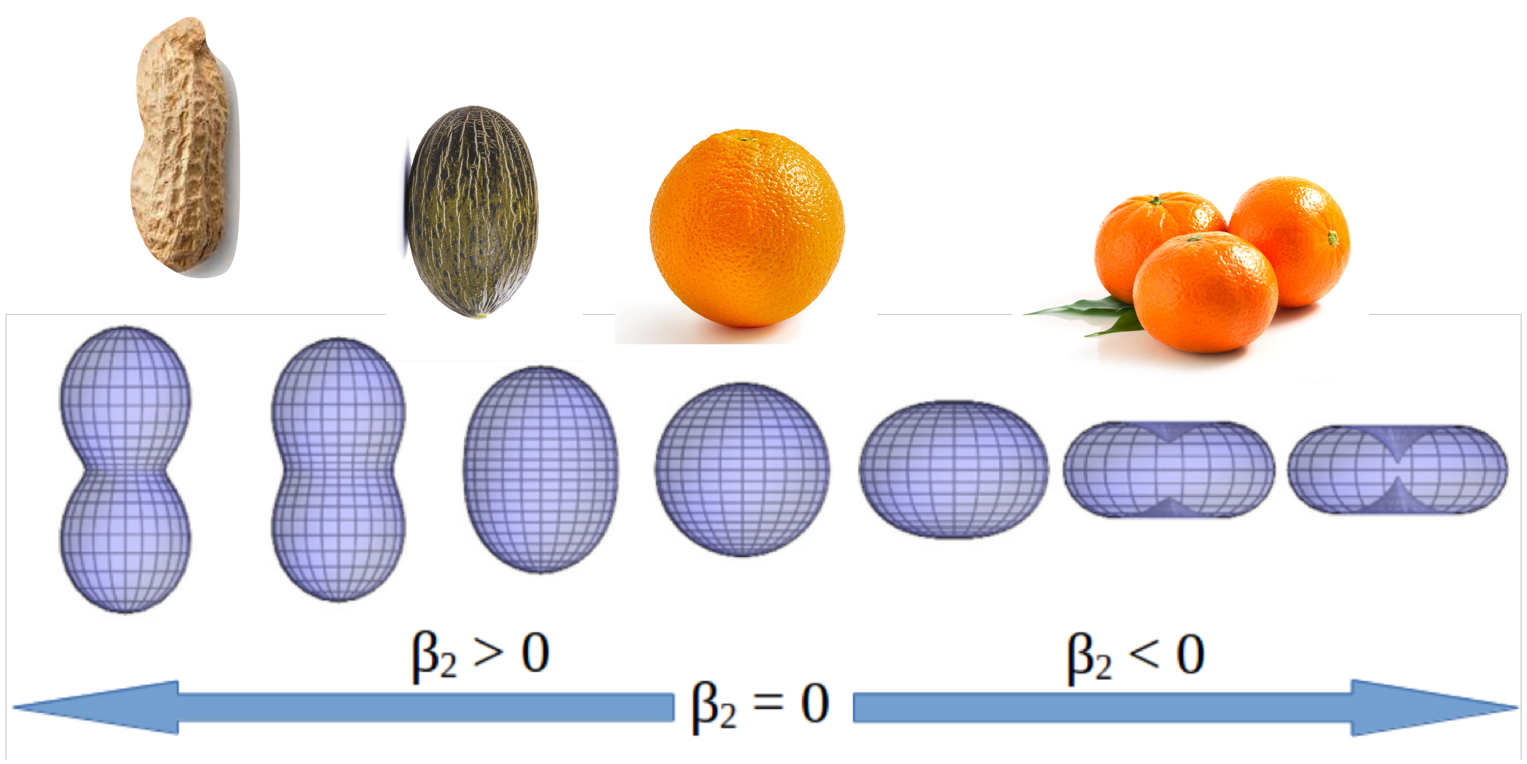
axial quadrupole shapes



P. A. Butler, W. Nazarewicz, Rev. Mod. Phys. 68, 349 (1996)

Introduction

Can we provide a **microscopic** description of these collective phenomena?



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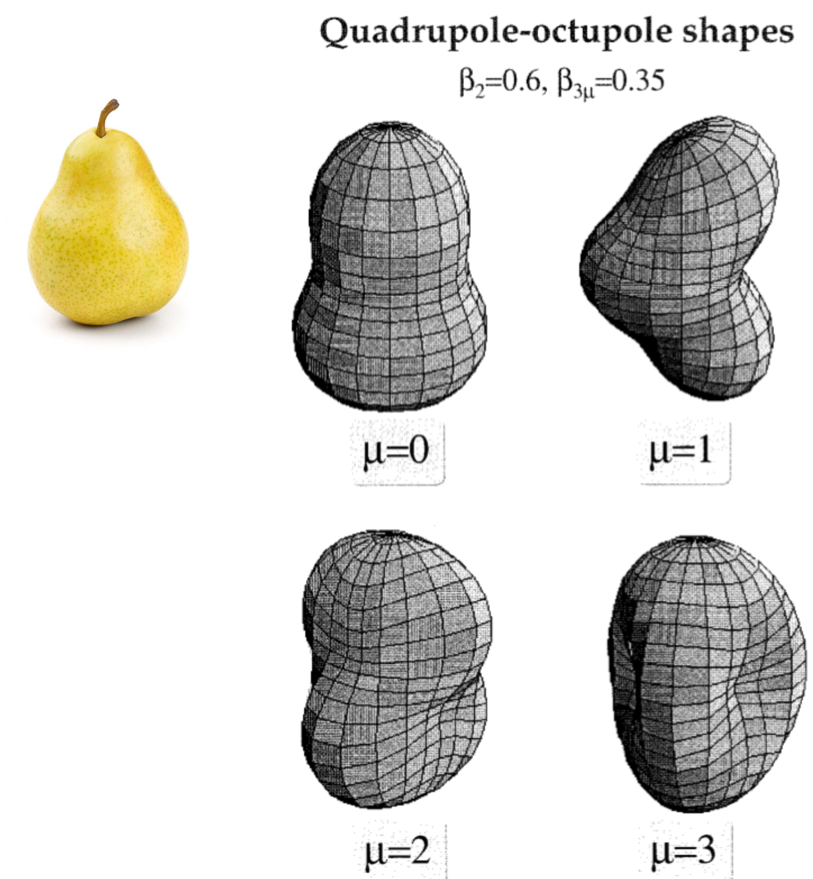

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Introduction

Let us assume that *we know* the nuclear interaction. Exact nuclear wave functions and energies cannot be obtained in general because of:

a) the exploding dimensionality of the many-body Hilbert space

b) the huge amount of two-, three- (eventually, *N*-) body matrix elements that are impossible to store

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

??

Some of the most widely used *solutions* to attack these problems:

- **Valence-space (Shell Model) calculations** with phenomenological (or normal-ordered, SRG evolved) two-body Hamiltonians

- **Approximate methods (variational)** with phenomenological interactions (or energy density functionals)

Introduction

- Valence-space (Shell Model) calculations with phenomenological (or normal-ordered, SRG evolved) two-body Hamiltonians

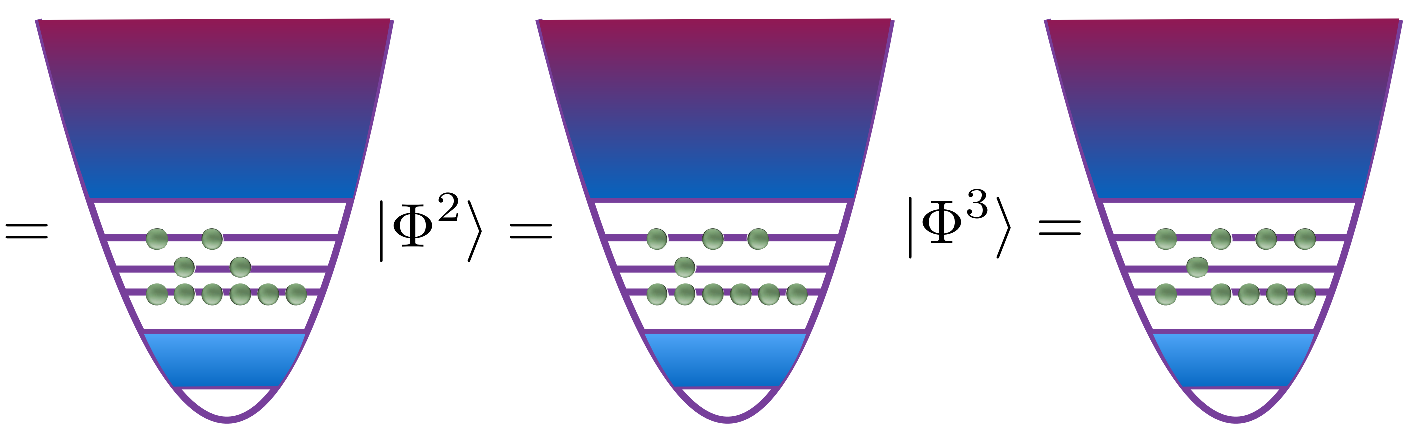
Full diagonalization of an *adapted* Hamiltonian within a valence space

$$\hat{H}_{v.s.}|\Psi^n_{v.s.}\rangle = E_n\,|\Psi^n_{v.s.}\rangle$$

Nuclear wave functions are linear combinations of Slater determinants written in terms of occupations of spherical orbits

$$|\Psi^n_{v.s.}\rangle = \sum_{k\in\, v.s.} C^n_k|\Phi^k\rangle$$

$$|\Phi^1\rangle = \qquad |\Phi^2\rangle = \qquad |\Phi^3\rangle = \qquad \ldots$$



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Introduction

- Approximate methods (variational) with phenomenological interactions (or energy density functionals)

Variational space of trial wave functions

Hamiltonian machine

Variational approach to the exact solution

Introduction

- Approximate methods (variational) with phenomenological interactions (or energy density functionals)

Variational spaces

Full Variational space of trial wave functions

Mean field approach

Hartree-Fock

HF-Bogoliubov

Beyond mean field approach

Configuration Mixing

Self-consistent mean-field: HFB

We use the variational method to find an approximate solution to the many-body problem defined by the Hamiltonian (non-relativistic, two-body):

$$\hat{H} = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{4} \sum_{abcd} \bar{v}_{abcd} c_a^\dagger c_b^\dagger c_d c_c$$

where $c_a^\dagger|-\rangle \equiv |a\rangle$; $\langle\vec{r}st|a\rangle = \Phi_a(\vec{r})\chi_{1/2,m_{s_a}}\chi_{1/2,m_{t_a}}$ are single-particle states

$\{c_a, c_b\} = \{c_a^\dagger, c_b^\dagger\} = 0; \{c_a^\dagger, c_b\} = \delta_{ab}$ (Fermions)

$t_{ab} = \langle a|\hat{T}|b\rangle$ one-body single-particle matrix elements of the kinetic energy

$\bar{v}_{abcd} = \langle ab|\hat{V}|cd\rangle - \langle ab|\hat{V}|dc\rangle$ two-body matrix elements of the interaction

Self-consistent mean-field: HFB

We use the variational method to find an approximate solution to the many-body problem defined by the Hamiltonian (non-relativistic, two-body):

$$\hat{H} = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{4} \sum_{abcd} \bar{v}_{abcd} c_a^\dagger c_b^\dagger c_d c_c$$

We define a set of generalized product-like wave functions $\{|\Phi\rangle\}$ which are vacua of certain quasiparticle operators $\beta^\dagger, \beta$

$$|\Phi\rangle = \prod_q \beta_q |-\rangle$$

The quasiparticle operators are defined as (**HFB transformation**):

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l$$

variational parameters

with $\{\beta_k, \beta_l\} = \{\beta_k^\dagger, \beta_l^\dagger\} = 0; \{\beta_k^\dagger, \beta_l\} = \delta_{kl}$

and $W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}; W^\dagger W = \mathbb{I}$

Self-consistent mean-field: HFB

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Hartree-Fock-Bogoliubov equations

We want to find the parameters (*U*,*V*), or equivalently, the one-body density matrix and pairing tensor that minimize the HFB energy.

However, the HFB transformation mixes creation and annihilation single-particle operators. Hence, the particle number symmetry can be broken by the HFB wave function

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l$$

Therefore, instead of minimizing the HFB energy, constraints on the number of particles are introduced through Lagrange multipliers:

$$\delta E'_{\mathrm{HFB}}\left[|\Phi\rangle\right] = 0 \quad \text{with} \quad E'_{\mathrm{HFB}}\left[|\Phi\rangle\right] = \langle\Phi|\hat{H} - \lambda_N \hat{N} - \lambda_Z \hat{Z}|\Phi\rangle$$

- $\beta_k|\Phi\rangle = 0$ trial wave functions are quasiparticle vacua
- $\lambda_N \rightarrow \langle\Phi|\hat{N}|\Phi\rangle = N$ Lagrange multiplier for neutrons
- $\lambda_Z \rightarrow \langle\Phi|\hat{Z}|\Phi\rangle = Z$ Lagrange multiplier for protons

Self-consistent mean-field: HFB

Constrained Hartree-Fock-Bogoliubov equations

We can generalize the introduction of constraints in the HFB calculations to study not only one single solution but an energy landscape

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l$$

Therefore, we now minimize:

$$\delta E'_{\mathrm{HFB}}\left[|\Phi(\vec{q})\rangle\right] = 0 \text{ with } E'_{\mathrm{HFB}}\left[|\Phi(\vec{q})\rangle\right] = \langle\Phi(\vec{q})|\hat{H} - \lambda_N \hat{N} - \lambda_Z \hat{Z} - \vec{\lambda}_{\vec{q}} \cdot \hat{\vec{Q}}|\Phi(\vec{q})\rangle$$

- $\beta_k(\vec{q})|\Phi(\vec{q})\rangle = 0$ trial wave functions are quasiparticle vacua
- $\lambda_N \rightarrow \langle\Phi(\vec{q})|\hat{N}|\Phi(\vec{q})\rangle = N$ Lagrange multiplier for neutrons
- $\lambda_Z \rightarrow \langle\Phi(\vec{q})|\hat{Z}|\Phi(\vec{q})\rangle = Z$ Lagrange multiplier for protons
- $\vec{\lambda}_{\vec{q}} \rightarrow \langle\Phi(\vec{q})|\hat{\vec{Q}}|\Phi(\vec{q})\rangle = \vec{q}$ Lagrange multipliers for collective coordinates

Self-consistent mean-field: HFB

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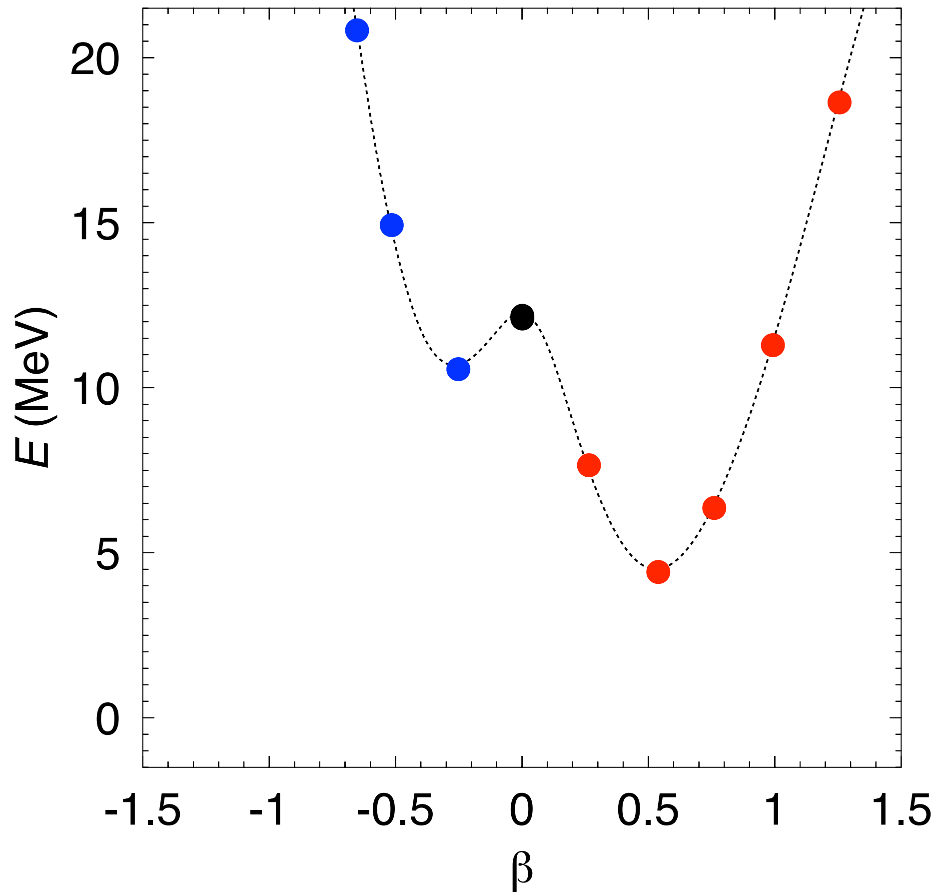
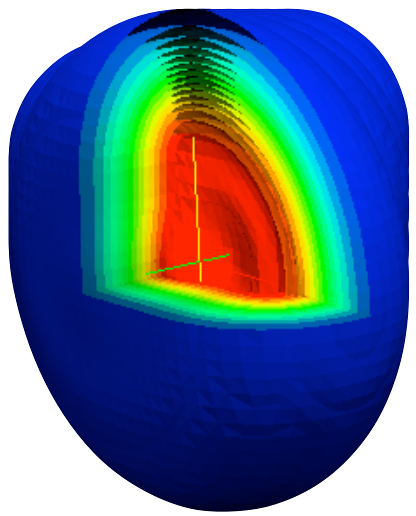
Constrained Hartree-Fock-Bogoliubov equations

Example: ^{24}Mg





Self-consistent mean-field: HFB

Constrained Hartree-Fock-Bogoliubov equations

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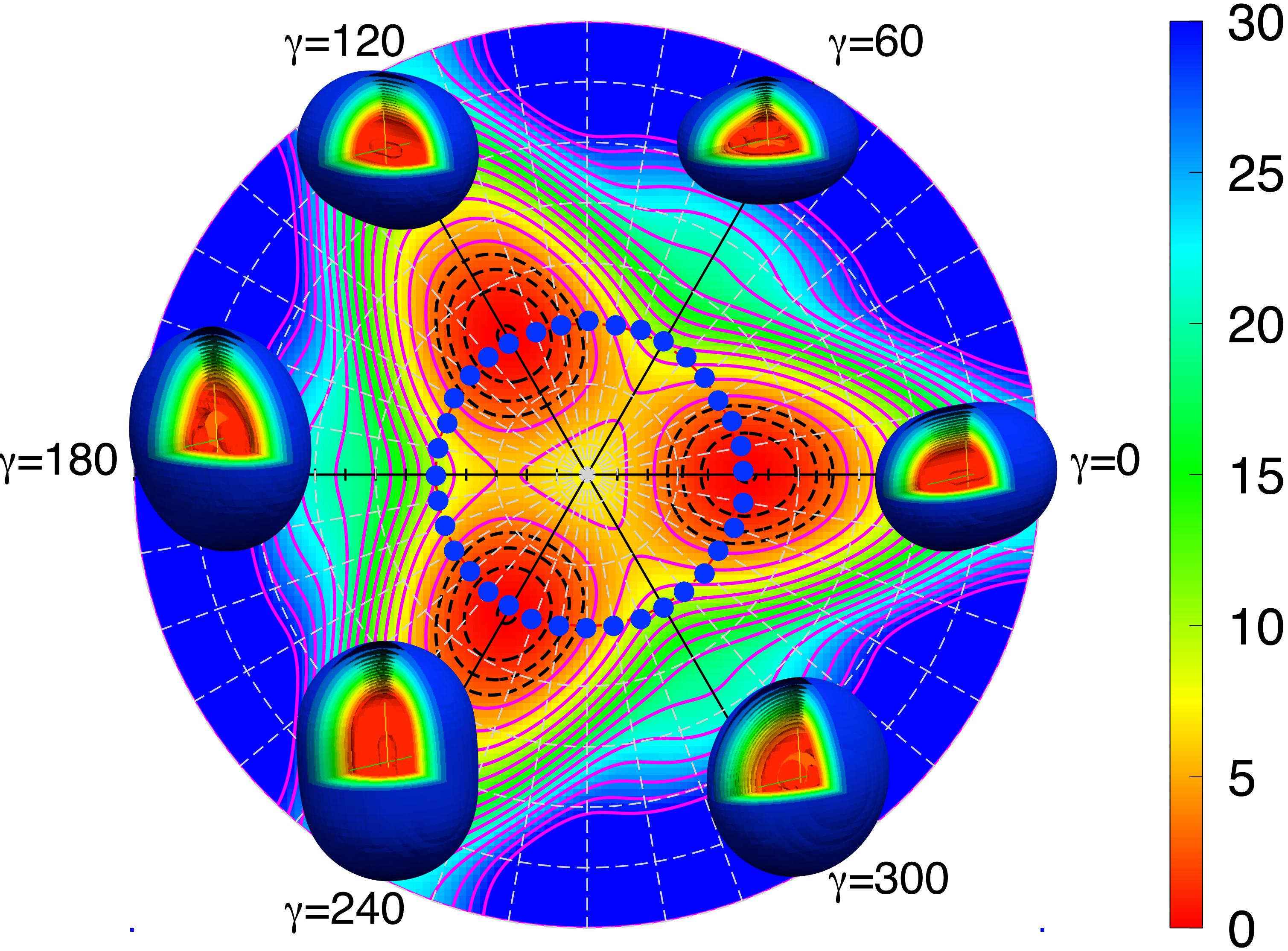
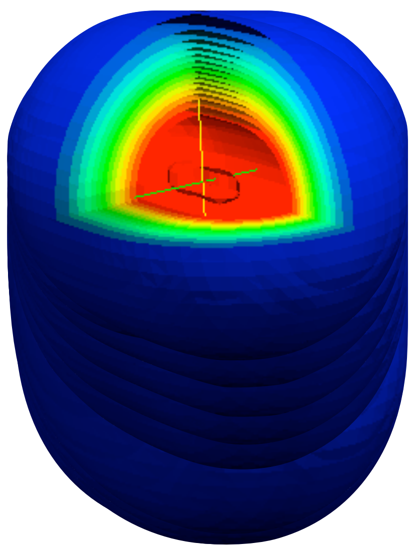
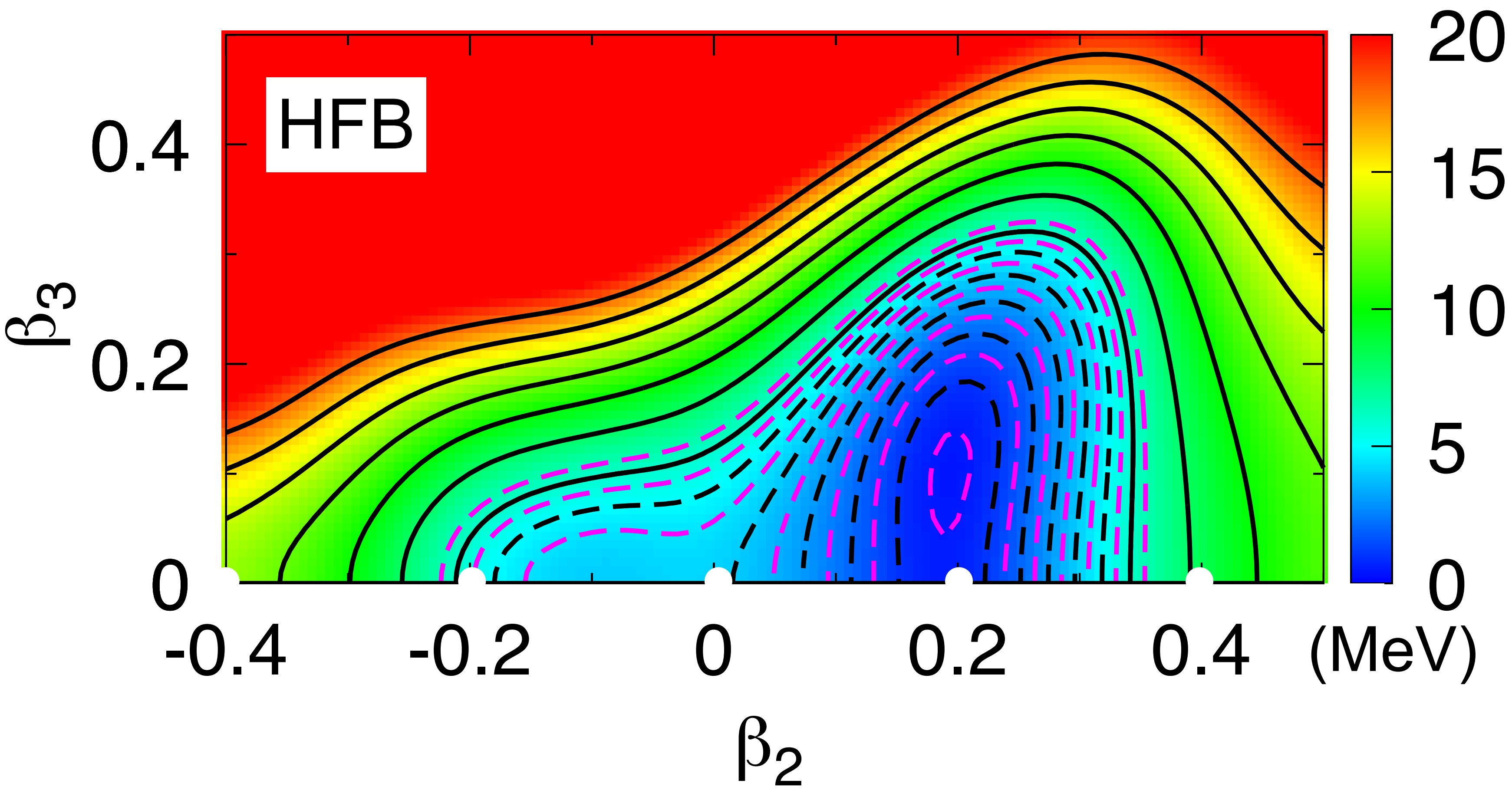


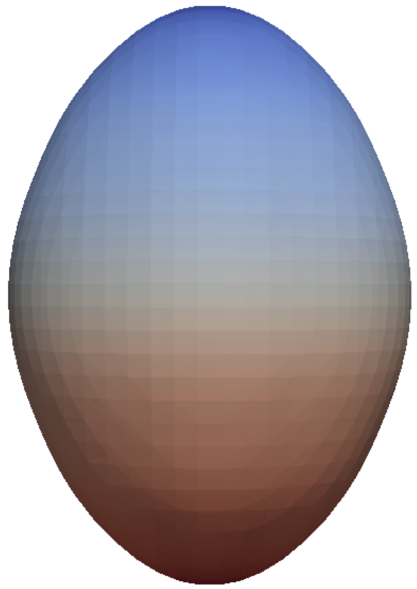
- Symmetry corresponding to the different orientation of the axes
- All configurations are included between γ∈[0º,60º]



Self-consistent mean-field: HFB

Example: ^{144}Ba axial calculations





R. Bernard, L. M. Robledo, T. R. R., PRC (2016)

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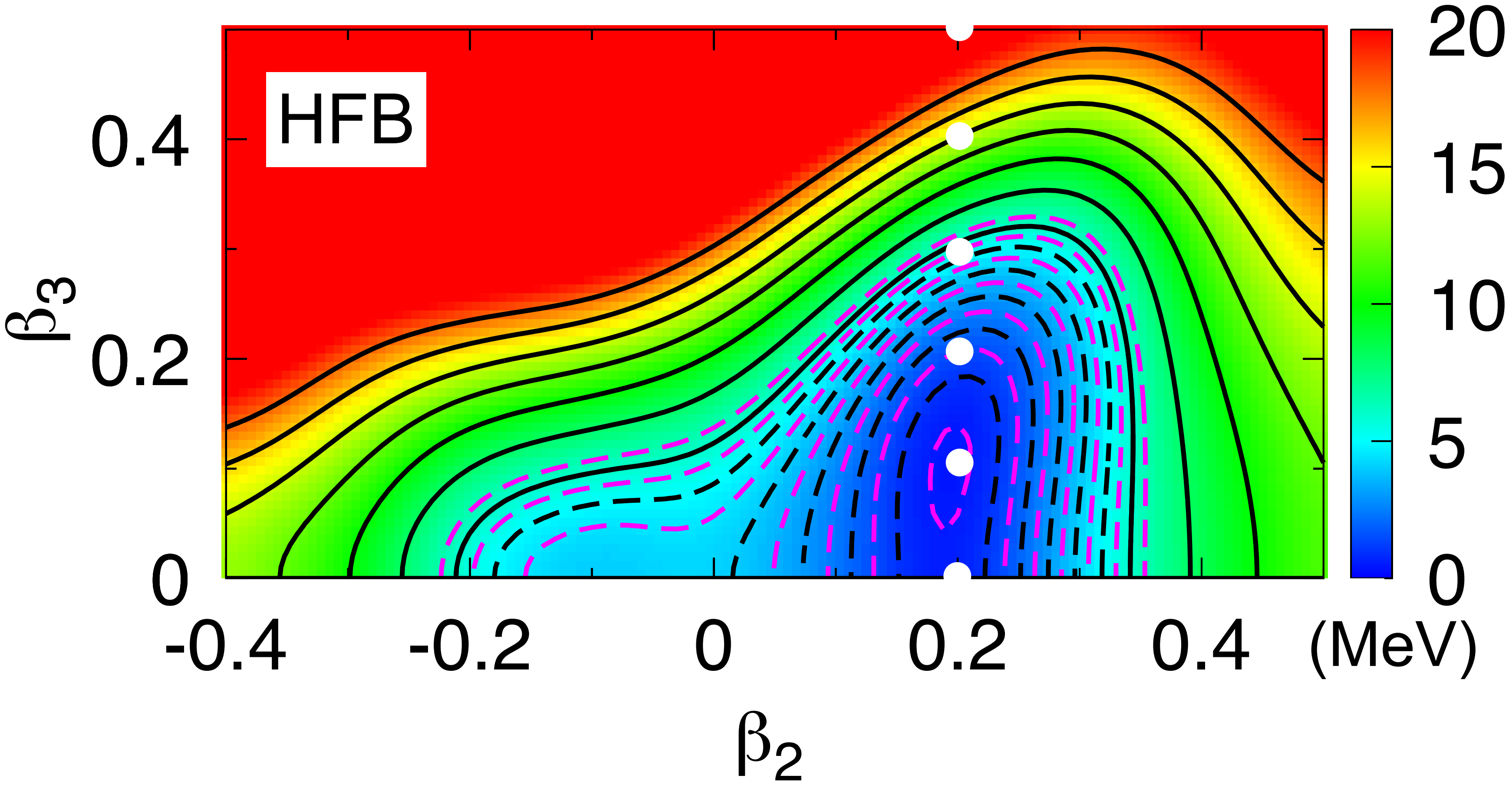

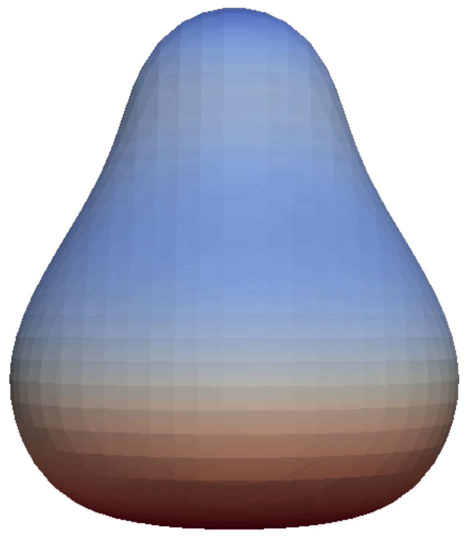

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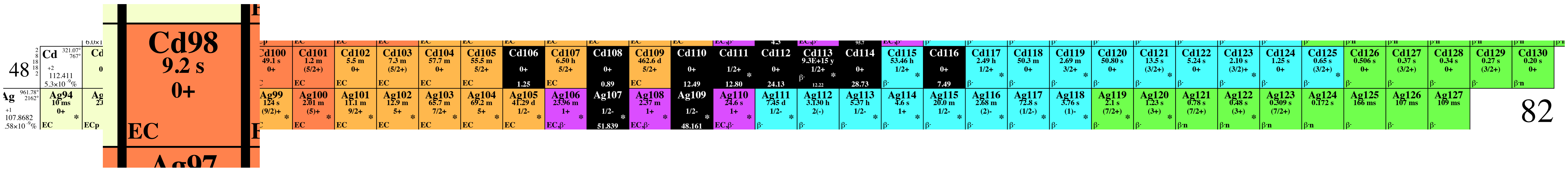
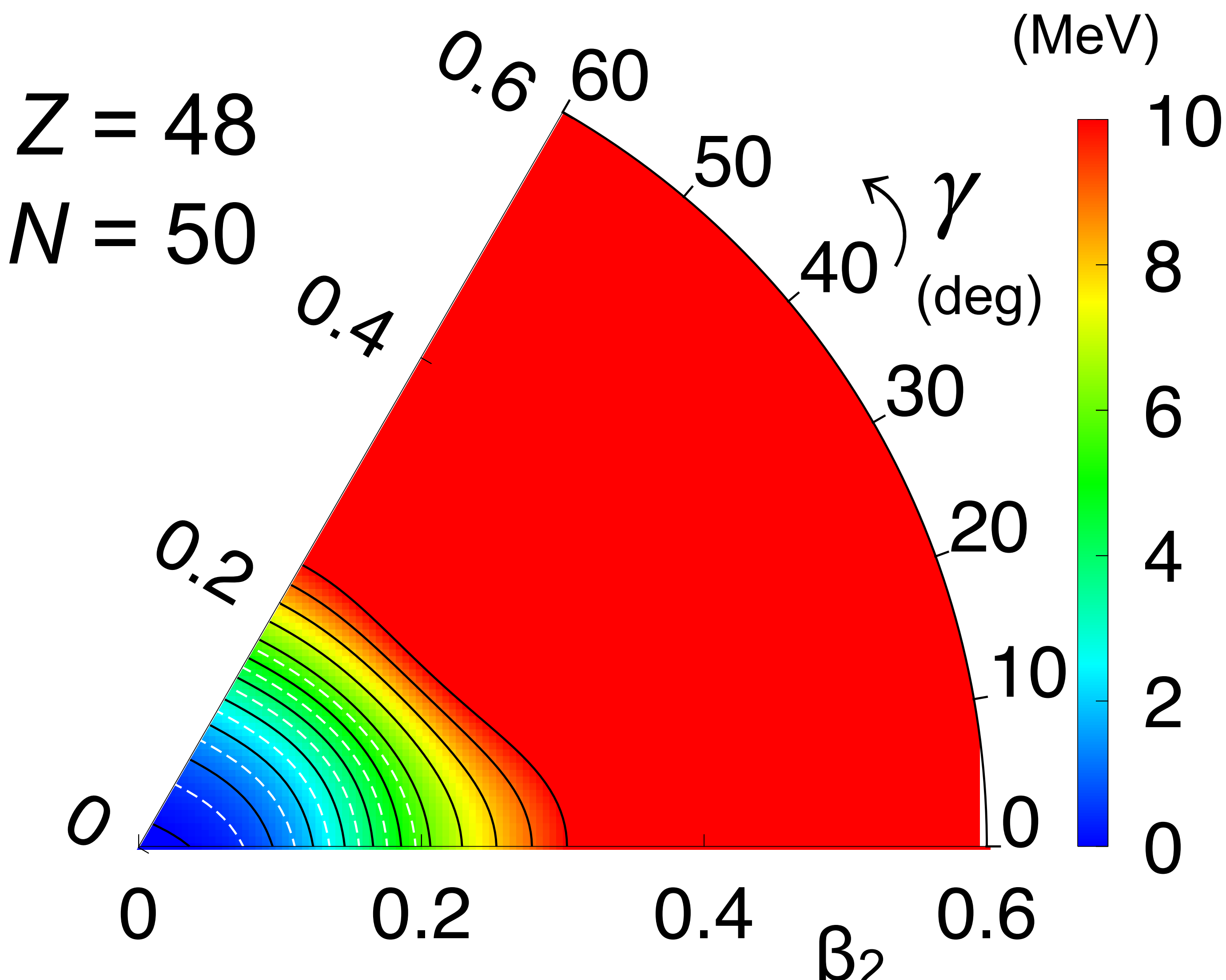
PN-VAP energy surfaces





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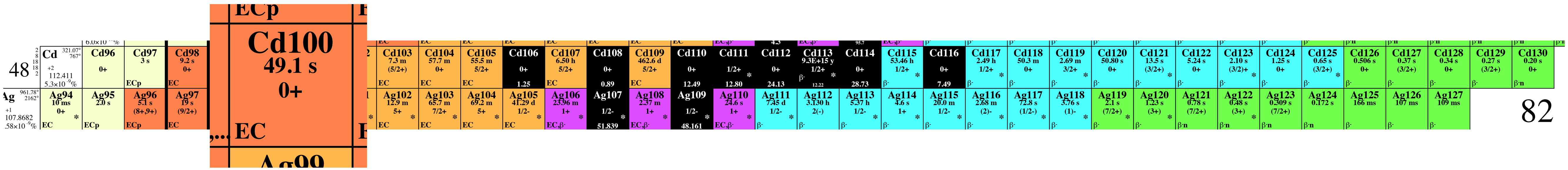

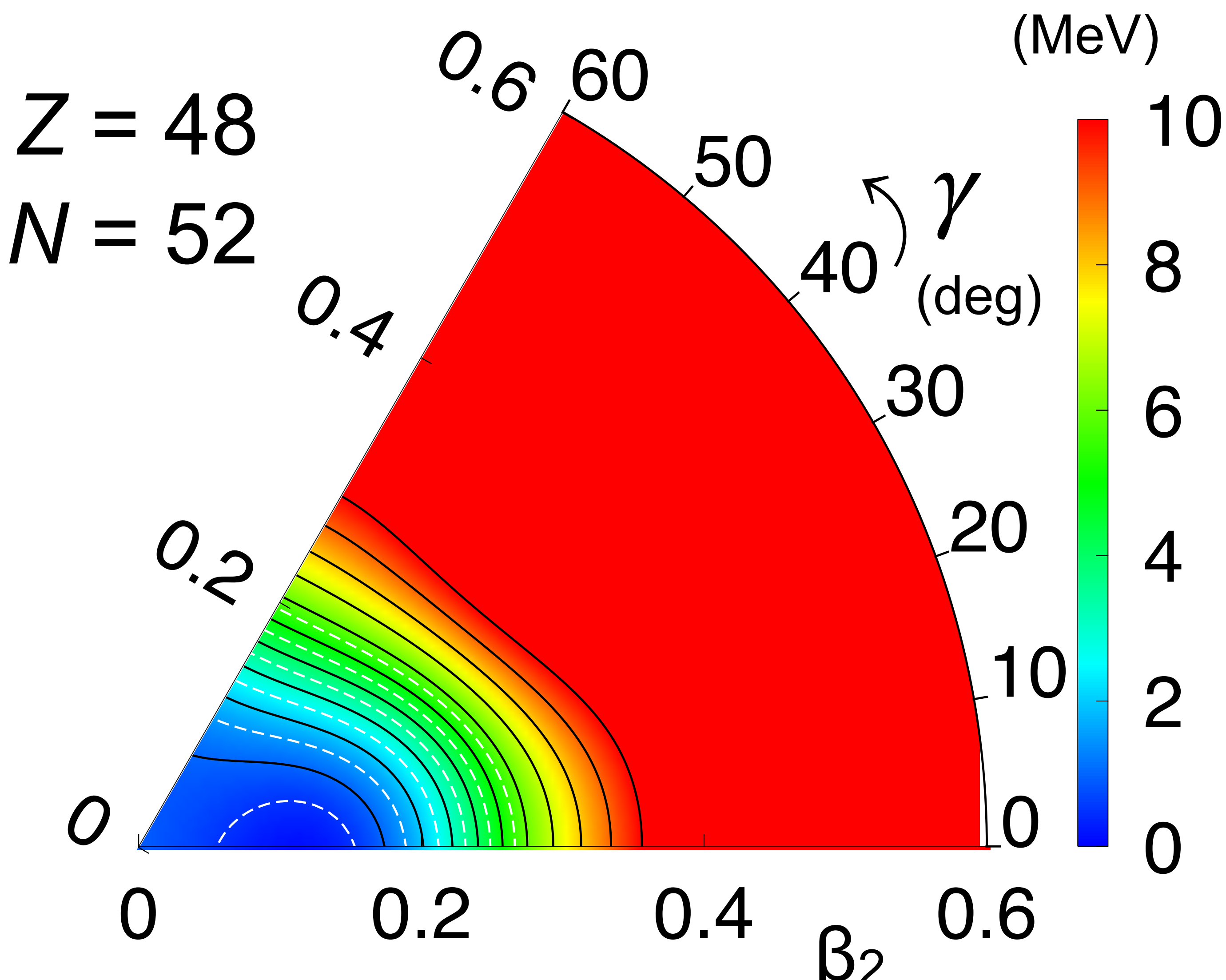

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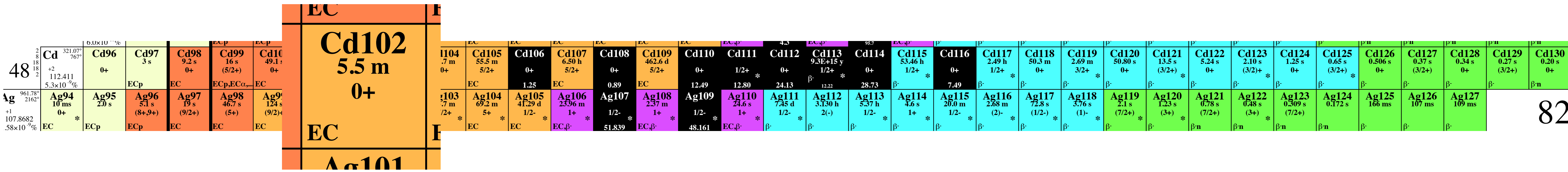

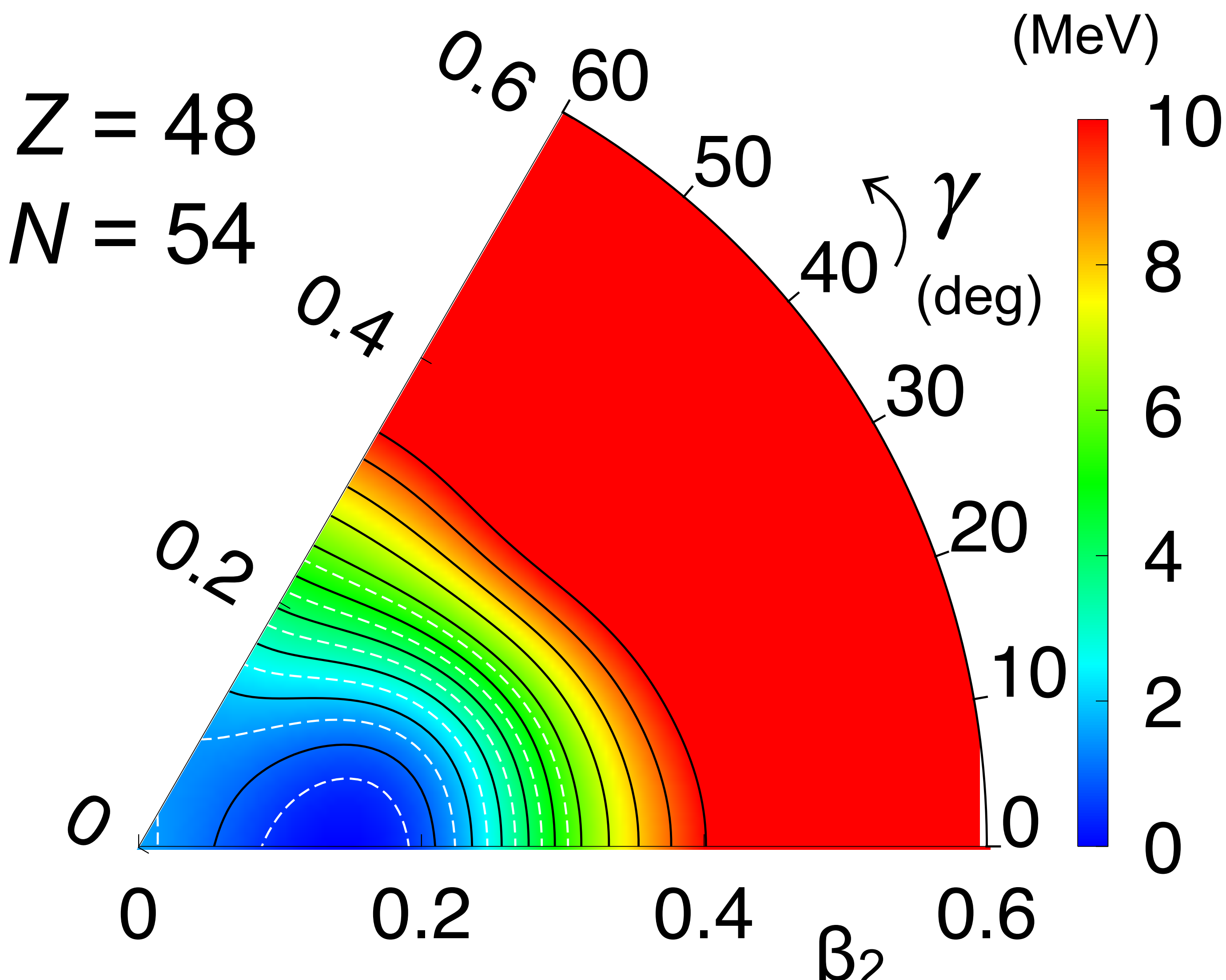

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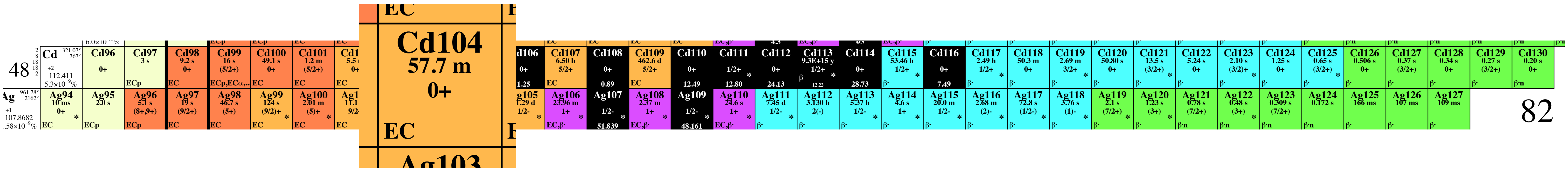

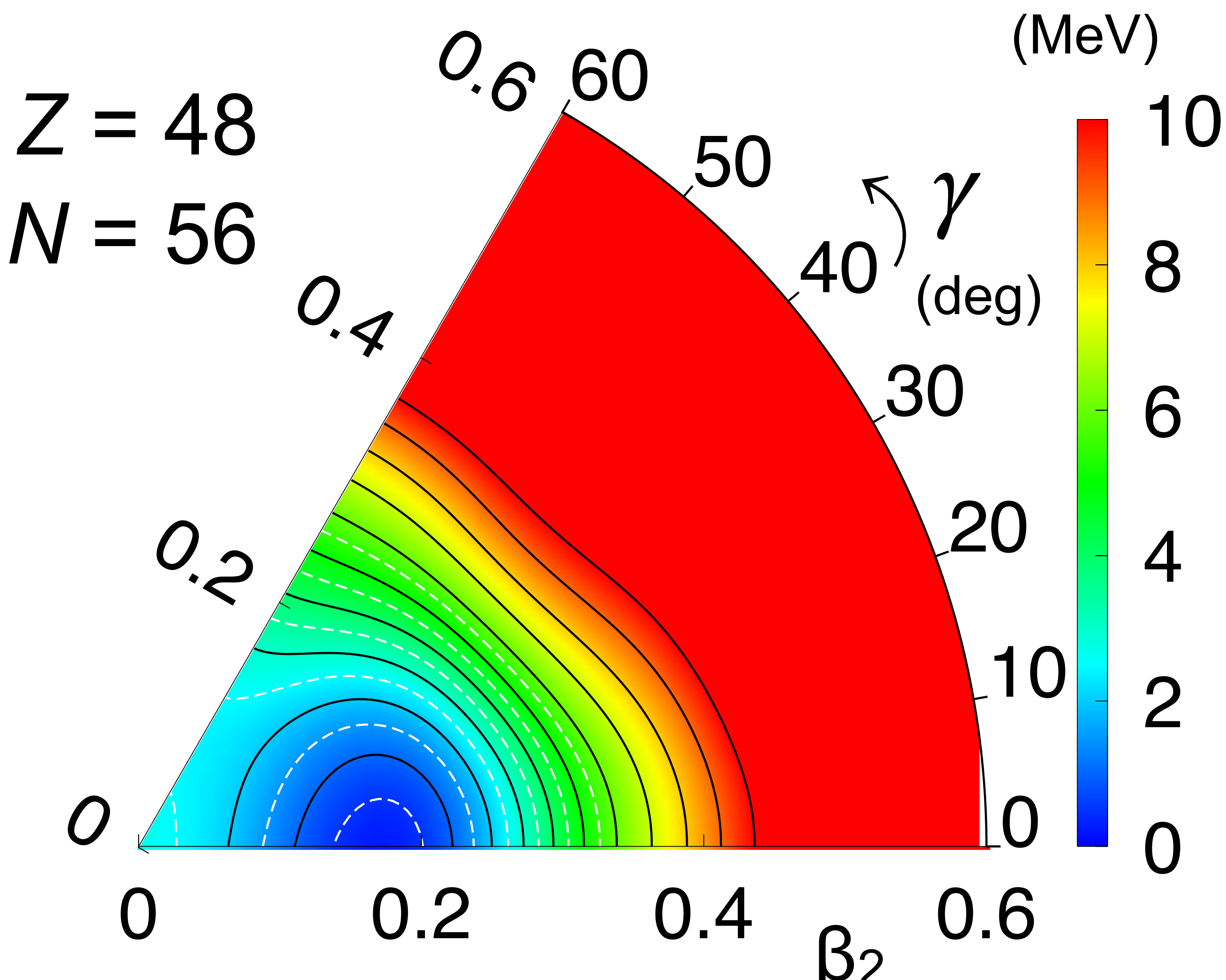

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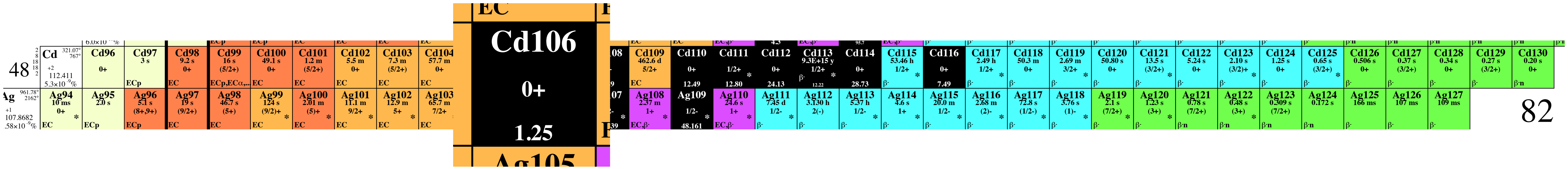

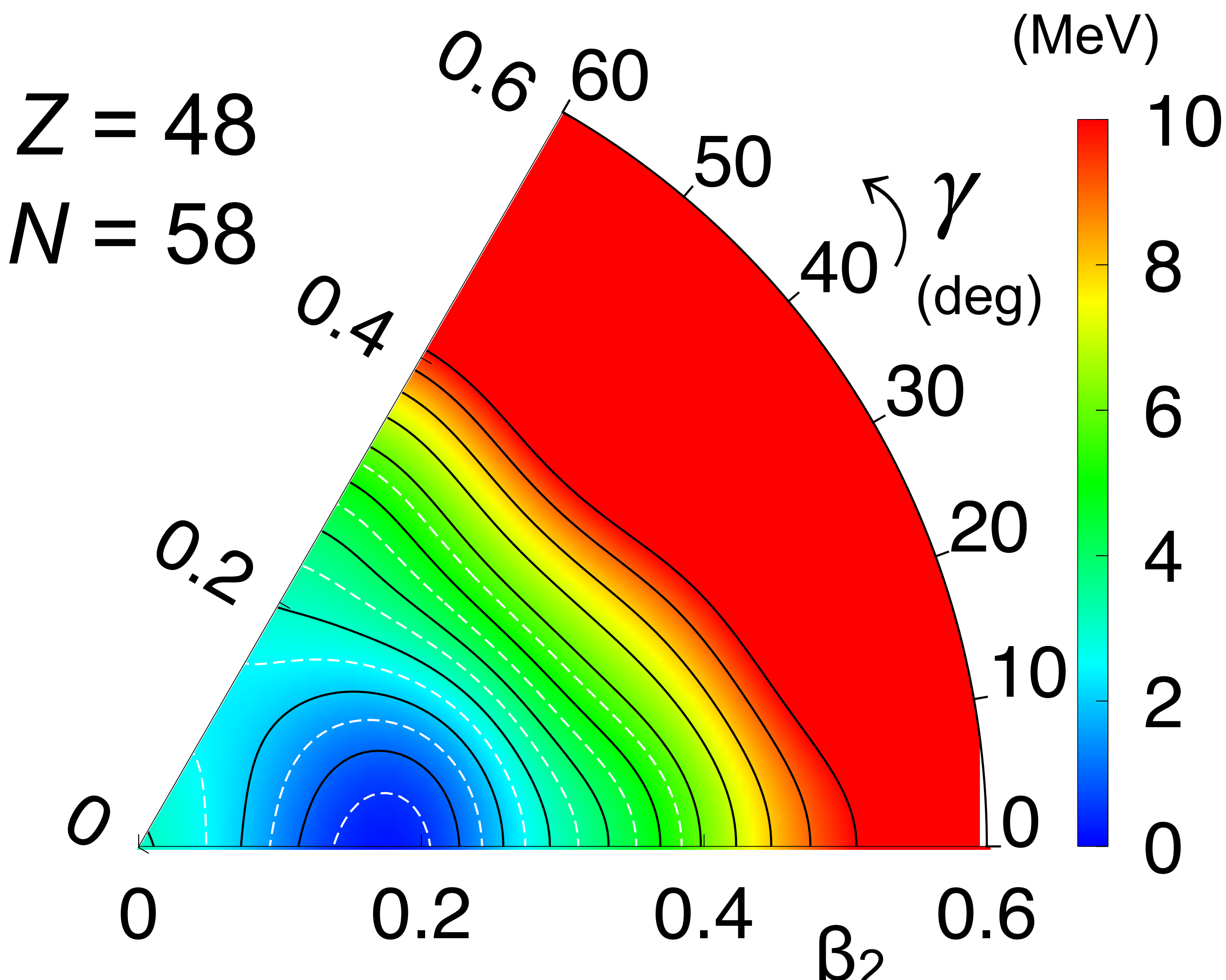

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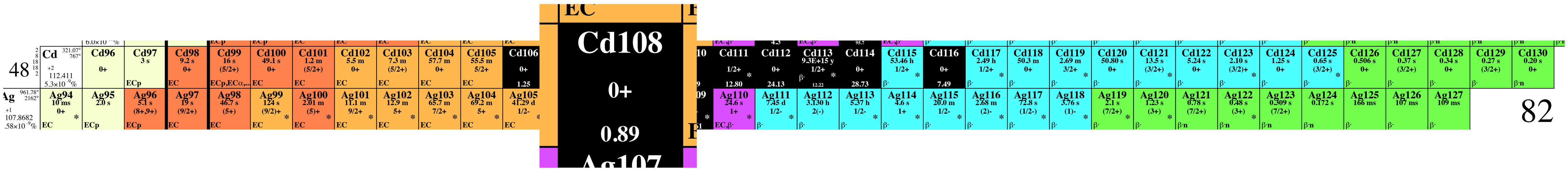

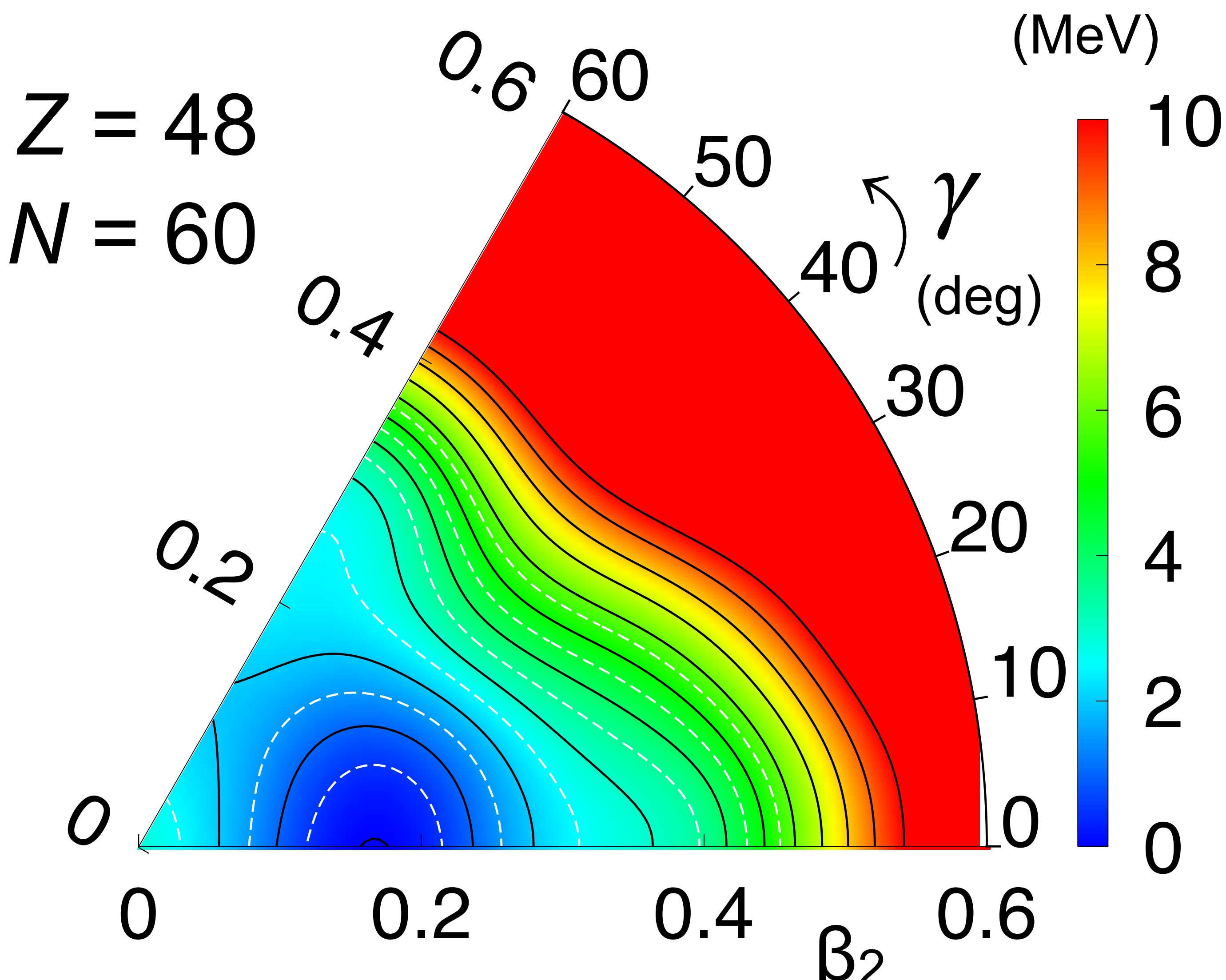

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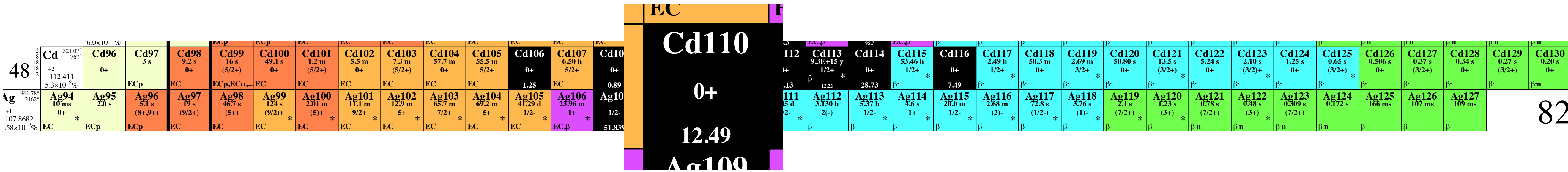

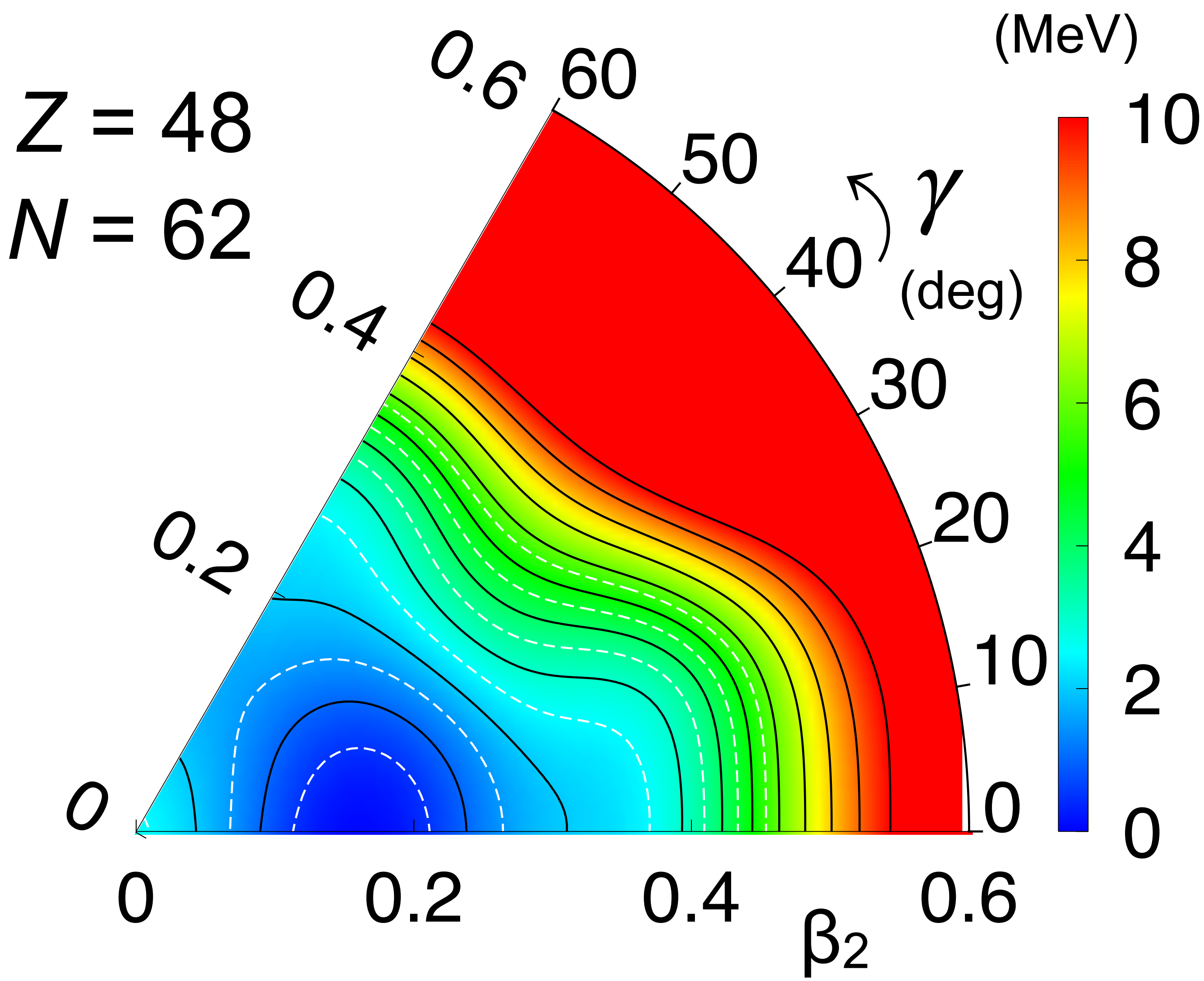

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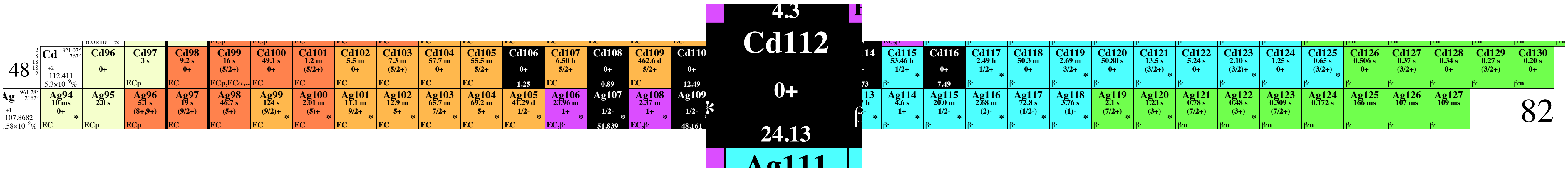

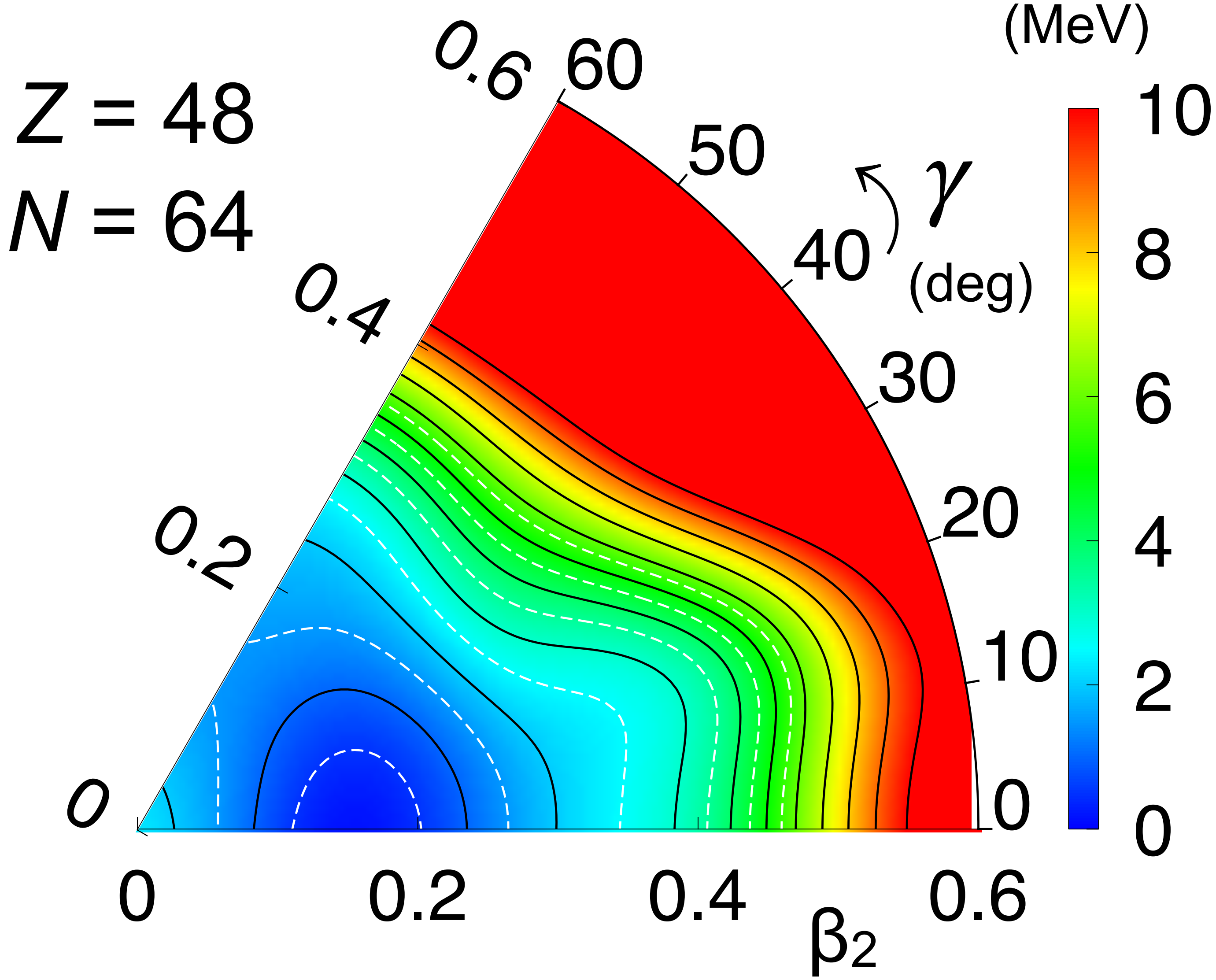

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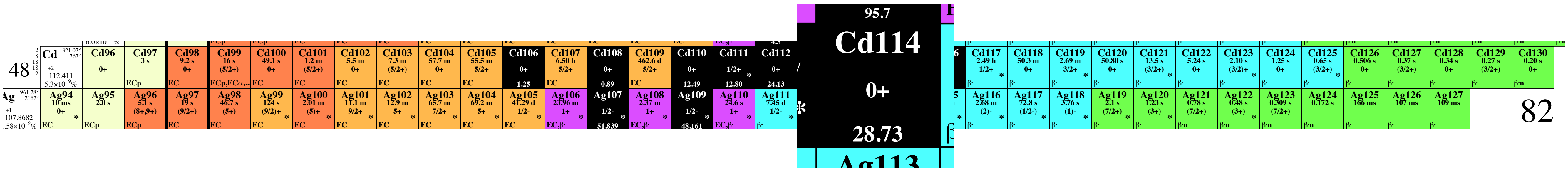

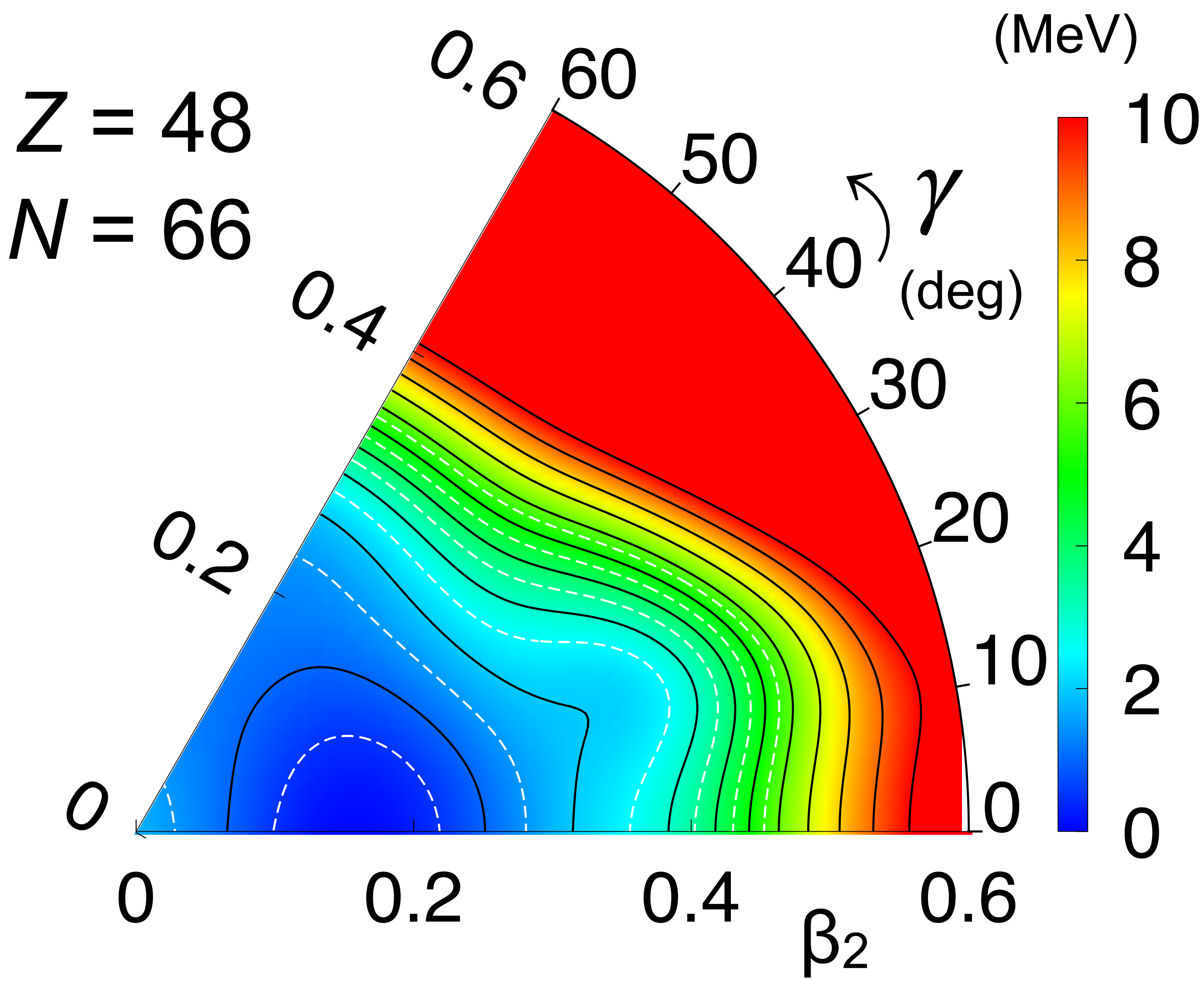

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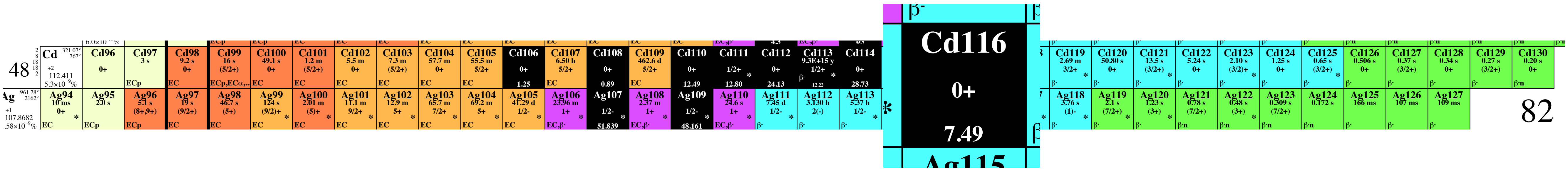

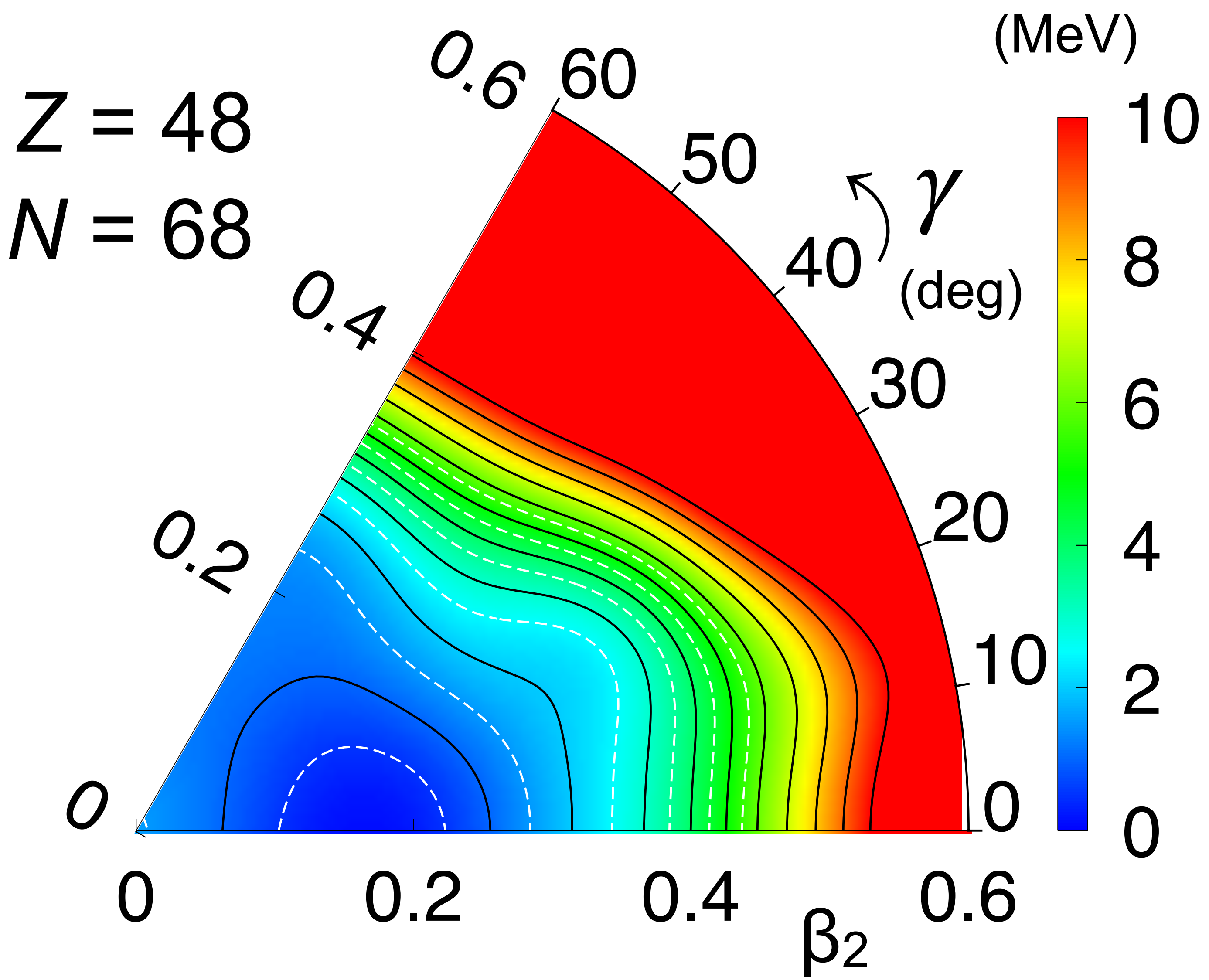

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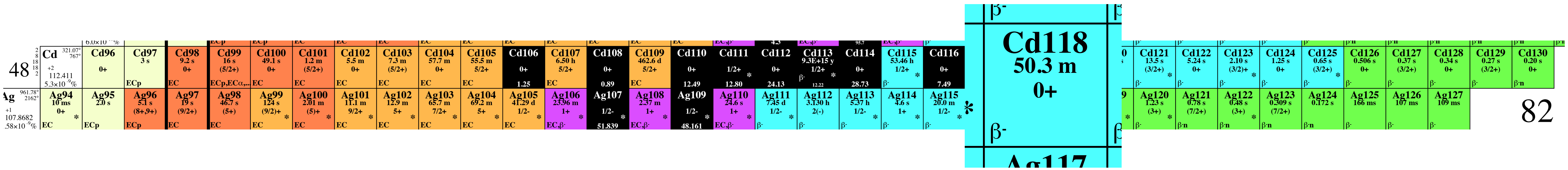

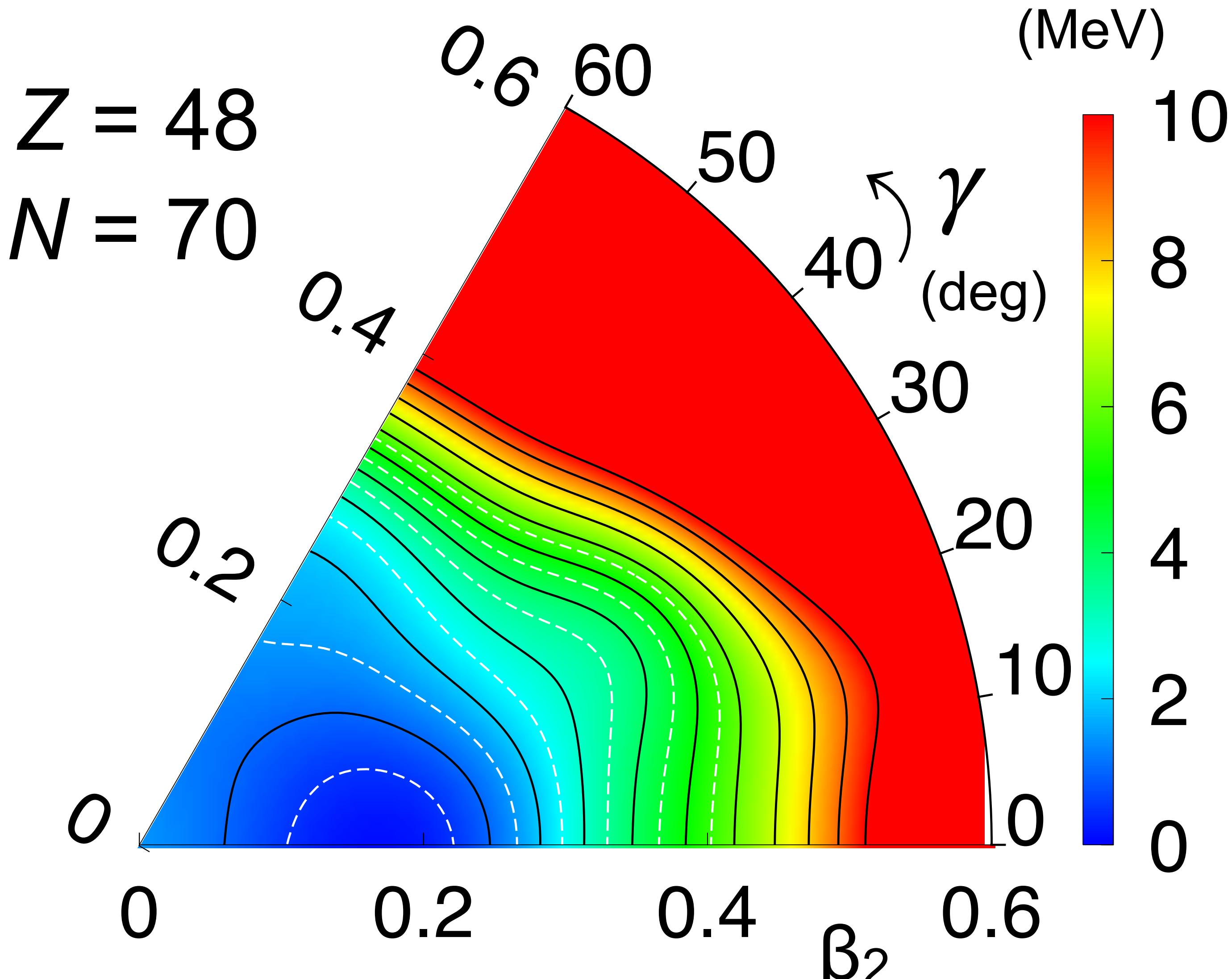

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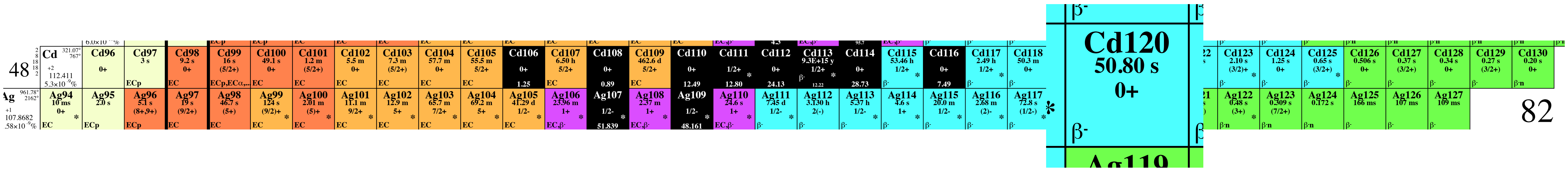

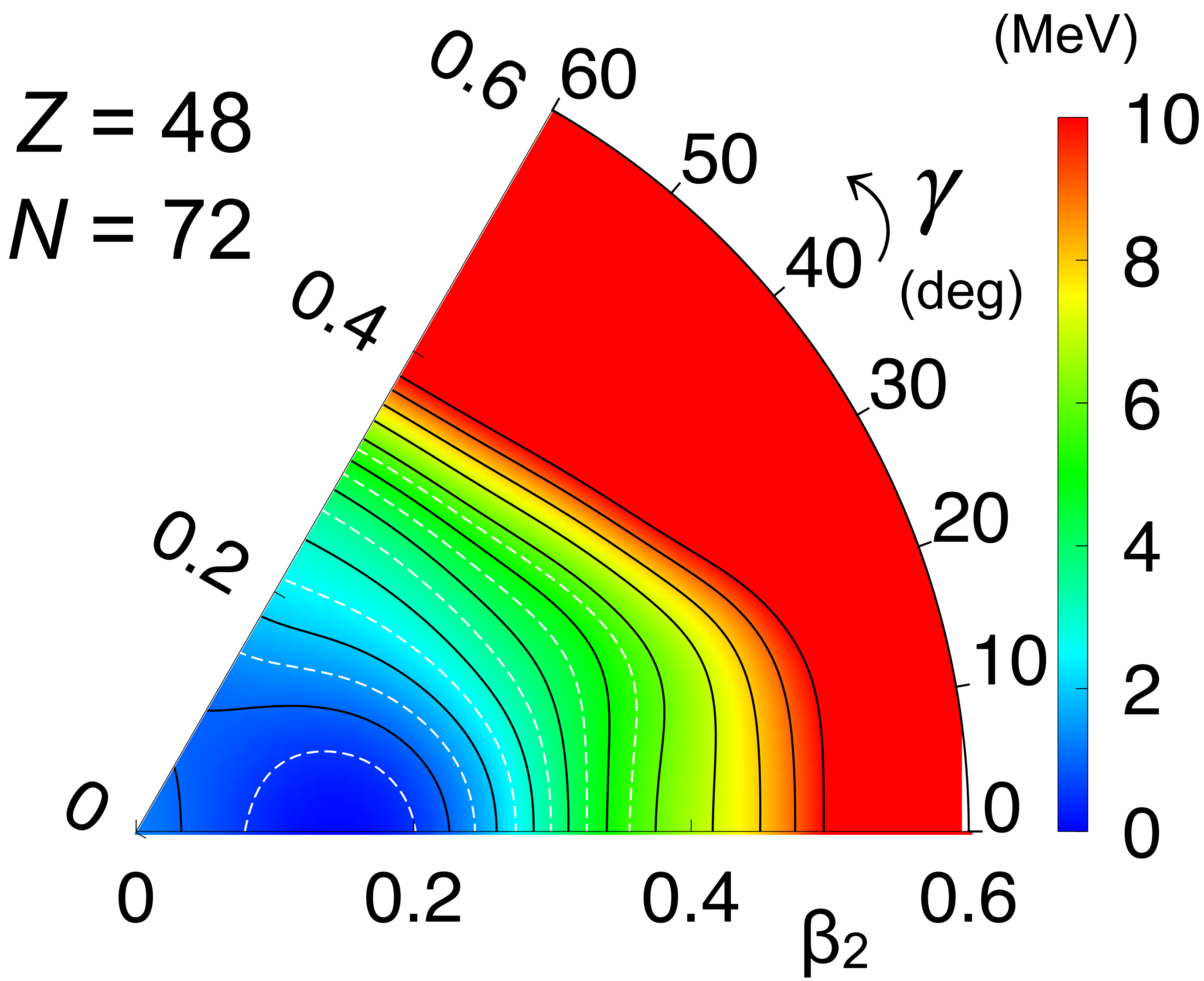

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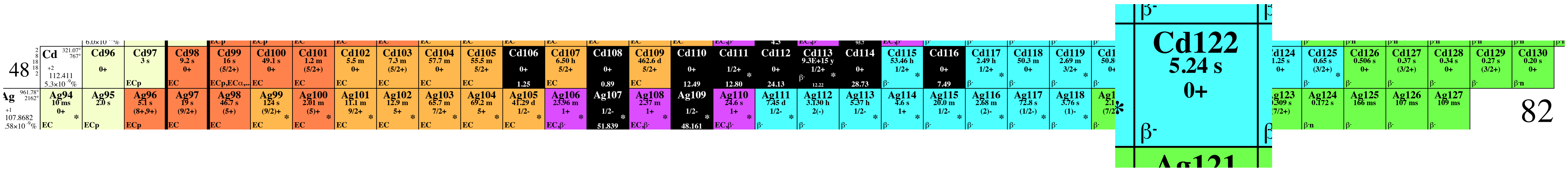

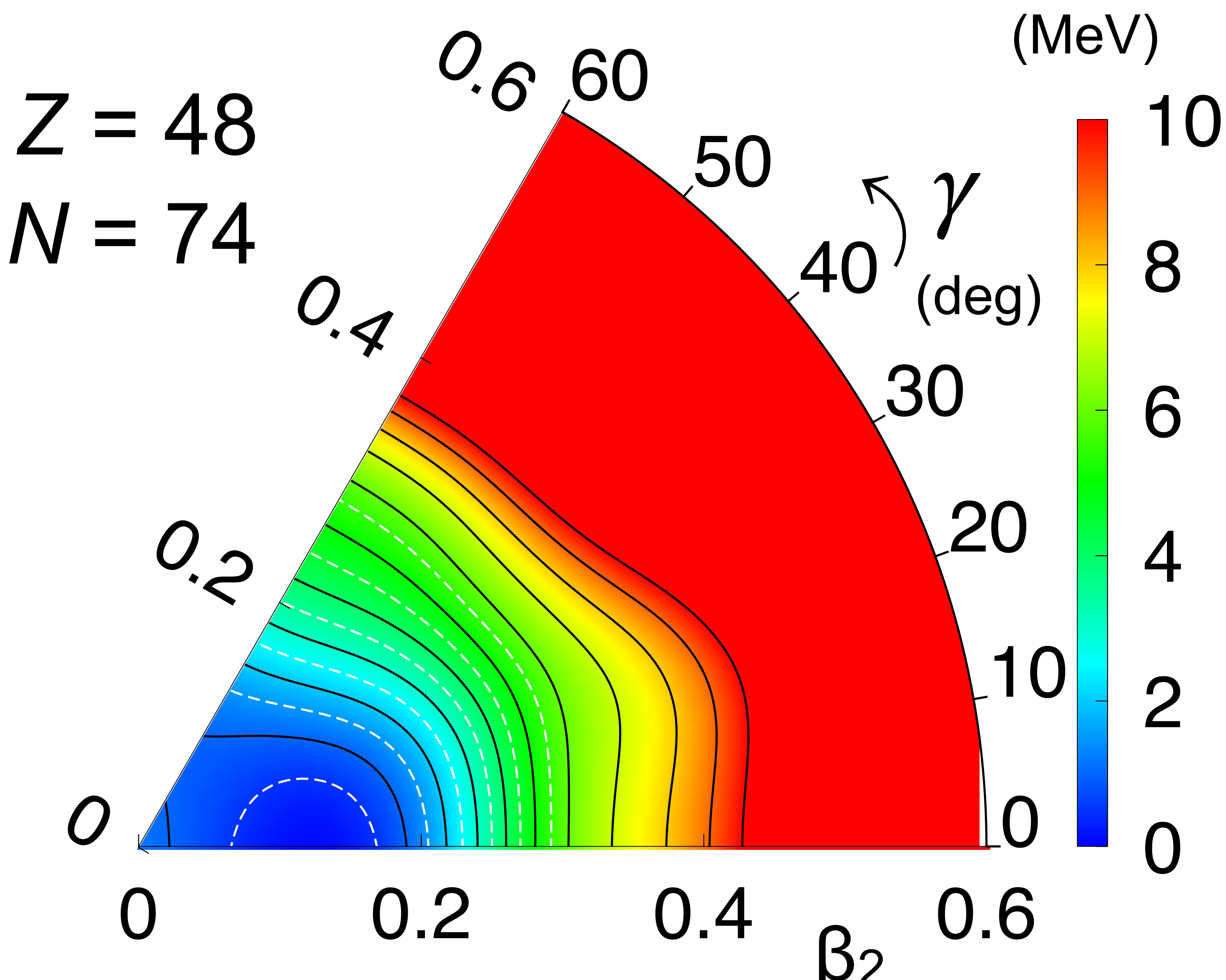

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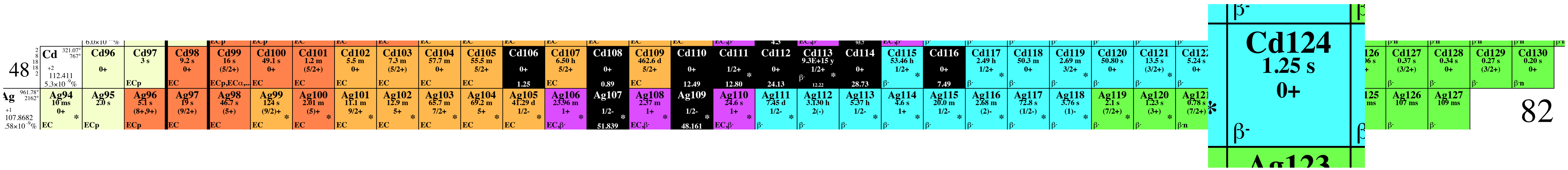

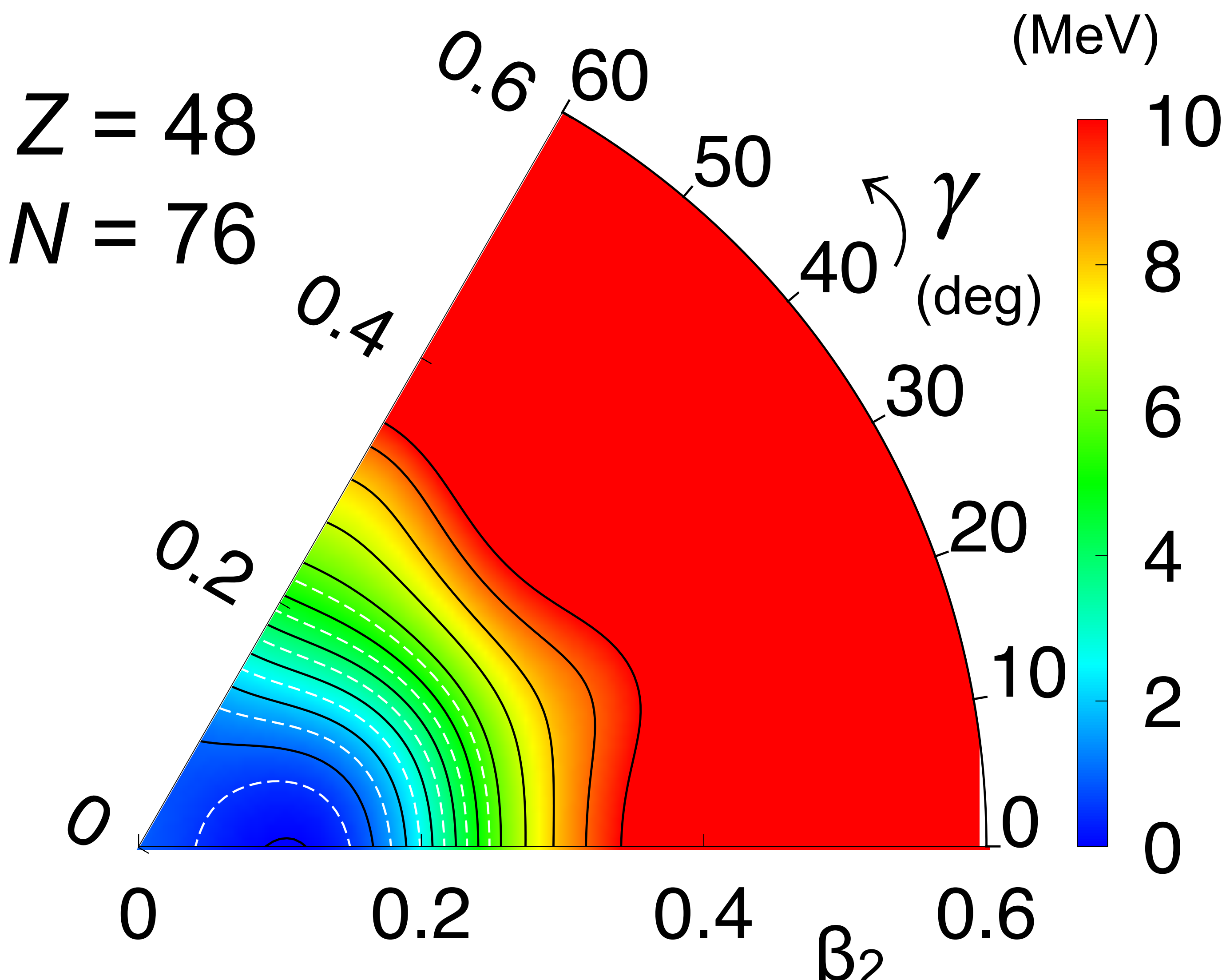

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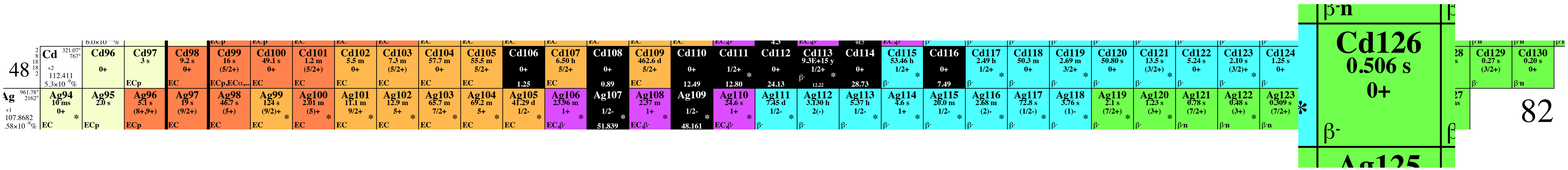

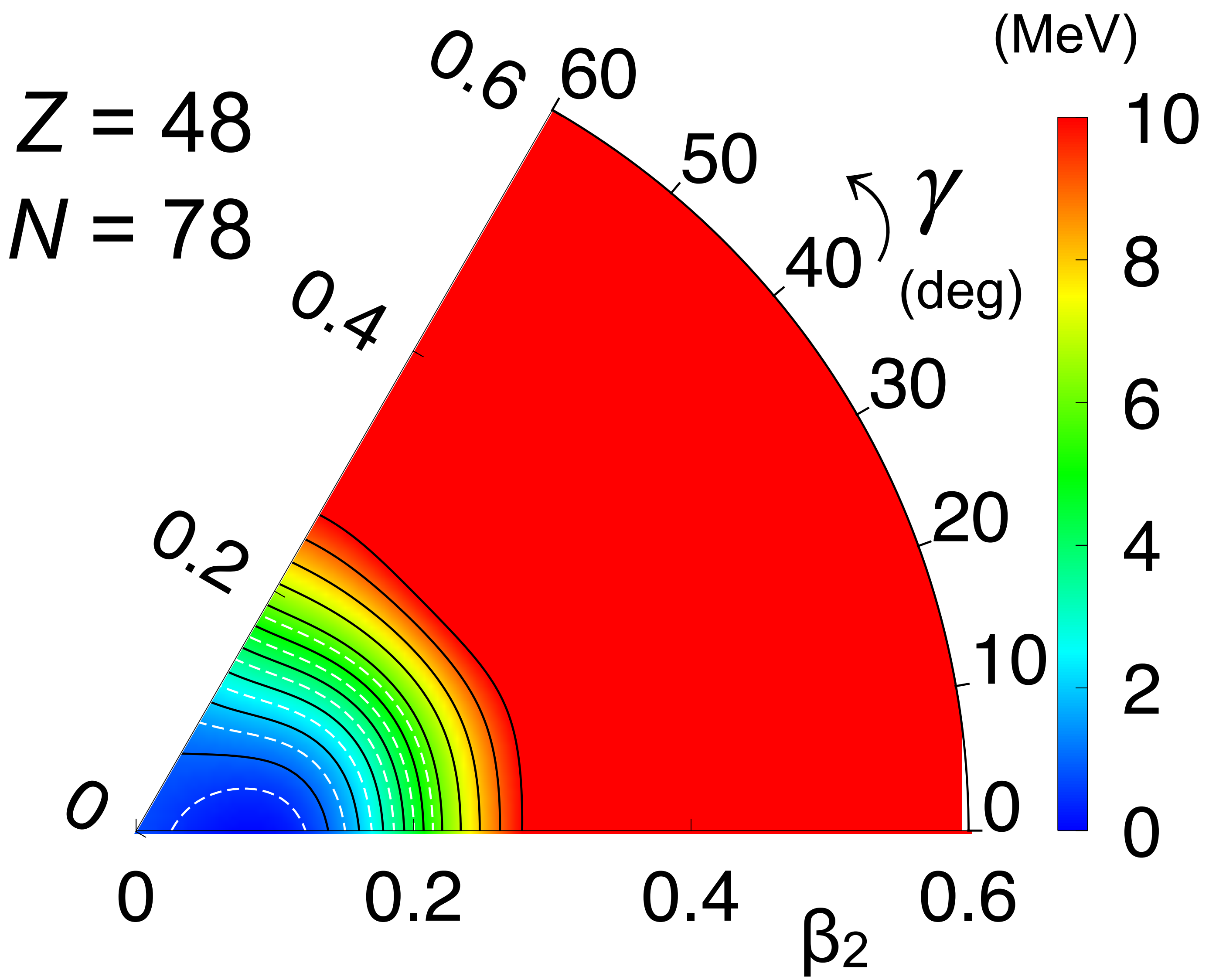

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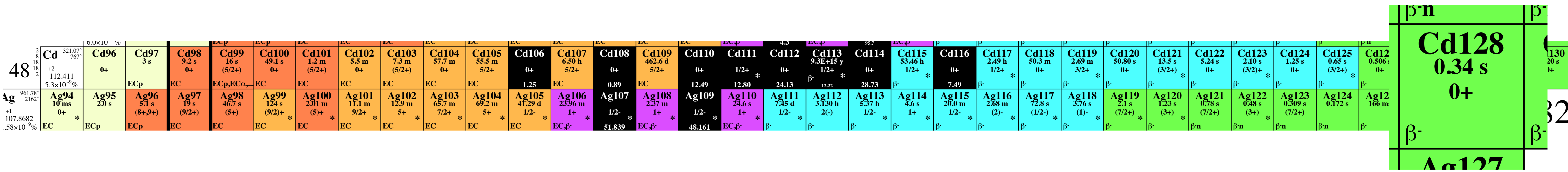

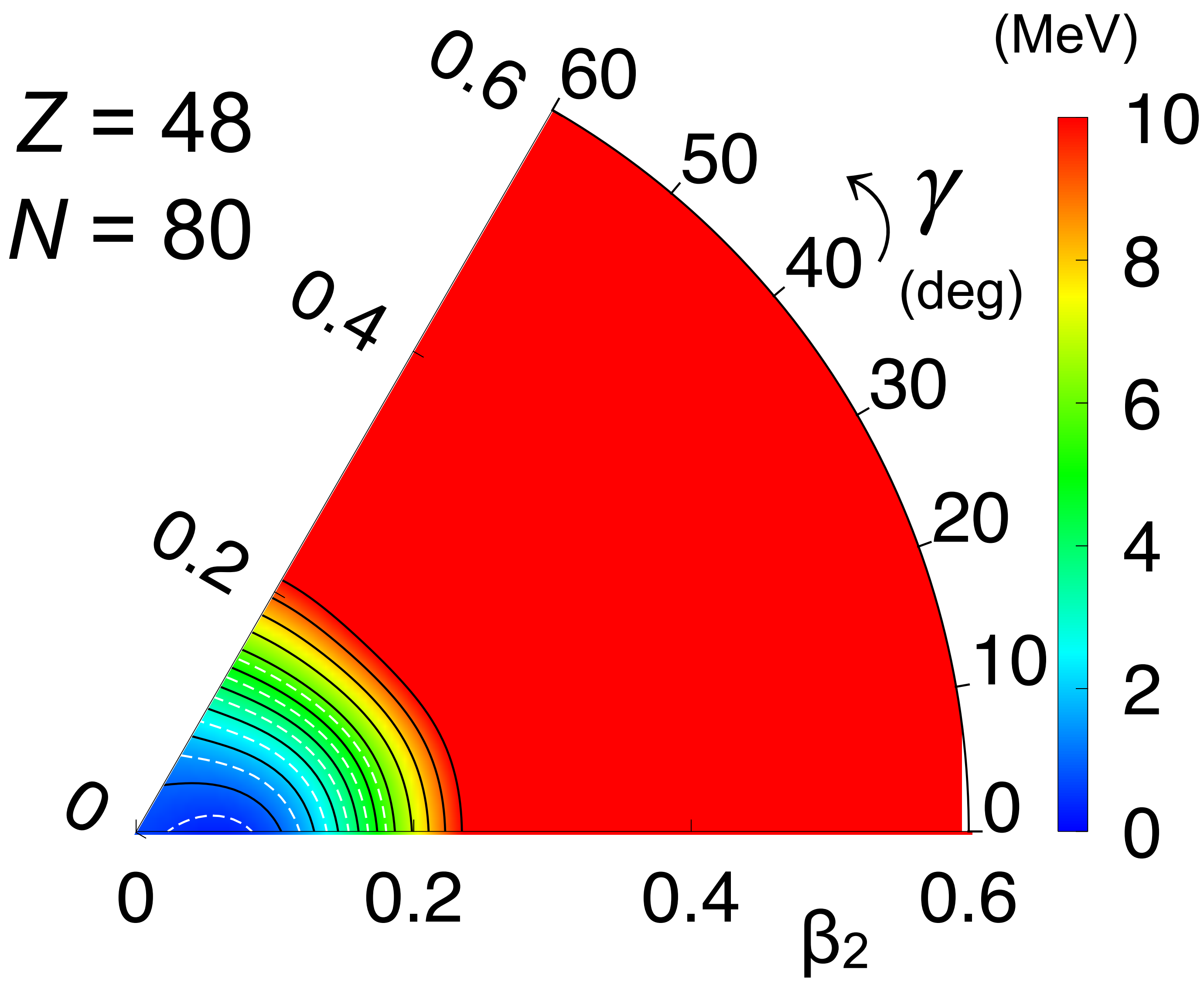

PN-VAP energy surfaces

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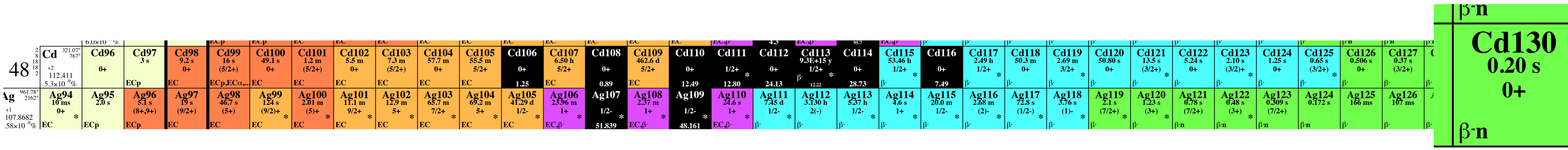

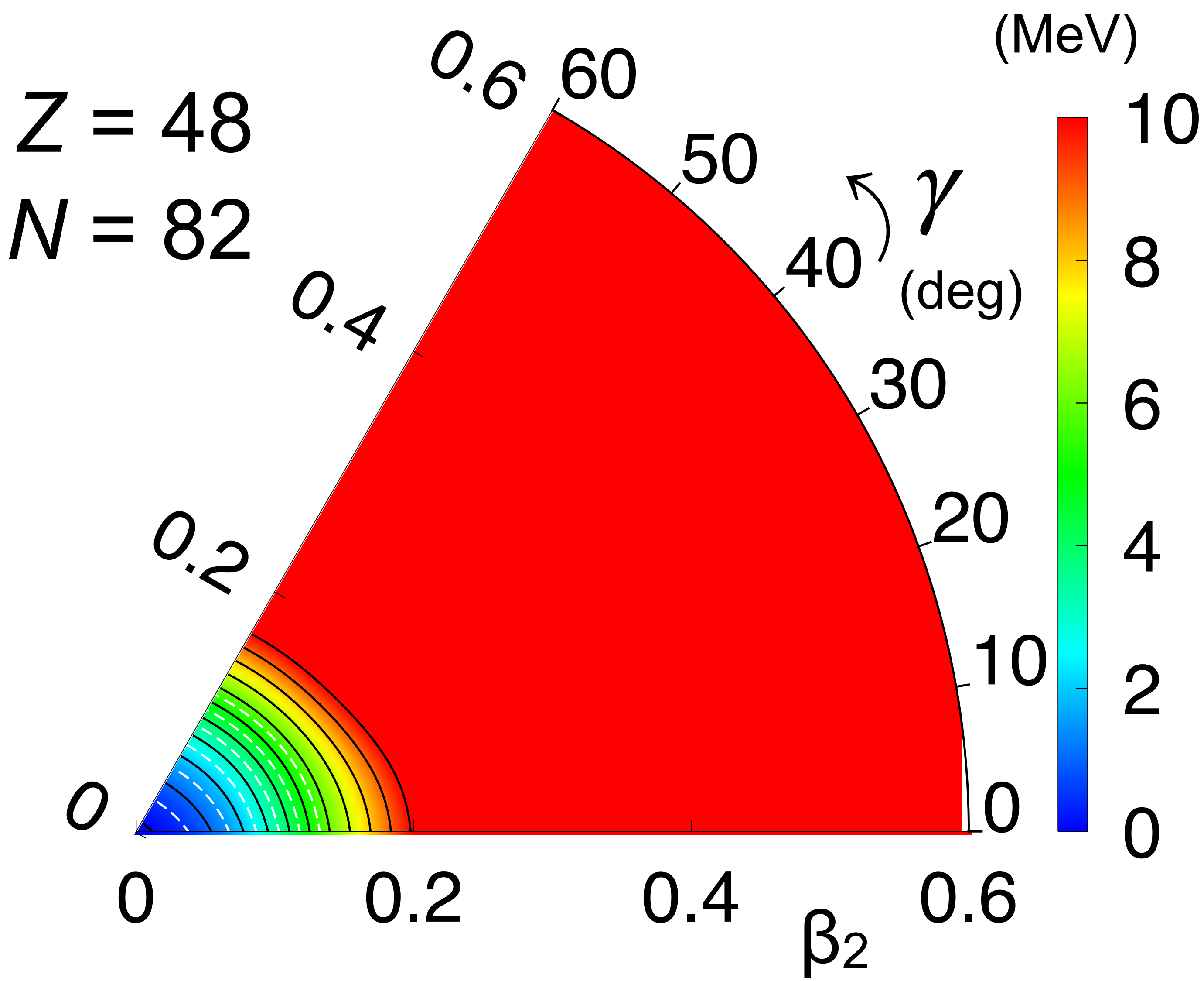

PN-VAP energy surfaces

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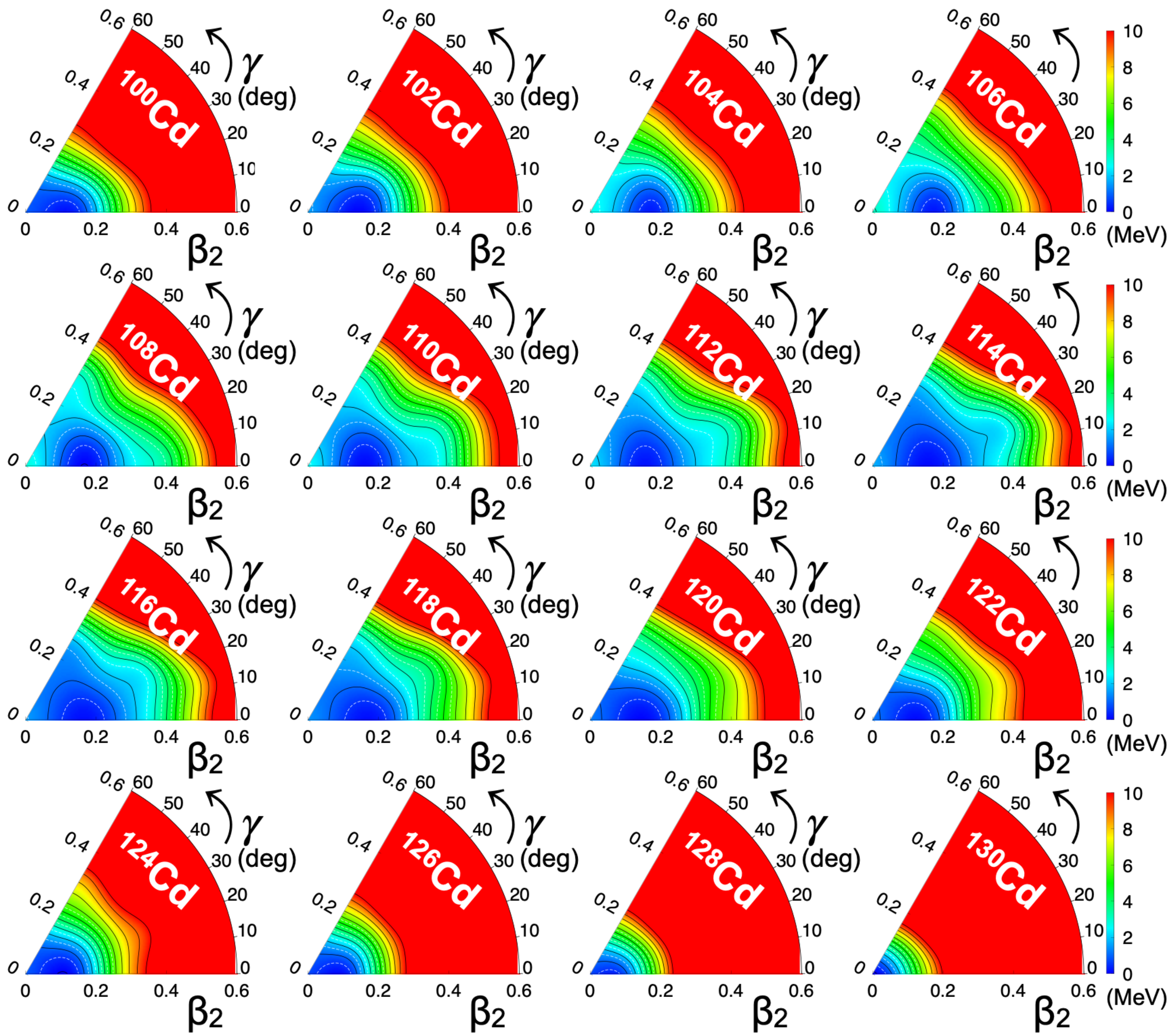
- Shape evolution in cadmium isotopes



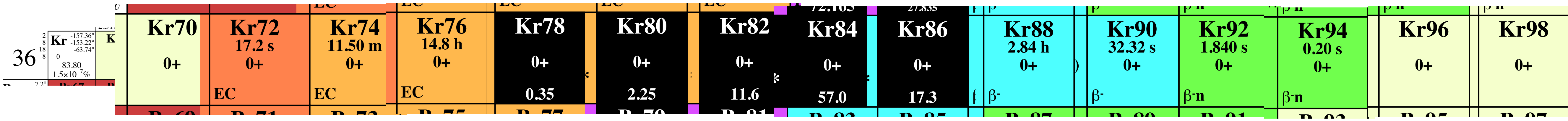
➡ Slightly prolate deformed minima are found along the whole isotopic chain.

➡ Deformation is larger (and almost constant) in the mid-shell and smaller when approaching to the magic neutron numbers (N = 50, 82).

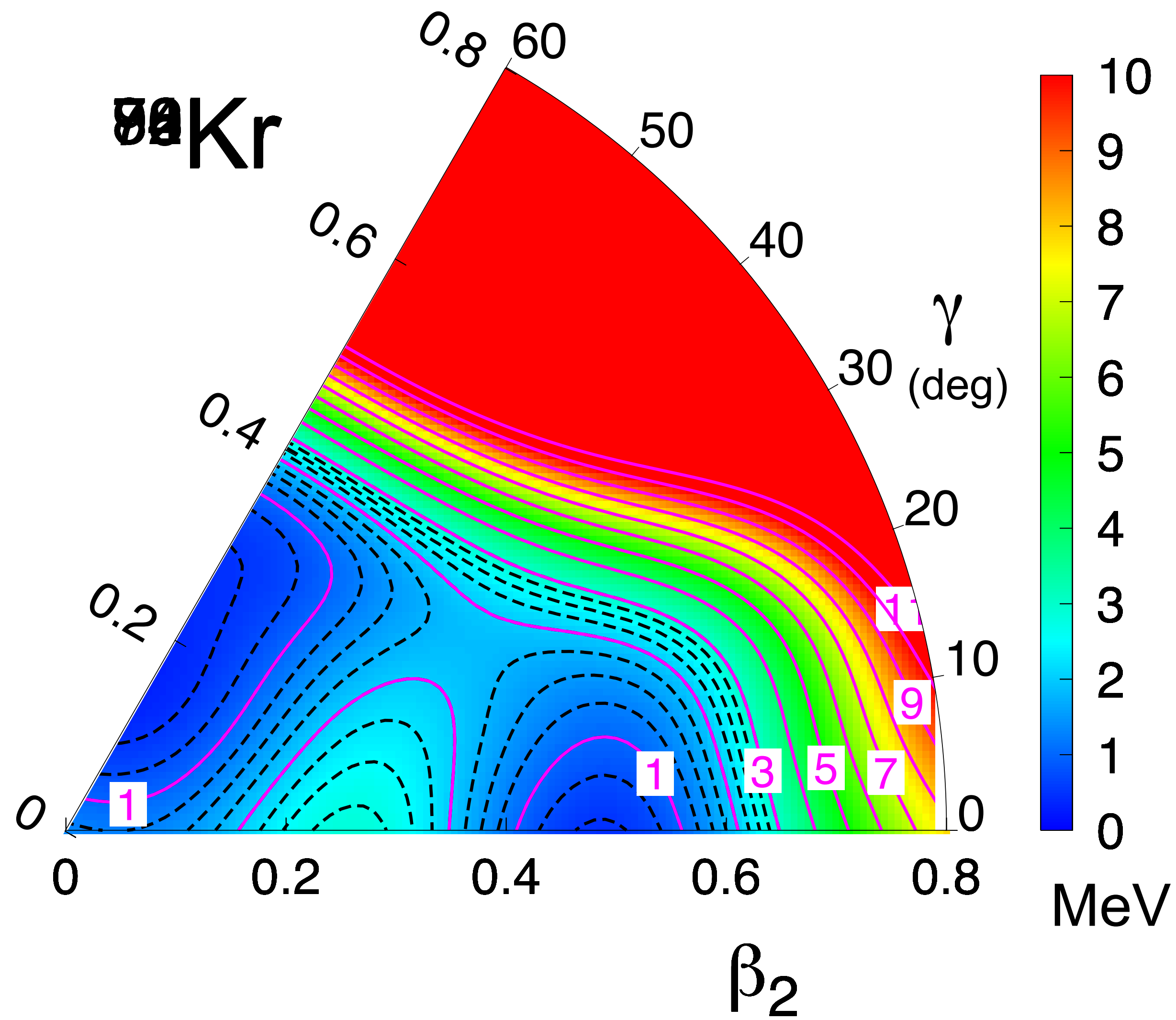
➡ A depression at β_2~0.35, γ~20 is found in $^{110-118}$Cd.

M. Siciliano et al., Physical Review C 104, 034320 (2021)

PN-VAP energy surfaces

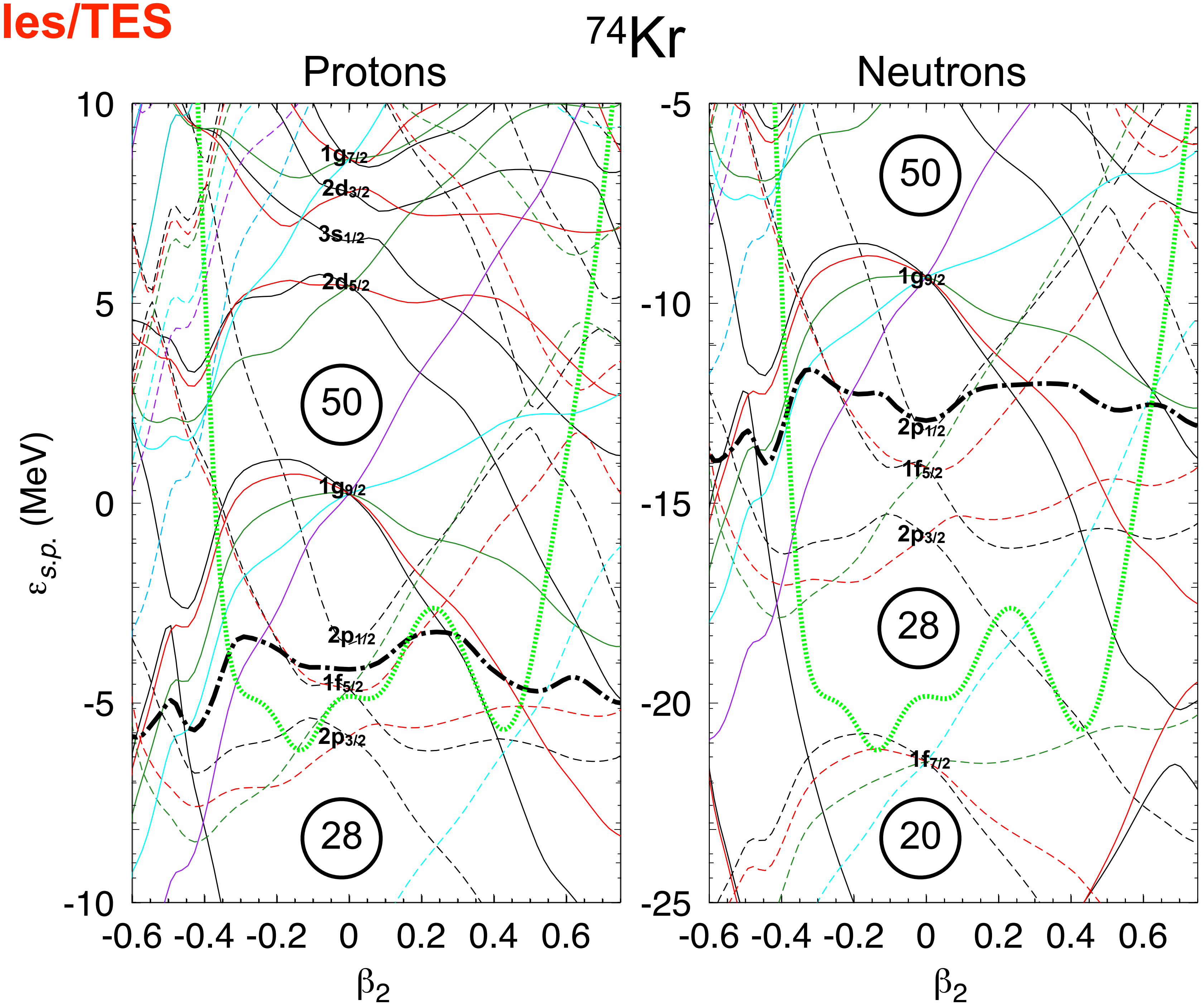


- ✓ Oblate shape in ^{70}Kr
- ✓ Two minima in $^{72-76}$Kr
- ✓ γ-softness in $^{78-80}$Kr
- ✓ Slightly prolate deformation in $^{82-84}$Kr
- ✓ Spherical semi-magic ^{86}Kr
- ✓ γ-softness in $^{88-92}$Kr
- ✓ Oblate shape in ^{94}Kr
- ✓ Oblate/prolate minima in $^{96-98}$Kr



Shell structure

Single particles/TES



Symmetry breaking

Let me be provocative: Nuclear shape comes as a non-observable degree of freedom (or an 'artifact') of the variational approximation at the mean-field level (one-body density approximation)

Remember: $$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l$$

$\delta E'_{\rm HFB}\left[|\Phi(\vec{q})\rangle\right] = 0$ with $E'_{\rm HFB}\left[|\Phi(\vec{q})\rangle\right] = \langle\Phi(\vec{q})|\hat{H} - \lambda_N \hat{N} - \lambda_Z \hat{Z} - \vec{\lambda}_{\vec{q}} \cdot \hat{\vec{Q}}|\Phi(\vec{q})\rangle$

- $\beta_k(\vec{q})|\Phi(\vec{q})\rangle = 0$ trial wave functions are quasiparticle vacua
- $\lambda_N \rightarrow \langle\Phi(\vec{q})|\hat{N}|\Phi(\vec{q})\rangle = N$ Lagrange multiplier for neutrons
- $\lambda_Z \rightarrow \langle\Phi(\vec{q})|\hat{Z}|\Phi(\vec{q})\rangle = Z$ Lagrange multiplier for protons
- $\vec{\lambda}_{\vec{q}} \rightarrow \langle\Phi(\vec{q})|\hat{\vec{Q}}|\Phi(\vec{q})\rangle = \vec{q}$ Lagrange multipliers for collective coordinates

Beyond self-consistent mean-field

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Symmetry restoration

- The Hamiltonian $\hat{H}$ has certain symmetries

$$\left[\hat{H},\hat{S}_i\right]=0 \quad \text{with} \quad \hat{S}_i=\left(\hat{N},\hat{Z},\hat{J}^2,\hat{J}_z,\hat{\Pi},...\right)$$

- However, the HFB wave function is not an eigenstate of the operators $\hat{S}_i$ (in general)

$$\hat{S}_i|\Phi\rangle \neq c_{s_i}|\Phi\rangle$$

- A better approach to the actual eigenvalues/eigenstates of the Hamiltonian should recover the symmetries of the Hamiltonian ☛ **PROJECTION TECHNIQUES**

$$|\Phi\rangle \rightarrow \hat{P}^{s_i}|\Phi\rangle = |\Psi^{s_i}\rangle \quad \text{with} \quad \hat{S}_i|\Psi^{s_i}\rangle = c_{s_i}|\Psi^{s_i}\rangle$$

Projection operator

Beyond self-consistent mean-field

- **Examples of projection operators**
  - Particle number: $$P^N = \frac{1}{2\pi}\int_0^{2\pi} e^{i\varphi(\hat{N}-N)}d\varphi$$
  - Parity: $$P^\pi = \frac{1}{2}\left(\mathbb{I} - \pi\hat{\Pi}\right)$$
  - Angular Momentum: $$P^I_M = \sum_{K=-I}^{+I} g^I_K P^I_{MK}$$

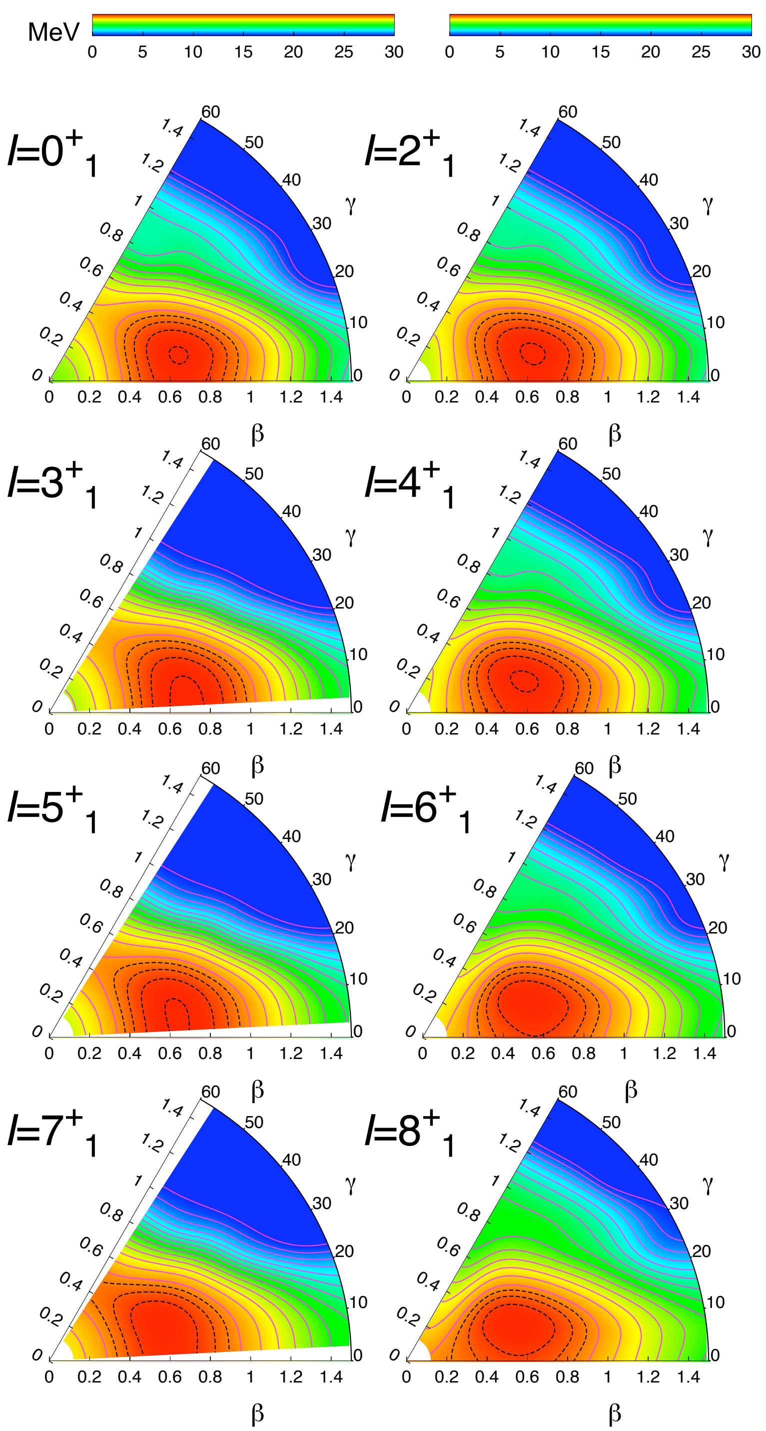
$$P^I_{MK} = \frac{2I+1}{8\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma \mathcal{D}^{I*}_{MK}(\Omega)\hat{R}(\Omega)$$ with $\Omega = (\alpha, \beta, \gamma)$ Euler angles

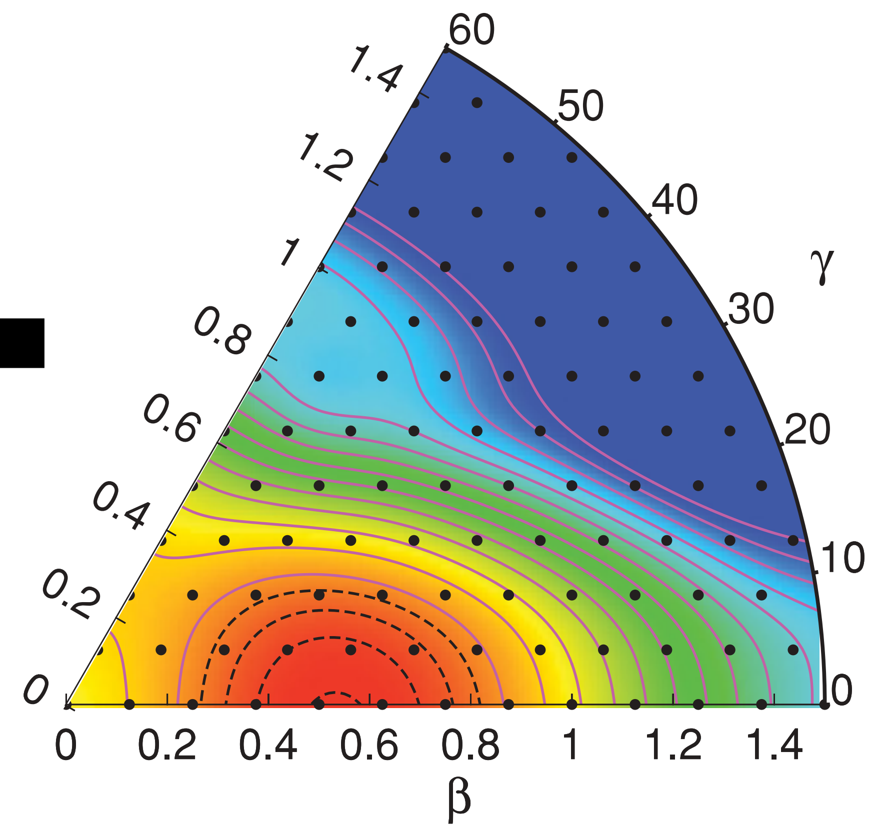
$$\hat{R}(\Omega) = e^{-i\alpha\hat{J}_z}e^{-i\beta\hat{J}_y}e^{-i\gamma\hat{J}_z}$$ Rotation operator

$$\mathcal{D}^I_{MK}(\Omega) = \langle IM|\hat{R}(\Omega)|IK\rangle = e^{-i\gamma K}e^{-i\alpha M}d^I_{MK}(\beta)$$ Wigner matrices

Beyond self-consistent mean-field

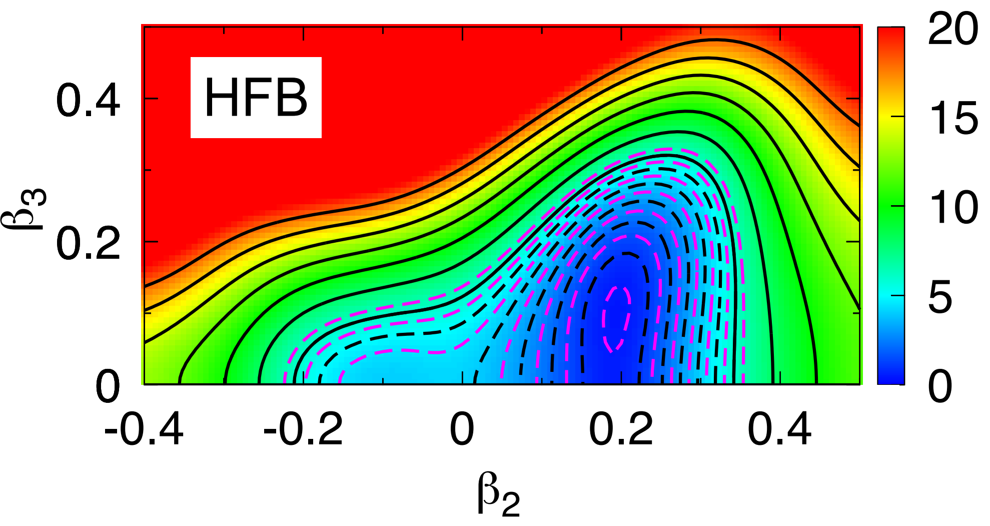
^{24}Mg triaxial calculations



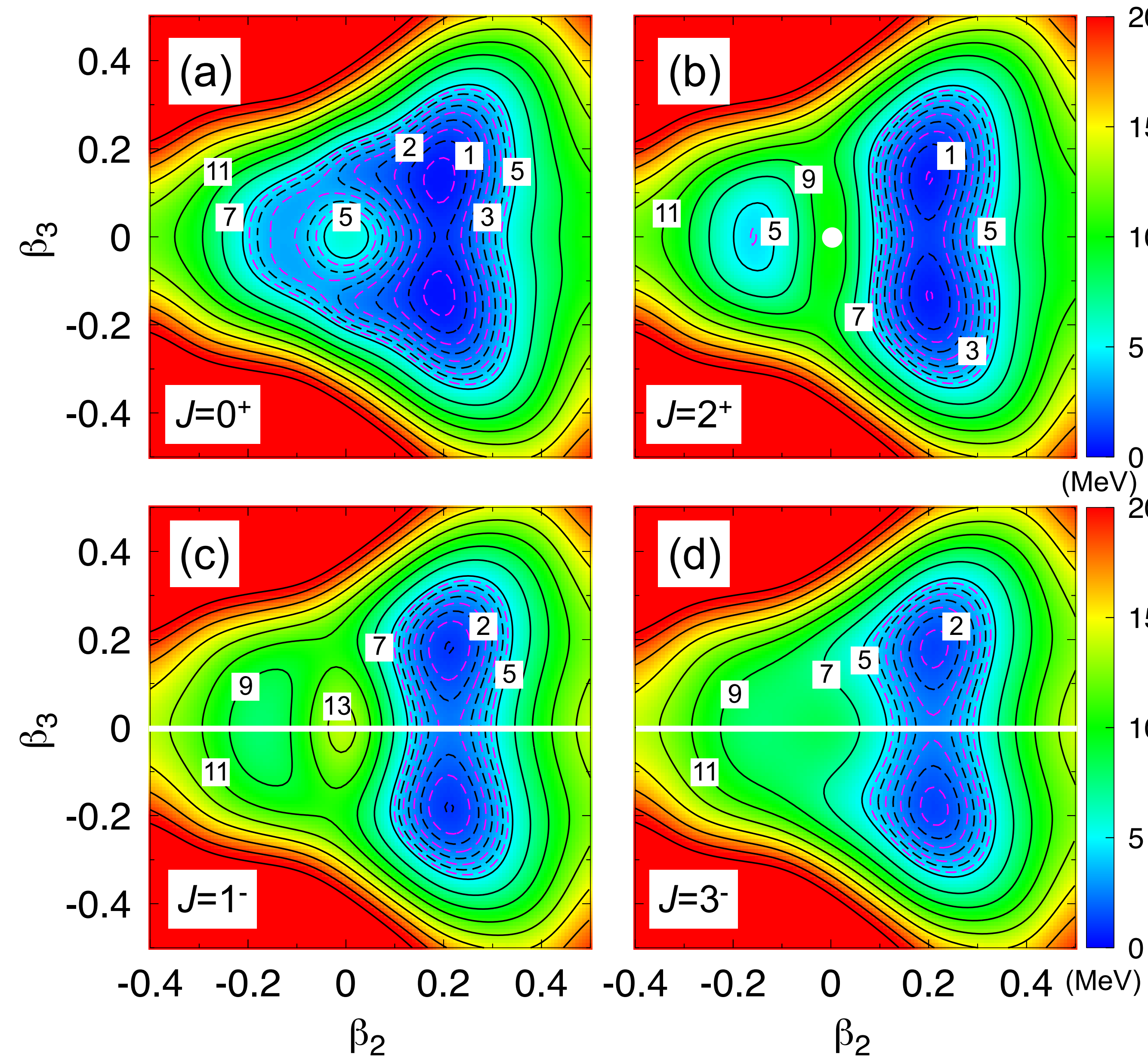


Beyond self-consistent mean-field

^{144}Ba axial calculations



Particle number, angular momentum and parity projected TES



R. Bernard, L. M. Robledo, T. R. R., PRC (2016)

Configuration mixing: PGCM

Nuclear wave functions: Generator Coordinate Method (GCM) ansatz

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} P^{J}_{MK} P^{N} P^{Z} P^{\pi} |\Phi(q)\rangle$$

$$\Gamma \equiv (JMNZ\pi)$$

linear combination — coefficients of the linear combination — "basis" states

Configuration mixing: PGCM

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Nuclear wave functions: Generator Coordinate Method (GCM) ansatz

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coefficients of the linear combination

The coefficients are obtained by minimizing the expectation value of the Hamiltonian (energy) with those coefficients as the variational parameters:

$$\sum_{q'K'} \left(\mathcal{H}_{qK,q'K'}^{\Gamma} - E_{\sigma}^{\Gamma} \mathcal{N}_{qK,q'K'}^{\Gamma}\right) f_{\sigma;q'K'}^{\Gamma} = 0$$

Hill-Wheeler-Griffin (HWG) equation

$$\mathcal{H}_{qK,q'K'}^{\Gamma} = \langle \Phi(q)|\hat{H} P_{KK'}^{J} P^{N} P^{Z} P^{\pi}|\Phi(q')\rangle,$$
$$\mathcal{N}_{qK;q'K'}^{\Gamma} = \langle \Phi(q)|P_{KK'}^{J} P^{N} P^{Z} P^{\pi}|\Phi(q')\rangle$$

Hamiltonian and norm kernels

Configuration mixing: PGCM

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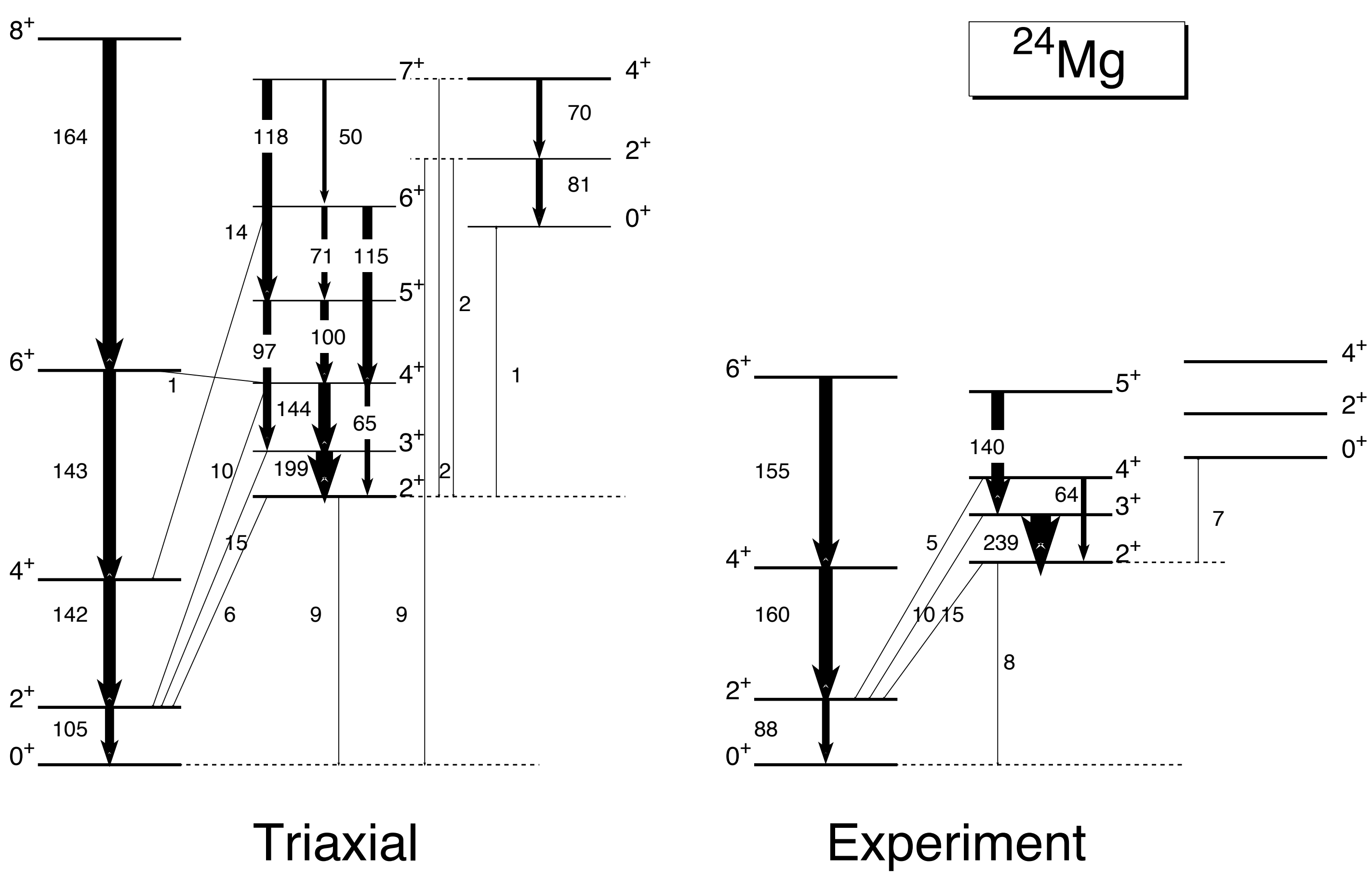
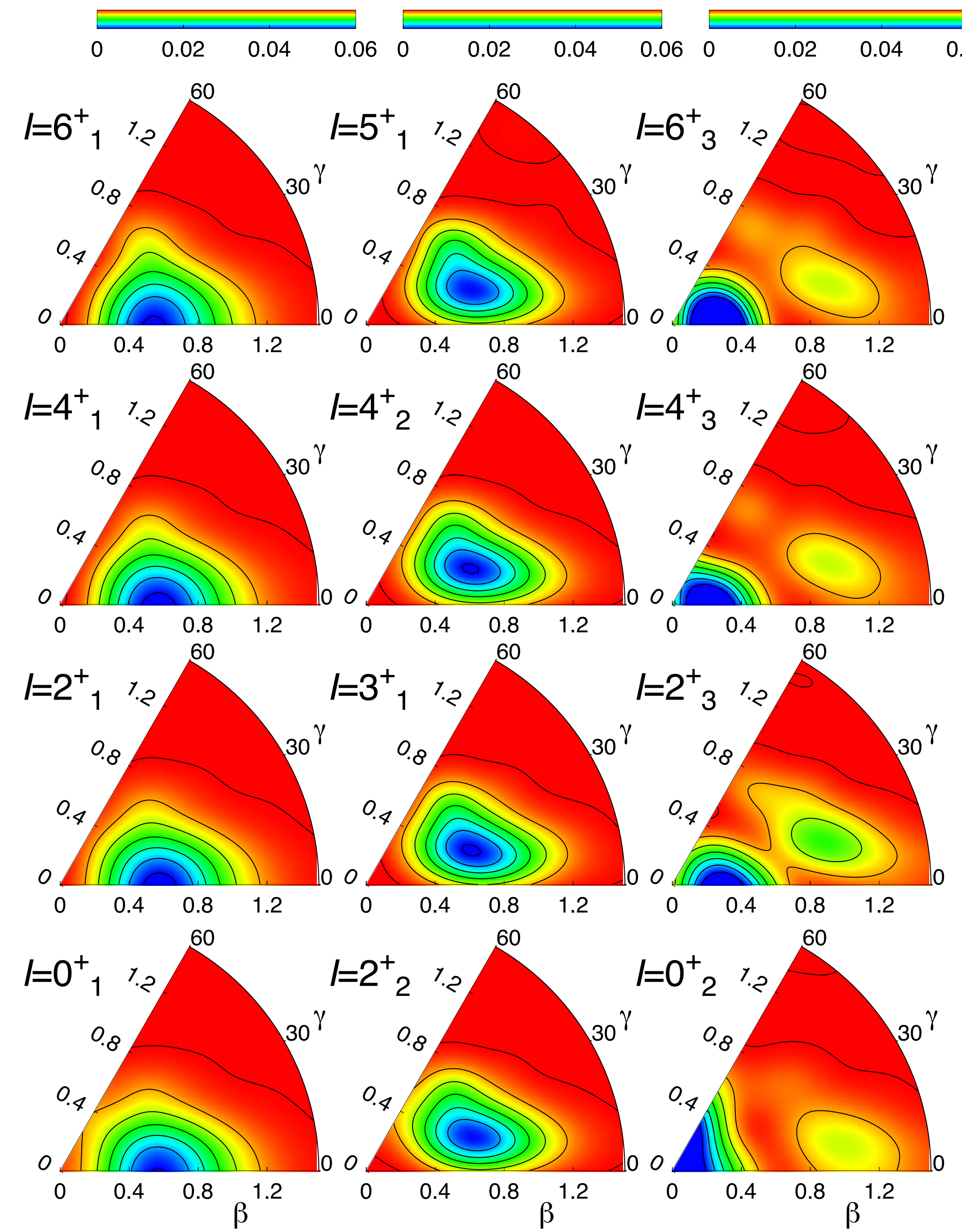
collective wave functions

^{24}Mg triaxial calculations





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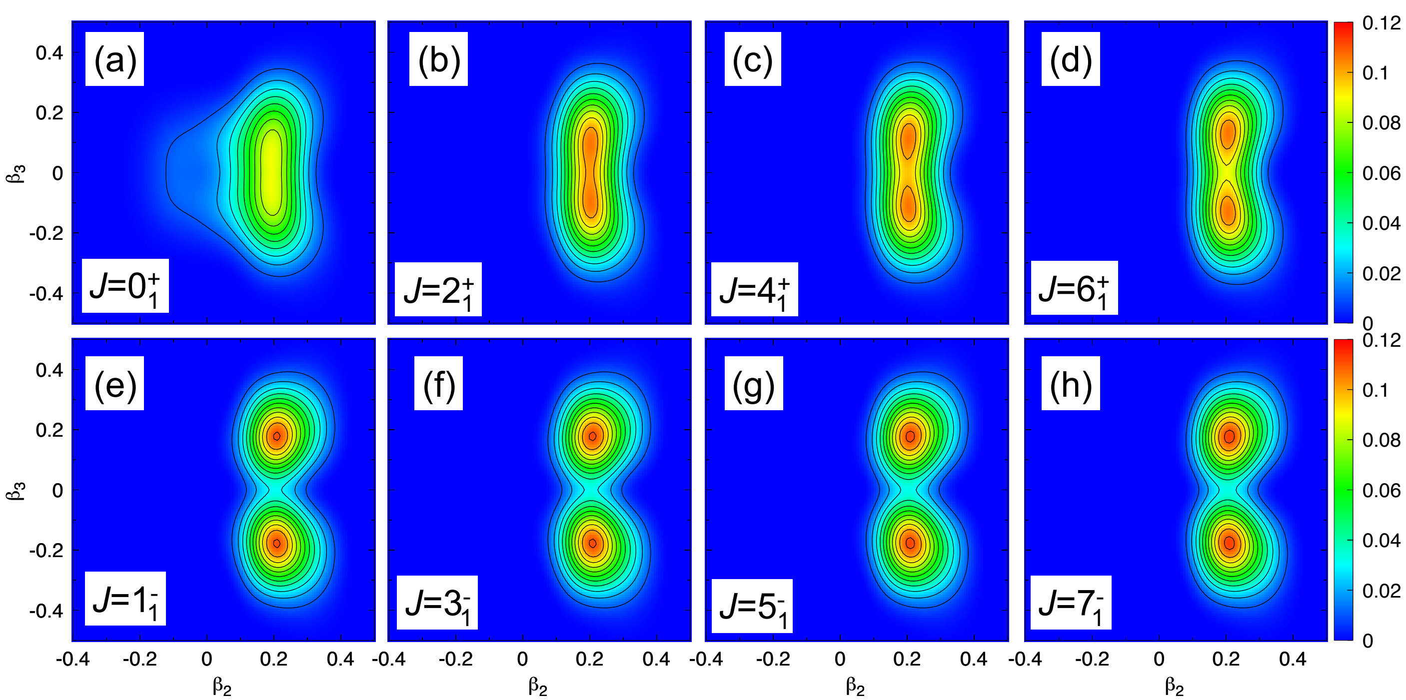

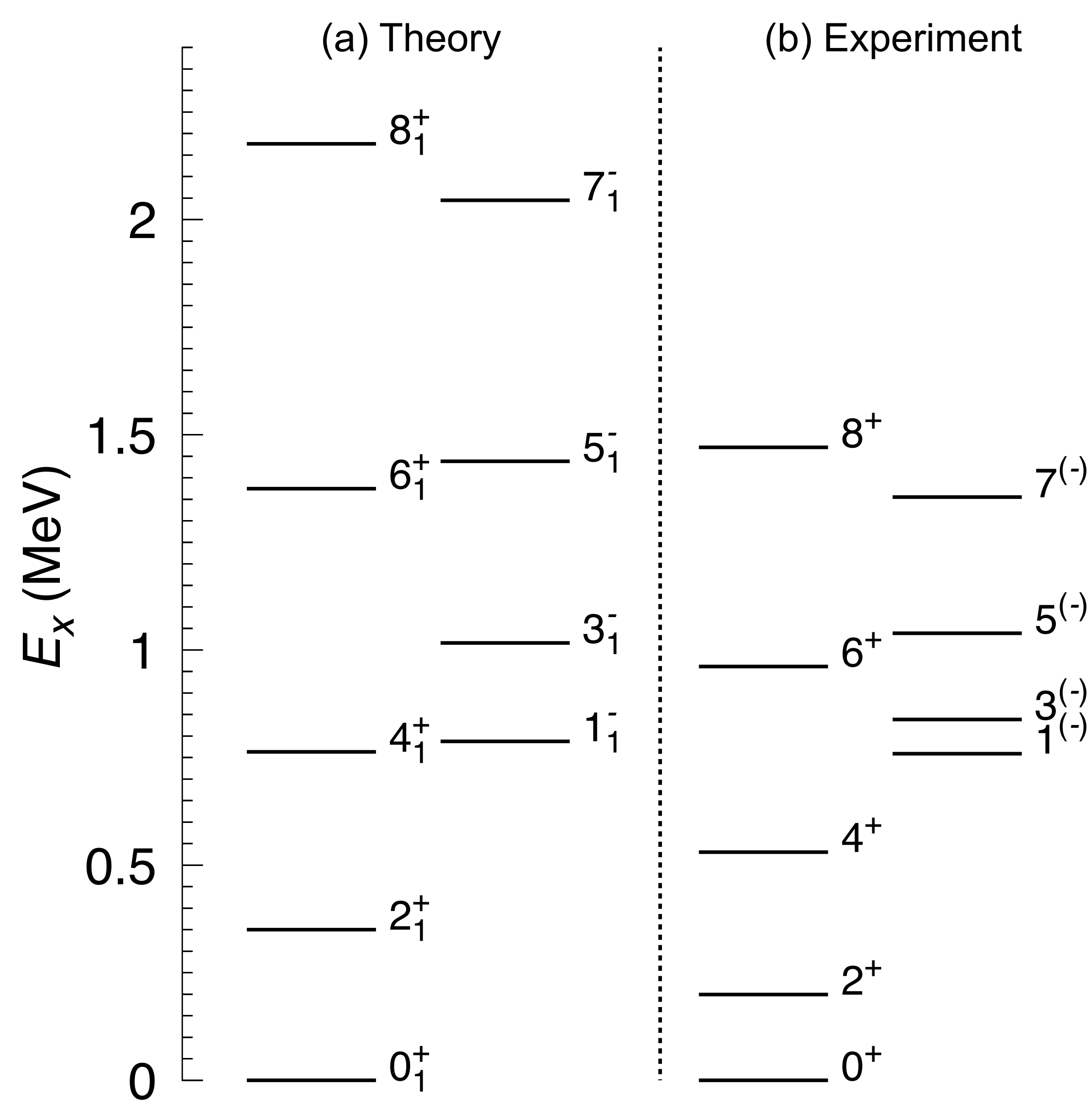

Configuration mixing: PGCM

- Nuclear wave functions wave functions: Generator Coordinate Method (GCM) ansatz

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$$\Gamma \equiv (JMNZ\pi)$$

Remark: we are (computational) limited to explore only certain degrees of freedom