High-Performance Algorithm for Calculating Non-Spurious Spin- and Parity-Dependent Nuclear Level Densities

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Year-5 deliverables

- Develop and test the Moments Method nuclear level density code that removes the center-of-mass spurious states

- Use the new Moments Method code to calculate nuclear level densities and reaction rates in the rp-process path
Nuclear Level Densities

- need to know nuclear level densities (NLD) for nuclear reactions, astrophysics, and applications

- theories and methods:
  - Fermi Gas Model: combinatorics of single-particle excitations near the Fermi surface. H. A. Bethe, 1936
    \[ \rho(E, J, \pi) = \frac{1}{2} F(U, J) \rho_{FG}(U), \text{ where } U = E - \Delta \]
  - Hartree-Fock-Bogolyubov model: also combinatorics
  - Shell Model calculations. Moments Method: describes statistical properties of nuclei
    M. Horoi et al.: PRC 69 041307(R), (2004); NPA 785, 142 (2005); PRL 98, 262503 (2007)
Moments Method. Statistical Spectroscopy

\[ \rho(E, \alpha) = \sum_{\kappa} D_{\alpha \kappa} \cdot G(E + E_{gs} - E_{\alpha \kappa}, \sigma_{\alpha \kappa}) \]

\[ \alpha = \{ n, J, T_z, \pi \} - \text{set of quantum numbers, } G(E, \sigma) - \text{Gaussian function} \]

\[ \kappa - \text{configurations, e.g. 6 particles in } sd \text{ shell:} \]

\[
\begin{array}{c|cccc}
\kappa & d^5_2 & s^1_2 & d^3_2 \\
1 & 6 & 0 & 0 \\
2 & 5 & 1 & 0 \\
3 & 5 & 0 & 1 \\
4 & 4 & 2 & 0 \\
\cdots & \cdots & \cdots & \cdots \\
15 & 0 & 2 & 4 \\
\end{array}
\]

\[ D_{\alpha \kappa} - \text{number of many-body states with given } J \text{ that can be built for a given configuration } \kappa \]

Moments of \( H \) for each configuration \( \kappa \):

\[ E_{\alpha \kappa} = \frac{\text{Tr}(\alpha \kappa)[H]}{D_{\alpha \kappa}} \]

\[ \sigma_{\alpha \kappa}^2 = \frac{\text{Tr}(\alpha \kappa)[H^2]}{D_{\alpha \kappa}} - \left( \frac{\text{Tr}(\alpha \kappa)[H]}{D_{\alpha \kappa}} \right)^2 \]

M. Horoi, M. Ghita, and V. Zelevinsky, PRC 69 (2004) 041307(R)

it is important to know the \( E_{gs} \) and cut-off parameter \( \eta \).
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it is important to know the \( E_{gs} \) and cut-off parameter \( \eta \)
Results for $^{52}$Fe, $^{52}$Cr, parity=$+1$, some $J. \; pf$-shell

Comparison of nuclear level densities between exact Shell Model (solid line), Moments Method (dashed line), and HFB method (dotted line). Cut-off parameter $\eta = 2.6$, interaction GXPF1A.

Removal of the center-of-mass spurious states

Lawson method

\[
H \rightarrow H' = H + \beta \left[ \left( H_{CM} - \frac{3}{2} \hbar \omega \right) \frac{A}{\hbar \omega} \right]
\]


Recursive method

3D-Harmonic oscillator:

\[
N_{\text{pure}}(A, K \hbar \omega) = N_{\text{tot}}(A, K \hbar \omega) - \sum_{K' = 1}^{K} C_{K'} N_{\text{pure}}(A, (K - K') \hbar \omega)
\]

\[
N_{\text{pure}}(A, 0 \hbar \omega) = N_{\text{tot}}(A, 0 \hbar \omega), \quad C_{K'} = (K' + 1)(K' + 2)/2
\]


Nuclear level density:

\[
\rho^{(0)}(E, J, K) = \rho(E, J, K) - \sum_{K' = 1}^{K} \sum_{J + J' = J_{\text{step 2}}} \sum_{J_{K'} = J_{\text{min}}}^{J_{K'} = J - |J - J_{K'}|} \rho^{(0)}(E, J', K - K')
\]

$N\hbar\omega$ restriction and Width calculation

Before (no restriction):

\[
\text{Tr}^{(\alpha \kappa)}[H] = \sum_{\lambda \in \kappa} \langle \lambda | H | \lambda \rangle
\]

\[
\text{Tr}^{(\alpha \kappa)}[H^2] = \sum_{\lambda \in \kappa} \sum_{\mu} \langle \lambda | H | \mu \rangle \langle \mu | H | \lambda \rangle = \sum_{\lambda \in \kappa} \langle \lambda | H^2 | \lambda \rangle
\]

Now (restricted):

\[
\text{Tr}^{(\alpha \kappa)}[H] = \sum_{\lambda \in \kappa} \langle \lambda | H | \lambda \rangle
\]

\[
\text{Tr}^{(\alpha \kappa)}[H^2] \Rightarrow \sum_{\lambda \in \kappa} \sum_{\mu \in R} \langle \lambda | H | \mu \rangle \langle \mu | H | \lambda \rangle \neq \sum_{\lambda \in \kappa} \langle \lambda | H^2 | \lambda \rangle
\]

Example: $^{20}\text{Ne}$, (s-p-sd-pf)-model space, $1\hbar\omega$

$^{20}\text{Ne} (1\hbar\omega)$

$J^\pi = 1^-$

$^{20}\text{Ne} (1\hbar\omega)$

$J^\pi = 2^-$

- are shell model calculations with $\beta = 0$ and $\beta = 4$,
- moments method: $\rho$, $\rho^{(0)}$, and $\delta\rho = \rho - \rho^{(0)}$

$J = 1$

$\rho^{(0)}(E, 1, 1\hbar\omega) = \rho(E, 1, 1\hbar\omega) - \sum_{J' = 0}^{2} \rho(E, J', 0\hbar\omega)$

$J = 2$

$\rho^{(0)}(E, 2, 1\hbar\omega) = \rho(E, 2, 1\hbar\omega) - \sum_{J' = 1}^{3} \rho(E, J', 0\hbar\omega)$
$^{22}\text{Mg, (s-p-sd-pf)-model space, } 1\hbar\omega, \beta \cdot A = 110\text{MeV}$
$^{26}$Al and $^{28}$Si, (s-p-sd-pf)-model space, both parities, all $J$
Code scaling (NERSC/Hopper)

Moments Method Code = “PreCalc” + “Calc”

“PreCalc” $\rightarrow N_p + N_n \approx 5.3 \cdot 10^3$ conf. – scales not good
“Calc” $\rightarrow N_p \cdot N_n \approx 7.1 \cdot 10^6$ conf. – scales good

at Number of cores = 1,500: “PreCalc” = 1min, “Calc” = 2.5 min

How to improve the “PreCalc” part?

Dynamic load balancing: one Master $\Rightarrow$ several Masters (ADLB)
Nuclear data needs:
- Masses (proton separation energies)
- $\beta$-decay rates
- Reaction rates (p-capture and $\alpha,p$)

Some recent mass measurements
$\beta$-endpoint at ISOLDE and ANL Ion trap (ISOLTRAP)

Separation energies
Experimentally known up to here

Many lifetime measurements at radioactive beam facilities
(for example at LBL, GANIL, GSI, ISOLDE, MSU, ORNL)
- Know all $\beta$-decay rates (earth)
- Location of drip line known (odd Z)

Indirect information about rates
from radioactive and stable beam experiments
(Transfer reactions, Coulomb breakup, …)

Direct reaction rate measurements
with radioactive beams have begun
(for example at ANL, LLN, ORNL, ISAC)

slide from H. Schatz
NLD and Hauser-Feshbach

talys 1.2: www.talys.eu

**NLD-M1**

- *ldmodel 1*: Constant temperature + Fermi gas model
- *ldmodel 2*: Back-shifted Fermi gas model
- *ldmodel 3*: Generalised superfluid model
- *ldmodel 4*: Microscopic level densities from Goriely’s table
- *ldmodel 5*: Microscopic level densities from Hilaire’s table

**NLD-M5**


\[58\text{Fe} (^3\text{He}, \alpha)\]
\[\theta = 150^\circ\]

\[59\text{Co}(d, \alpha)\]
\[\theta = 150^\circ\]
Comparison with Moments Densities

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NLD-M1

ldmodel 1: Constant temperature + Fermi gas model
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NLD-M5

Interface:
Moments table -> Hilaire’s table


← $^{59}\text{Co}(d, \alpha)$

$\theta = 150^0$

← $^{58}\text{Fe}(^3\text{He}, p)$

$\theta = 150^0$
Example: reaction rates in rp-process path

\[ ^{25}\text{Al} (p,\gamma) ^{26}\text{Si} \]

\[ ^{26}\text{Si} (p,\gamma) ^{27}\text{P} \]

**TALYS 1.2**: [http://www.talys.eu/](http://www.talys.eu/)


Deliverables for year 5

- new algorithm of removal of the contribution of center-of-mass spurious states was successfully developed and tested
- the code is parallelized and was tested using up to 6,000 processors
- calculations of NLD in large model spaces were performed
- calculations of reaction rates in the rp-process path were made

What’s next?

- improve the scaling
- develop interface, scripts
- write documentation, examples. publish the code
- more applications: NLD, reaction rates, schematic interactions
CMU Personnel:

Mihai Horoi, PI
Roman Senkov, postdoc
Jagjit Kaur, student

Publications:


Invited talks:

4. M. Horoi, “Nuclear Structure Theory Relevant to the Facility for Rare Isotope Beams”, colloquium at Western Michigan University, Kalamazoo, MI, January 24, 2011.

Accepted talks: