Progress Report on Calculating Accurate Nuclear Level Densities Using Spin Projected Moments Method

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Nuclear Level Densities (NLD)

Hauser and Feshbach, Phys. Rev 87, 366 (1952),


\[ T(E,J,\pi) = \int_{E_{\text{min}}}^{E_{\text{max}}} T(E,J,\pi;E_x,J_x,\pi_x) \rho(E_x,J_x,\pi_x) dE_x \]

- See Erich Ormand’s talk

\[ \rho(E_x,J,\pi) = \frac{1}{2} \mathcal{F}(U,J) \rho_{\text{FG}}(U) \]

\[ U = E_x - \Delta \]

Equal contribution to both parities

Remedy by Alhassid, Bertsch, Liu,
Nakada, PRL 84, 4313 (2000) + Basel group (Rauscher)

\[ \text{HF+BCS} \rightarrow \rho_{\text{HF+BCS}}(U) \]

Accurate Nuclear Level Densities

Comparison of:
1. CI,
2. HF+BCS
   www-astro.ulb.ac.be/Html/nld.html
3. experimental data

Complete spectroscopy: sd-shell nuclei

Conclusions:
- HF+BCS overestimates the data
- CI accurately describes the data
NLD and Statistical Spectroscopy

M. Horoi et al.:
PRC 67, 054309 (2003),
PRC 69, 041307(R) (2004),
NPA 785, 142 (2005).

PRL 98, 265503 (2007)

Configurations: e.g. 4 particles in sd
d3 d5 s1
4 0 0
3 1 0
3 0 1 ...

preserve rotational invariance
and parity

\[ \rho(E_x, J, \pi) = \sum_{c \in \text{conf}} D_c(J, \pi) G_{FR}(E, E_c(J), \sigma_c(J)) \]

\[ E_c(J), \sigma_c(J) \leftarrow \text{Tr}_{SD_c} < M \mid H^q \mid M >_{SD_c} \]

\[ E_x = E - E_{\text{g.s.}} \]

\[ E_c(J), \sigma_c(J): \text{computational intensive} \]

Configurations can be calculated in parallel

Conclusion:
- Moments method NLD reproduces very well the CI NLD

\( ^{28}\text{Si} \ \pi = + \) staircase: CI, USD

E_g.s. from CI, PCI, Exponential Convergence Method (PRL 82, 2064 (1999)), CC, etc.
NLD Comparison: CI, Moments, HF+BCS
NuShellX: coupled-J code


Can calculate a large number of non-yrast states: ideal for level density

- Hardware: 3.2 GHz, dual-quad Intel, 16 GB RAM, 700 GB SATA II HD
- Maximum 8 threads
- **HPC equivalent**: computes five J=0 states in $^{56}$Ni (m-scheme dim = $10^9$) in 4 hours !!!

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![Graph](image)
NLD of $^{56}\text{Fe}$: CI, Moments, HF+BCS

Ohio data: PRC 74, 014314 (2006)
Ratio of unnatural to natural NLD of different parities at low energies

\[ \rho(E_x, J, \pi) = \frac{1}{2} \mathcal{F}(U, J) \rho_{FG}(U) \]

\[ U = E_x - \Delta \]

Equal contribution to both parities


Configurations: e.g. 4 particles in fpg

- f5 p3 p1 g9 \pi
- 4 0 0 0 +
- 3 1 0 0 +
- 3 0 1 0 +
- 3 0 0 1 -

... preserve rotational invariance and parity
NLD for the rp-process

the rp-process path

$^{68}\text{Se}$
$^{64}\text{Ge}$


$^{65}\text{Ge}, J=9/2$

$^{65}\text{Ge}, J=1/2$

$Ioroi CM^1$
Publications


Presentations

Status of the NLD Project

Moments Code for NLD:
- Serial Code: finalized
- Parallel Code: in progress
- HPC resources: up to 100,000 CPU-hour

NuShellX CI Code (W. Rae):
- Serial Code: finalized, adapted to Unix environment
- Parallel Code: OpenMP - proved to scale to 32 threads, depending on J
- HPC resources: up to 100,000 thread-hour
Plan for the rest of Year 2

- Finish the parallelization of the Moments code
- Calculate nuclear level densities around the “waiting-point nucleus” $^{68}\text{Se}$

Plan for Year 3

- Calculate the nuclear level densities for most of the nuclei in the rp-process path
- Provide input to HF code (LLNL) to calculate reaction rates
- Investigate algorithm efficiency
- HPC resources needed: up to 300,000 thread-hour

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- Investigate level densities for the r-process path. Calculate the relevant reaction rates.

- Improve the efficiency of the algorithm to scale to over 1,000 cores

- Restrict the class of intermediate configuration for second moments $\sigma_c(J)$; useful for removal of center-of-mass spurious components (PRL 98, 265503 (2007))
NLD and Statistical Spectroscopy

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\[ \rho(E_x,J,\pi) = \sum_{p \in \text{conf}} D_p(J,\pi) G_{FR}(E, E_p(J), \sigma_p(J)) \]

\[ E_p(J), \sigma_p(J) \leftarrow \text{Tr}_{SD} < M \mid H^q \mid M >_{SD} \]

\[ E_x = E - E_{g.s.} \]

\( E_{g.s.} \) from CI, PCI, Exponential Convergence Method (ECM), PRL 82, 2064 (1999), etc.

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Fixed spin and parity nuclear level density for restricted shell model configurations

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\[ \langle\langle H \rangle\rangle m_{nM}T_z = \sum_i \epsilon_i D^i(m_{nM}T_z) + \sum_{i<j} V_{ij ij} D^{ij}(m_{nM}T_z) \]

\[ \langle\langle H^2 \rangle\rangle m_{nM}T_z = \sum_i \epsilon_i^2 D^i(m_{nM}T_z) + \sum_{i<j} \left[ 2\epsilon_i \epsilon_j + 2(\epsilon_i + \epsilon_j)V_{ij ij} + \sum_{k<l} V_{ijkl}^2 \right] D^{ij}(m_{nM}T_z) + \sum_{(i<j)\neq l} \left[ (2V_{iikk}V_{jj kj} - V_{i jkl}^2) + 2\epsilon_i \epsilon_j V_{ij ij} \right] D^{ij l}(m_{nM}T_z) + \sum_{(i<j)\neq (k<l)} \left[ V_{ij kl}^2 + V_{ij ij} V_{kl kl} - 4V_{ki ij} V_{kj kl} \right] D^{ij kl}(m_{nM}T_z) \]

\[ E_{\tilde{m}}(J) = \langle\langle H \rangle\rangle m_{nM}JT_z = \left( \langle\langle H \rangle\rangle m_{nM} = JT_z - \langle\langle H \rangle\rangle m_{nM} = (J+1)T_z \right) / D(m_{nM}JT_z) \]

\[ \langle H^2 \rangle m_{nM}JT_z = \left( \langle\langle H^2 \rangle\rangle m_{nM} = JT_z - \langle\langle H^2 \rangle\rangle m_{nM} = (J+1)T_z \right) / D(m_{nM}JT_z) \]

\[ \sigma_{\tilde{m}JT_z} = \sqrt{\langle H^2 \rangle m_{nM}JT_z - \langle H \rangle^2 m_{nM}JT_z} \]

\[ m \] is the number of particles
\[ D^i(m_{nM}T_z) \] is the number of determinants in a partition \( \tilde{m} \) with \( nMT_z \) and state \( i \) occupied,
Removal of Spurious Center-of-Mass Excitations

\( \rho(E, J, 0+2) \): total density in a model space including all 0+2 h.o. excitations

\( \rho_{\text{nsp}}(E, J, 0+2) \): center-of-mass excitations removed

\[
\rho_{\text{nsp}}(E,J = 2, 0 + 2) =
\rho(E,2,0 + 2) - \sum_{J_k = 0}^{2} \sum_{J' = |2 - J_k|}^{2+J_k} \rho_{\text{nsp}}(E,J',0) - \sum_{J' = 1}^{3} \rho_{\text{nsp}}(E,J',1)
\]

\(^{10}\text{B} \): 10 particles in \( s-p-sd-pf \) shell model space

Horoi and Zelevinsky, PRL 98, 265503 (2007)