Benchmarking mean-field approximations to level densities

G.F. Bertsch, Y. Alhassid, C.N. Gilbreth, and H. Nakada
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Motivation
--need to know accurate level densities for Hauser-Feshbach reaction theory
--computational considerations favor finite-temperature HF and HFB for systematic surveys.
--we don’t know the accuracy of the mean-field approximations at finite temperature

Outline of the talk
1. Level densities--present state of the art
2. The SMMC benchmark
3. Hurdles: grand canonical to canonical, dealing with condensates
4. HF performance in Dy162 (deformed, weak pairing)
5. HFB performance in Sm148 (spherical, strong pairing)
6. Lessons learned
State of the art

The backshifted Fermi Gas beats global mean field.

Other methods:
   - Shell-Model Monte Carlo
   - Moments of Cl shell-model Hamiltonians
   - Static path
What about the CI shell model?

1. Matrices too large for brute-force diagonalization.
2. Moment methods might work, but still need an accurate ground-state energy.
Sample the operator

\[ \hat{P}_N \hat{P}_P e^{-\beta \hat{H}} \]

to estimate expectation values in the canonical ensemble:

\[
\langle \hat{O} \rangle = \frac{\langle \hat{O} \hat{P}_N \hat{P}_P e^{-\beta \hat{H}} \rangle}{\langle \hat{P}_N \hat{P}_P e^{-\beta \hat{H}} \rangle}
\]

\[
\langle \hat{O} \rangle_\beta = \frac{\langle \hat{O} \hat{P}_N \hat{P}_P e^{-\beta \hat{H}} \rangle}{\langle \hat{P}_N \hat{P}_P e^{-\beta \hat{H}} \rangle}
\]

Comments:
Hamiltonian must have good sign.
Statistical quantities are calculated from \( E(\beta) = \langle \hat{H} \rangle_\beta \)
Results available up to and including lanthanides, but not yet actinides.
Important Equations

Entropy from canonical energy

\[ S(\beta) = \int_{E(\infty)}^{E(\beta)} \beta dE \]

1-D saddle point for the canonical state density

\[ \rho(E) = \left( 2\pi \left| \frac{\partial E}{\partial \beta} \right| \right)^{-1/2} e^{S_c(\beta)} \]

where

\[ E = -\frac{\partial \ln Z_c}{\partial \beta} \]

Project quantum numbers

\[ P_N = \left( 2\pi \sigma^2 \right)^{-1/2} e^{-\left( N - \langle N \rangle \right)^2 / 2\sigma^2} \]

where

\[ \sigma^2 = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 \]
The 1-D saddle point is remarkably accurate.

Canonical level density for the Hamiltonian

$$H = \delta \sum_{i=0}^{\Omega-1} (i + 1/2) a_i^\dagger a_i$$

Filled circles: actual number of states.
Solid line: 1-D saddle point with exact number projection
Dotted line: 2-D saddle point
Dash-dot: 1-D saddle point with approximate number projection
SMMC benchmark

The benchmark nuclei are $^{162}$Dy (deformed) and $^{148}$Sm (spherical).

The Hamiltonian has the form

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + \sum_{i<j} \sum_{k<l} v_{ij,kl} a_i^\dagger a_j^\dagger a_l a_k$$

where $\varepsilon_i$ is from a Woods-Saxon potential and

and $v_{ij,kl}$ has the form

$$v(r_1, r_2) = \sum_L v_L f_L(r_1) f_L(r_2) \sum_M Y_{LM}(\hat{r}_1) Y_{LM}(\hat{r}_2)$$

Limiting energies

<table>
<thead>
<tr>
<th>nucleus</th>
<th>$\beta$</th>
<th>SMMC</th>
<th>HF</th>
<th>HFB</th>
<th>correlation energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{148}$Sm</td>
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<td>-119.15</td>
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SMMC results

Despite very different structure, D’s are nearly equal.

Resonance spacing at neutron threshold

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>$E_x$ (MeV)</th>
<th>$J^\pi$</th>
<th>$D$ (eV)</th>
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<tbody>
<tr>
<td>$^{148}\text{Sm}$</td>
<td>8.1</td>
<td>$(3^-, 4^-)$</td>
<td>3.7±0.6</td>
</tr>
<tr>
<td>$^{162}\text{Dy}$</td>
<td>8.2</td>
<td>$(2^+, 3^+)$</td>
<td>2.4±0.3</td>
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</table>
State and level densities from finite-temperature HF(B)

Start with grand canonical ensemble

\[ \langle H \rangle, \langle N_p \rangle, \langle N_n \rangle, \langle \Pi \rangle, \langle J^2_{x,y,z} \rangle, S \]

at inverse temperature \( \beta \)

\[ \log(Z) = \beta \langle H \rangle - S - \beta \mu_p \langle N_p \rangle - \beta \mu_n \langle N_n \rangle \]

\( \rightarrow \rho_{gc}(E) \)

3-D saddle-point or

\[ Z_c \approx Z P_{N_p} P_{N_n} \]

Project onto canonical ensemble for fixed nucleon number \( N_p, N_n \).

\[ \langle H \rangle_c, \langle \Pi \rangle_c, \langle J^2_{x,y,z} \rangle_c, S_c \]

\[ \log(Z_c) = \beta \langle H \rangle_c - S_c \]

\( \rightarrow \rho_c(E) \)

4-D saddle-point or

\[ Z_M \approx Z P_M \]

Project onto \( M \) for level densities.

\[ \langle H \rangle_M, S_M \]

\( \rightarrow \rho_M(E) \)
**HF for \(^{162}\text{Dy}\)**

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<td>-371.91</td>
<td>11.41</td>
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Limiting energies

Sharp HF phase transition is completely smoothed out.

HF misses the finite S at low temperature (due to rotational band structure).
Performance on state density: $^{162}$Dy

State density is a factor of 10 too low, due to rotational band physics.
T. Dossing, private communication
The independent-particle approximation

Generate the single-particle spectrum from the ground-state HF, and assume it doesn’t change at finite beta.

Agrees with the full HF to better than a factor of 2 up to neutron threshold.
Level density, $^{162}\text{Dy}$

Attempt to correct for rotational band degeneracy:

$$\rho_K(E) = P_K \rho_{HF}(E) \quad \rho_{J^\pi}(E) \approx \frac{1}{2} \sum_{K=0}^{J} \rho_K$$

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<td>SMMC HF HFB Exp.</td>
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</tr>
</tbody>
</table>
| $^{162}\text{Dy}$ | 8.2       | $(2^+, 3^+)$ | $2.3 \pm 0.3 0.67$ | 2.4

too much!
HFB for $^{148}\text{Sm}$

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<td></td>
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Limiting energies

HF and SMMC have very similar $E(\beta)$ functions, provided they are offset by their respective ground-state values.

The entropy function

All tested approximations fail at one end or the other.
Mild kinks due to pairing phase transition are completely suppressed. Canonical entropy too low at T=0. Grand canonical entropy looks much better near T=0.
State density -- Sm-148

HFB = HF above phase transition--justifies “back-shift” parametrization

Factor-of-three problem remains at $E_x \sim 1-4$ MeV
Conclusions (tentative, of course)

0) There are no visible signatures of mean-field phase transitions.
1) Back-shifted HF is a good approximation for spherical nuclei above the HFB pairing phase transition.
2) The independent-particle approximation is acceptable for excitation energies below ~15 MeV.
3) The Bjørnholm-Bohr-Mottelson enhancement for deformed nuclei only affects the state densities at low excitation energies. The level density at low J is not affected.
4) We could not extract a reliable level density from HF in the presence of strong deformation.
5) Difficulties with number projection prevented us from getting a reliable state density in HFB below the pairing transition.
Can we do better?

1) Try exact PAV number projection to address point 5) above (in progress by YA).
2) The static path approximation does not distinguish between spherical and deformed nuclei; it might help for point 4) above.
3) Moment methods are promising; they should be benchmarked and compared with HF(B).
Final Comments


2. What about soft nuclei? Besides SMMC, only candidate for a theory is the static path approximation, so far only used for well-deformed nuclei.

3. Where did Bjornholm, Bohr, and Mottelson go wrong?
Thermodynamic Consistency

\[ dS = \beta dE \]

A sum rule for the canonical entropy:

\[ \int_0^{E(\infty)} \beta dE = \ln \left( \frac{\Omega_p}{N_p} \right) + \ln \left( \frac{\Omega_n}{N_n} \right) \]

Useful as a computational check