Particle-number projection in finite-temperature mean-field approximations to level densities

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- Motivation
- Finite-temperature mean-field theory for level densities
- Particle-number projection in the finite-temperature Hartree-Fock-Bogoliubov approximation with time-reversal symmetry
- Benchmarking mean-field results against shell model Monte Carlo calculations in heavy nuclei
- Symmetry restoration in Hartree-Fock-Bogoliubov theory without time-reversal symmetry
- Conclusions and outlook

Motivation

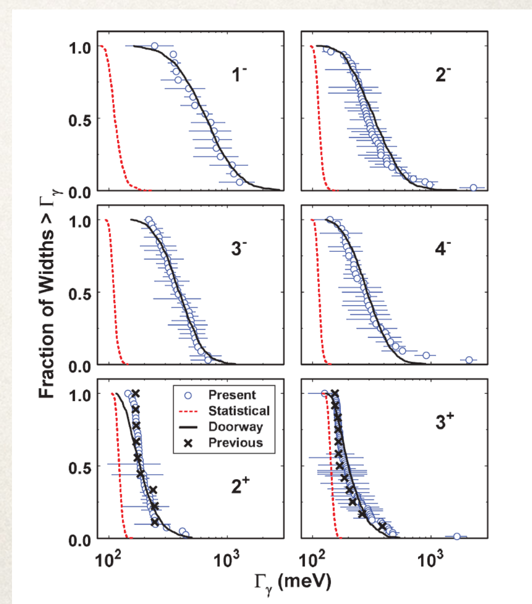
- The nuclear level density is a crucial input to the Hauser-Feshbach theory of compound nucleus reactions. Applications in astrophysical reaction rate calculations, nuclear technologies, etc.

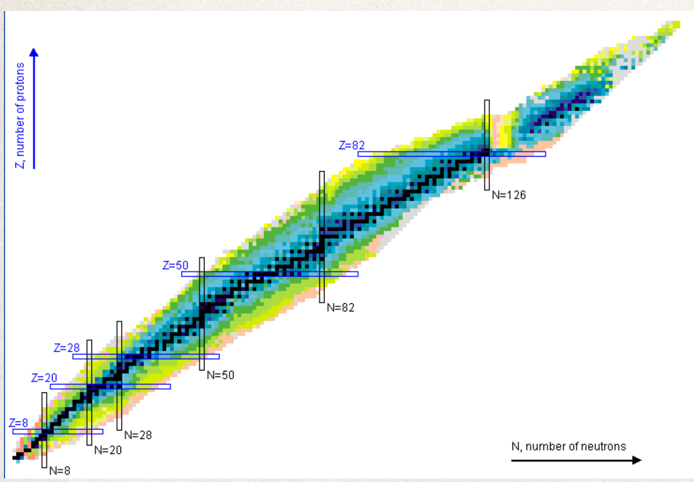
$$T_c(E,J,\Pi) = \sum_{\text{known levels}} \underbrace{T_{cf}(E,J,\Pi)}_{\text{transmission coefficients}} + \int dE_f \sum_{J_f,\Pi_f} T_{cf}(E,J,\Pi)\underbrace{\rho(E_f,J_f,\Pi_f)}_{\text{level density}}$$

Rauscher and Thielemann At. Data Nucl. Data. Table (2000)

- Theoretical level densities are necessary in cases where no experimental data exists, e.g., nuclei far from stability.
- Theoretical level densities are crucial for interpretation of experimental results: fluctuation properties of neutron resonances, normalization and spin distribution in Oslo method.

Koehler et al., PRC (2013)





$$\underbrace{\langle \Gamma_{\lambda\gamma f}(XL)\rangle}_{\text{Average partial radiation width}} = \frac{\overbrace{f_{XL}(E_\gamma)}^{\text{gamma strength function}} E_\gamma^{2\lambda+1}}{\rho(E_\lambda, J_\lambda, \Pi_\lambda)}$$

Configuration-interaction (CI) shell-model approach

- Phenomenological level density (LD) models: back-shifted Fermi gas, Gilbert-Cameron constant temperature
  - Advantage: simple analytical expressions.
  - Disadvantage: parameters must be adjusted for each nucleus to fit data well.
- It is useful to predict LD microscopically from underlying nuclear interactions.
- Thermodynamic approach to state density:

$$\rho(E, N_p, N_n) = \frac{1}{(2\pi i)^3} \int d\beta d\alpha_p d\alpha_n e^{\beta E - \sum_{i=p,n} \alpha_i N_i} \underbrace{Z_{gc}}_{\text{grand-canonical partition function}} \approx \frac{e^{S_c}}{\sqrt{2\pi T^2 C}}$$

e^{S_c} ← canonical entropy

C ← heat capacity

$$\alpha_i = \beta \mu_i$$

- CI shell model approach provides an accurate framework for calculating the LD in the presence of correlations.
- Limited by the combinatorial growth of the many-particle model space dimension.

Finite-temperature mean-field theory

- Basic idea: replace the two-body nucleon-nucleon interaction with an average single-particle potential.
- Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) theory: the mean-field potential is derived self consistently with respect to the single-particle density matrix ρ and pairing tensor κ.

$$\hat{V} = \frac{1}{4}\sum_{ijkl} \bar{v}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \rightarrow \hat{V}_{mf} = \sum_{ij} \Gamma(\rho)_{ij} a_i^\dagger a_j + \frac{1}{2}\left(\sum_{ij} \Delta(\kappa)_{ij} a_i^\dagger a_j^\dagger - \Delta^*(\kappa)_{ij} a_i^\dagger a_j^\dagger\right)$$

HF $\rho_{ij} = \left\langle a_j^\dagger a_i \right\rangle$ HFB $\kappa_{ij} = \langle a_j a_i \rangle$

- Relations between ρ, κ, Γ, and Δ are derived variationally by minimizing the grand thermodynamic potential.
- Advantage: thermodynamic quantities are calculated easily.
- Challenges:
  - Correlations beyond the mean-field are neglected.
  - Mean-field solutions often break symmetries of the underlying Hamiltonian (e.g., rotational symmetry in the deformed phase of HF/HFB, particle-number conservation in the pairing phase of HFB).

Benchmarking the mean-field level density

Alhassid, Bertsch, Gilbreth, Nakada, PRC (2016)

- The level density can be calculated exactly in the shell model Monte Carlo (SMMC, c.f. Yoram's talk). However, this method requires more computational effort than mean-field theory, as well as "good-sign" interactions. Recent review: Alhassid, arXiv:1607:01870 in a review book ed. K.D. Launey
- Mean-field theory is widely used, but its inherent accuracy vs. exact methods is not well understood.
- Benchmark: compare the mean-field results against SMMC results using the same model space and the same interaction.
- Model space for rare-earth nuclei: protons: 50-82 shell plus $1f_{7/2}$, neutrons: 82-126 shell plus $0h_{11/2}$ and $1g_{9/2}$.
- Hamiltonian: Woods-Saxon plus spin orbit, pairing plus multipole-multipole interactions. Alhassid, Fang, Nakada, PRL (2008)

Ensemble reduction

- The HF and HFB potentials are determined in the grand-canonical ensemble, but the LD is defined within the microcanonical ensemble.
- Two-step process: 1. grand-canonical —> canonical.
  2. canonical —> microcanonical. Focus of this work is on step 1.

Step 1. $Z_c(\beta, N_p, N_n) = \int d\alpha_p d\alpha_n e^{-\sum_{i=p,n} \alpha_i N_i} Z_{gc}$ Step 2. $\rho(E) \approx \frac{e^{S_c}}{\sqrt{2\pi T^2 C}}$

- Usual method: saddle-point approximation of the integral in Step 1.

$$Z_c \approx \zeta^{-1} Z_{gc} e^{-\sum_{i=p,n} \alpha_i N_i}$$

- Discrete Gaussian (DG) approximation: modify saddle point correction ζ to account for the fact that N is a discrete integer.

$$\zeta = \sum_{N_i', N_j' \mid i,j=p,n} \exp\left[-\frac{1}{2} \sum_{i,j=p,n} \left. \frac{\partial N}{\partial \alpha} \right|_{i,j}^{-1} (N_i' - N_i)(N_j' - N_j) \right]$$

Alhassid et al. PRC, (2016).

- Problems with DG: oscillations at low temperatures and computational effort.

Particle-number projection and symmetry restoration

Rossignoli and Ring, Ann. Phys. (1991)

- Approximate canonical partition function found by taking trace of mean-field Gibbs operator $e^{-\beta \hat{H}_{mf}}$ over only N particle-states. $N = (N_p, N_n)$, H_{mf} is the grand-canonical mean-field Hamiltonian.

- This is known as particle-number projection (PNP) after variation.

- Particle-number projection is given by Fourier sum in a finite model space of N_s single-particle states.

$$Z_c \approx \mathrm{Tr}\, \hat{P}_N e^{-\beta \hat{H}_{mf}} = \frac{e^{-\beta\mu N}}{N_s} \sum_{n=1}^{N_s} e^{-i\phi_n N} \mathrm{Tr}\left[e^{i\phi_n \hat{N}} e^{-\beta(\hat{H}_{mf} - \mu \hat{N})} \right] \qquad \phi_n = \frac{2\pi n}{N_s}$$

- HF is particle-number-conserving, so evaluation of above trace is straightforward.

- In the HFB, particle-number conservation is broken in the pairing phase. PNP is equivalent to symmetry restoration.

  - The same techniques can be applied to restoration of rotational symmetry in deformed nuclei.

- To find LD: obtain canonical thermal energy and canonical entropy from Z_c by the usual thermodynamic relations.

$$E_c == -\frac{\partial \ln Z_c}{\partial \beta} \qquad S_c = \beta E_c + \ln Z_c$$

Particle-number projection in HFB with time-reversal symmetry

PF, Alhassid, and Bertsch, arXiv:1610.08954 (2016), accepted to PRC.

- General formula for projection trace in HFB involves a phase ambiguity for each term in the Fourier sum. Rossignoli and Ring, (1993)
- If the HFB energies come in degenerate time-reversed pairs, then the traces in the Fourier sum can be evaluated unambiguously by matrix algebra in the single-particle space
- This is possible because using only half the single-particle states fully defines the operators of interest.

q.p. operators $\xi^\dagger = \left(\alpha^\dagger_{k_1}, \ldots, \alpha^\dagger_{k_{N_s/2}}, \alpha_{\bar{k}_1}, \ldots, \alpha_{\bar{k}_{N_s/2}}\right)$

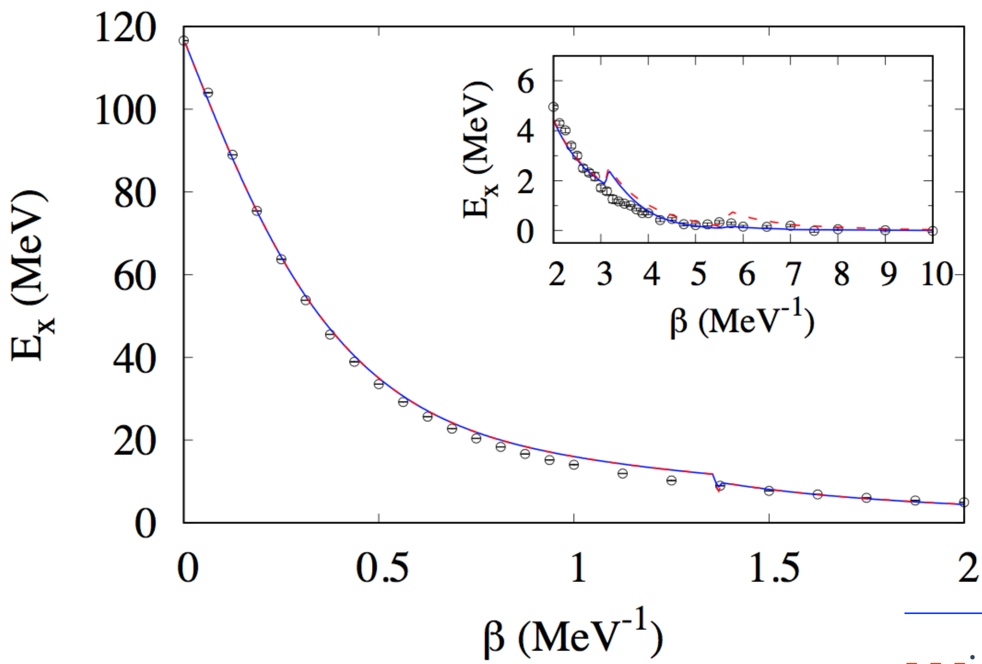
"Reduced" Bogoliubov transformation $\begin{pmatrix} \alpha_k \\ \alpha^\dagger_{\bar{k}} \end{pmatrix} = \mathcal{W}^\dagger \begin{pmatrix} a_k \\ a^\dagger_{\bar{k}} \end{pmatrix}$

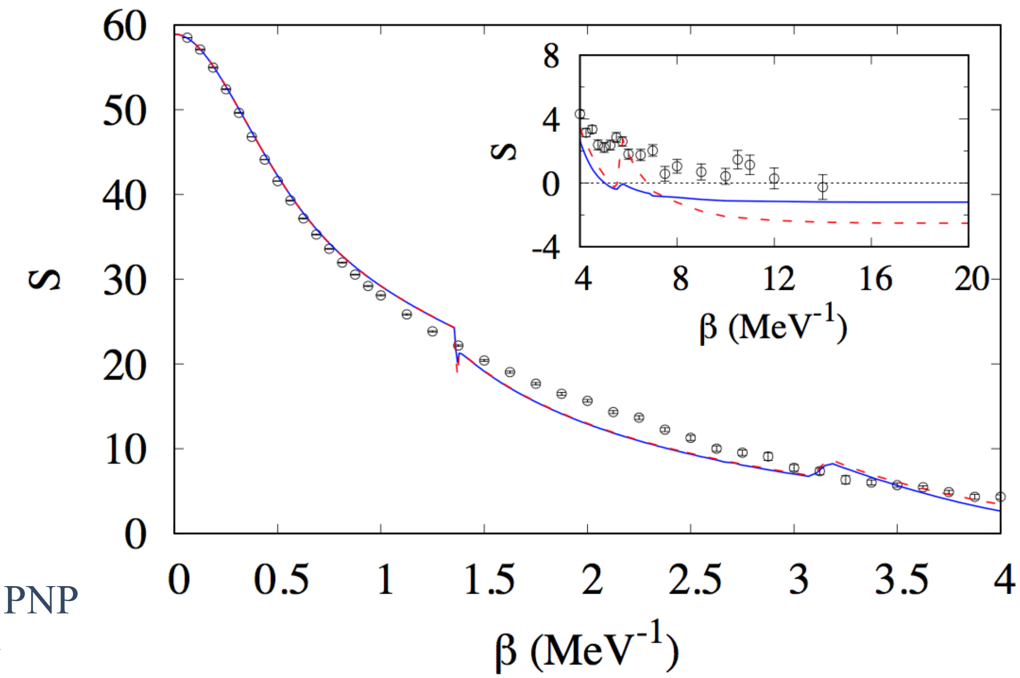
$$\hat{H}_{HFB} - \mu \hat{N} = \xi^\dagger \mathcal{E} \xi + \text{ const.} \qquad \hat{N} = \xi^\dagger \left(\mathcal{W}^\dagger \mathcal{N} \mathcal{W}\right) \xi + N_s/2$$

Group property $e^{i\phi_n \xi^\dagger (\mathcal{W}^\dagger \mathcal{N} \mathcal{W}) \xi} e^{-\beta \xi^\dagger \mathcal{E} \xi} = e^{\xi^\dagger C(\beta,\phi_n) \xi}$ $\quad e^{C(\beta,\phi_n)} = e^{i\phi_n \mathcal{W}^\dagger \mathcal{N} \mathcal{W}} e^{-\beta \mathcal{E}}$

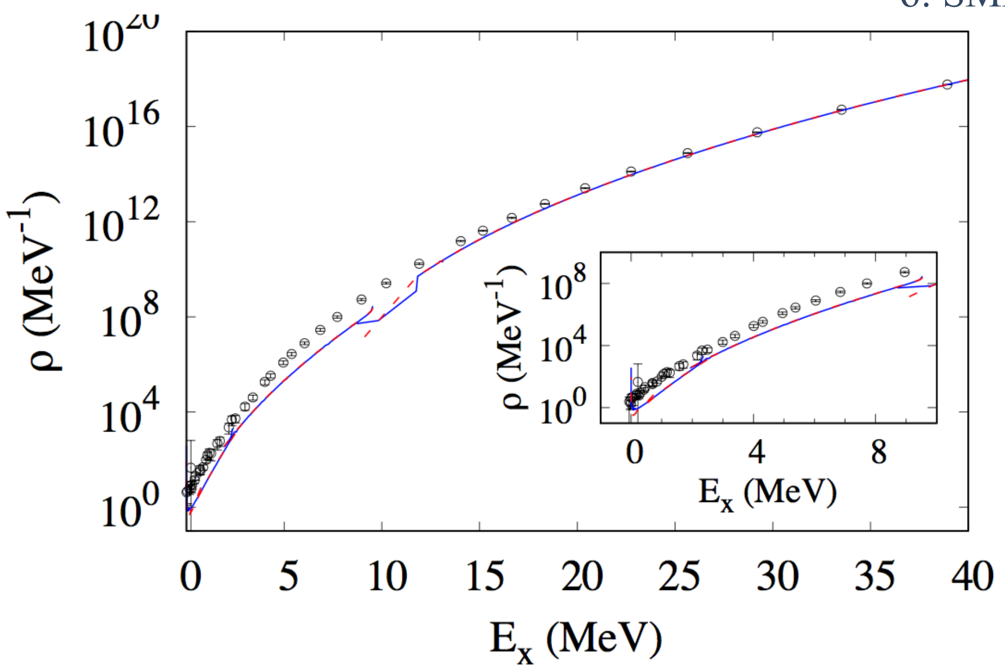
$$\Rightarrow \boxed{\mathrm{Tr}\left[e^{i\phi_n \hat{N}} e^{-\beta(\hat{H}_{HFB} - \mu \hat{N})}\right] \propto (-)^n \det\left(1 + \mathcal{W}^\dagger e^{i\phi_n \mathcal{N}} \mathcal{W} e^{-\beta \mathcal{E}}\right)}$$

^{150}Sm: transitional nucleus, deformed in the ground state



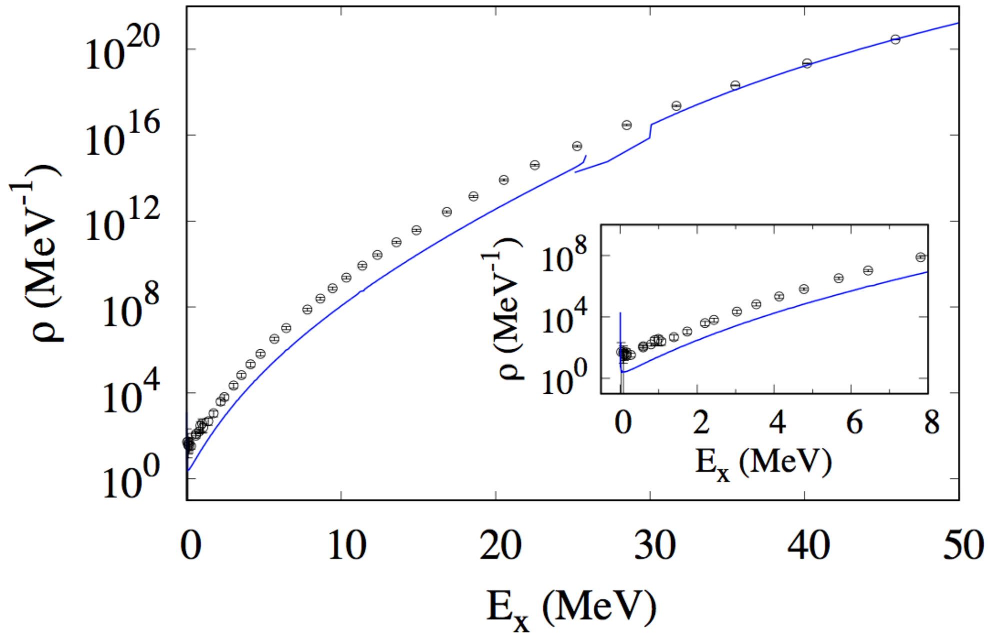


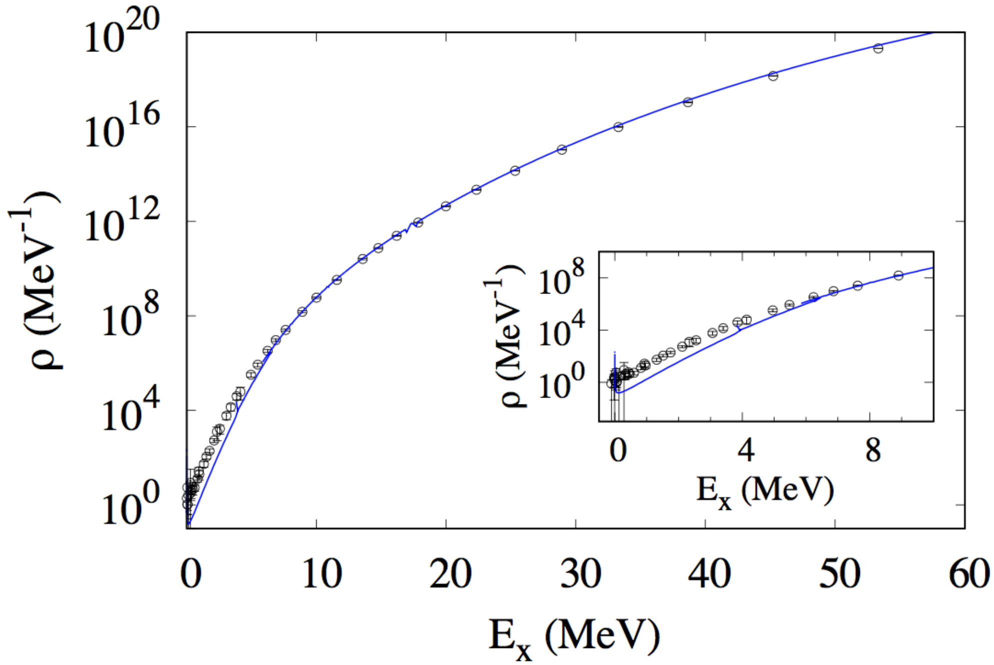
: PNP
: DG
o: SMMC



- Reduction of mean-field state density in deformed phase because mean-field theory describes only the intrinsic states, not rotational bands.
- Unphysical negative mean-field entropy at low temperatures due to violation of particle-number conservation in HFB.

Finite-temperature HF and BCS: ^{162}Dy and ^{148}Sm





——: PNP

o: Open circles: SMMC

^{162}Dy: strong deformation, weak pairing, HF. See even more clearly enhancement in SMMC due to inclusion of rotational bands.

^{148}Sm: spherical, BCS. Unphysical reduction of mean-field entropy causes reduction of mean-field state density in pairing phase.

Low-temperature limit of the HFB

- Why does the mean-field approximate canonical entropy become negative below the pairing phase transition?
- At sufficiently low temperatures, the system is in the HFB ground state, which does not conserve particle number.

$$|\Phi\rangle = \sum_{N'} \alpha_{N'} |\psi_{N'}\rangle \qquad\qquad |\alpha_{N'}|^2 < 1$$

$$\Rightarrow S_c = \beta E_0 - \ln Z_c = \ln[|\alpha_N|^2] < 0$$

- Can extend this logic to higher temperatures in the pairing phase.
- This is a fundamental limitation on symmetry restoration projection after variation in finite-temperature mean-field theory.

Projection in general HFB using pfaffians

Robledo, PRC (2009). Bertsch and Robledo, PRL (2012). Fanto, in preparation.

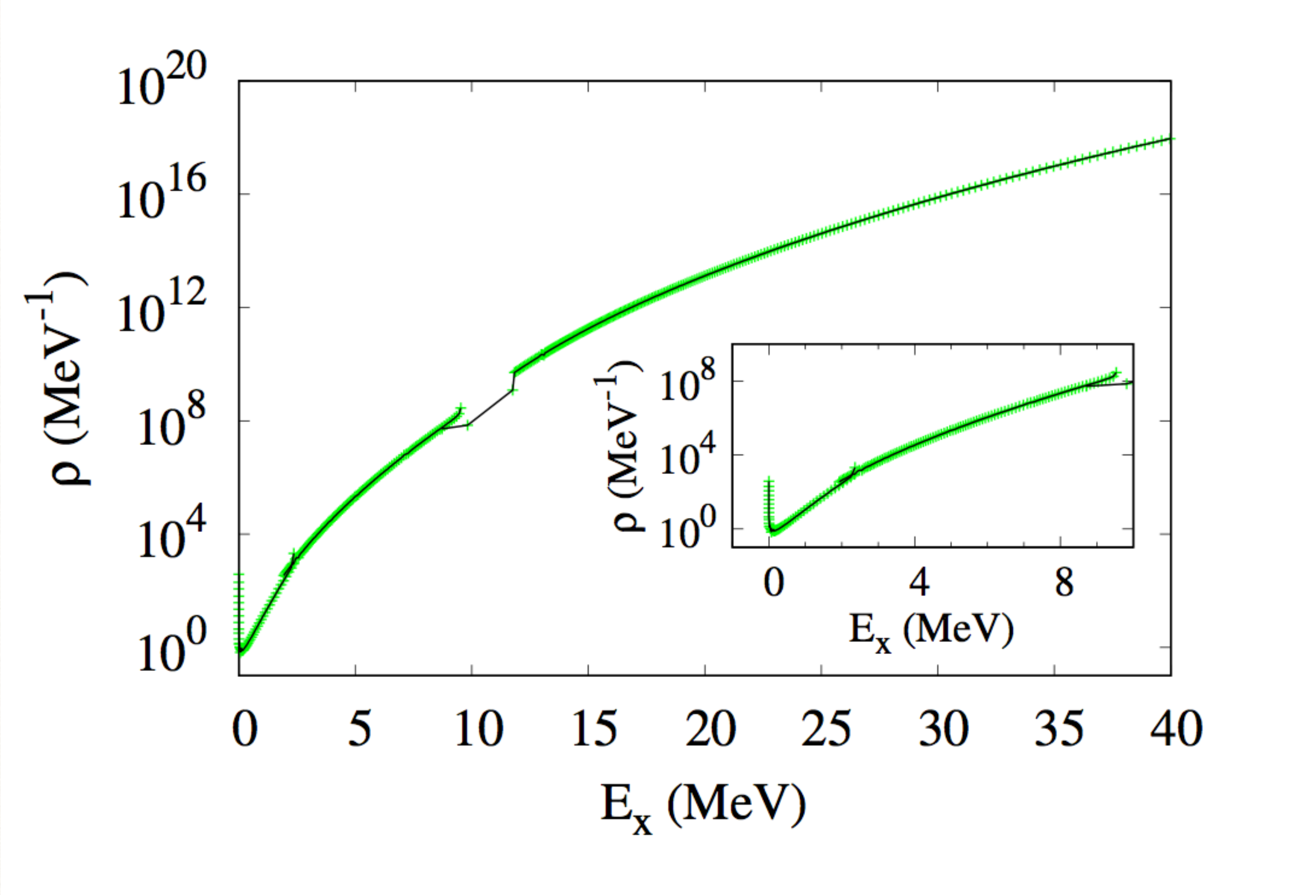
- Consider cases in which the HFB Hamiltonian breaks time-reversal symmetry, e.g., for odd nuclei and triaxial nuclei.
- The general symmetry projection formula involves an undetermined phase in traces in Fourier sum. This phase problem can be circumvented by a new formula involving the pfaffian: the square root of a determinant of a skew-symmetric matrix with a well-defined phase.
- This new formula allows symmetry restoration projection after variation for any HFB Hamiltonian.
- Highlights of the formula: $T = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} = W^\dagger e^{i\phi_n \mathcal{N}} W e^{-\beta\mathcal{E}}$ $\quad W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$

full Bogoliubov transformation, $2N_s$ dimensional

$$\mathrm{Tr}\left[e^{i\phi_n \hat{N}} e^{-\beta(\hat{H}_{HFB} - \mu\hat{N})}\right] \propto (\det T_{22})^{-\frac{1}{2}} \mathrm{pf}\begin{pmatrix} T_{12}T_{22}^{-1} & -(1+T_{22}^T) \\ 1+T_{22} & T_{21}T_{22}^T \end{pmatrix}$$

$$(\det T_{22})^{\frac{1}{2}} \propto \langle\Phi| e^{i\phi_n \hat{N}} |\Phi\rangle \propto \frac{1}{\langle\Phi|\Phi\rangle} \mathrm{pf}\begin{pmatrix} V^T U & e^{i\phi_n} V^T V^* \\ -e^{i\phi_n} V^\dagger V & U^\dagger V^* \end{pmatrix}$$

Validating the pfaffian method: particle-number projection in ^{150}Sm
Preliminary



———: pfaffian PNP
+: time-reversal PNP

- Work in progress: application to a model with broken time-reversal symmetry in the HFB.

Conclusions

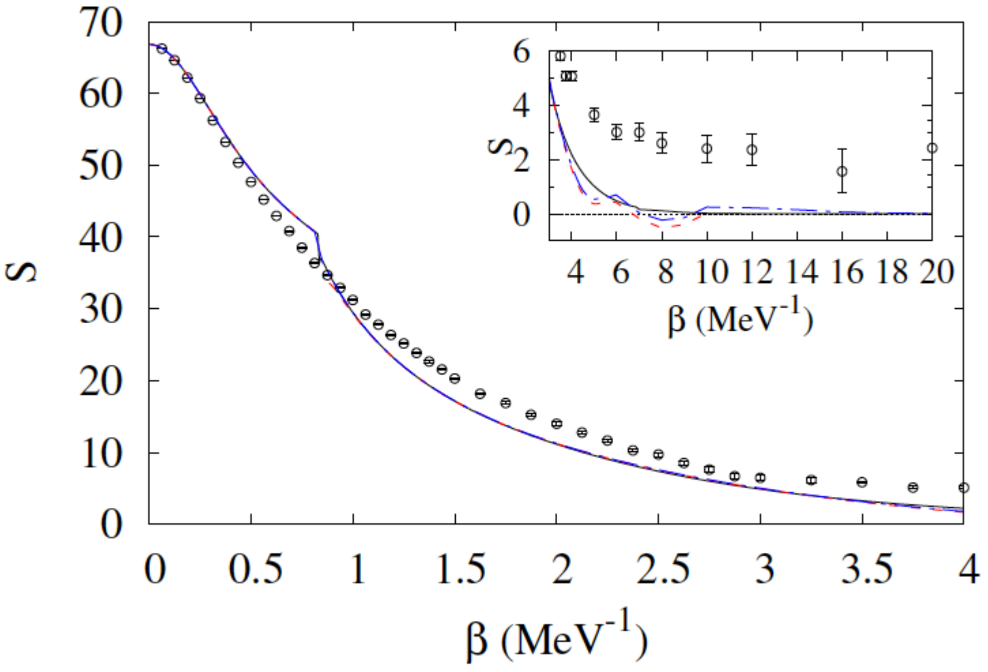
- The finite-temperature mean-field approximation works well for the calculation of level densities at excitation energies above the shape or pairing transitions.
- At energies below the shape transition, the mean-field state density is reduced due to the lack of rotational bands.
- At energies below the pairing transition in the HFB, the mean-field density is further reduced because of the inherent violation of particle-number conservation in the grand-canonical ensemble.
- We introduce a particle-number projection formula in the finite-temperature HFB approximation with time-reversal symmetry without a destructive phase ambiguity.
- We introduce and validate a formula for symmetry restoration projection for the most general HFB Hamiltonian without a destructive phase ambiguity.

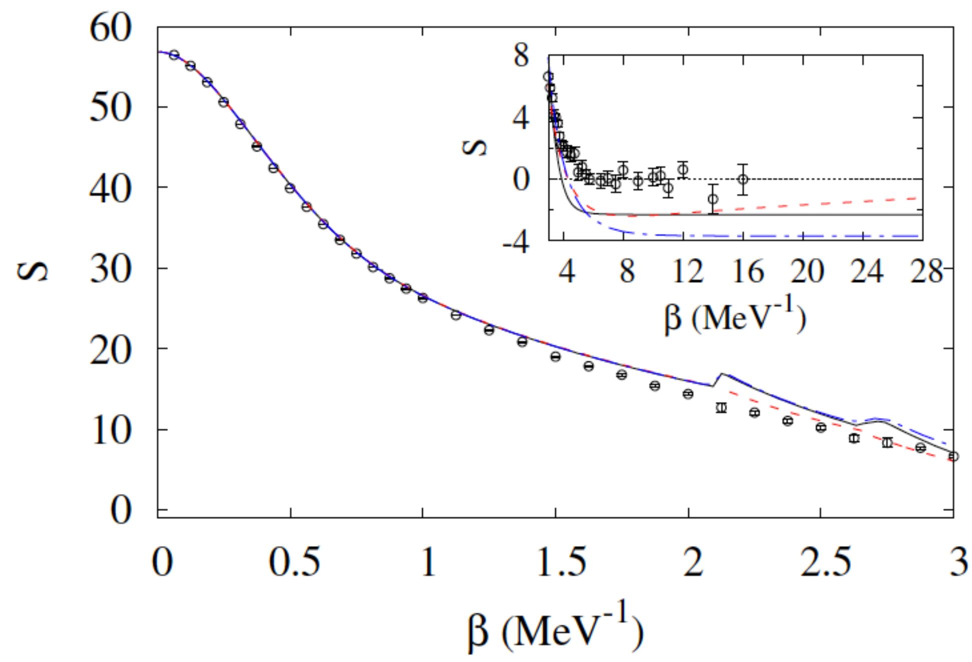
Outlook

- Develop variation after projection methods to avoid negative entropies at low temperatures.
- Spin dependence of level density in finite-temperature mean-field theory.

Finite-temperature HF and BCS: ^{162}Dy and ^{148}Sm

———: PNP
- - -: Red dashed: DG1
-.-.-:Blue dashed-dotted: DG2
o :Open circles: SMMC





^{162}Dy: strong deformation, weak pairing.

Rossignoli and Ring, (1993)

^{148}Sm: spherical, BCS

Esebbag and Egido, Nucl. Phys. A (1993).
H. Flocard, Les Houches LXXIII (2001)

DG1 and DG2 refer to different ways of calculating $\left.\frac{\partial N}{\partial \alpha}\right|_{ij}$

DG1: calculate derivatives numerically. DG2: $\left.\frac{\partial N}{\partial \alpha}\right|_{ij} \approx \left\langle (\Delta N_i)^2 \right\rangle \delta_{ij}$

- State density vs. level density: state density counts 2J+1 degenerate states for ea

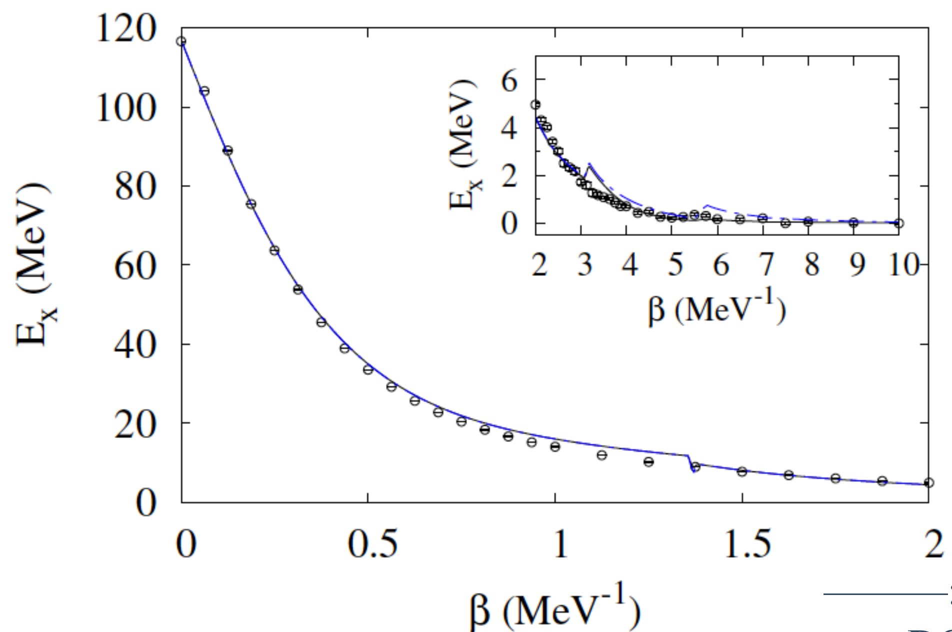
level density $\tilde{\rho}(E) = \begin{cases} \rho_{M=0}(E) \text{ even-mass nuclei} \\ \rho_{M=1/2}(E) \text{ odd-mass nuclei} \end{cases}$ ρ(E) = state density

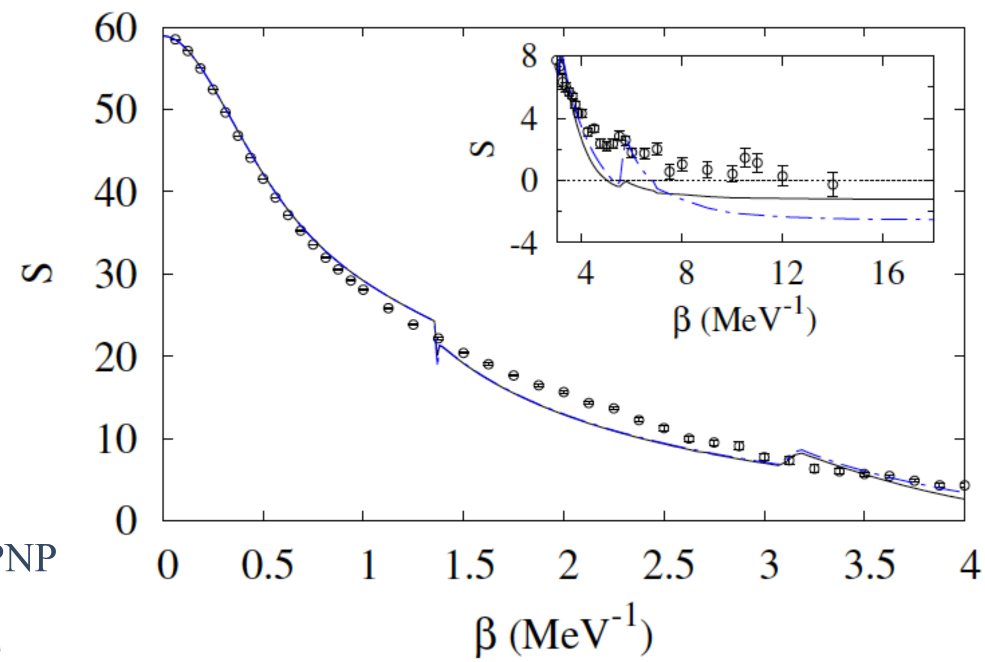
$$\mathcal{E} = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$$

$$\mathcal{N} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

particle operators

^{150}Sm: transitional nucleus deformed in the ground state





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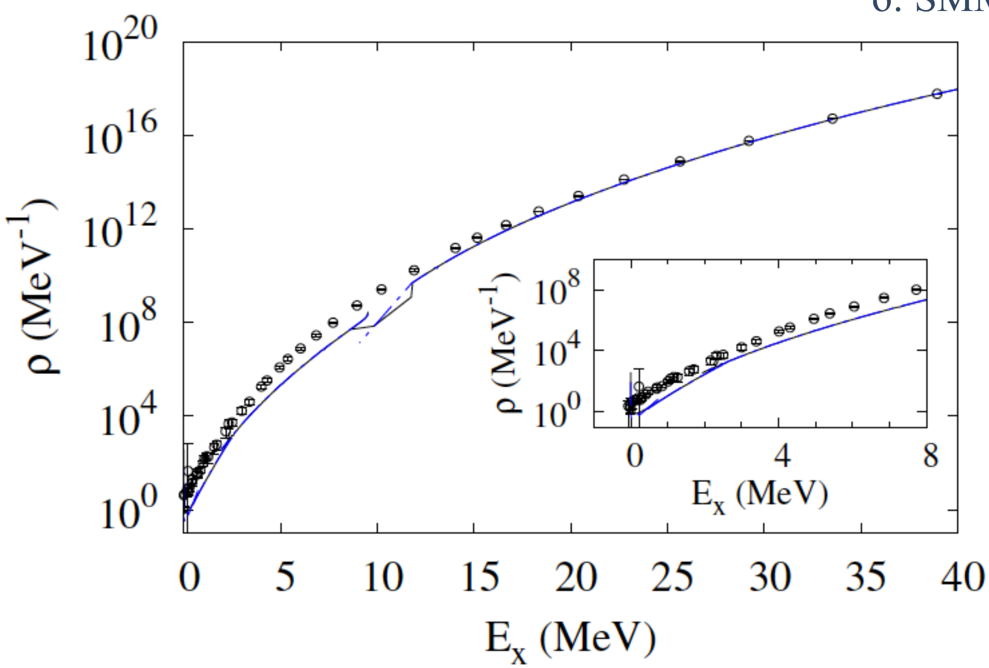

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