Benchmarking the Hartree-Fock and Hartree-Fock-Bogoliubov approximations to level densities

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Motivation

--need to know structure of the levels to model dynamic processes; HF and HFB give better windows on the structure than other methods.

--computational considerations favor finite-temperature HF and HFB for systematic surveys.

--breaking and restoring symmetries is a universal problem of mean-field theory

Outline of the talk

1. Thermodynamic consistency
2. The SMMC benchmark nuclei: Dy162 (deformed) and Sm148 (spherical)
3. Canonical vs grand canonical ensembles
4. HF performance in Dy162
5. HFB performance in Sm148

Thermodynamic Consistency

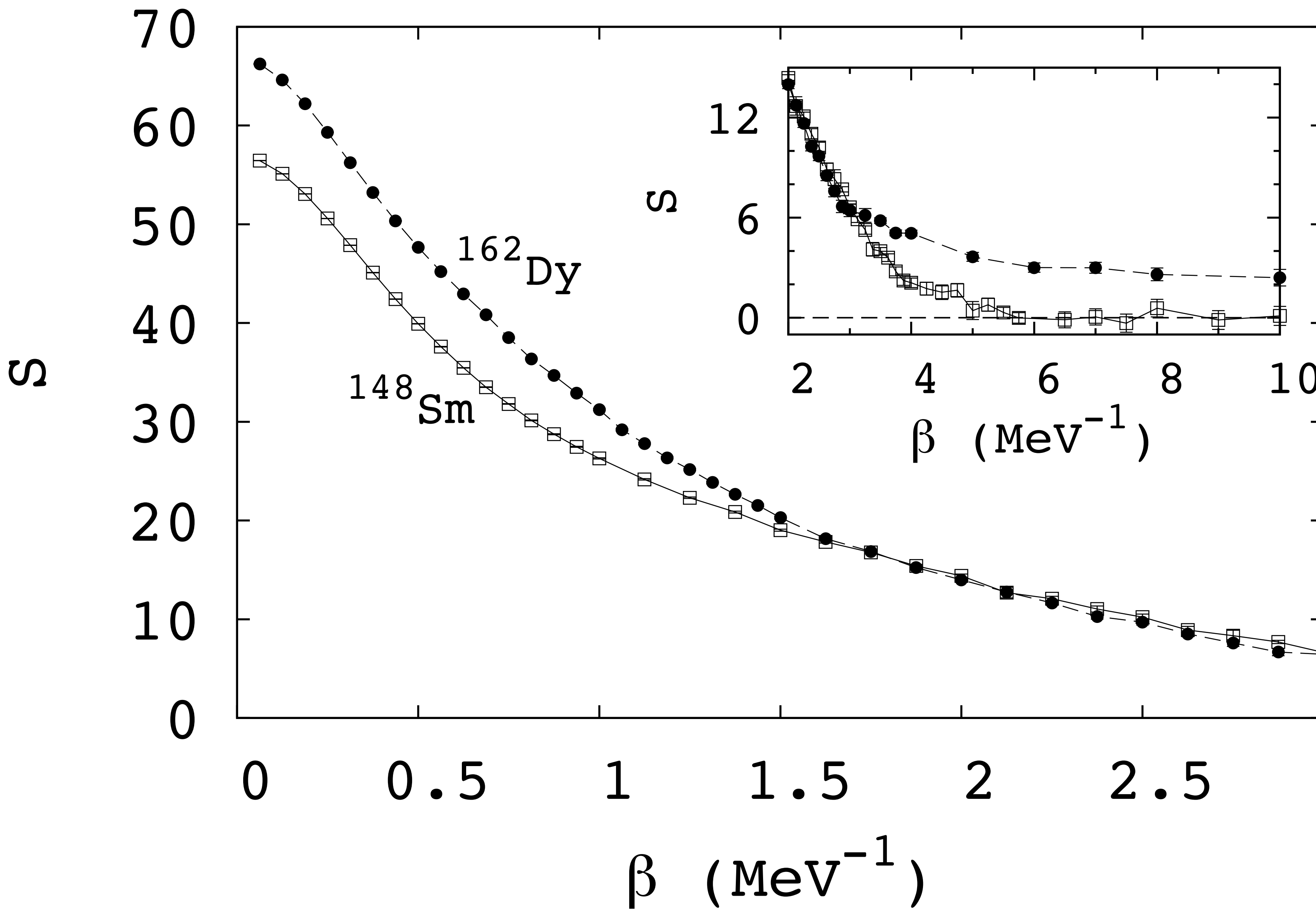
$$dS = \beta dE$$

A sum rule for the canonical entropy:

$$\int_0^{E(\infty)} \beta dE = \ln \binom{\Omega_p}{N_p} + \ln \binom{\Omega_n}{N_n}$$

Useful as a computational check

Entropy functions in SMMC



Resonance spacing at neutron threshold

Nucleus	E (MeV)	J^π	D (eV)			
			SMMC	HF	HFB	Exp.
^{148}Sm	8.1	$(3^-, 4^-)$	3.8 ± 0.6		4.7	5.7
^{162}Dy	8.2	$(2^+, 3^+)$	2.3 ± 0.3	0.67		2.4

From grand canonical to canonical

$$S_c(\beta, N_0) \approx S_{gc}(\beta, \alpha_0) - \ln \zeta(\beta, N_0) + \beta \frac{\partial \ln \zeta}{\partial \beta}$$

where ζ^{-1} is the probability of N_0 particles in the ensemble.

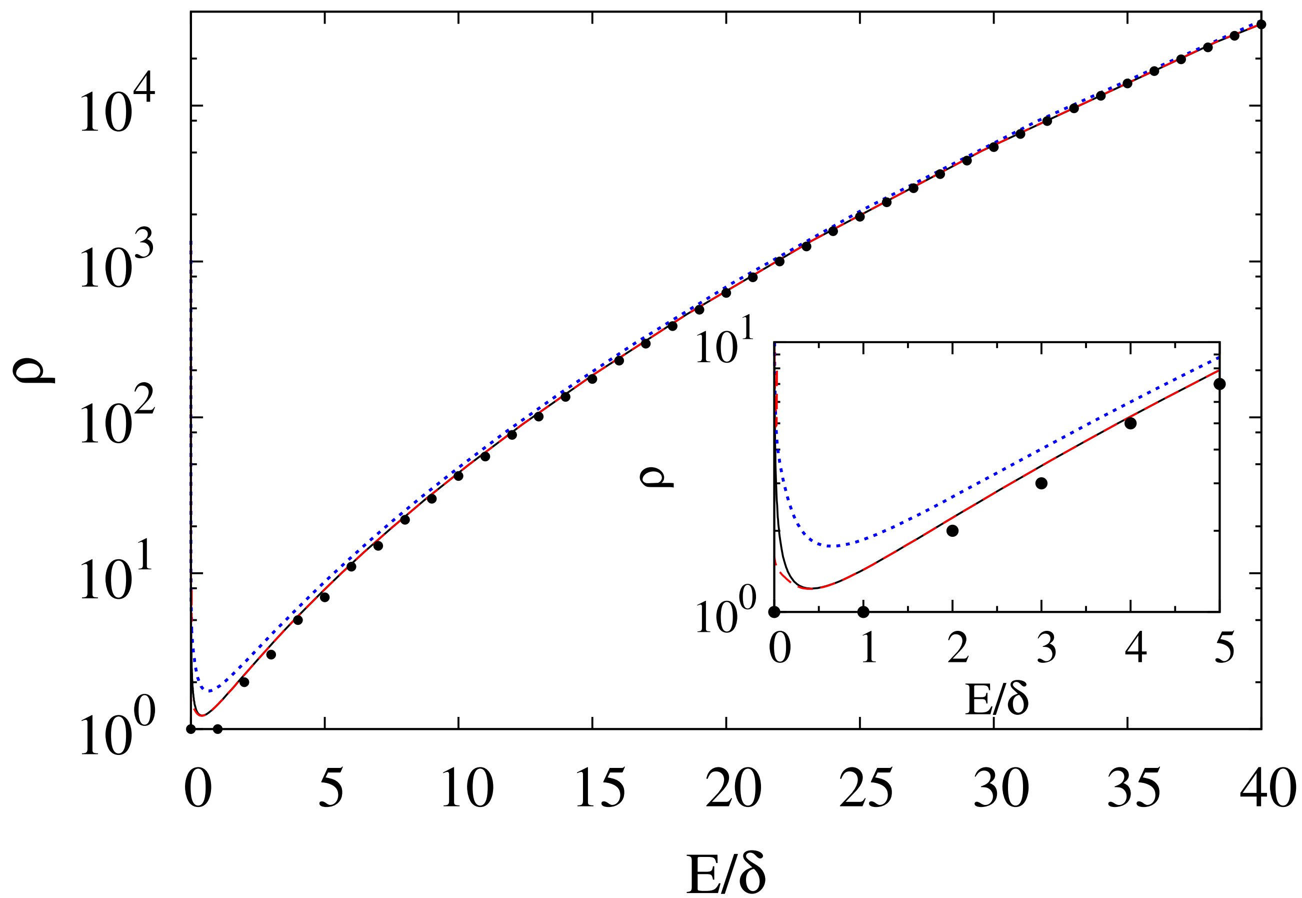
We have tested 3 approximations for ζ^{-1}

State density

$$\rho_s(E) \approx \left(-2\pi \frac{dE_c}{d\beta}\right)^{-1/2} \exp\left(S_c(\beta_c(E))\right)$$

A simple model to verify saddle-point approximation and reduction to canonical entropy.

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



Conclusions:

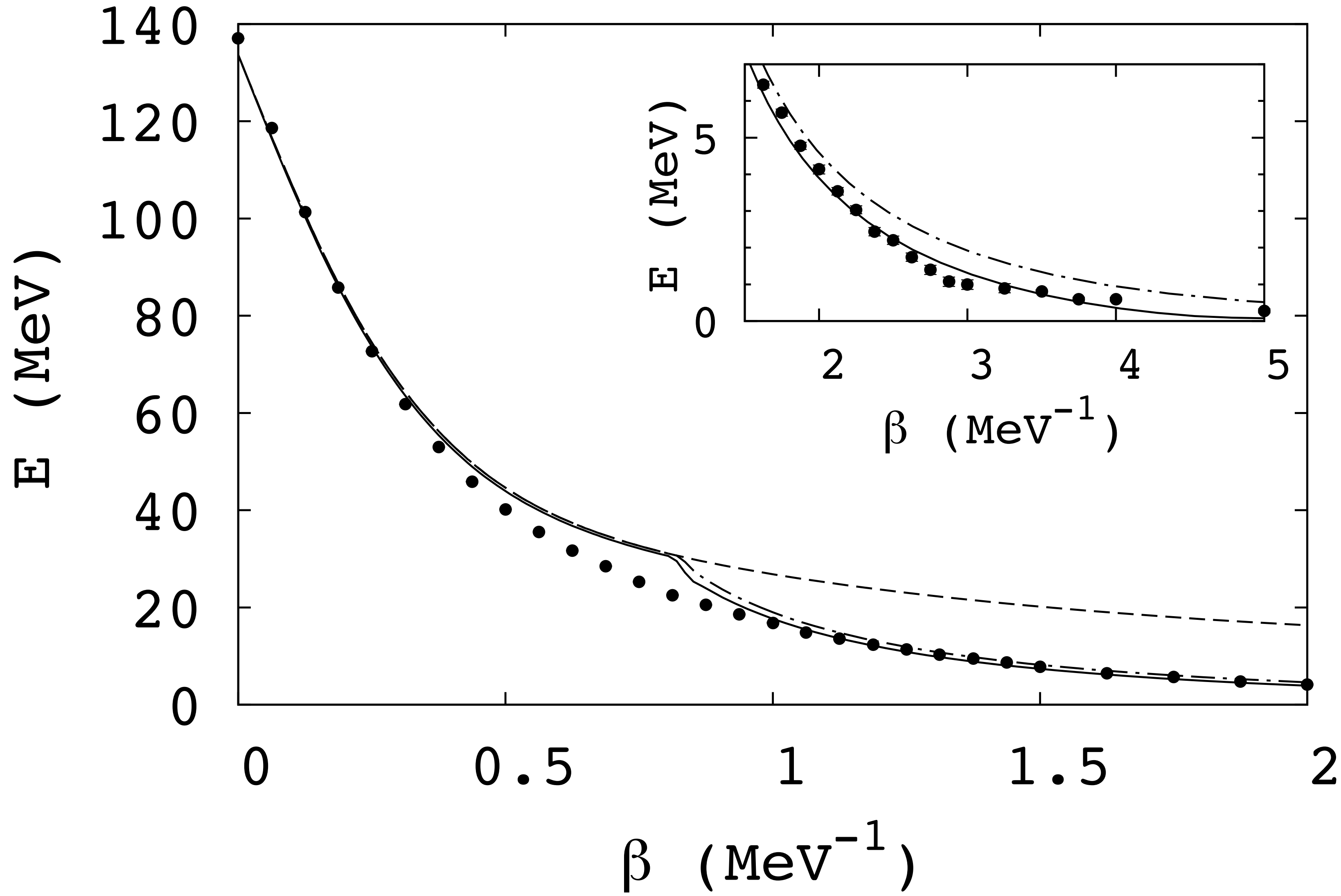
--canonical saddle-point state density is amazingly accurate;

--similar accuracy can be extracted from grand canonical in this model.

Preliminaries: Performance of HF and HFB at zero and infinite temperature

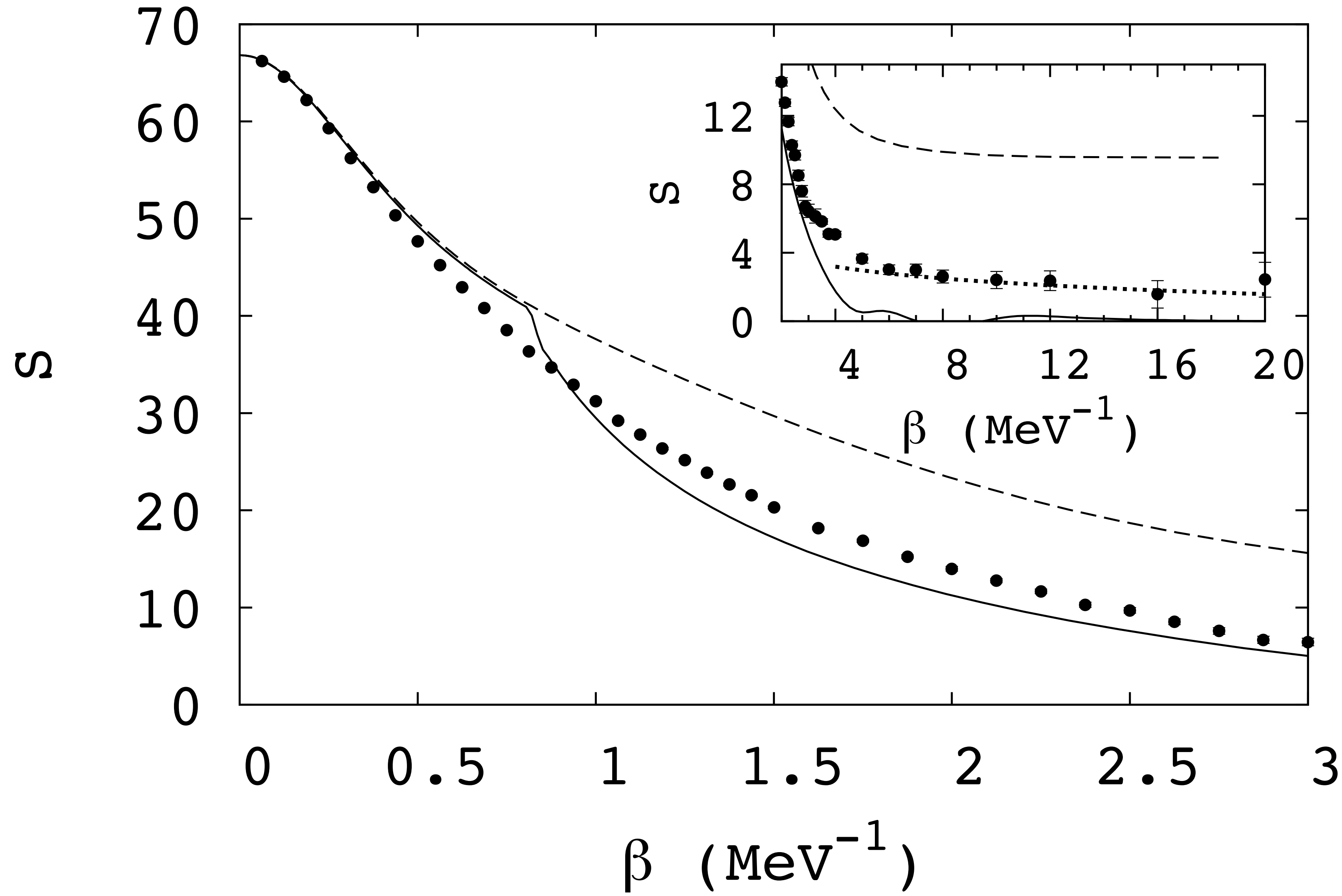
nucleus	β	SMMC	HF	HFB	correlation energy: condensation	correlation energy: other
		Units are MeV				
^{148}Sm	0	-119.16	-119.1	-119.1		
	∞	-235.65 ± 0.015	-230.83	-232.51	1.68	3.14
^{162}Dy	0	-238.35	-238.39	-238.39		
	∞	-375.39 ± 0.02	-371.78	-371.91	11.41	3.48

HF thermal energy --Dy-162



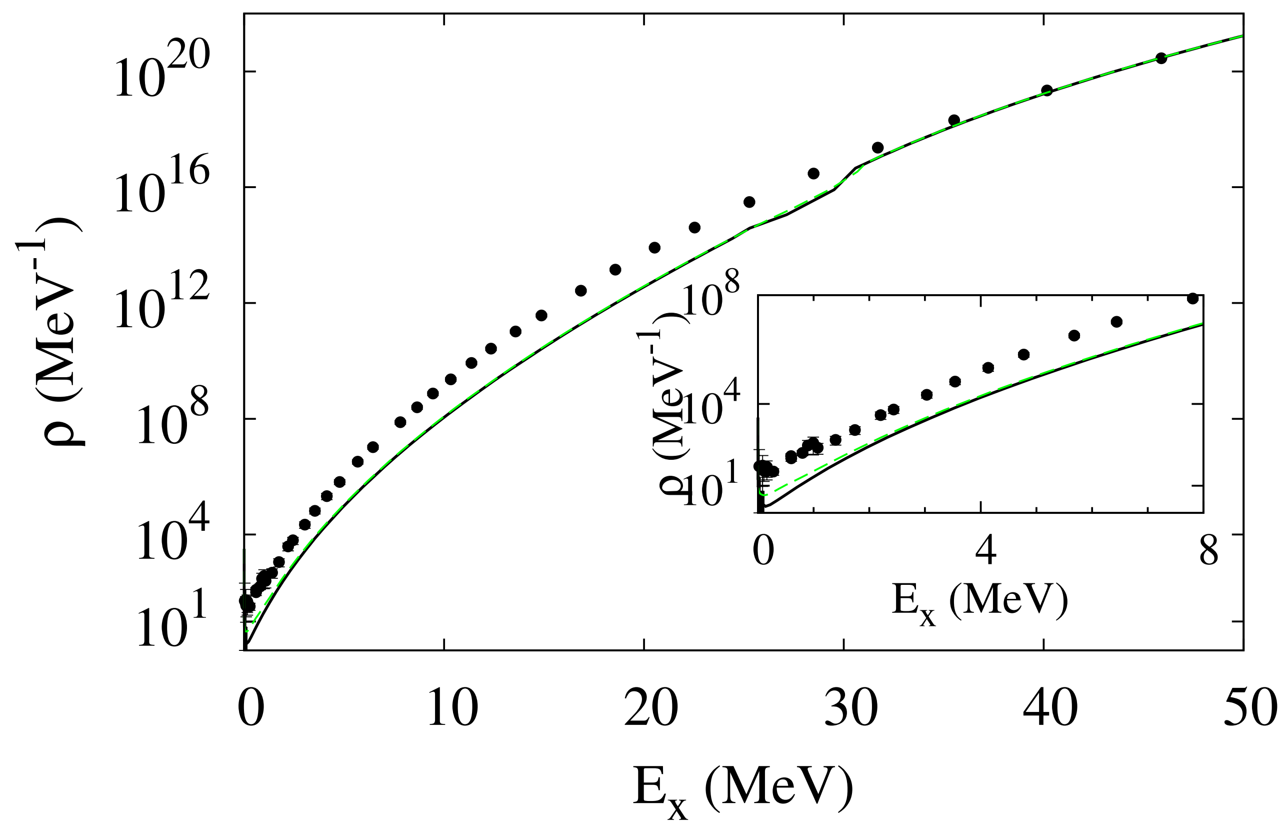
Sharp HF phase transition is completely smoothed out.

HF Entropy -- Dy162



Dashed line: HF sph.
Solid line: HF def.
Circles: SMMC
Dotted line: g.s. rotational band correction

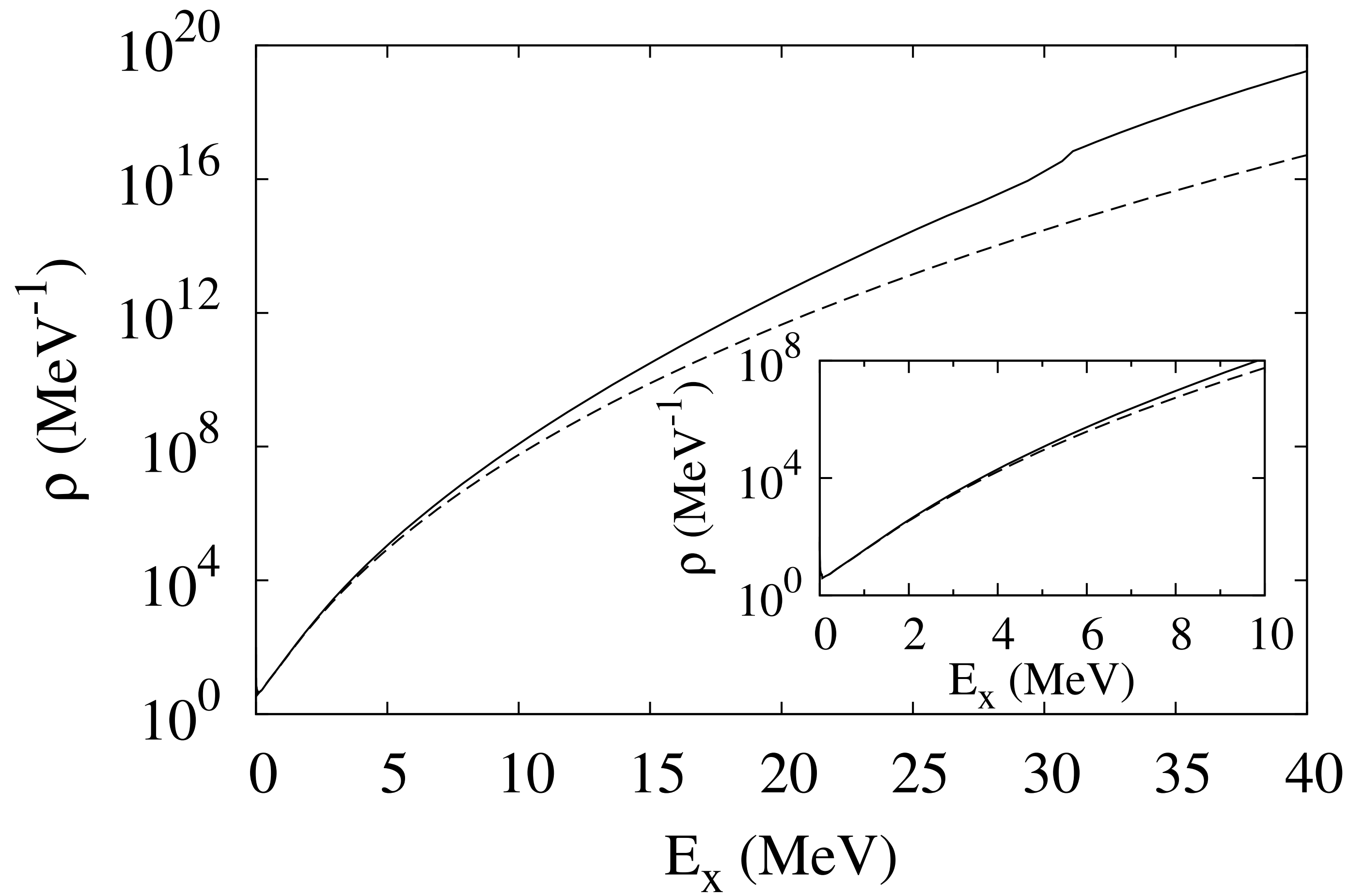
HF state density -- Dy-162



Factor of 10 too low without rotational band correction.

Performance of independent-particle model -- Dy-162

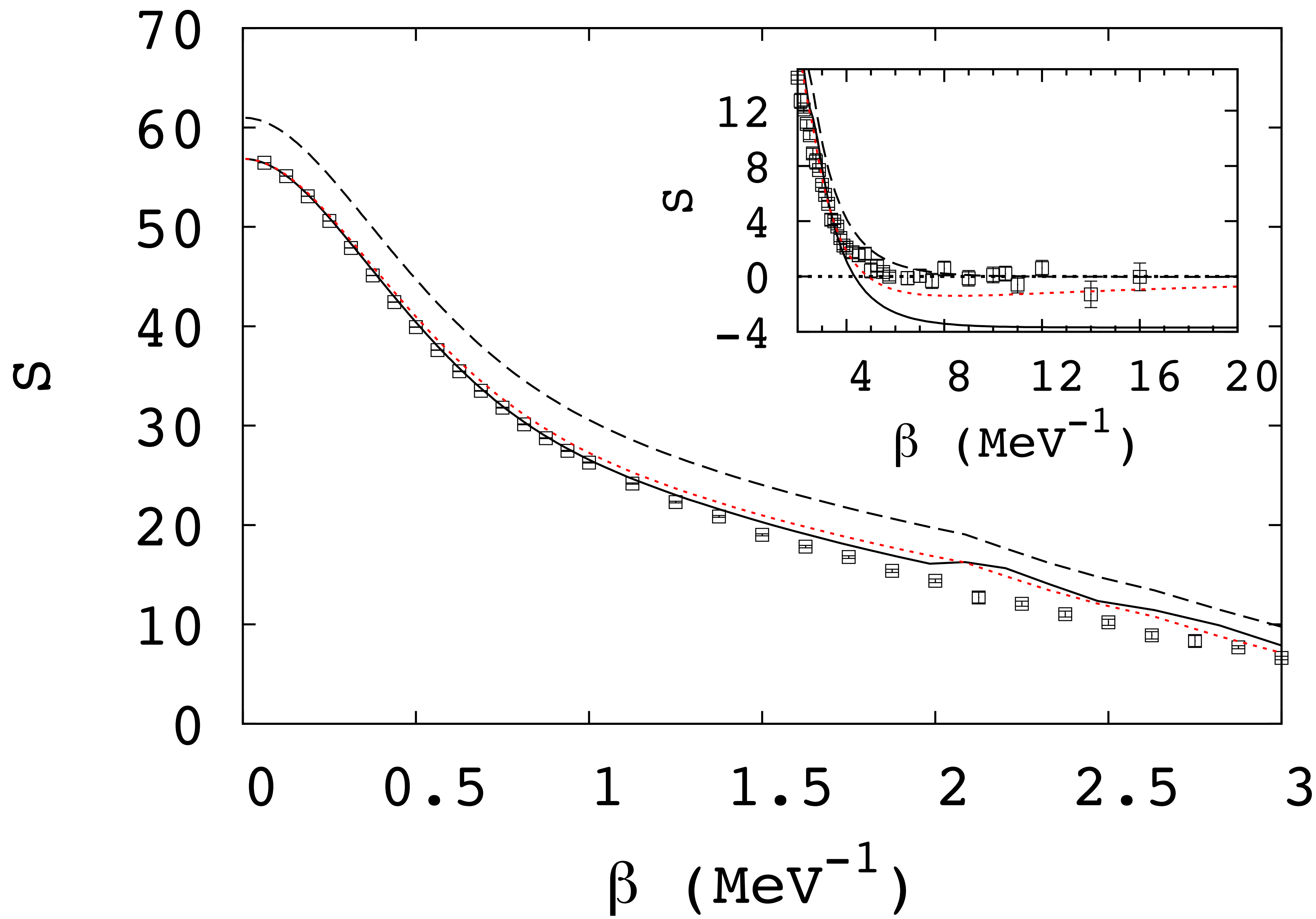
Excitations are independent particle and holes in the HF ground-state single-particle potential.



Works well up to neutron resonance energy; error less than a factor of 2 at 8 MeV.

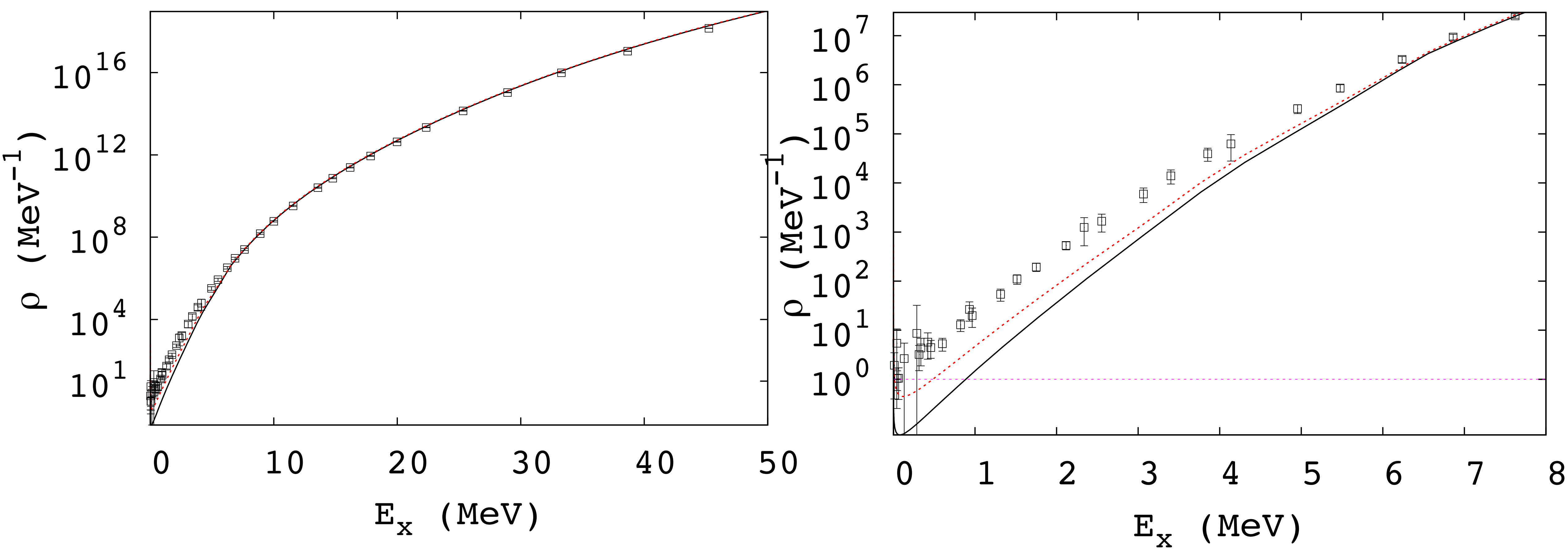
Sign of error is easy to understand: $\frac{1}{2} v \rho^2$

HFB entropy -- Sm-148



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 ~ 1-4 MeV

Final Comments

1. Number projection for HFB is not trivial, but may be doable. E.g. Uhrenholt, Aberg, et al., Nucl. Phys. A 913 127 (2013).

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?

Three possibilities for zeta

$$\zeta \approx [2\pi\langle(\Delta N)^2\rangle]^{1/2}$$

Gaussian distribution of N

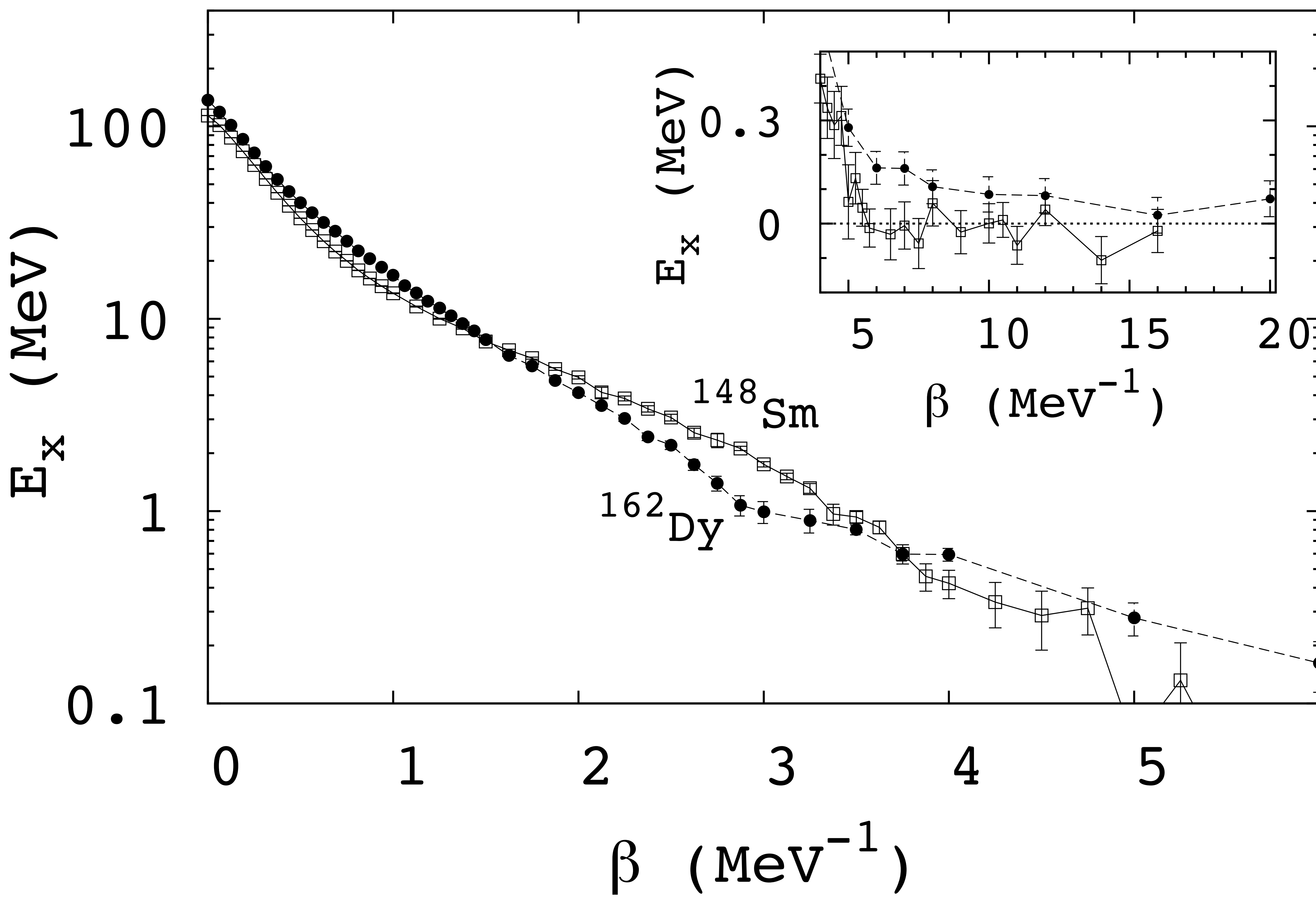
$$\zeta \approx \left[2\pi \frac{\partial N}{\partial \alpha}\right]^{1/2}$$

multidimensional saddle-point

$$\zeta \approx \sum_N e^{-(N-N_0)^2/2\langle(\Delta N)^2\rangle}$$

discrete Gaussian

Thermal energy in SMMC -- Dy-162 and Sm-148



Angular momentum in Dy-162 ensemble

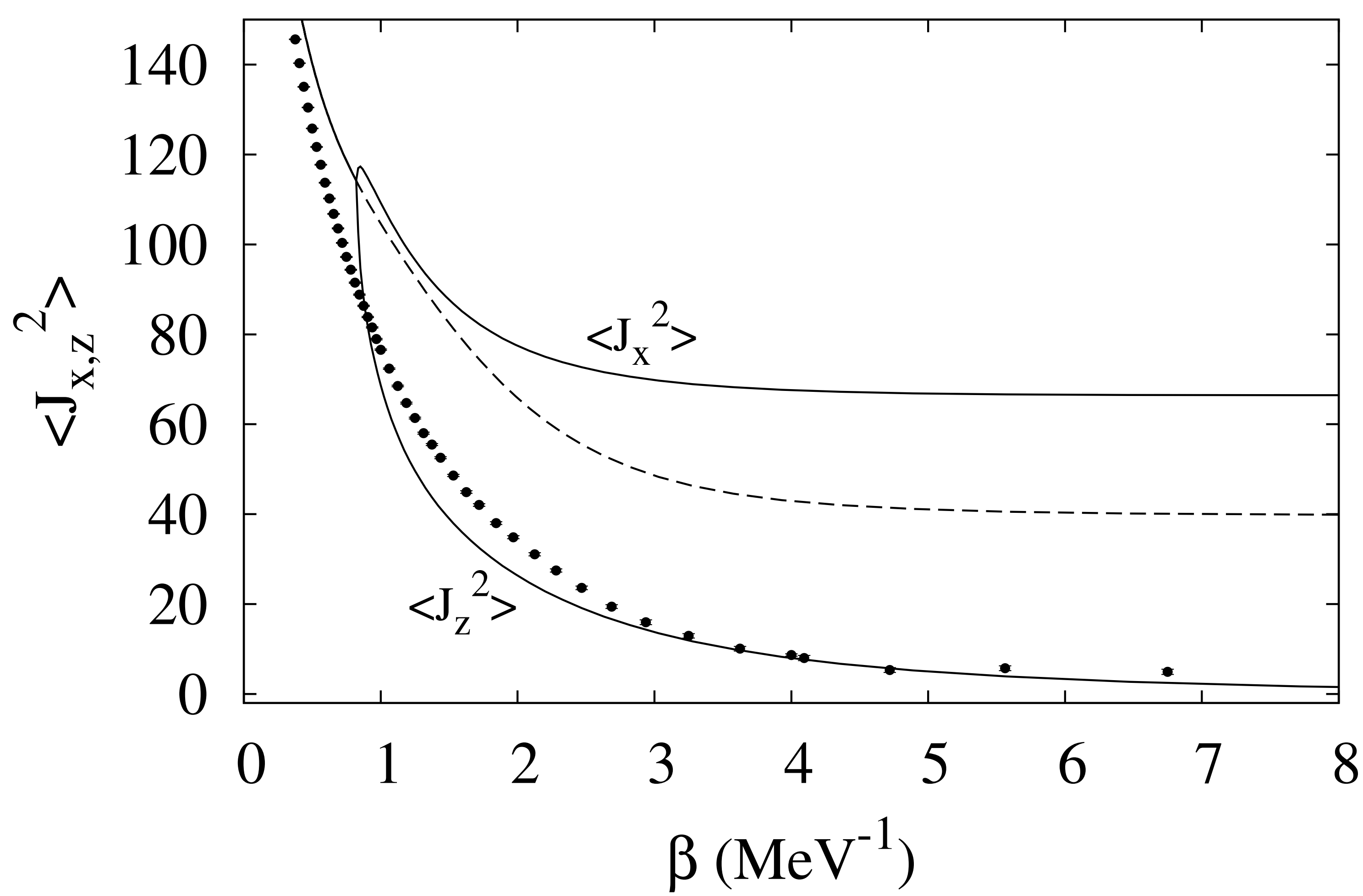


FIG. 9: Second moments of the angular momentum in ^{162}Dy. The solid lines are the HF results and exhibit a kink at the shape transition point. The dashed line describes the spherical HF solution for temperatures where the lowest equilibrium solution is deformed. These HF moments may be compared with the SMMC moments shown by solid circles. The SMMC moments satisfy $\langle J^2_{x,y}\rangle = \langle J^2_z\rangle = \langle \vec{J}^2\rangle/3$.