Shell model
Fermi Gas calculations
of Nuclear Leve Densities

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(with codes by I. Stetcu, LSU/UW and J. Staker, SDSU)

supported by US Dept of Energy

The nuclear LEVEL DENSITY (or STATE DENSITY*):
an important input into statistical neutron capture
(e.g. Hauser-Feshbach theory)

* State density: count all M_J states (2J+1 degeneracy)
  Level density: do not include 2J+1 degeneracy
In fact I will be mostly talking about the *state density*

The Strategy

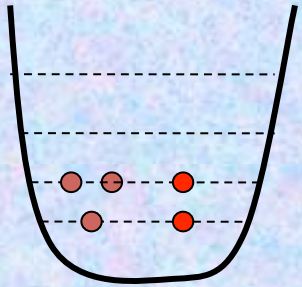
I'm going to compare "exact" numerical results (from full shell-model diagonalization) against approximation schemes

So I have two theoretical tools:
full shell-model diagonalization
and
Hartree-Fock / mean-field

The key idea is to use **the exact same input for both**

The "Full" interacting shell model

What an interacting shell-model code does:



Input into shell model:

- set of *single-particle states* ($1s_{1/2}$,$0d_{5/2}$, $0f_{7/2}$ etc)
- *many-body configurations* constructed from s.p. states: $(f_{7/2})^8$, $(f_{7/2})^6(p_{3/2})^2$, etc.
- *two-body matrix elements* to determine Hamiltonian between many-body states: $<(f_{7/2})^2$ J=2, T=0| V| $(f_{5/2}\ p_{3/2})$ J=2, T=0> (assume someone else has already done the integrals)

Output: eigenenergies and wavefunctions
(vectors in basis of many-body Slater determinants)

The "Full" interacting shell model

What an interacting shell-model code does:

Input into shell model:

"*sd*"-shell: Inert ^{16}O core; valence space $0d_{5/2} - 1s_{1/2} - 0d_{3/2}$
-- 12 single-particle states

"*pf*"-shell: Inert ^{40}Ca core; valence space $0f_{7/2} - 1p_{3/2} - 0f_{5/2} - 1p_{1/2}$
-- 20 single-particle states

"*p-sd*$_{5/2}$"-shell: Inert ^{4}He core; valence space $0p_{3/2} - 0p_{1/2} - 0d_{5/2} - 1s_{1/2}$
-- 18 single-particle states

Basis states: Slater determinants in occupation space:

$0d_{5/2,-5/2}$	0
$0d_{5/2,-3/2}$	1
$0d_{5/2,-1/2}$	1
$0d_{5/2,+1/2}$	0
$0d_{5/2,+3/2}$	1
$0d_{5/2,+5/2}$	0

In *sd* shell: half-filled (^{28}Si) 93,000 states
In *pf* shell: half-filled (^{60}Zn) 2 billion states

The "Full" interacting shell model

What an interacting shell-model code does:

Input into shell model:

• *two-body matrix elements* to determine Hamiltonian between many-body states:
$\langle (f_{7/2})^2\ J=2,\ T=0|\ V|\ (f_{5/2}\ p_{3/2})\ J=2,\ T=0\rangle$
(assume someone else has already done the integrals)

These matrix elements generally start from a "realistic" two-body interaction, renormalized via G-matrix or Lee-Suzuki or SRG or...

Often phenomenological tweaks added to improve agreement in medium-mass nuclei

Interactions are intrinsically nonlocal, no restriction on form; 3-body possible (but challenging).

The "Full" interacting shell model

What an interacting shell-model code does:

The shell-model code BIGSTICK (successor to REDSTICK)
-M-scheme code (basis states have good M not good $\mathcal{J}$)
-Uses factorization of Hamiltonian to reduce memory storage
-Can handle 100 million basis states on a single processor
-Parallelized with MPI and OpenMP
-Three-body interactions being added (revision of algorithm)
- Uses Lanczos algorithm to get low-lying states

-Flexible; applied to electronic structure of atoms (M.Schuster, MS project)

Computing the Partition Function

Who's going to count all those states?

I'll use the full shell-model calculation to provide an "exact" result and compare against various approximations

Computing the Partition Function

The "thermodynamic method" centers around the *partition function*

$$Z(\beta) = \int_0^\infty dE \cdot e^{-\beta E} \rho(E)$$

(1) Construct the partition function
either from single-particle density of states
or from Monte Carlo evaluation of a path integral (Alhassid)

(2) Invert the Laplace transform through the saddle-point approximation

$$\rho(E) = \frac{1}{2\pi} \int_{-i\infty}^{i\infty} d\beta \cdot e^{\beta E} Z(\beta)$$

approximate integrand by a Gaussian

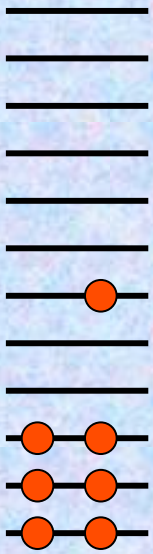
$$\rho(E) \cong \frac{Z(\beta_0) e^{\beta_0 E}}{\sqrt{2\pi D}}, E = -\frac{\partial \ln Z(\beta_0)}{\partial \beta}, D = \frac{\partial^2 \ln Z(\beta_0)}{\partial^2 \beta}$$

the "saddle-point condition" fixes
the value of β_0 for a given energy *E*

Computing the Partition Function

Start with (equally-spaced) single-particle levels and fill them like a Fermi gas (Bethe, 1936):

$$\rho_{BBFG}(E) = \frac{\sqrt{2\pi}}{12} \frac{\exp\sqrt{4a(E-\Delta)}}{(4a)^{1/4}(E-\Delta)^{5/4}}$$



Some modern version use "realistic" single-particle levels derived from Hartree-Fock (Goriely, Hilaire et al)

The single-particle levels arise from a mean field!

The parameter *a* reflects the density of *single-particle* states near the Fermi surface

Computing the Partition Function

Unfortunately, most of the Fermi-gas derived calculations need corrections to account for collectivity (vibrational and rotational motion)

These corrections are phenomenological, that is, *not* derived from an underlying Hamiltonian

The "combinatoric" level density appears to suffer from this same problem

My goal: to compute the single-particle energies *and* the collective corrections consistently from the same interaction

The "Full" interacting shell model

We also have a Hartree-Fock + RPA code
and (*new!*) a projected HF code

Code SHERPA (SHEll-model RPA) by CWJ + Ionel Stetcu

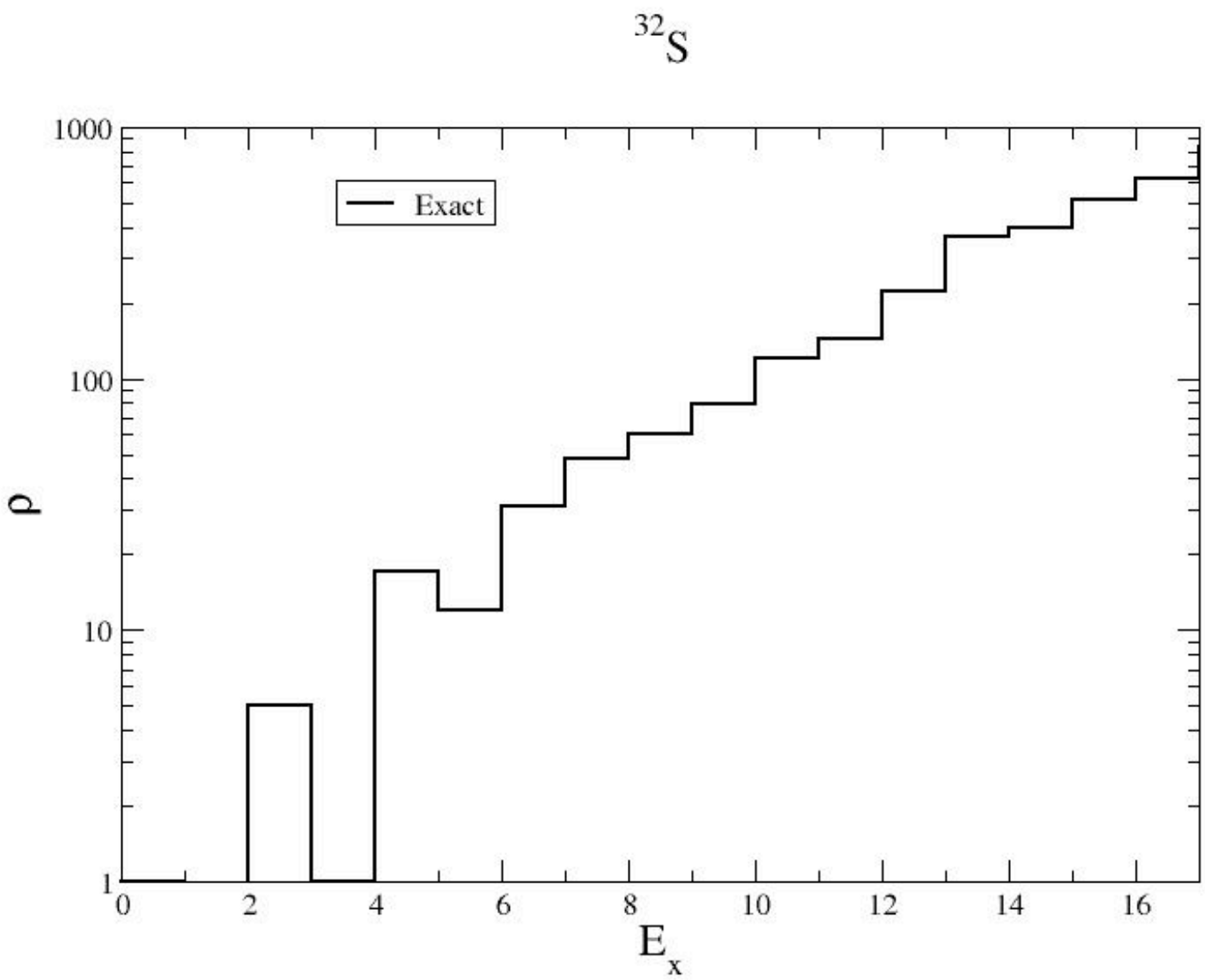
Uses *exactly* the same input as BIGSTICK code.

Does general Hartree-Fock by minimizing energy of a
Slater determinant in occupation space (e.g., *sd*, *pf* etc.)
--only restriction is assuming real wavefunctions (a problem when cranking)

From this we can get HF single-particle energies, can crank to get
moment of inertia, etc.

**Recent development (by Joshua Staker, SDSU PhD student):
Projected Hartree Fock allows us to precisely dissect
the intrinsic state.**

Mean-field Level densities



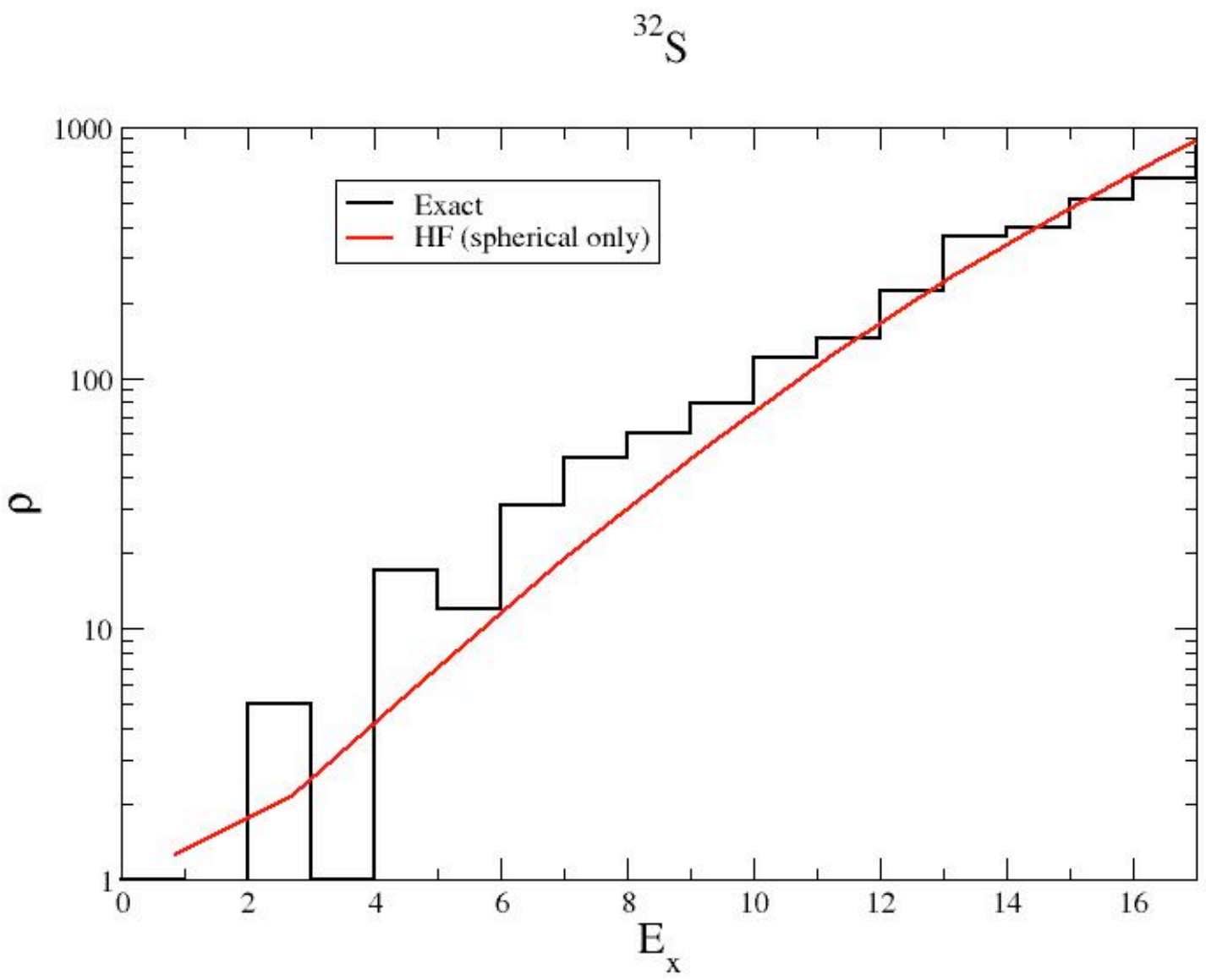
Mean-field Level densities

Now compute approximate partition function

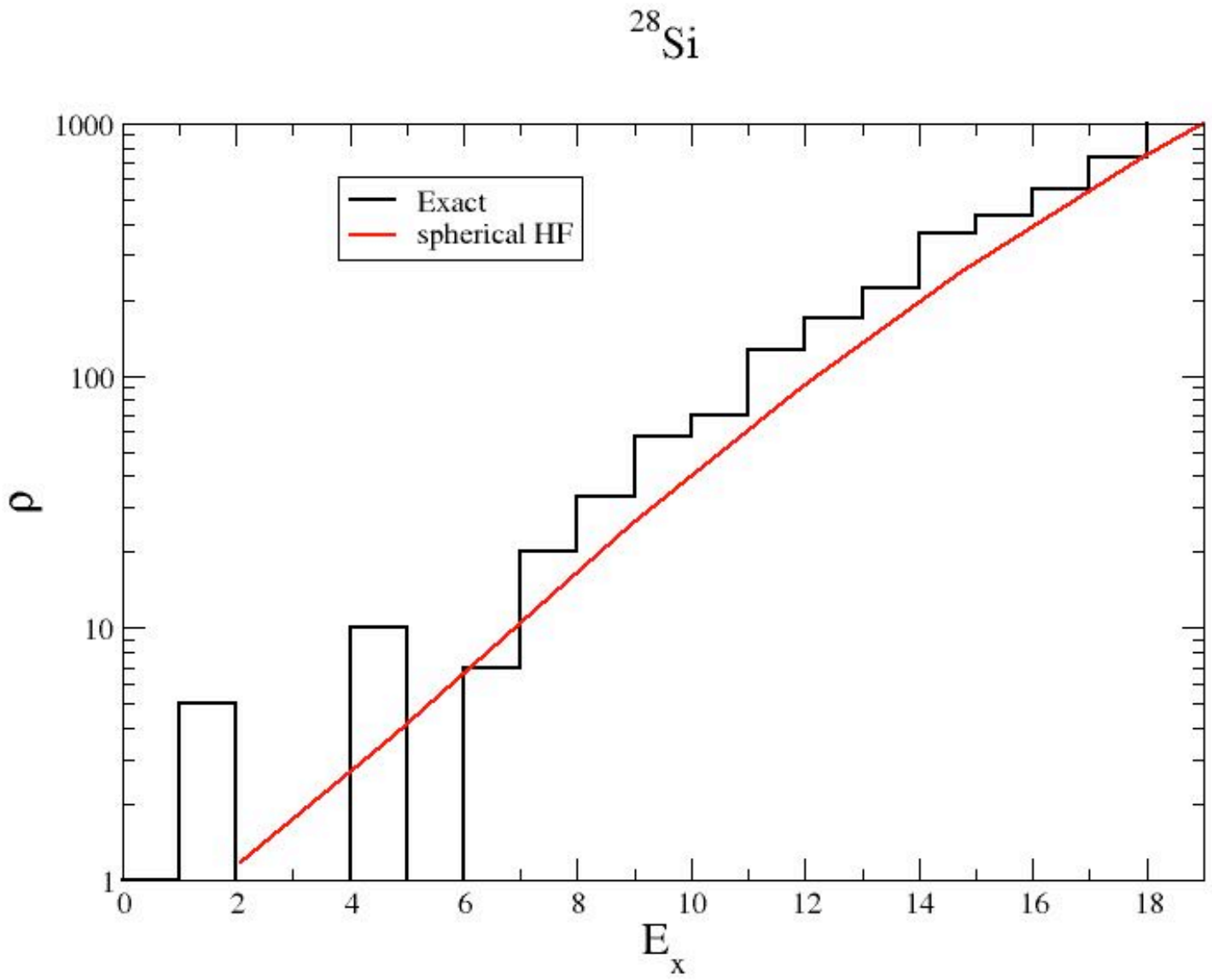
$$Z_{sp} = \prod (1 + \exp(-\beta\varepsilon_i + \alpha))$$

Hartree-Fock single-particle energies
(from shell-model interaction)

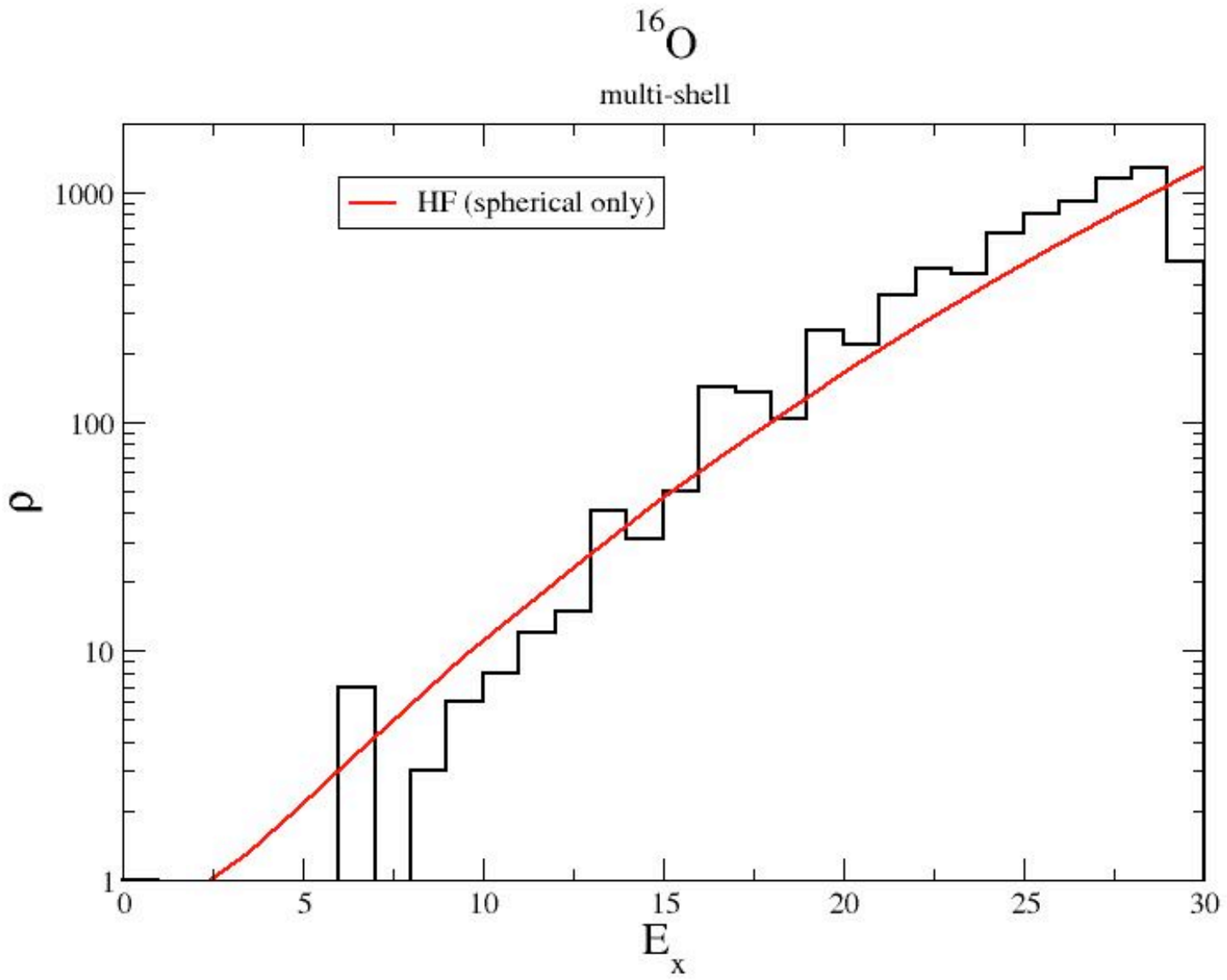
Mean-field Level densities



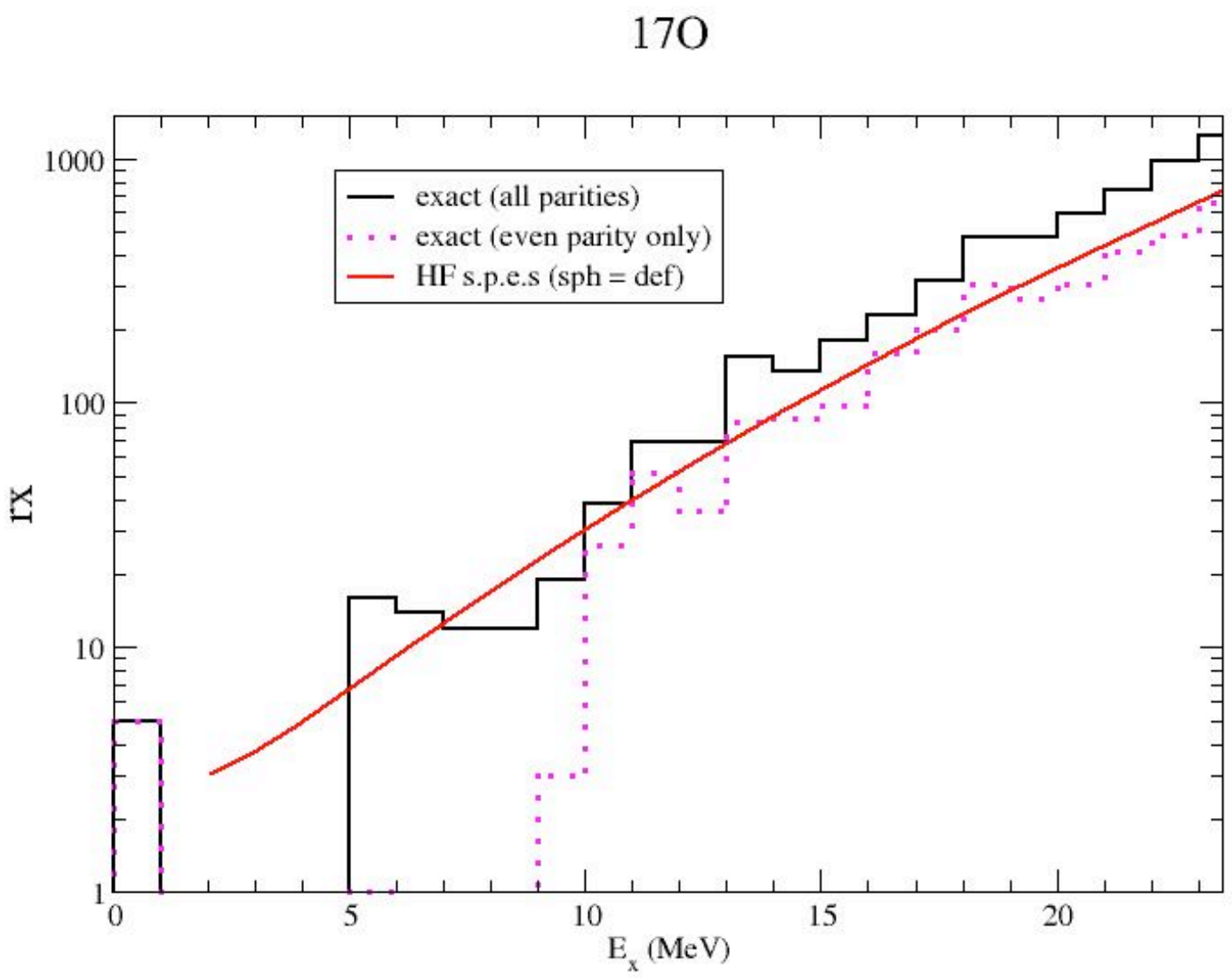
Mean-field Level densities



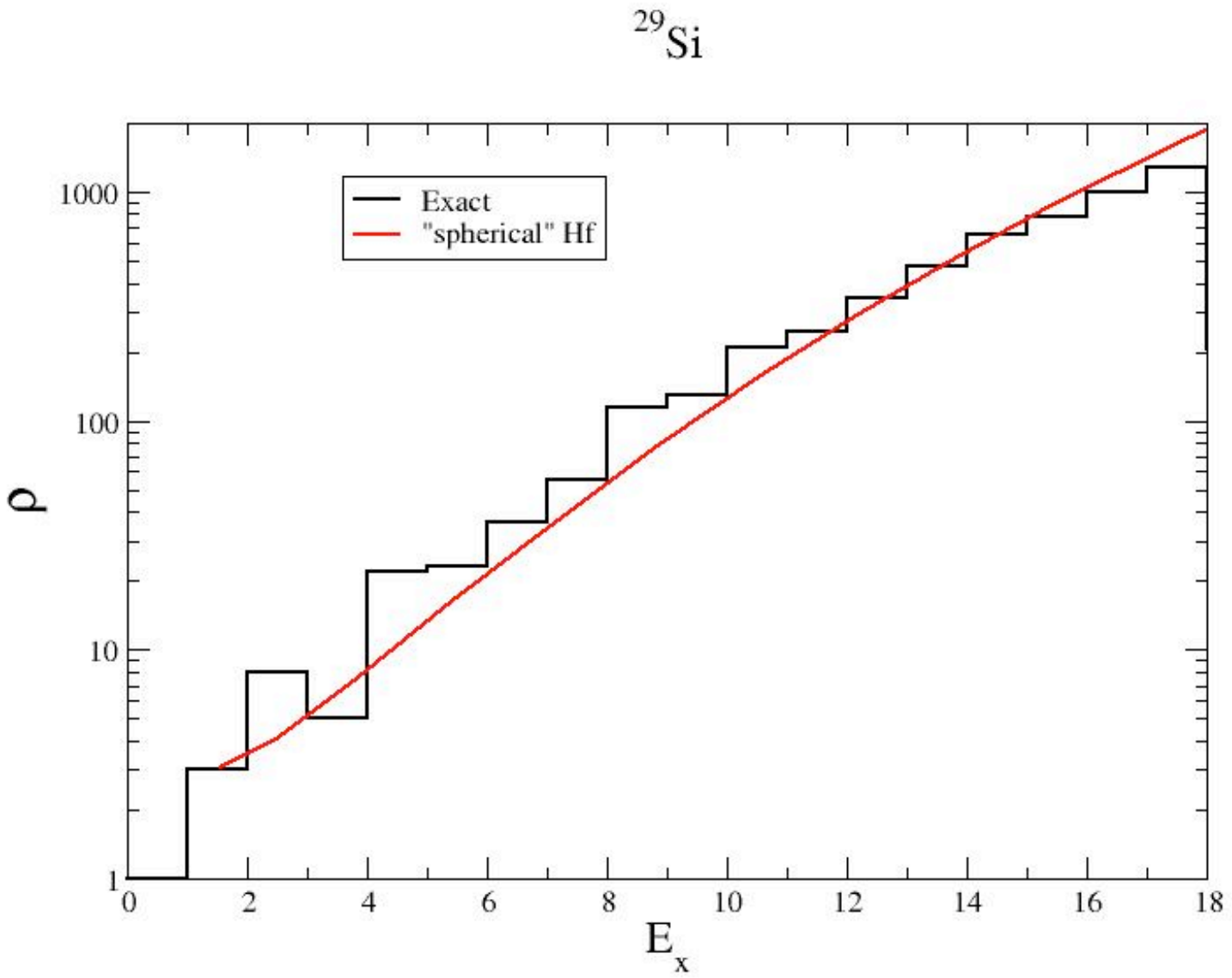
Mean-field Level densities



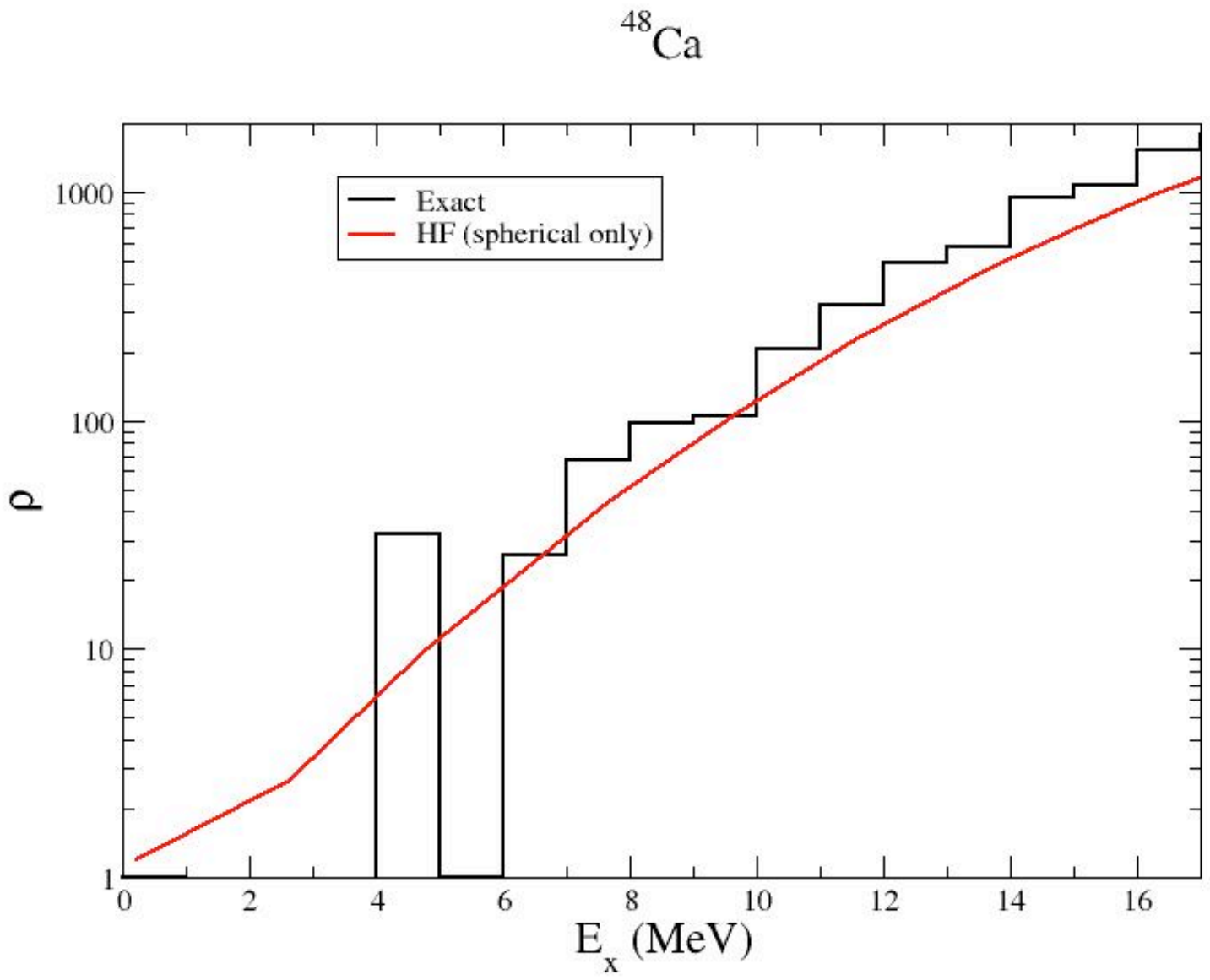
Mean-field Level densities



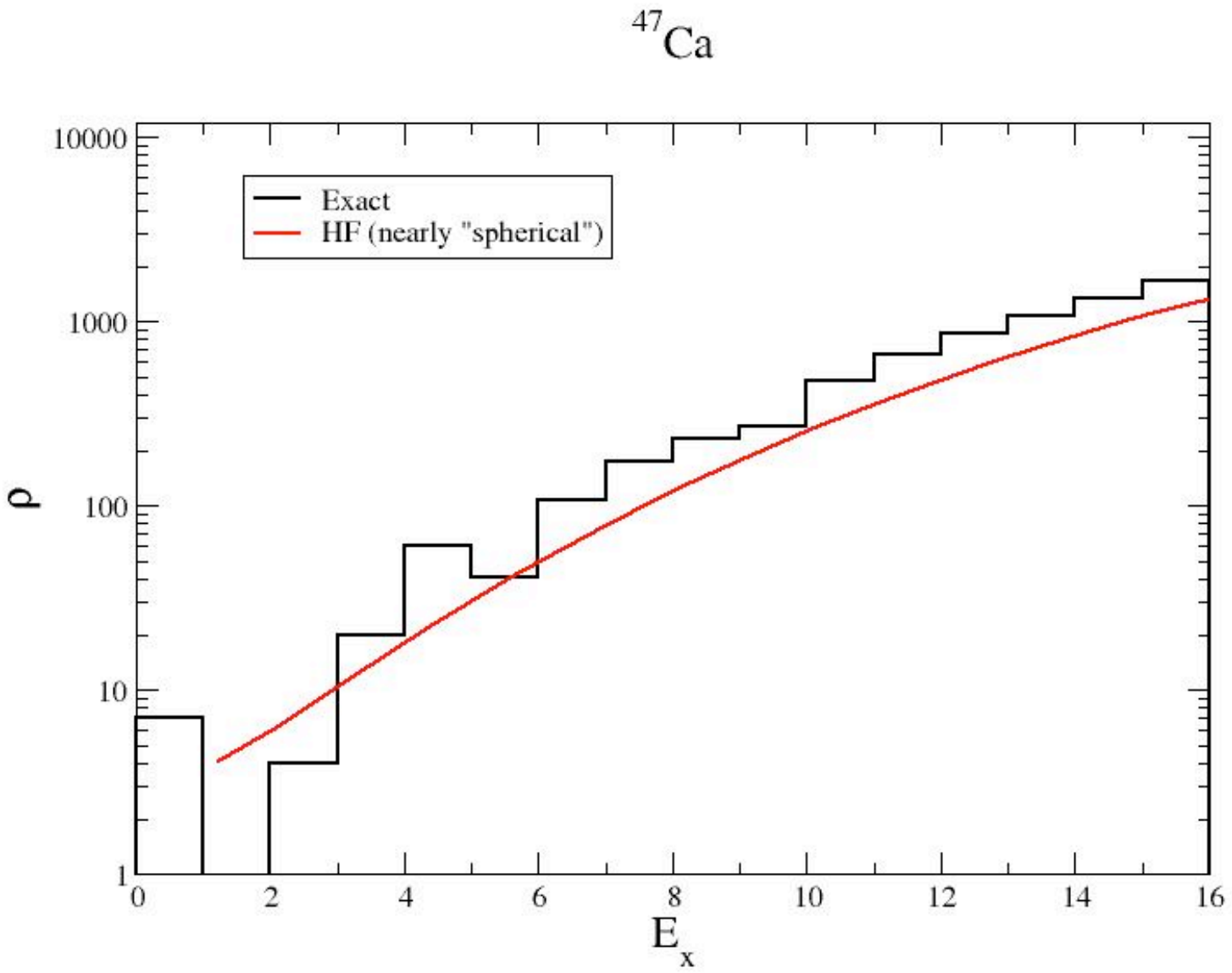
Mean-field Level densities



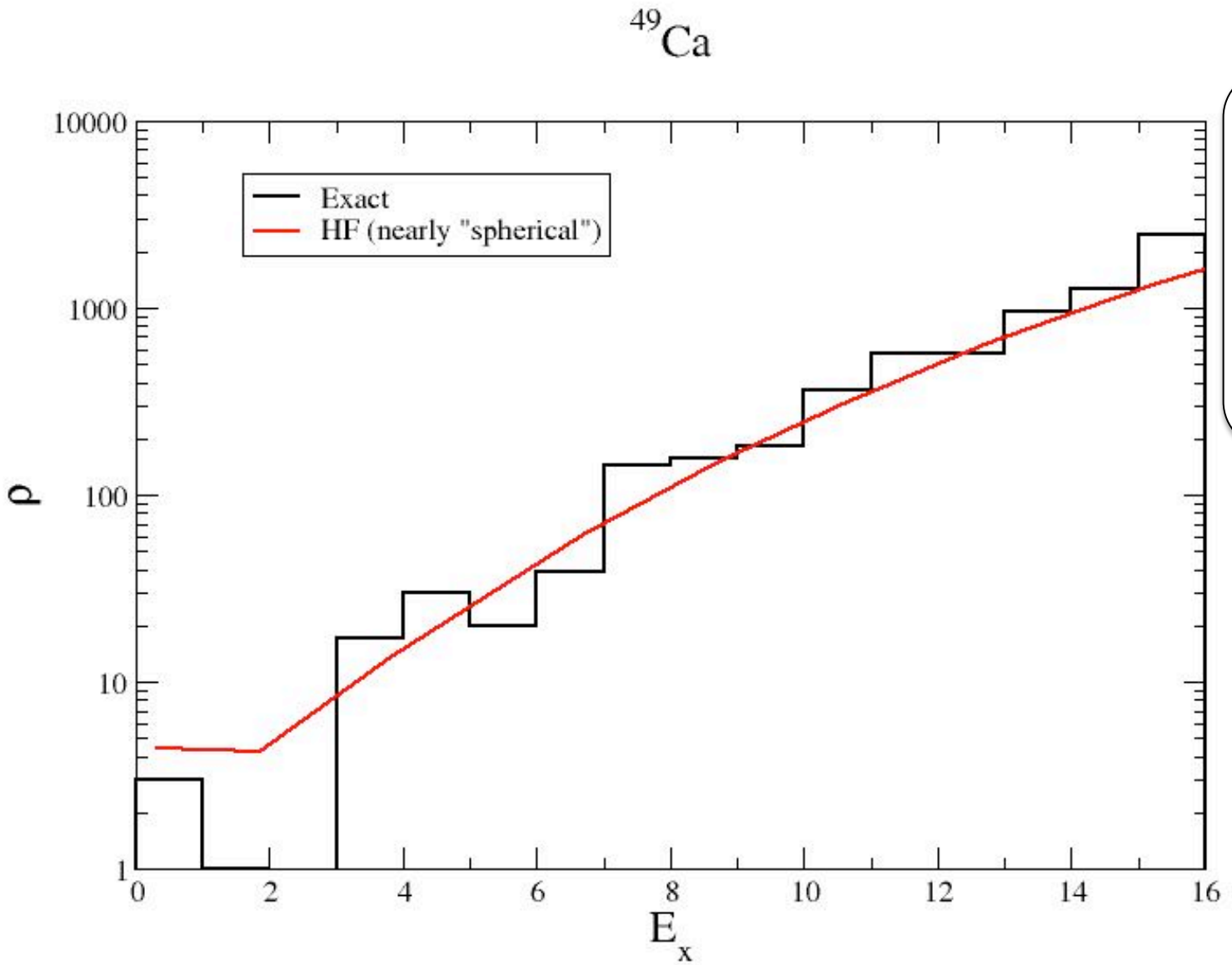
Mean-field Level densities



Mean-field Level densities

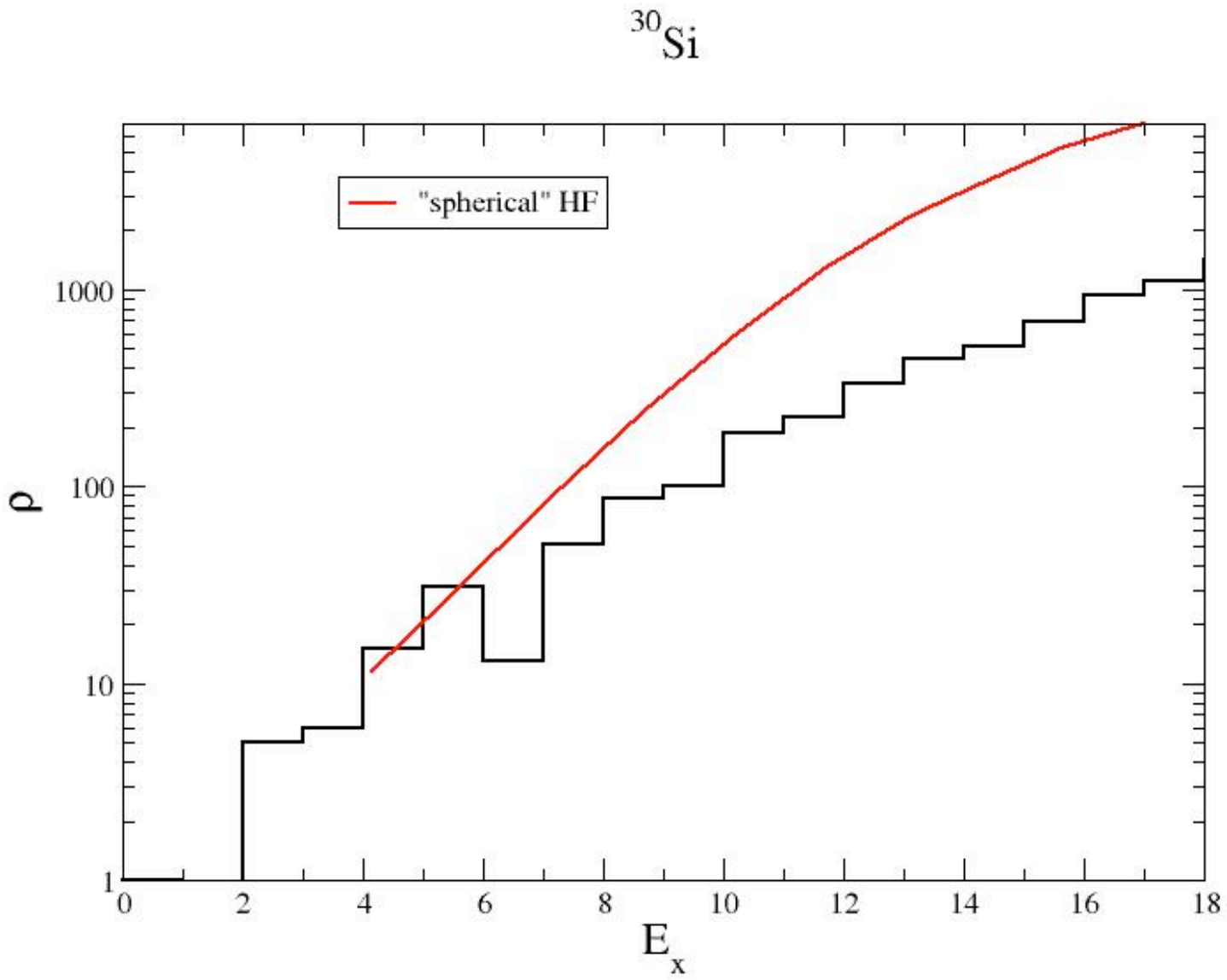


Mean-field Level densities

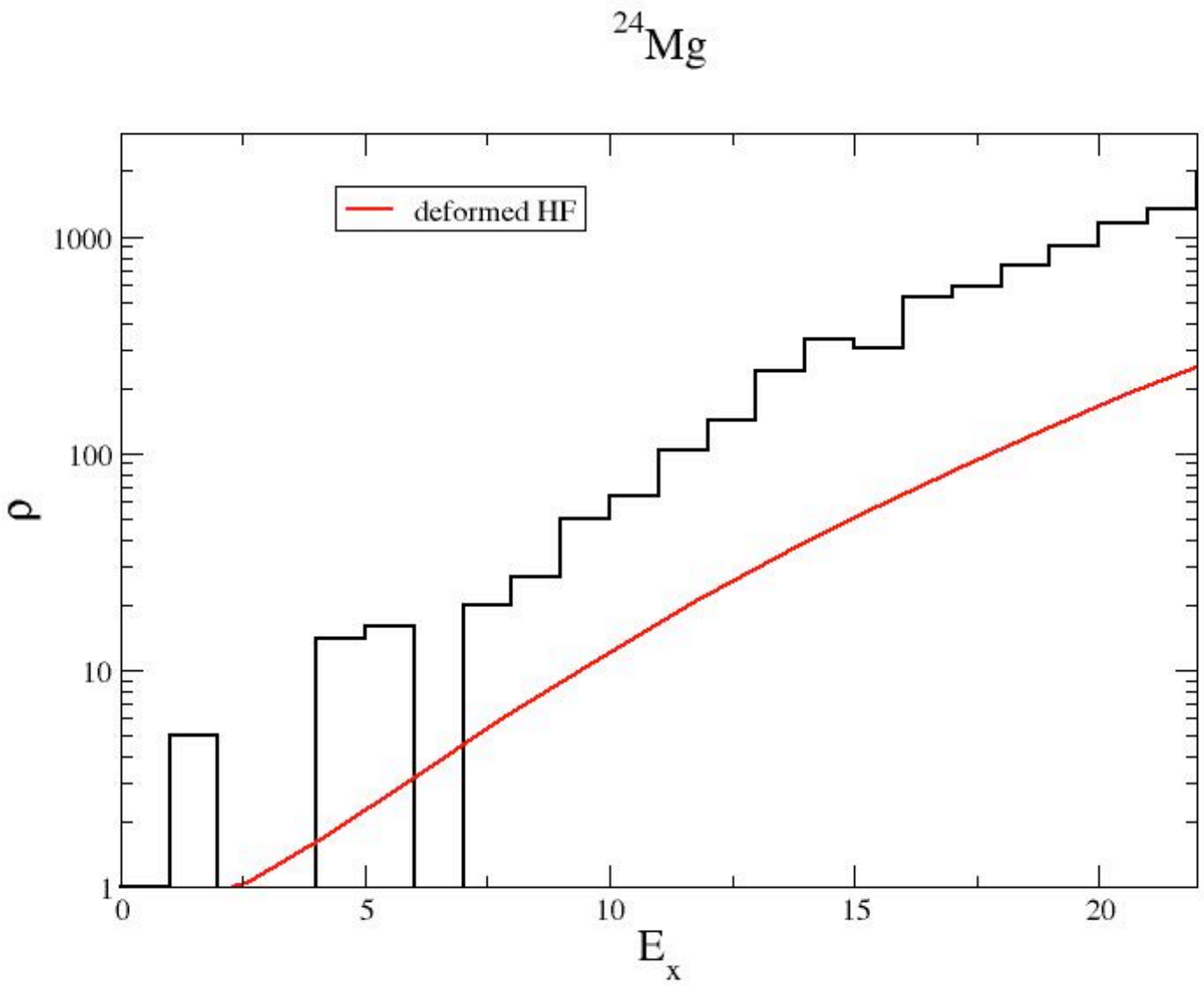


Does it ever not work?

Mean-field Level densities

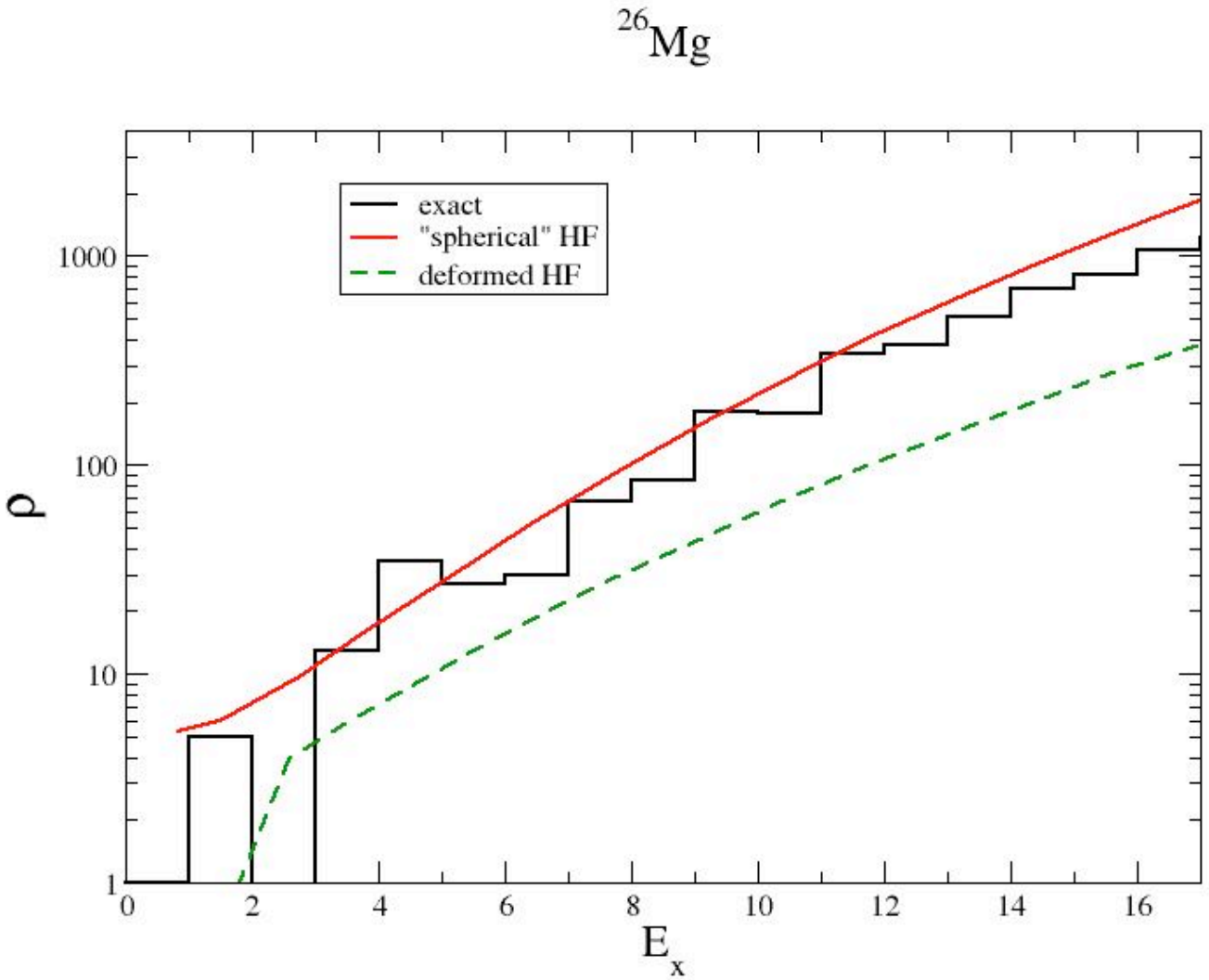


Mean-field Level densities



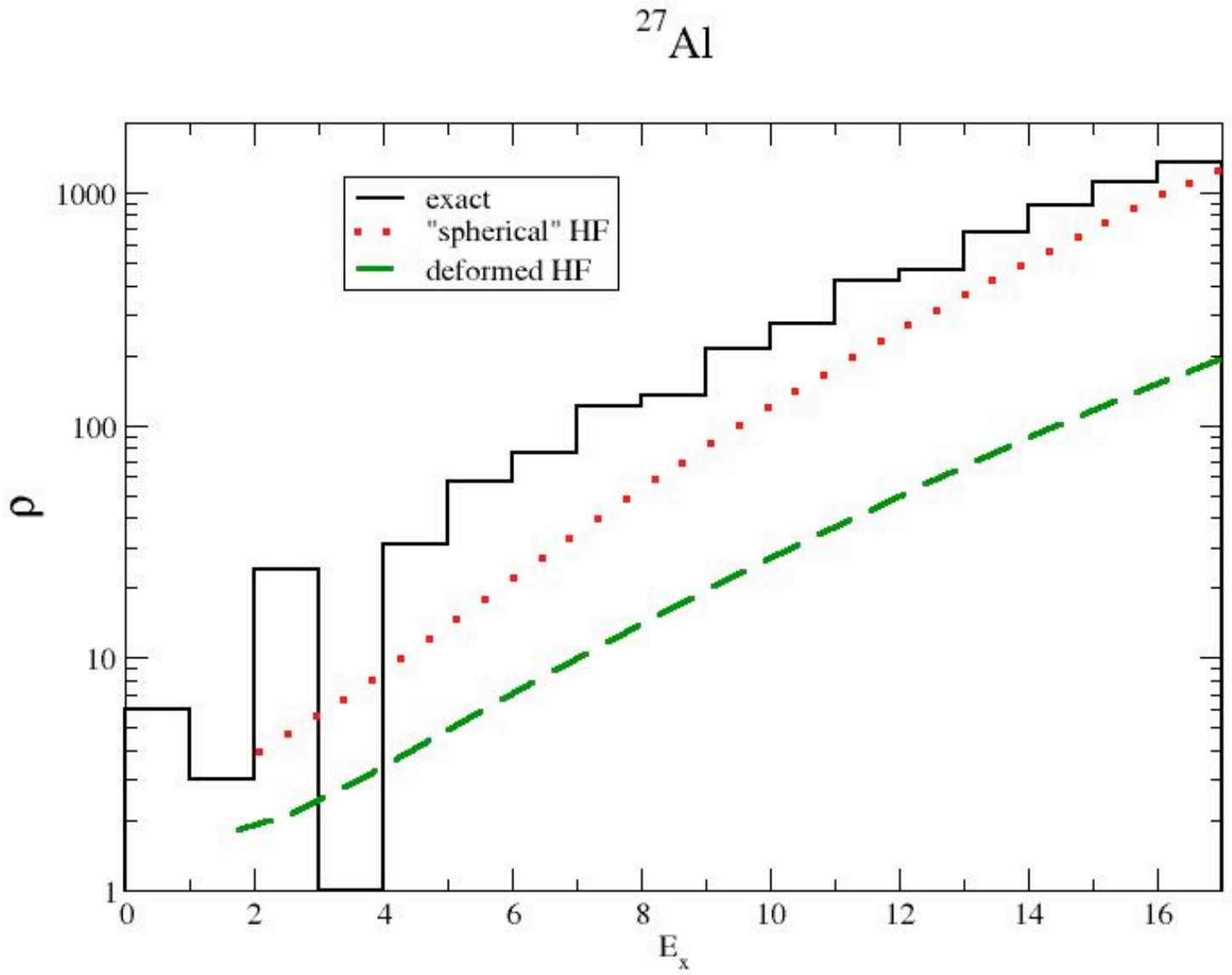
Oh-oh!

Mean-field Level densities



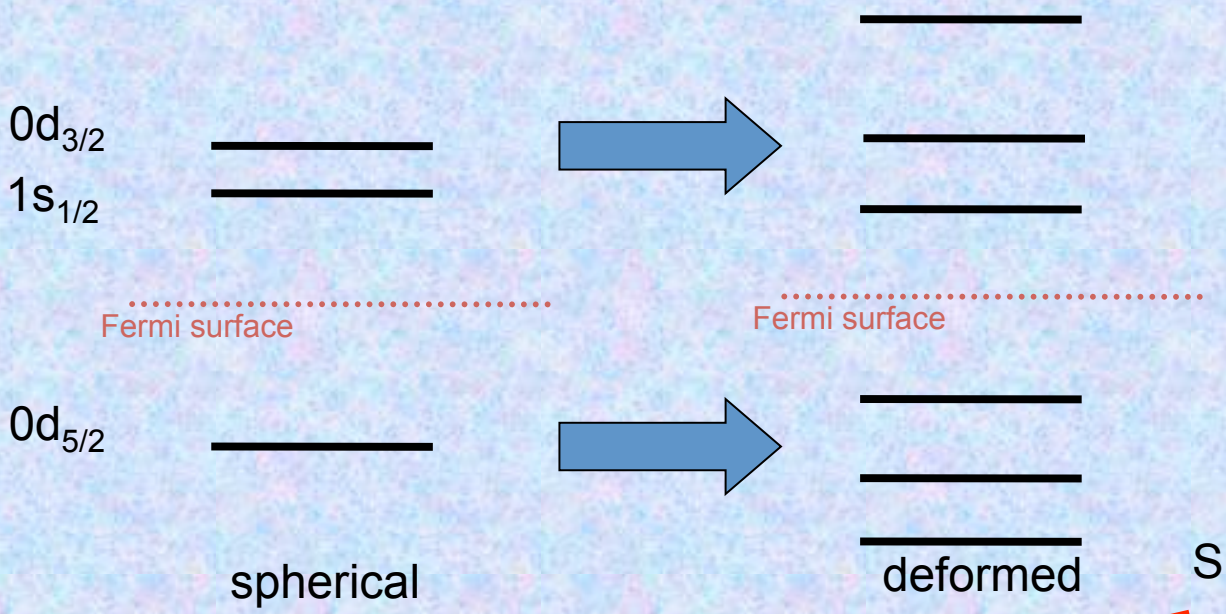
Oh-oh!

Mean-field Level densities



Mean-field Level densities

Difference is due to **fragmentation** of Hartree-Fock single-particle energies in deformed mean-field



This in turn is a manifestation of the residual interaction

Smaller s.p. level density → smaller nuclear level density

$$\rho_{BBFG}(E) = \frac{\sqrt{2\pi}}{12} \frac{\exp\sqrt{4a(E-\Delta)}}{(4a)^{1/4}(E-\Delta)^{5/4}}$$

Adding collective motion

Deformed HF state as an intrinsic state:

$$|\Psi_{HF}\rangle = \sum_J a_J |\Psi_J\rangle \qquad E_J = \langle \Psi_J | \hat{H} | \Psi_J \rangle$$

Now use Projected HF
(MS project of J. Staker, SDSU)
to dissect intrinsic state and
obtain rotational partition function:

$$Z_{rot} = \sum_J (2J+1) a_J^2 \exp(-\beta(E_J - E_0))$$

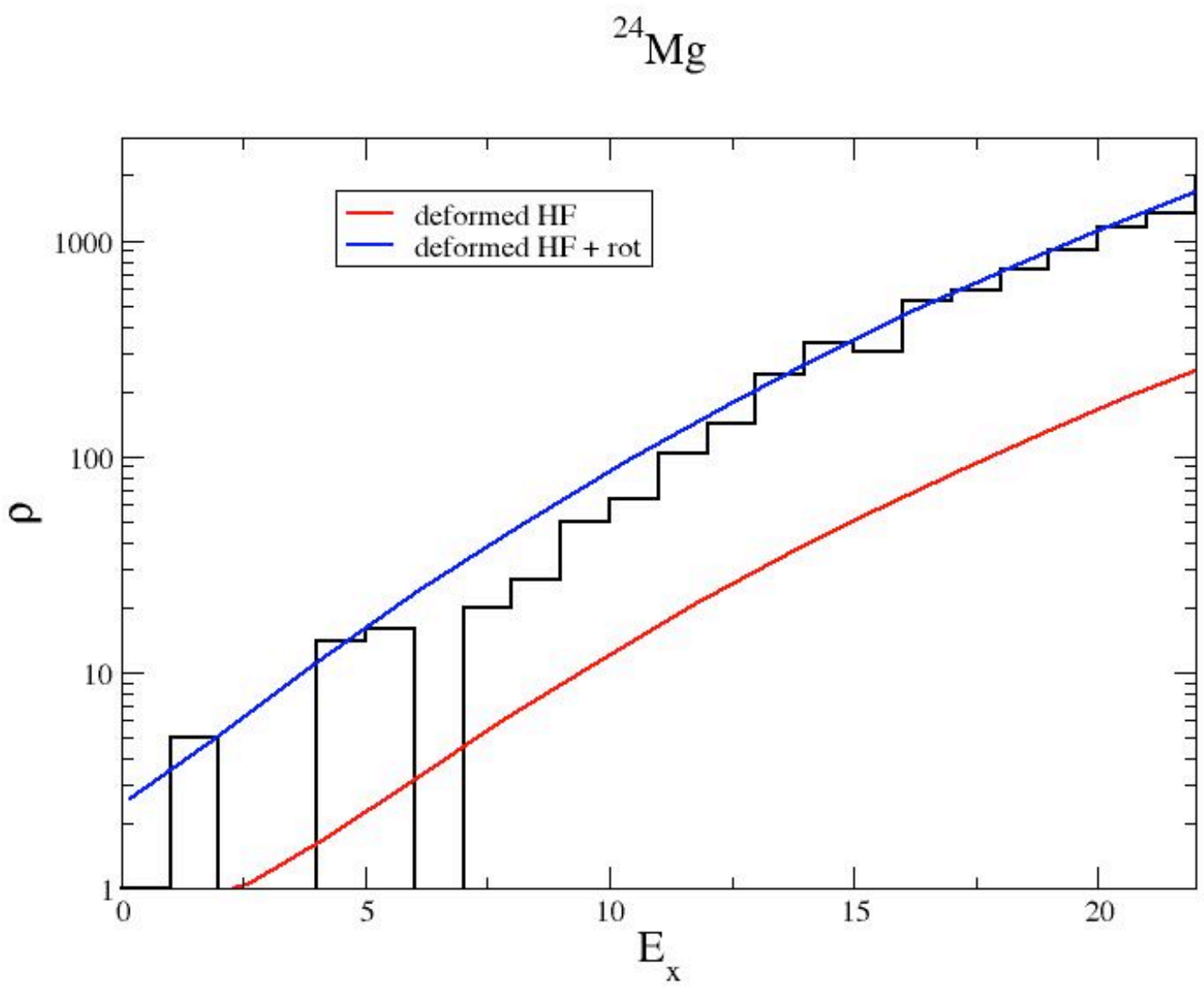
Adding collective motion

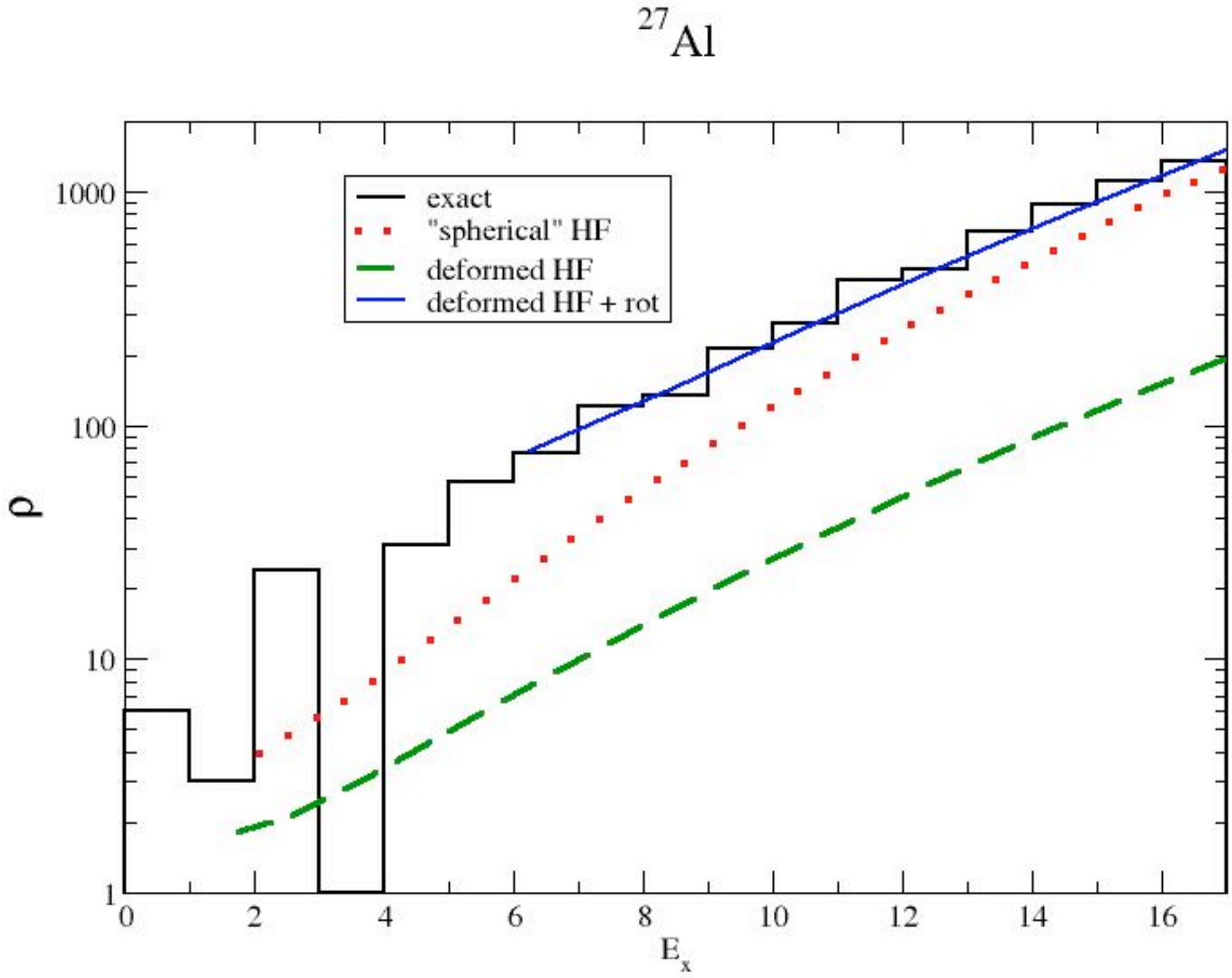
$$Z(\beta) = Z_{\pi}^{(sp)} \times Z_{\upsilon}^{(sp)} \times (Z_{rot})$$

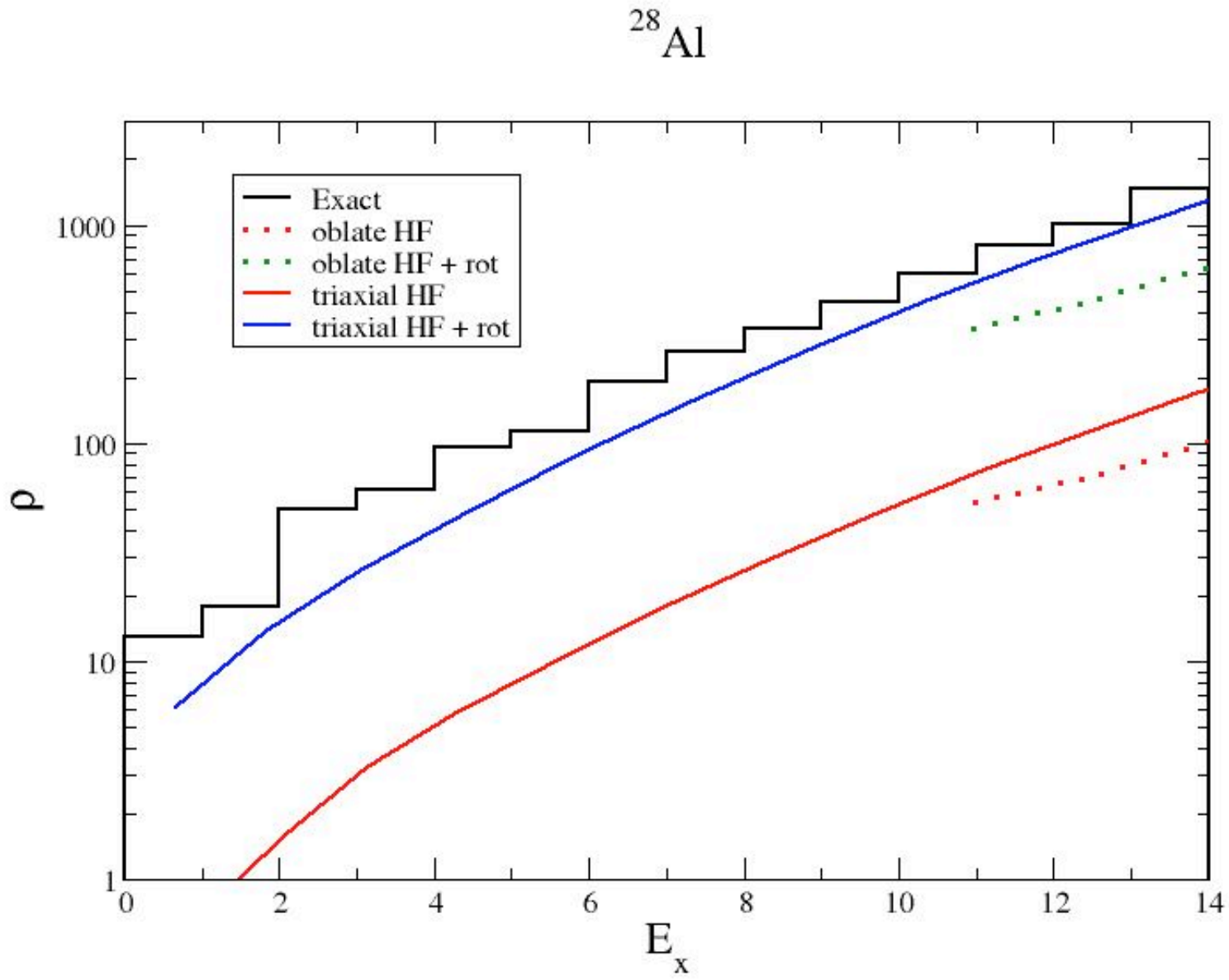
All of the parameters derived directly from HF calculation (s.p. energies) and PHF (dissection of intrinsic state)

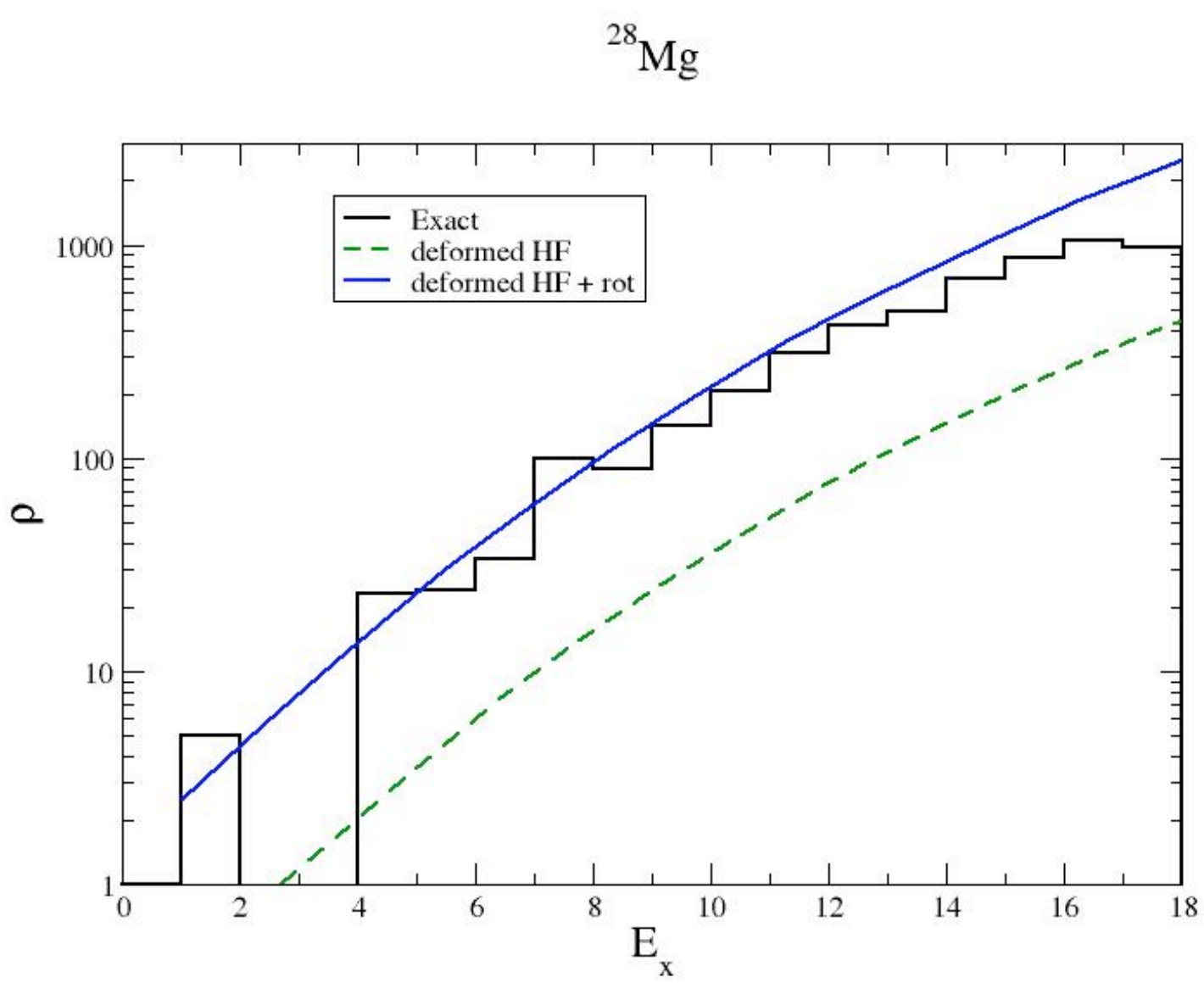
using CI shell-model interaction

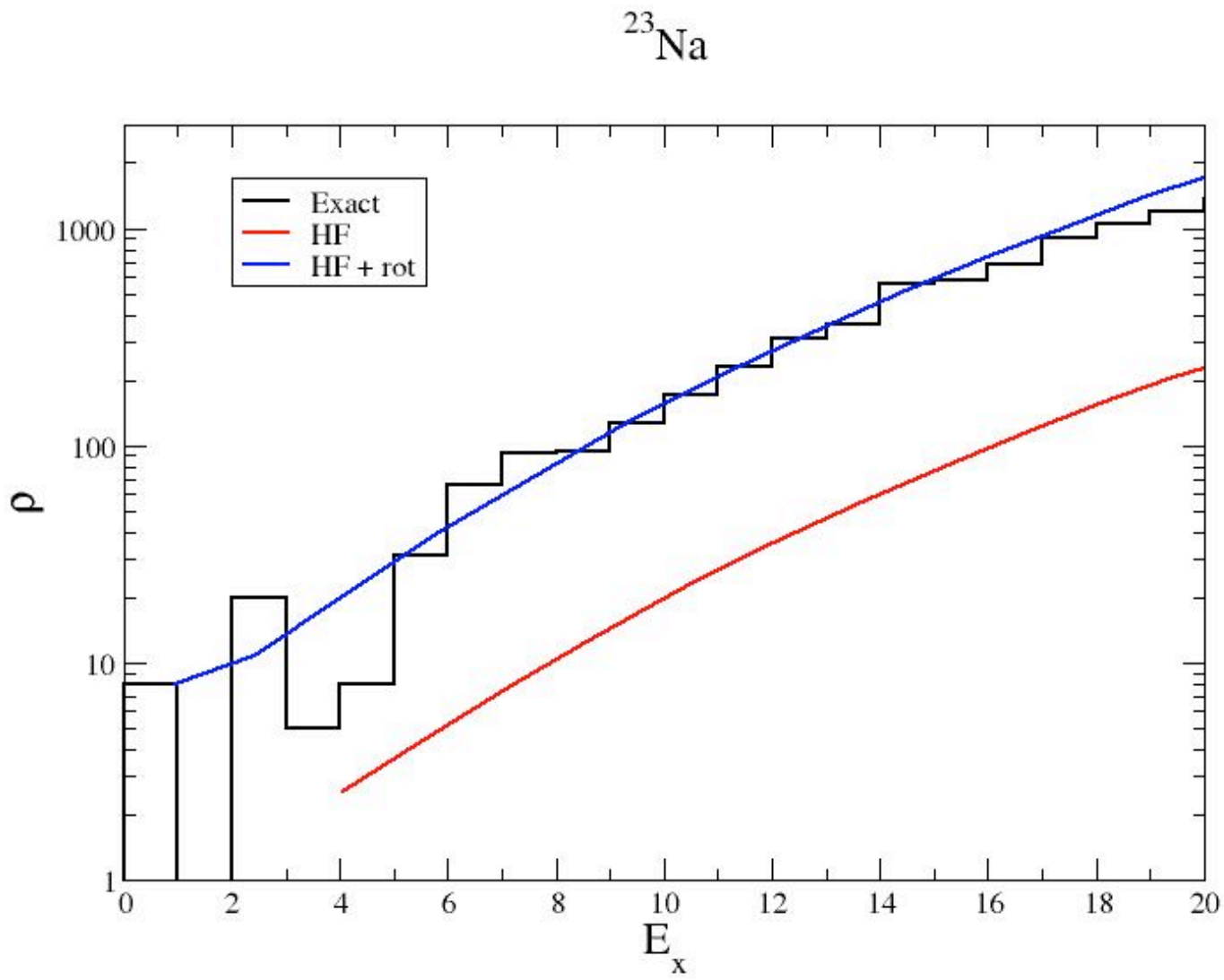
Computationally very cheap: a matter of a few seconds

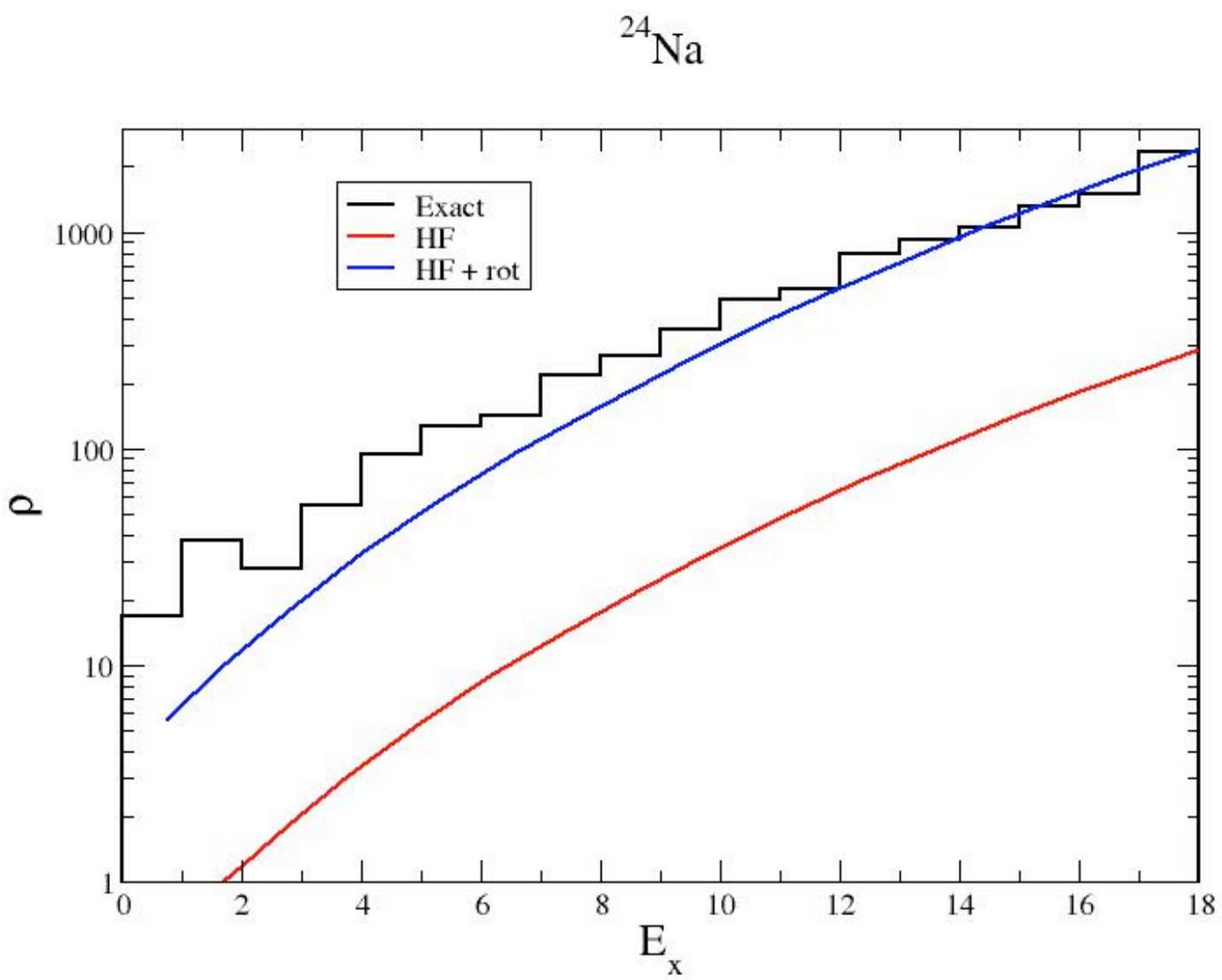

^{24}Mg
deformed HF
deformed HF + rot
1000
100
10
1
ρ
0
5
10
15
20
E$_x$

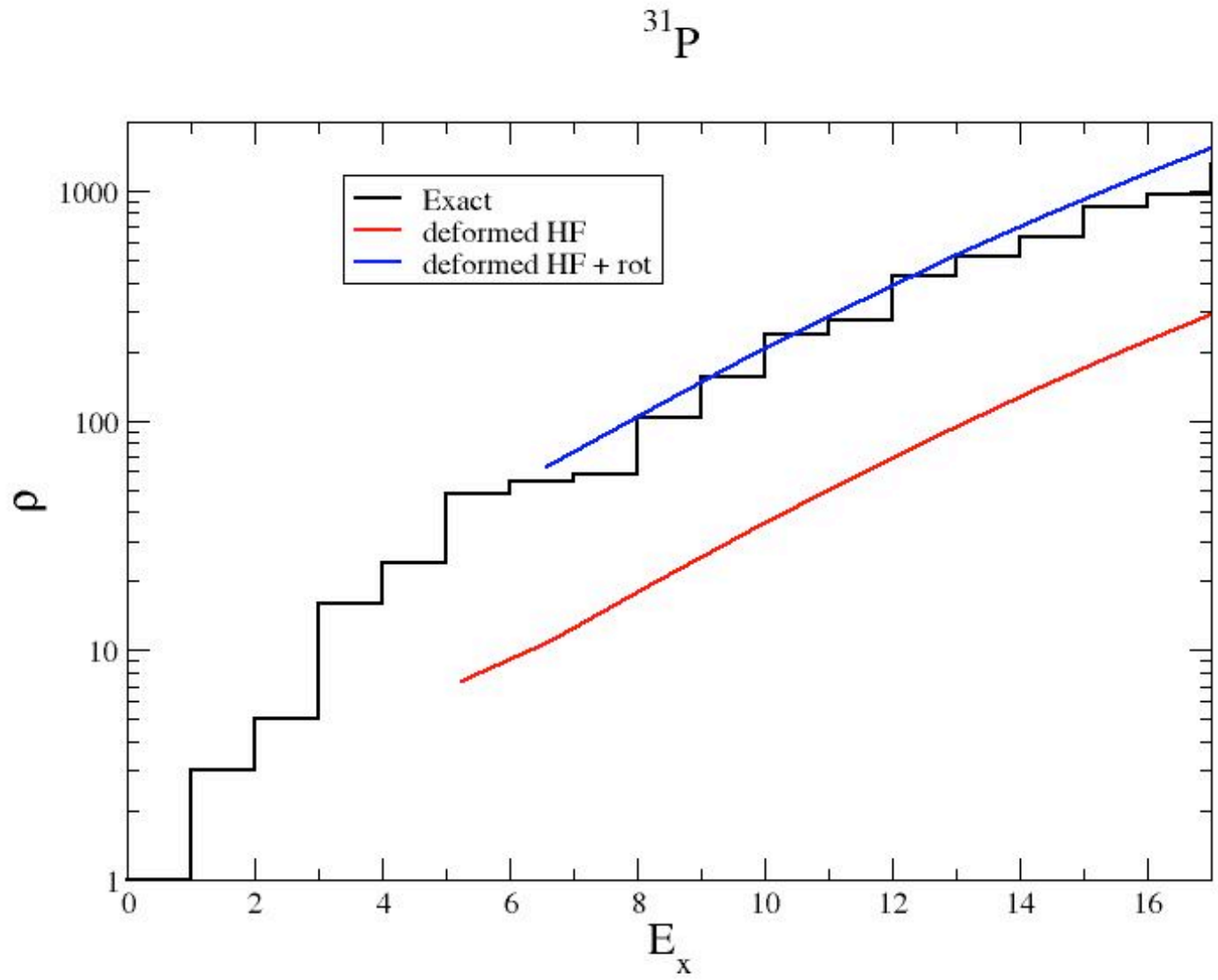

^{27}Al
exact
"spherical" HF
deformed HF
deformed HF + rot
ρ
1000
100
10
1
0
2
4
6
8
10
12
14
16
E$_x$

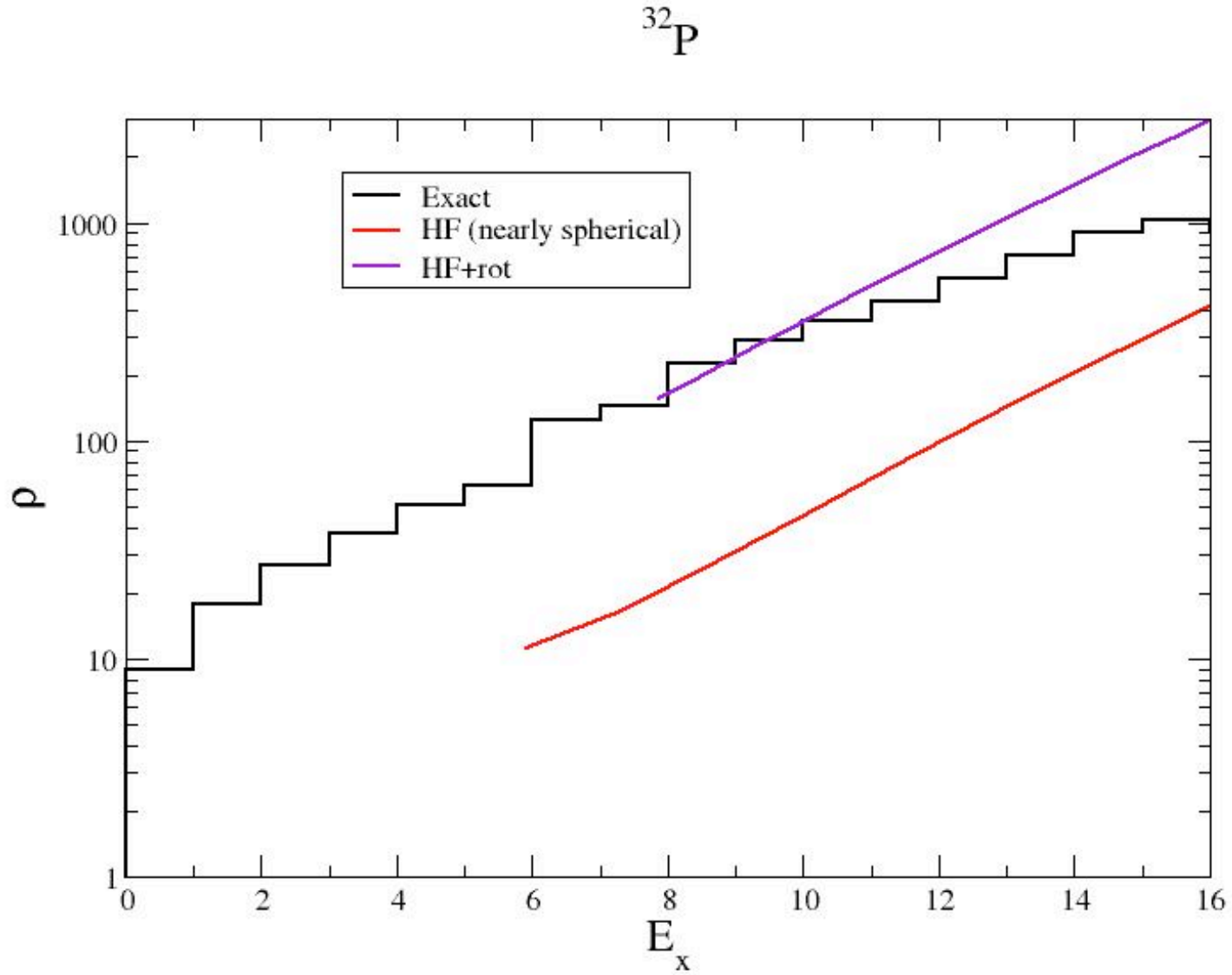

^{28}Al
Exact
oblate HF
oblate HF + rot
triaxial HF
triaxial HF + rot
ρ
1000
100
10
1
0
2
4
6
8
10
12
14
E$_x$

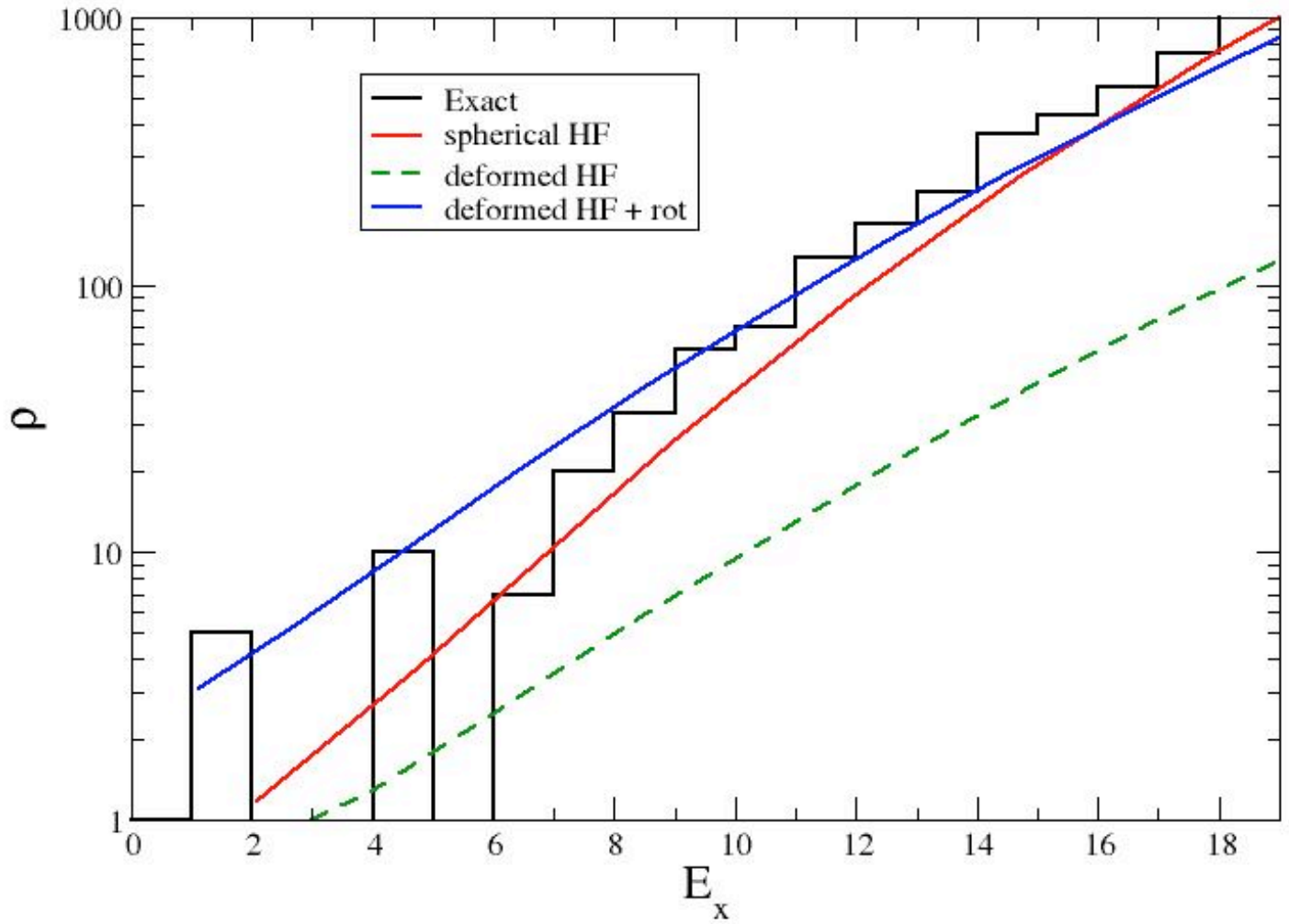

^{28}Mg
Exact
deformed HF
deformed HF + rot
1000
100
10
1
ρ
0
2
4
6
8
10
12
14
16
18
E$_x$

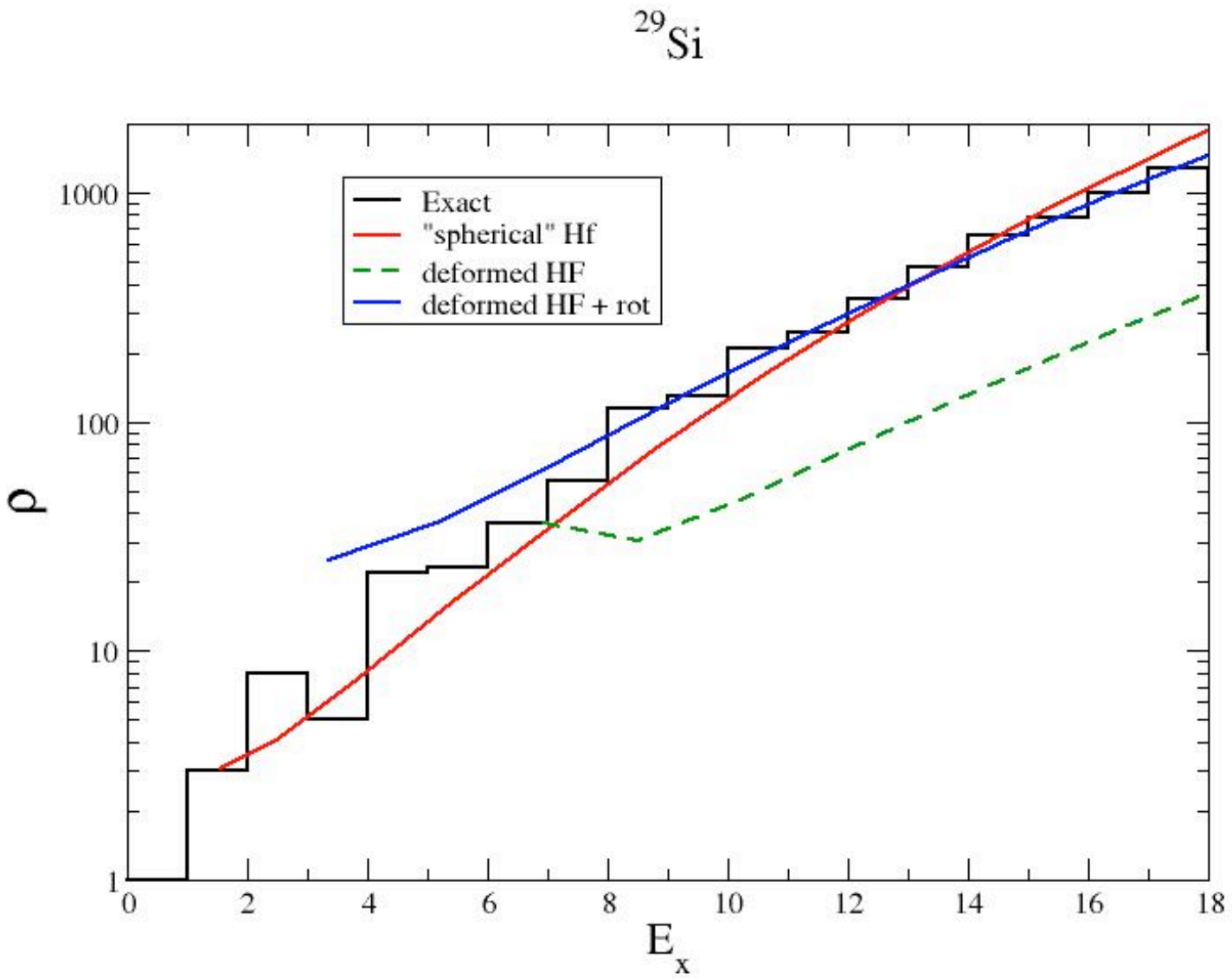

^{23}Na
Exact
HF
HF + rot
1000
100
10
1
ρ
0
2
4
6
8
10
12
14
16
18
20
E$_x$

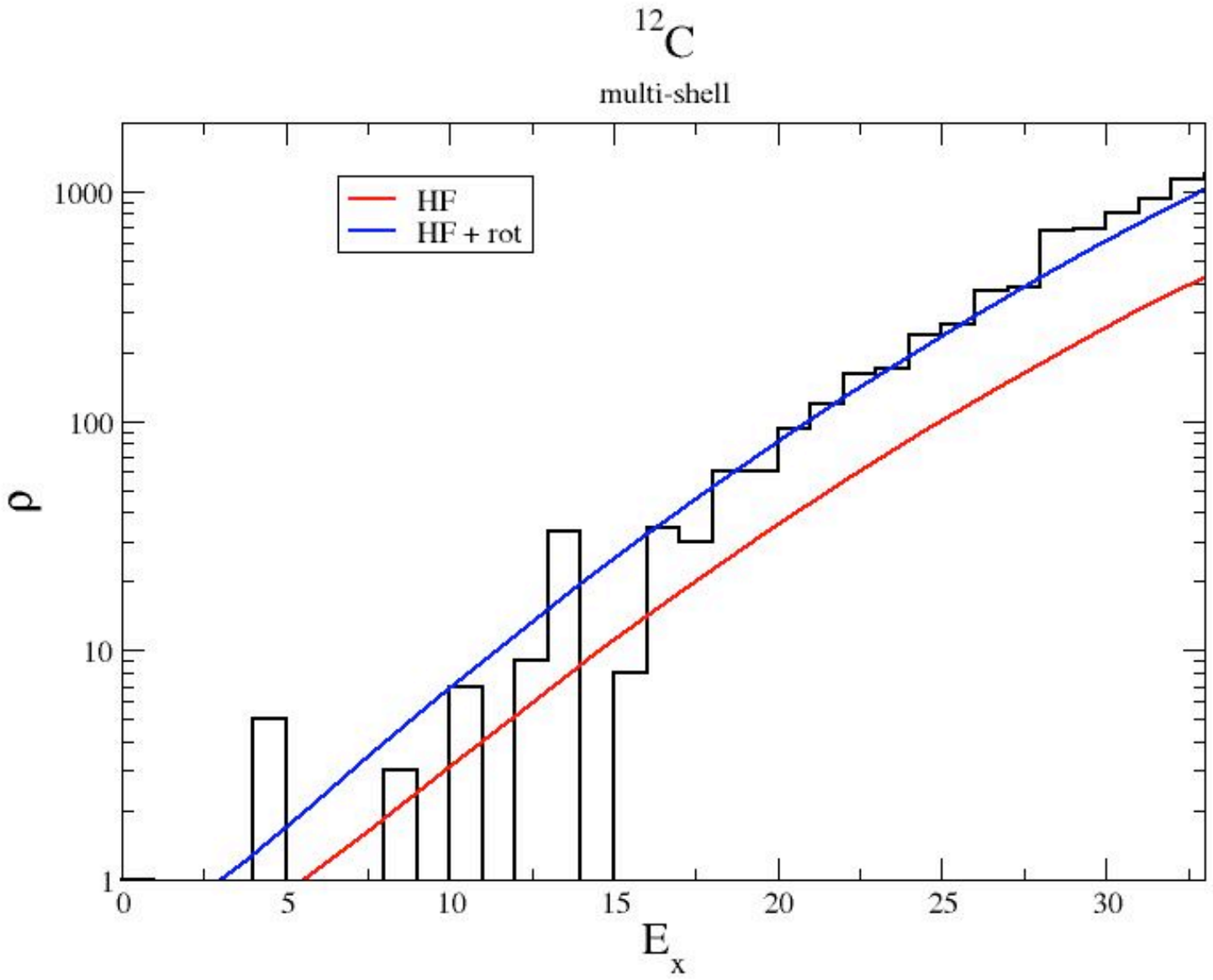

^{24}Na
Exact
HF
HF + rot
1000
100
10
1
ρ
0
2
4
6
8
10
12
14
16
18
E$_x$

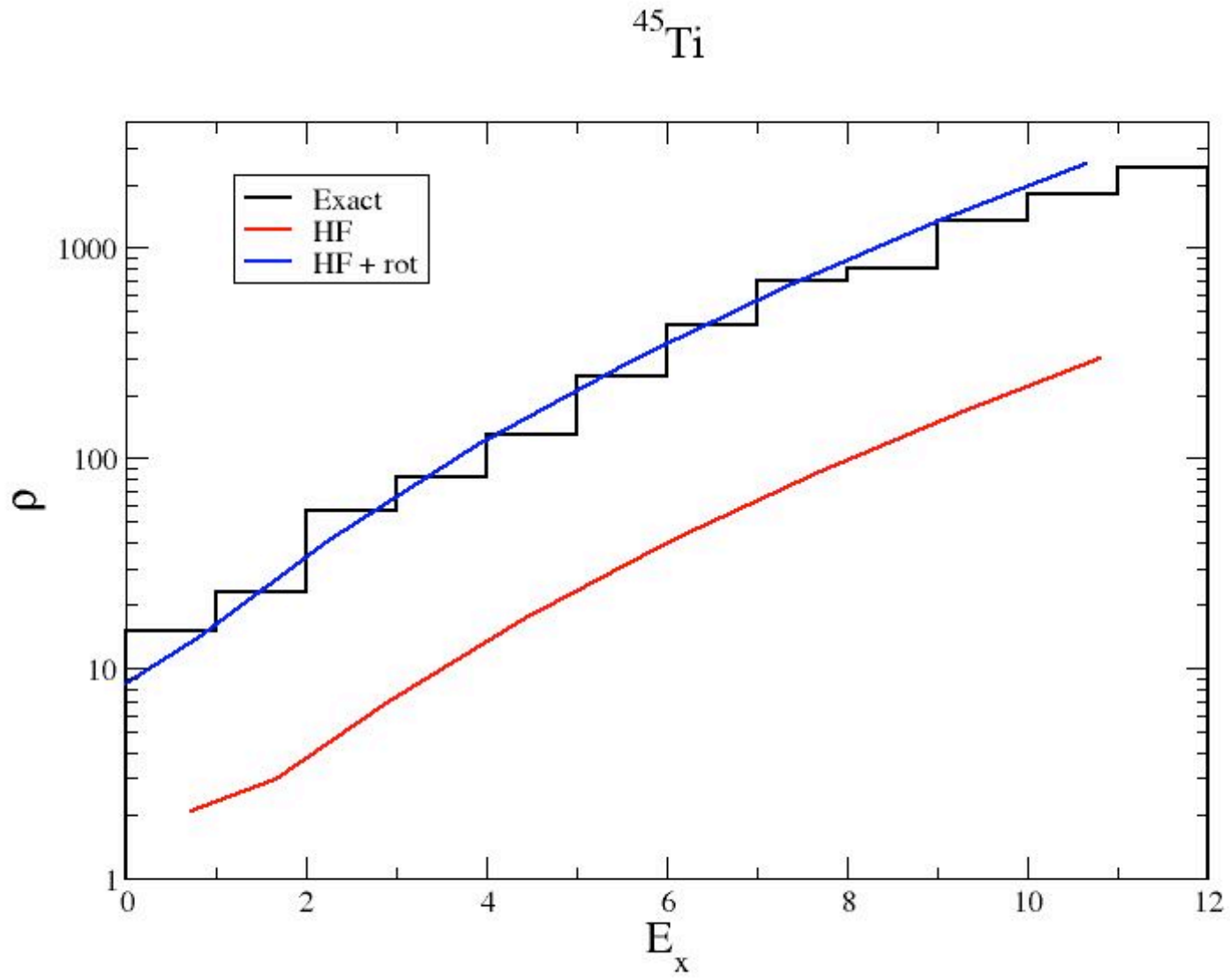

^{31}P
Exact
deformed HF
deformed HF + rot
1000
100
10
1
ρ
0
2
4
6
8
10
12
14
16
E$_x$

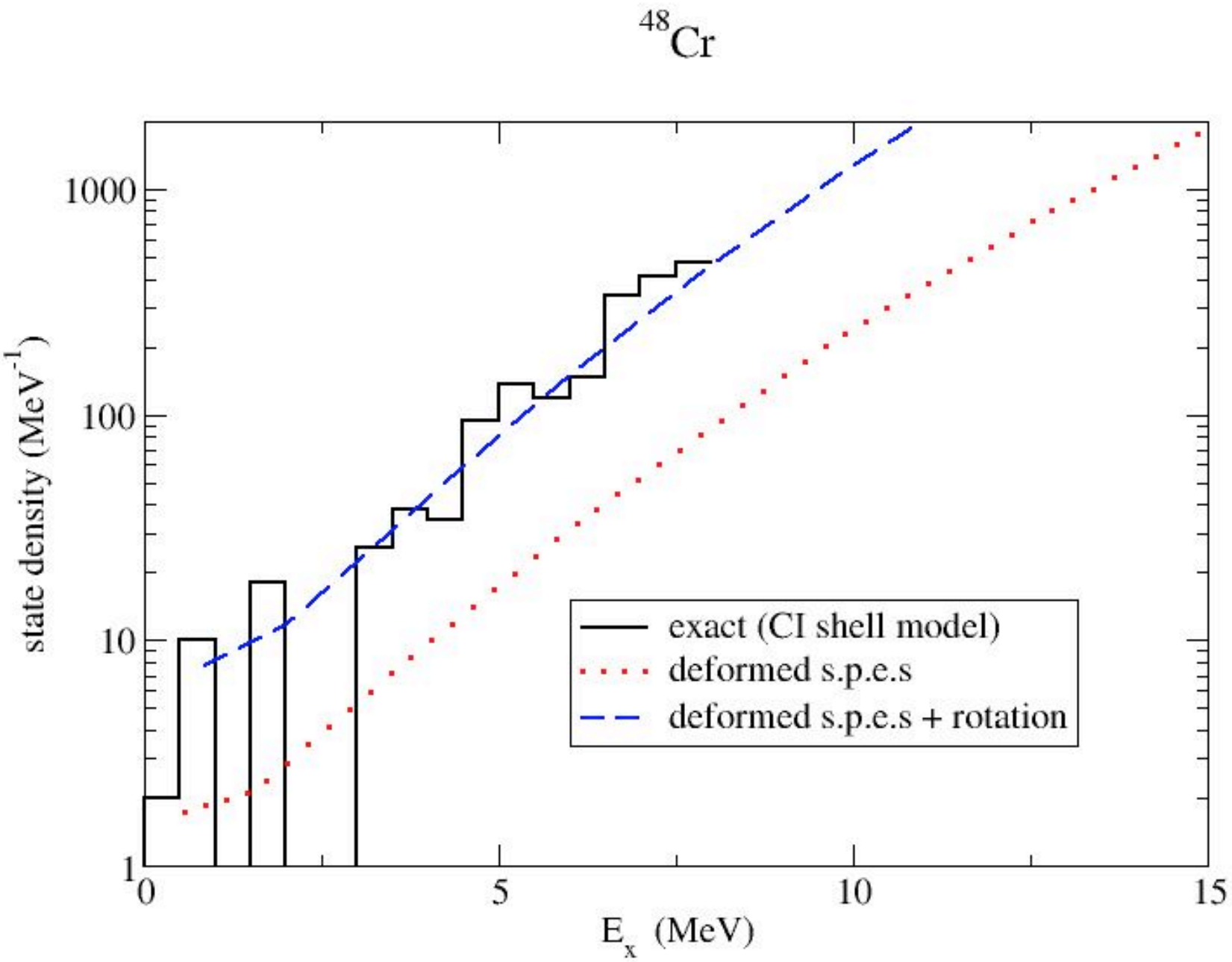

^{32}P
Exact
HF (nearly spherical)
HF+rot
1000
100
10
1
ρ
0
2
4
6
8
10
12
14
16
E$_x$

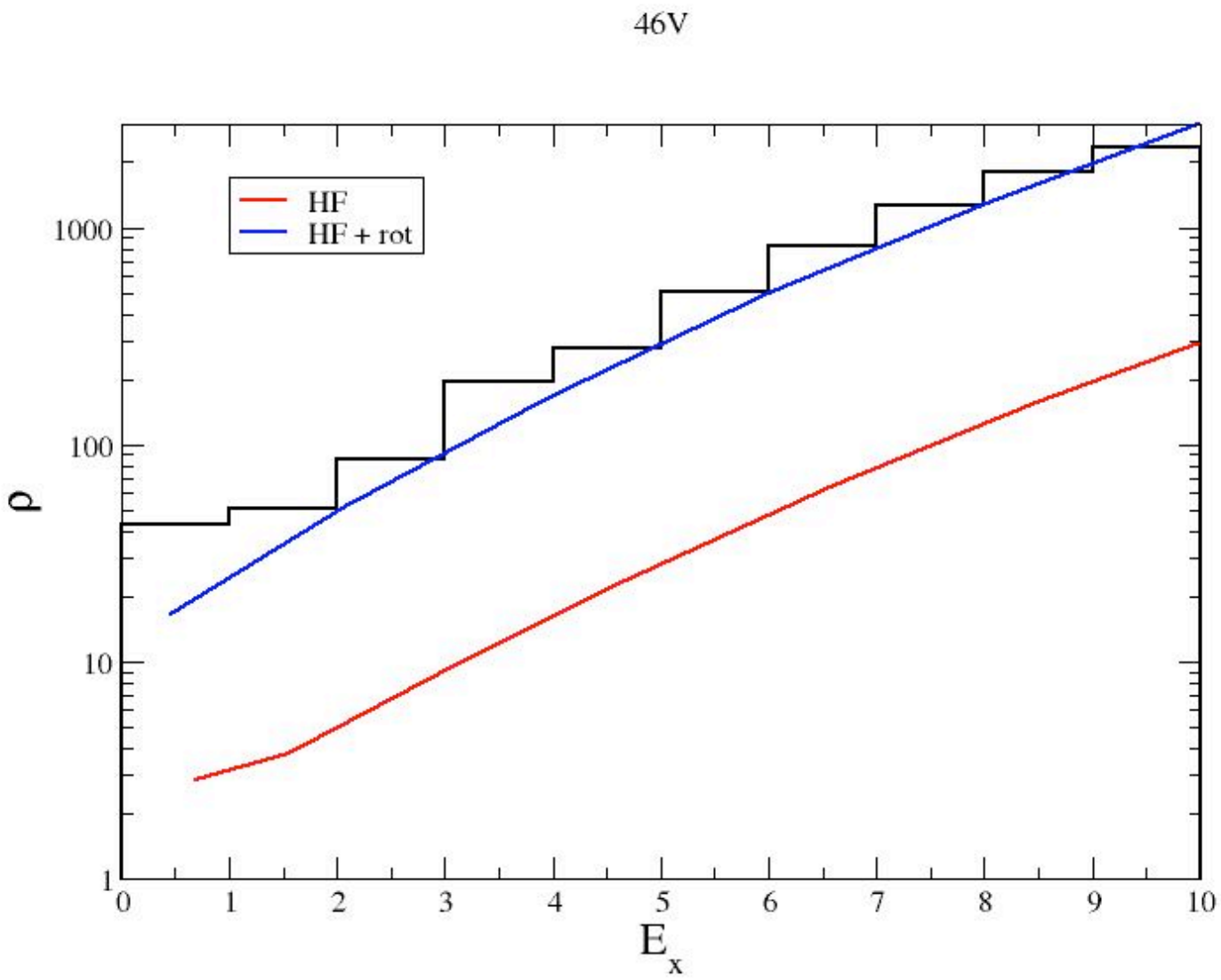

^{28}Si
1000
100
10
1
ρ
0
2
4
6
8
10
12
14
16
18
E_x
Exact
spherical HF
deformed HF
deformed HF + rot


^{29}Si
Exact
"spherical" Hf
deformed HF
deformed HF + rot
ρ
1000
100
10
1
0
2
4
6
8
10
12
14
16
18
E$_x$

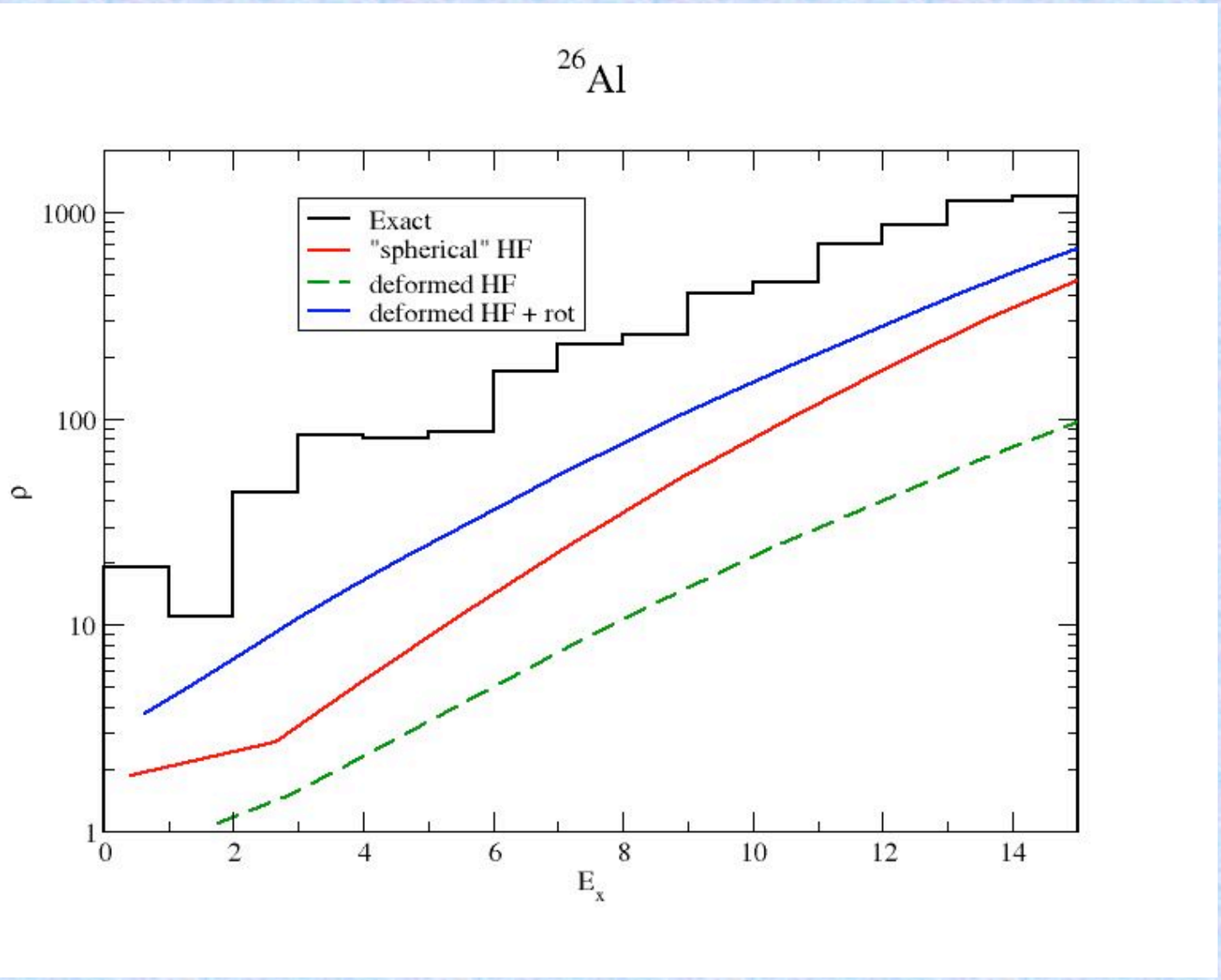

^{12}C
multi-shell
HF
HF + rot
1000
100
10
1
ρ
0
5
10
15
20
25
30
E$_x$

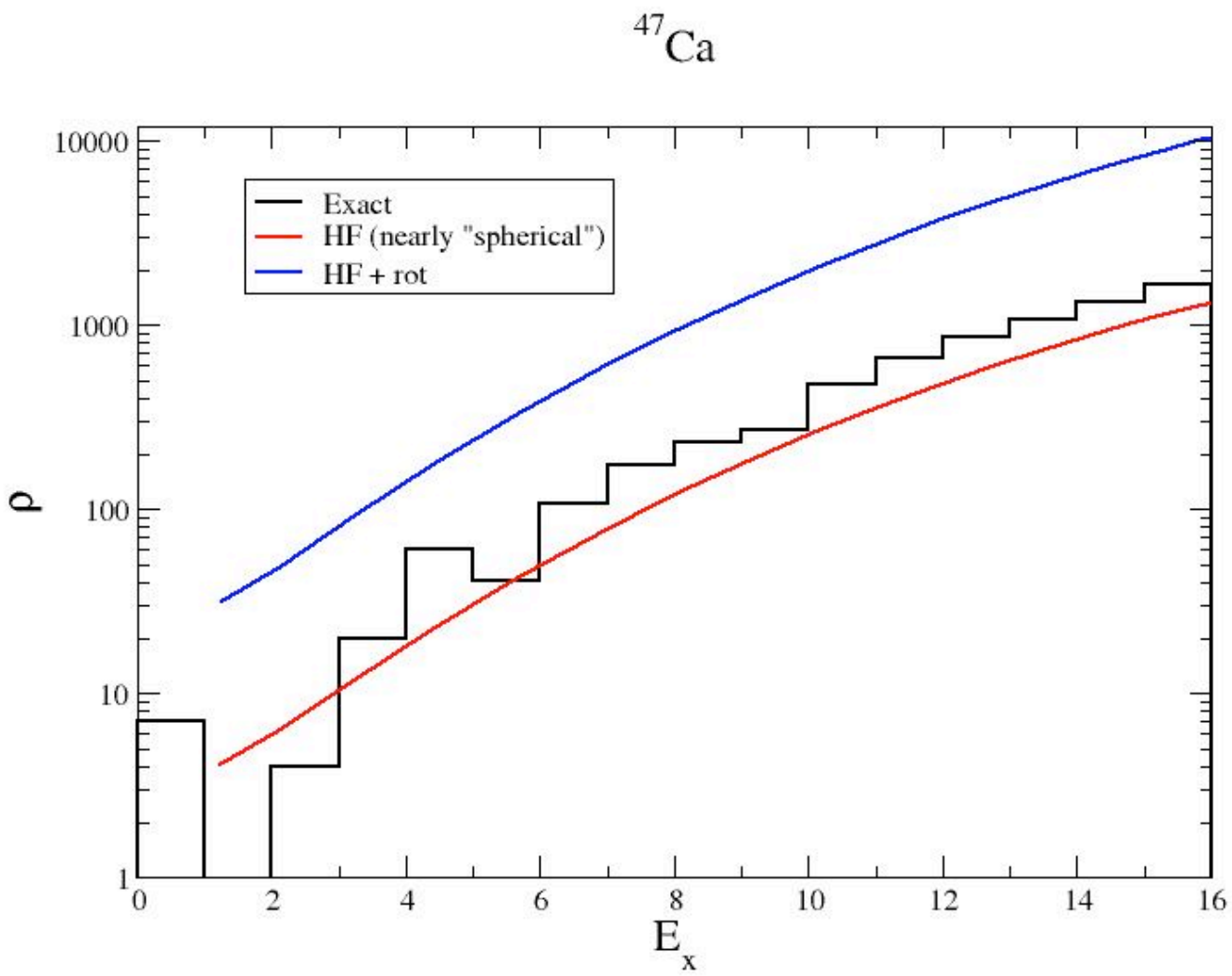

^{45}Ti
Exact
HF
HF + rot
1000
100
10
1
ρ
0
2
4
6
8
10
12
E$_x$

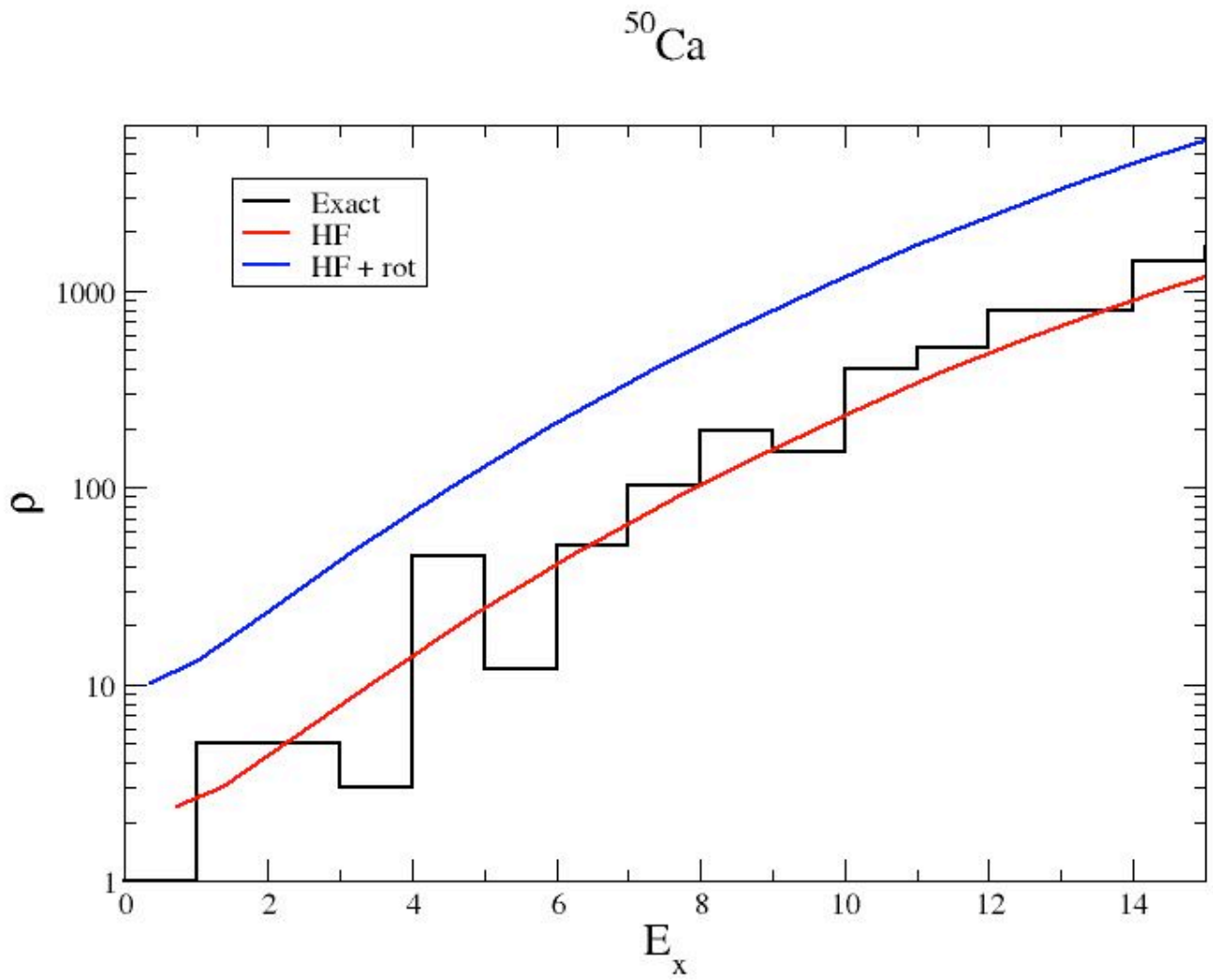

^{48}Cr
1000
100
10
1
0
5
10
15
state density (MeV^{-1})
E$_x$ (MeV)
exact (CI shell model)
deformed s.p.e.s
deformed s.p.e.s + rotation

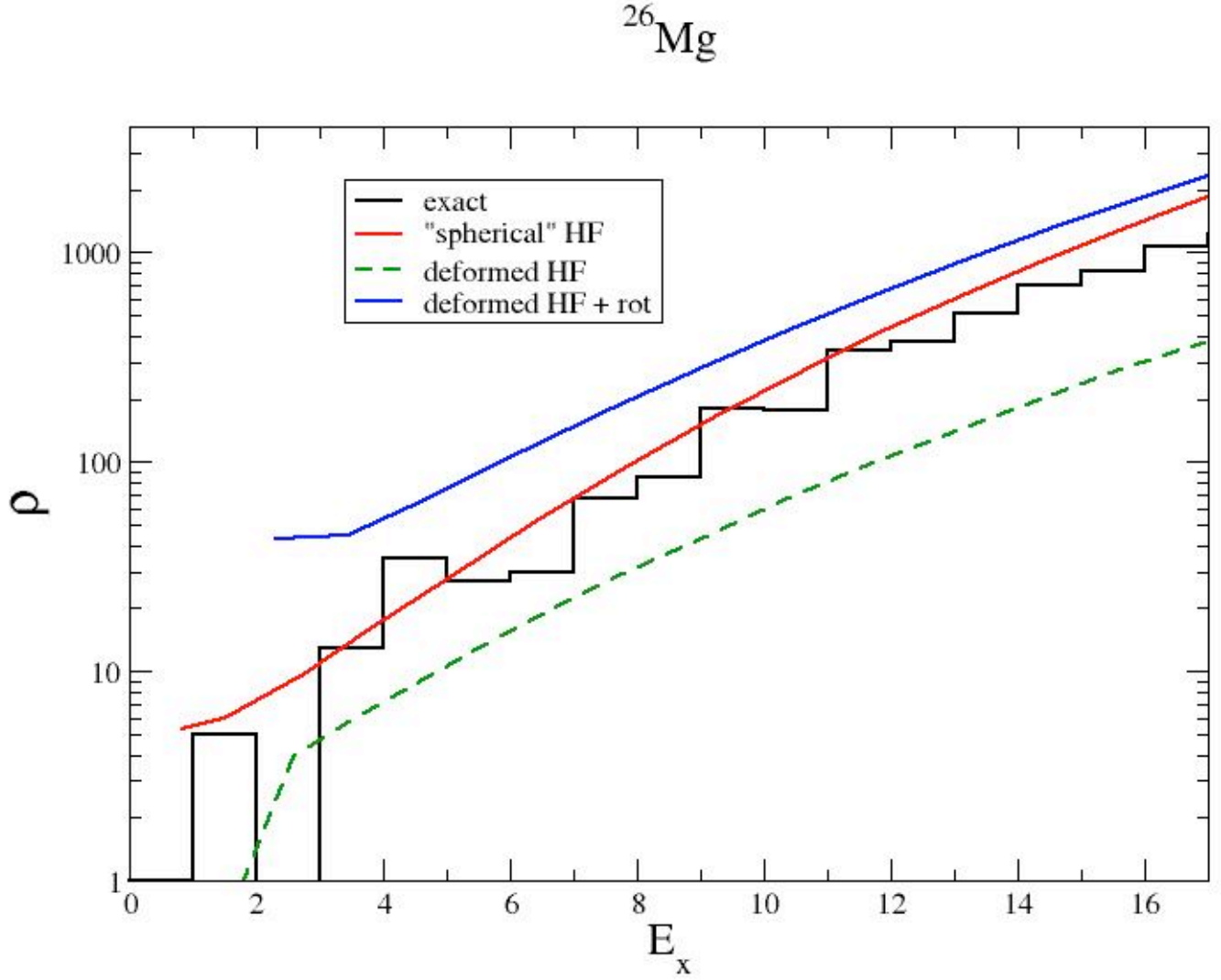


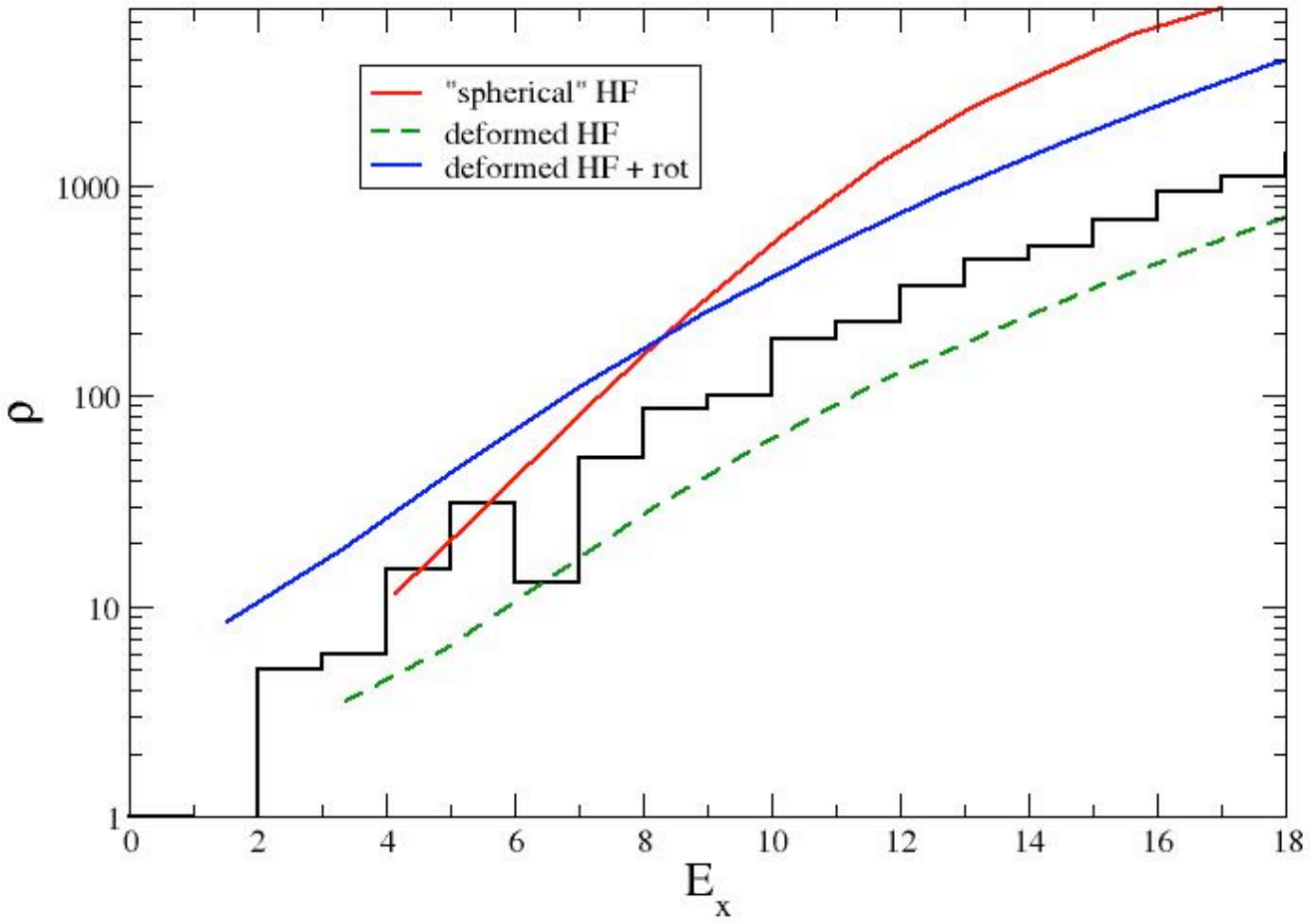
Does it ever not work?


^{26}Al
Exact
"spherical" HF
deformed HF
deformed HF + rot
1000
100
10
1
ρ
0
2
4
6
8
10
12
14
E$_x$


^{47}Ca
Exact
HF (nearly "spherical")
HF + rot
ρ
10000
1000
100
10
1
0
2
4
6
8
10
12
14
16
E$_x$


^{50}Ca
Exact
HF
HF + rot
1000
100
10
1
ρ
0
2
4
6
8
10
12
14
E$_x$


^{26}Mg
exact
"spherical" HF
deformed HF
deformed HF + rot
ρ
1000
100
10
1
0
2
4
6
8
10
12
14
16
E$_x$


^{30}Si
"spherical" HF
deformed HF
deformed HF + rot
ρ
1000
100
10
1
0
2
4
6
8
10
12
14
16
18
E$_x$

Our story so far....

I introduced a simple *ansatz* for the partition function, from mean-field single-particle energies + rotational partition function *derived from the same mean-field solution*.

-- while somewhat *ad hoc*, all nuclei use the same prescription. There is no "backshifting".

The methodology *mostly* works,

except when it doesn't.

What now?

Would be better to systematically derive corrections rather than guessing them.

Also obtaining J-dependence may be difficult.

Nonetheless, current methodology, though flawed, may be worth applying systematically throughout the chart of nuclides.

-> Isospin dependence?
-> What happens when continuum states are low-lying?