Signature of chaos in two-electron atoms

Motivations

- Classical three body problem is chaotic
- Classical-quantum correspondence principle
- Search for signatures of chaos in quantum case
- **No much success in helium up to now**

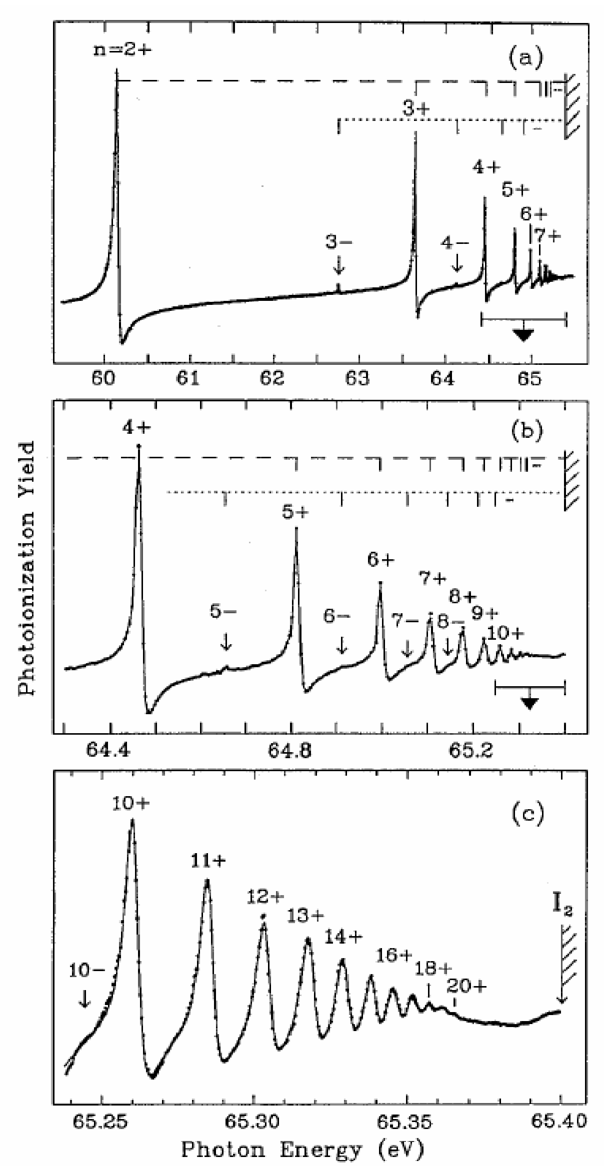
We want to look at the level statistics for helium

Regular
Poisson distribution

Irregular
Wigner distribution

Random-Matrix theory (Wigner 1957) ⟷ Bohigas *et al*. conjecture, PRL 1984

Double-excitation in He below N=2 threshold

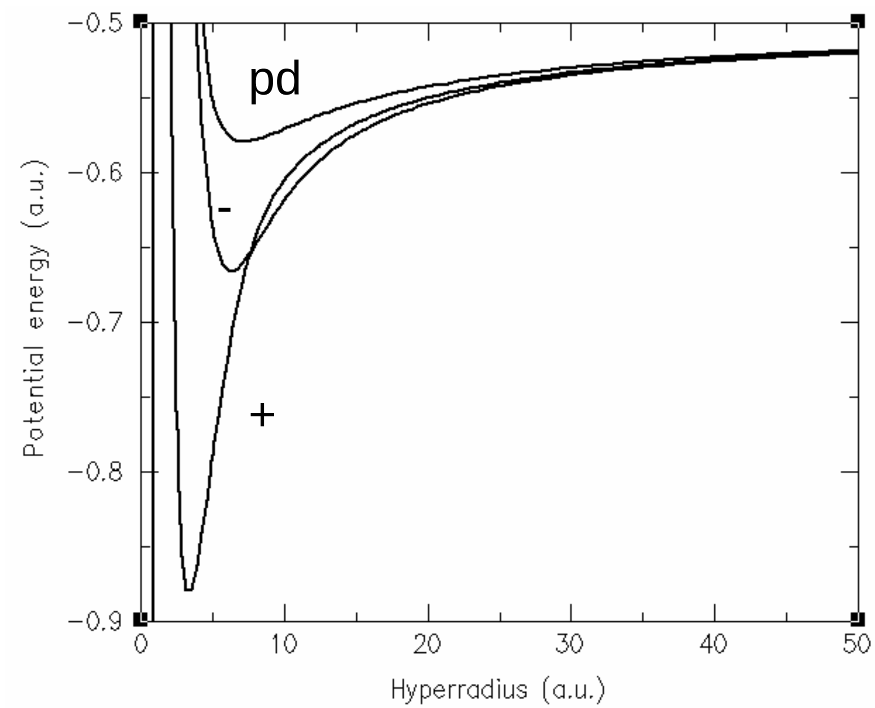


Domke *et al*, PRA **53**, 1424 1996

Three series:

$(K,T)^A=(0,1)^+$, $(1,0)^-$ and $(-1,0)^0$

or simply n+,n-, and 2pnd



Doubly excited states: low N

- Regular spectra
- Existence of approximate quantum numbers K, T

Success of Herrick & Lin’s classification scheme for low N

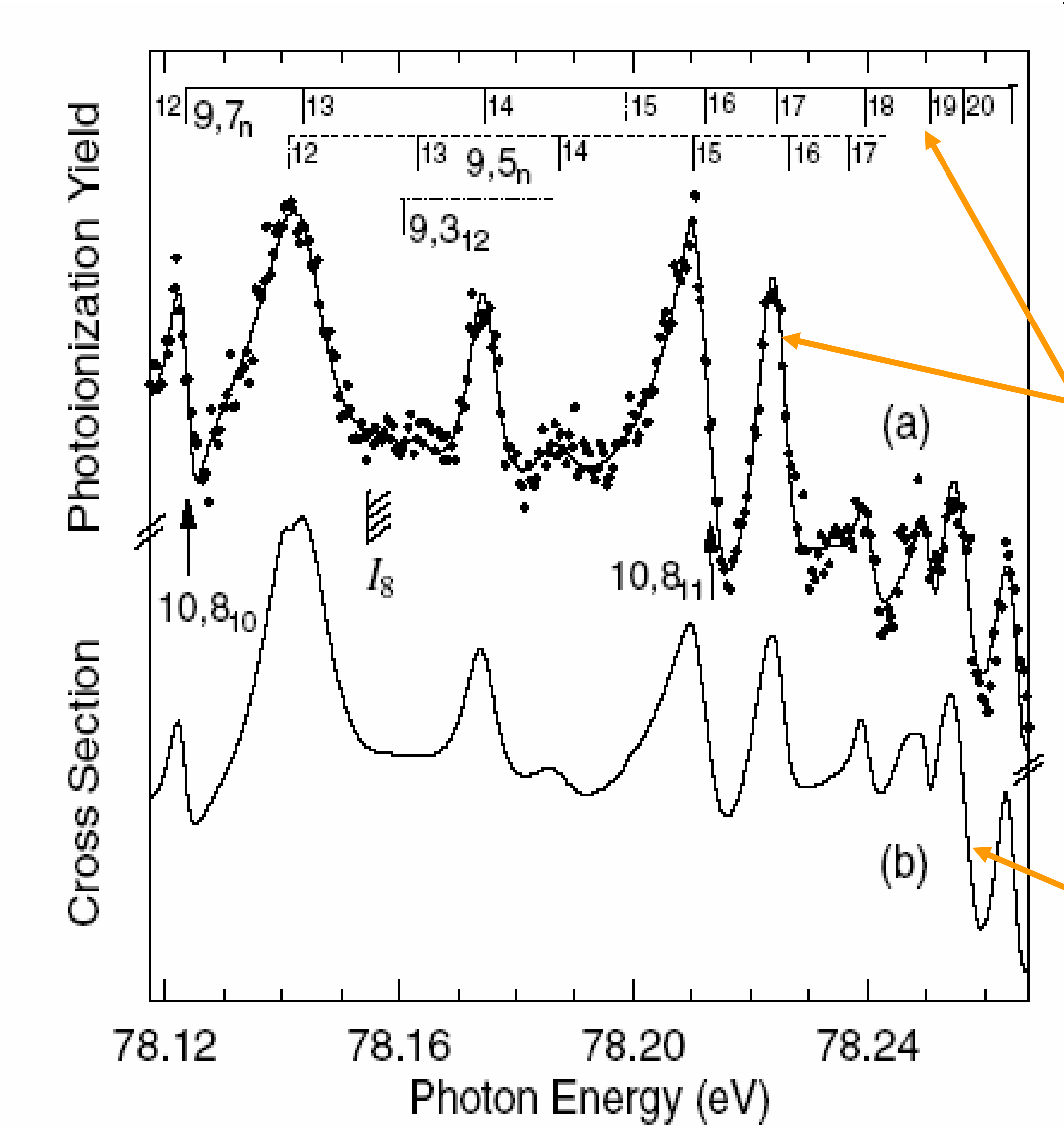
Notation ${}_N(K,T)_n^A$

Shorthand: $(N,K)_n$

Bottom line: **no signature of chaos at low N**

Double-excitation: high energy

(Puttner et al., PRL 2001)



Advanced Light Source (ALS) at Berkeley

Resolution ~ 2meV FWHM

Most intense series: K=N-2

Less regular as compared to lower energy. **Any chaos?**

Theory (complex-rotation method)

Hyperspherical close-coupling method

Main steps:

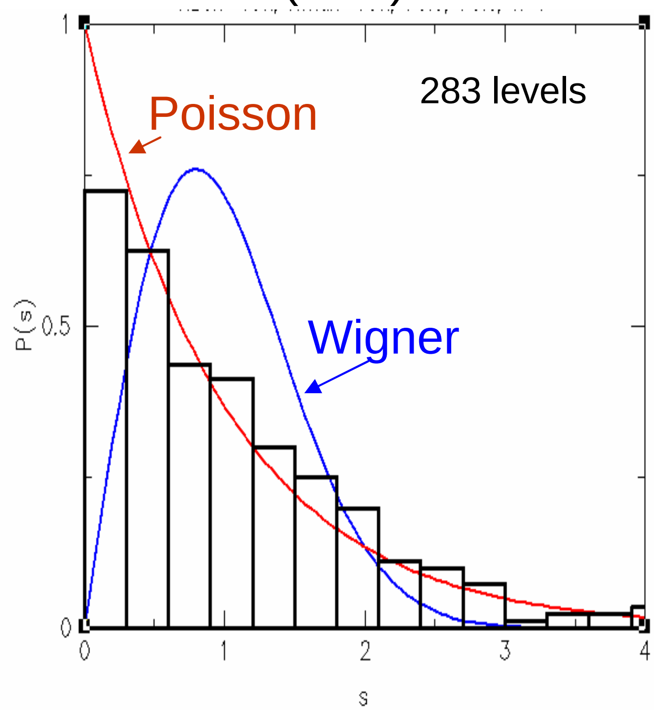
- Get the adiabatic curves by solving adiabatic Eq.
- Diabatization
- Choose the appropriate set of diabatized curves (i.e., truncation)
- Solve the coupled-channel Eqs.

- Statistical analysis of the energy levels

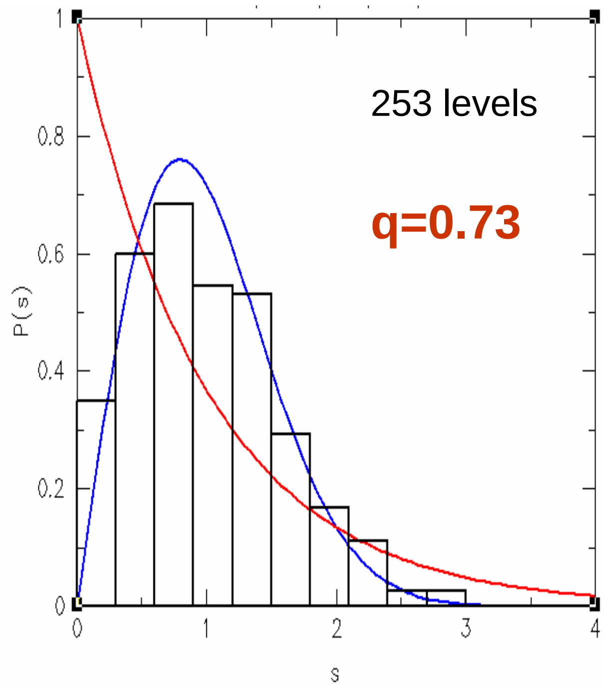
S^2 model: assume each electron has l=0

Nearest-neighbor-spacing distribution $I_{N=25}<E<I_{N=30}$

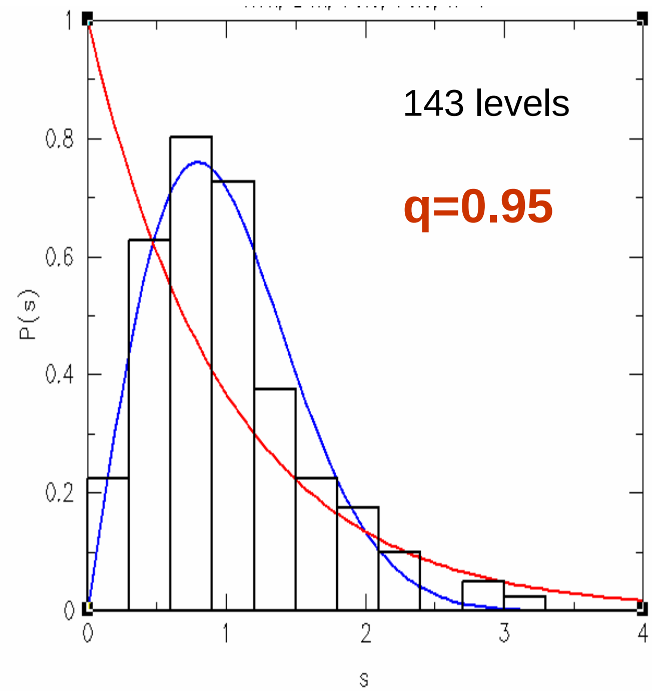
Independent electrons ($Z=\infty$)



C^{4+} (Z=6)

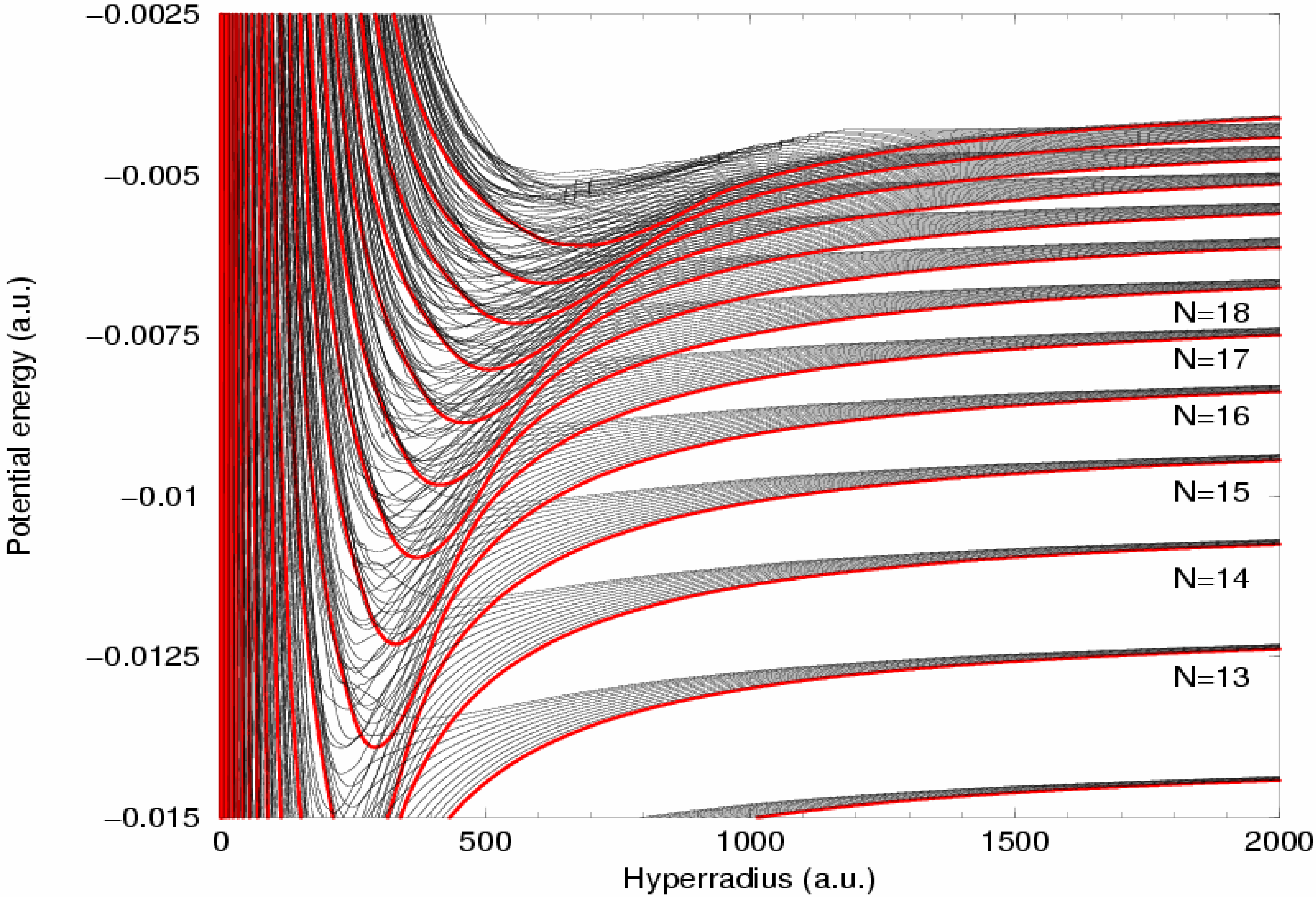


He (Z=2)



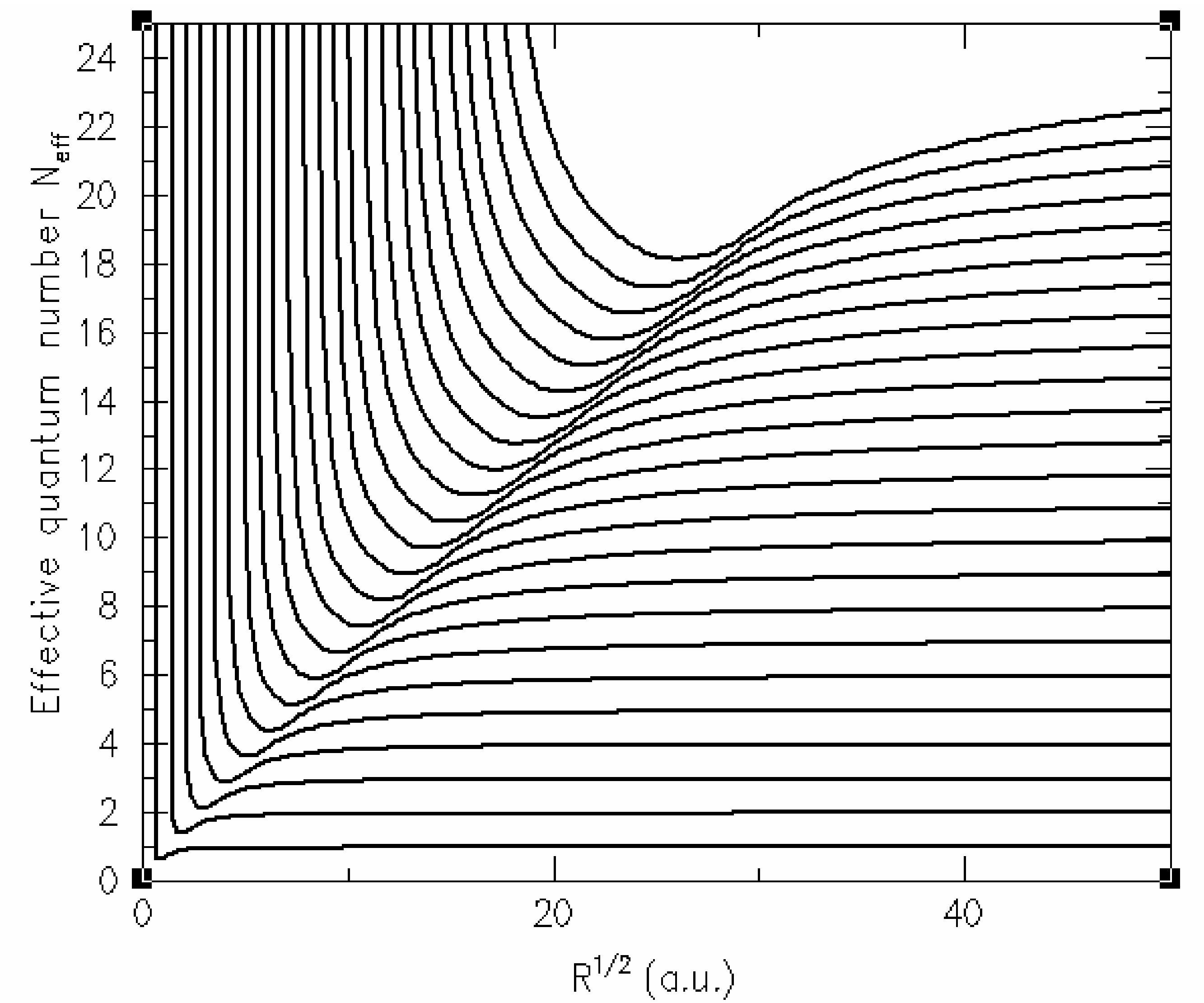
- For all: scaled R_{box}=10,000 au, Rmax=15,000 au
- Independent electron results are also calculated by HSCC (compare very well with exact solutions)

$^1S^e$ diabatized potential curves for real 3D helium



Lowest diabatized curves from each manifold of $^1S^e$ 3D helium

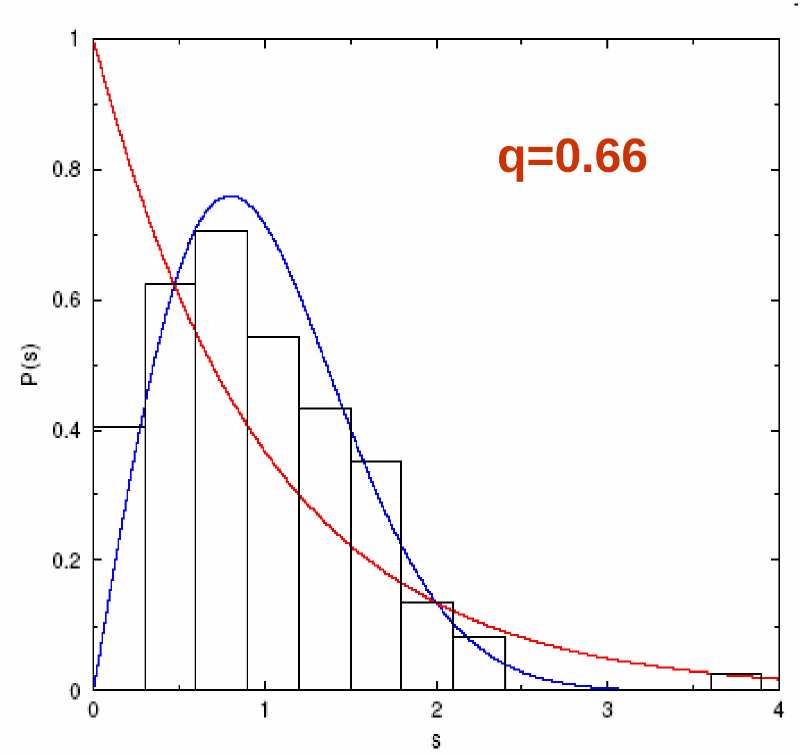
up to N=24

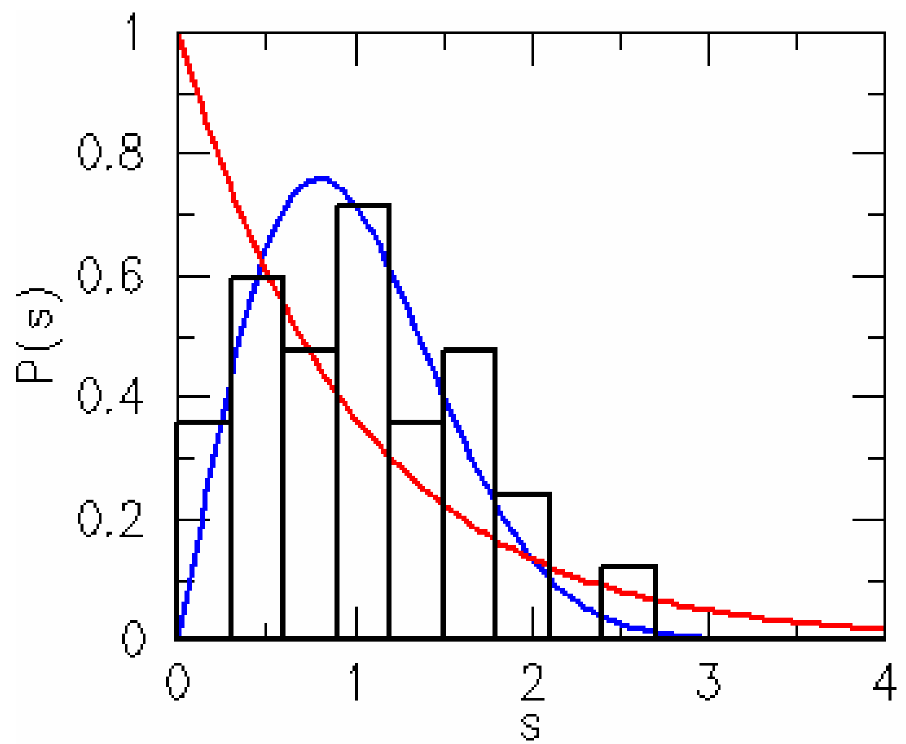


Resemblance to the s^2 model

3D He($^1S^e$): NNS distribution

$I_{15}<E<I_{20}$





$I_{15}<E<I_{20}$

139 levels

$I_{15}<E<I_{16}$

30 levels

R_{max}=3,000 au R_{box}=2,000 au

Summary & Outlook

- Simple method for calculating high-lying doubly excited states
- Evidence for the transition to chaotic regime

Future:

- Analysis of the S-matrix
- Photo-ionization cross section at high energy N>9 (positions & widths)
- Above three-body breakup threshold (Wannier threshold law vs. Temkin model)