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
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
Independent electrons
\( Z = \infty \)

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

Nearest-neighbor-spacing distribution \( I_{N=25} < E < I_{N=30} \)

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

\begin{itemize}
  \item Poisson
  \item Wigner
  \item \( q = 0.73 \)
  \item \( q = 0.95 \)
  \item 283 levels
  \item 253 levels
  \item 143 levels
\end{itemize}
$^1S^e$ 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

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

$q = 0.66$

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

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

$R_{\text{max}} = 3,000$ au  \hspace{1cm} R_{\text{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)