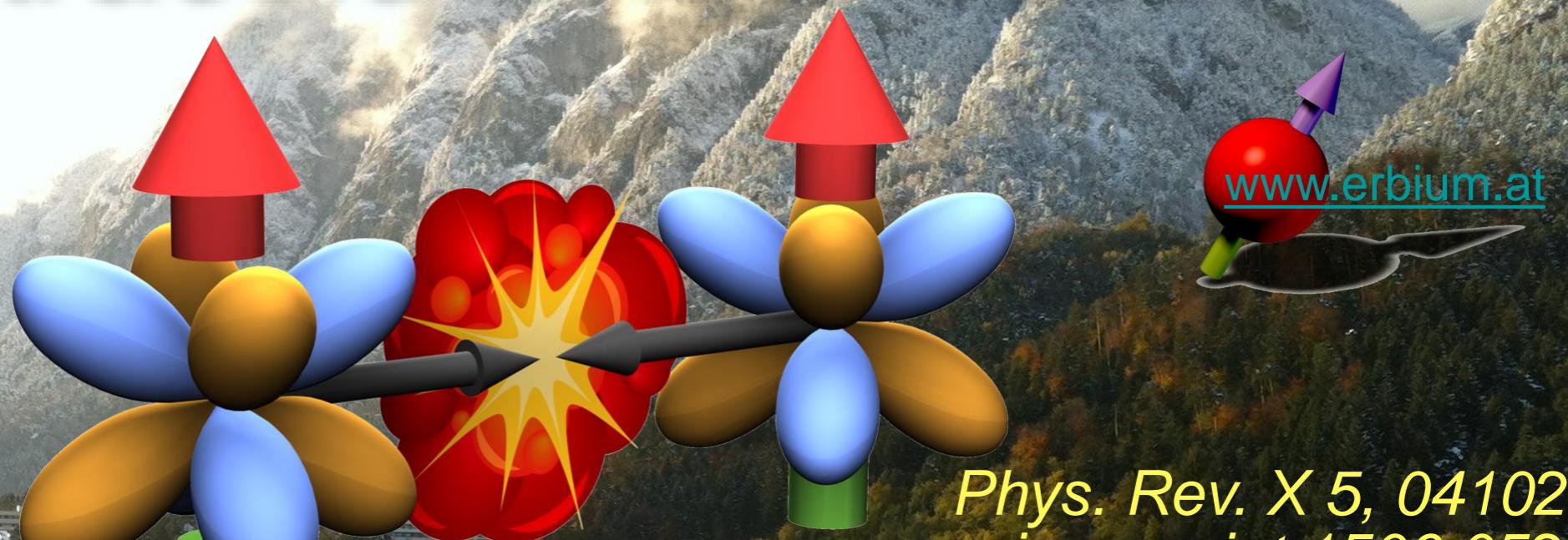
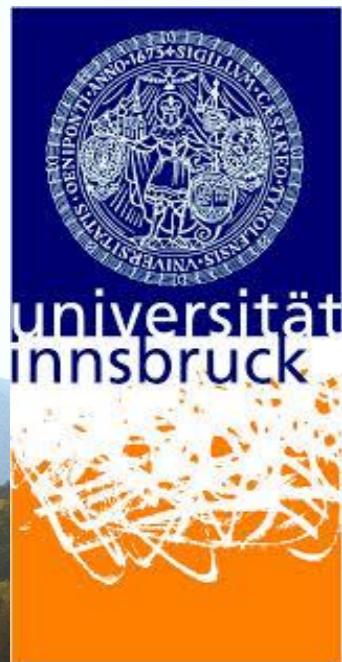


Emergence of chaotic scattering in ultracold lanthanides.



Phys. Rev. X 5, 041029
arxiv preprint 1506.05221

A. Frisch, S. Baier, K. Aikawa, L. Chomaz, M. J. Mark, F. Ferlaino
in collaboration with :

Dy group in Stuttgart: T. Maier, H. Kadau, M. Schmitt, M. Wenzel, I. Ferrier-Barbut, T. Pfau
Theory group in Temple/Maryland: C. Makrides, A. Petrov, and S. Kotochigova, E. Tiesinga.



Outline of the talk



- ◆ Toward non-alkali atoms, the quest for atomic richness and the case of magnetic atoms.
- ◆ Specificity of scattering of ultracold lanthanides
- ◆ Random Matrix Theory: Complex systems, dense spectra and chaos
- ◆ Chaos in Feshbach resonances of Lanthanides: First Erbium study and beyond, describing lanthanides chaoticity.
- ◆ Towards a theoretical understanding of the origin of chaos in lanthanides scattering

Experimental achievement of BEC



www.erbium.at

1 1 H hydrogen 1993	2 3 Li lithium 1995	4 beryllium 9.012	5 23 Ti titanium 47.87	6 24 Cr chromium 50.94	7 25 Mn manganese 54.94	8 26 Fe iron 55.85	9 27 Co cobalt 58.93	10 28 Ni nickel 58.69	11 29 Cu copper 63.55	12 30 Zn zinc 65.38(2)	13 31 Al aluminium 26.98	14 32 Si silicon 28.08; 28.09	15 33 P phosphorus 30.97	16 34 S sulfur 32.05; 32.08	17 35 Cl chlorine 35.44; 35.46	18 2 He helium 4.003 2001	
19 20 K potassium 39.10 1991 2009	21 Sc scandium 44.96	22 Ti vanadium 50.94	23 V chromium 52.00	24 Cr chromium 52.00 2004	25 Mn manganese 54.94	26 Fe iron 55.85	27 Co cobalt 58.93	28 Ni nickel 58.69	29 Cu copper 63.55	30 Zn zinc 65.38(2)	31 Ga gallium 69.72	32 Ge germanium 72.63	33 As arsenic 74.92	34 Se selenium 78.96(3)	35 Br bromine 79.90	36 Kr krypton 83.80	
37 38 Rb rubidium 85.47 1995 2009	39 Sr strontium 87.62 2009	40 Y yttrium 88.91	41 Zr zirconium 91.22	42 Nb niobium 92.91	43 Mo molybdenum 95.96(2)	44 Tc technetium	45 Ru ruthenium 101.1	46 Rh rhodium 102.9	47 Pd palladium 106.4	48 Ag silver 107.9	49 Cd cadmium 112.4	50 In indium 114.8	51 Sn tin 118.7	52 Sb antimony 121.8	53 Te tellurium 127.6	54 Xe xenon 131.3	
55 Cs cesium 132.9 2002	56 Ba barium 137.3	57-71 lanthanoids	72 Hf hafnium 178.5	73 Ta tantalum 180.9	74 W tungsten 183.8	75 Re rhenium 186.2	76 Os osmium 190.2	77 Ir iridium 192.2	78 Pt platinum 195.1	79 Au gold 197.0	80 Hg mercury 200.6	81 Tl thallium [204.3; 204.4]	82 Pb lead 207.2	83 Bi bismuth 209.0	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium	114 Fl flerovium	116 Lv livermorium				
57 La lanthanum 138.9	58 Ce cerium 140.1	59 Pr praseodymium 140.9	60 Nd neodymium 144.2	61 Pm promethium	62 Sm samarium 150.4	63 Eu europium 152.0	64 Gd gadolinium 157.3	65 Tb terbium 158.9	66 Dy dysprosium 162.5	67 Ho holmium 164.9	68 Er erbium 167.3	69 Tm thulium 168.9	70 Yb ytterbium 173.1	71 Lu lutetium 175.0			
89 Ac actinium	90 Th thorium 232.0	91 Pa protactinium 231.0	92 U uranium 238.0	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium			

The different condensed atoms



www.erbium.at

Bose-Einstein condensates

1 H hydrogen [1.008; 1.008]	1993
3 Li lithium [6.938; 6.997]	1995
11 Na sodium 22.99	1995
19 K potassium 39.10	2001
20 Ca calcium 40.08	2009
37 Rb rubidium 85.47	1995
38 Sr strontium 87.62	2009
55 Cs cesium 132.9	2002

One-electron atom
“simple” electronic structure ($L=0$),
tunable contact interaction!

$$U_c = \frac{4\pi\hbar^2 a}{m} \delta(r)$$

metastable state

2 He helium 4.003

$$V_{dd} = \frac{\mu_0 \mu^2}{4\pi} \frac{1 - 3 \cos^2 \theta}{r^3}$$

Multi-electron atom
“complex” electronic structure (L very large), tunable contact interaction and DDI!

66 Dy dysprosium 162.5

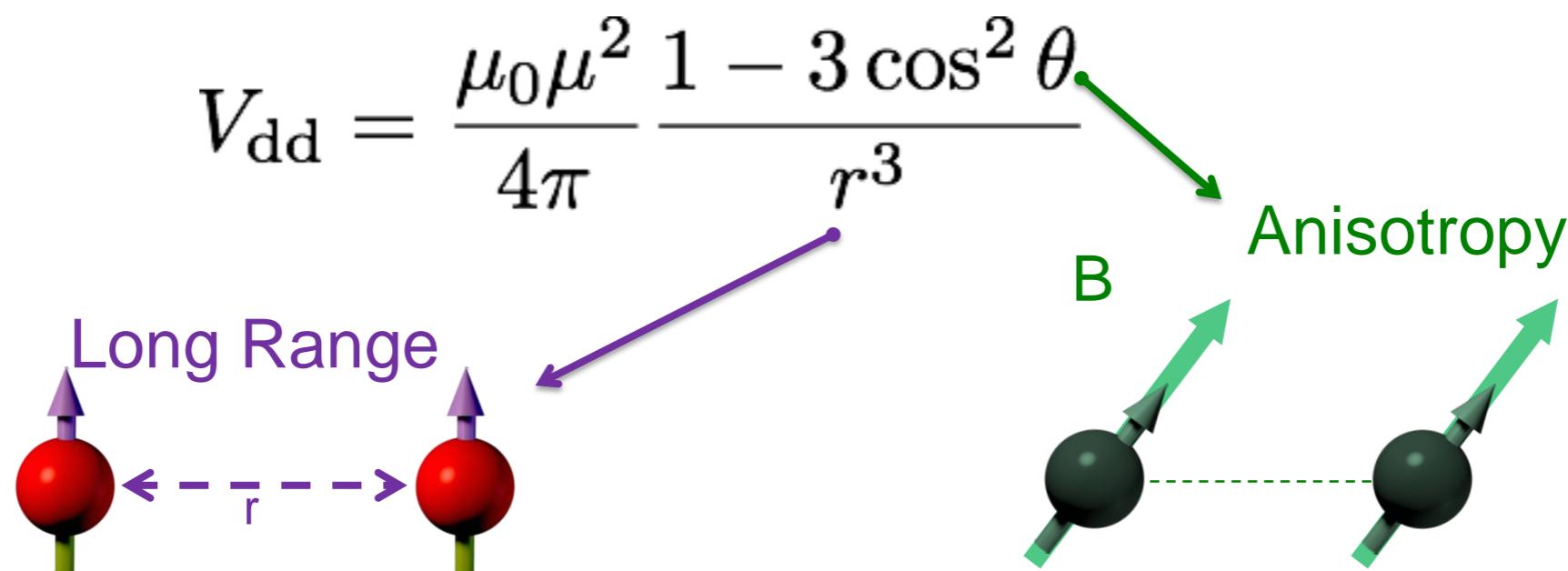
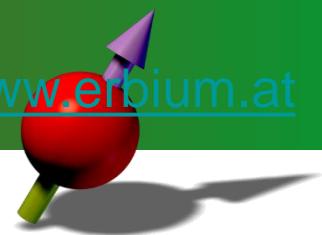
68 Er erbium 167.3

70 Yb ytterbium 173.1

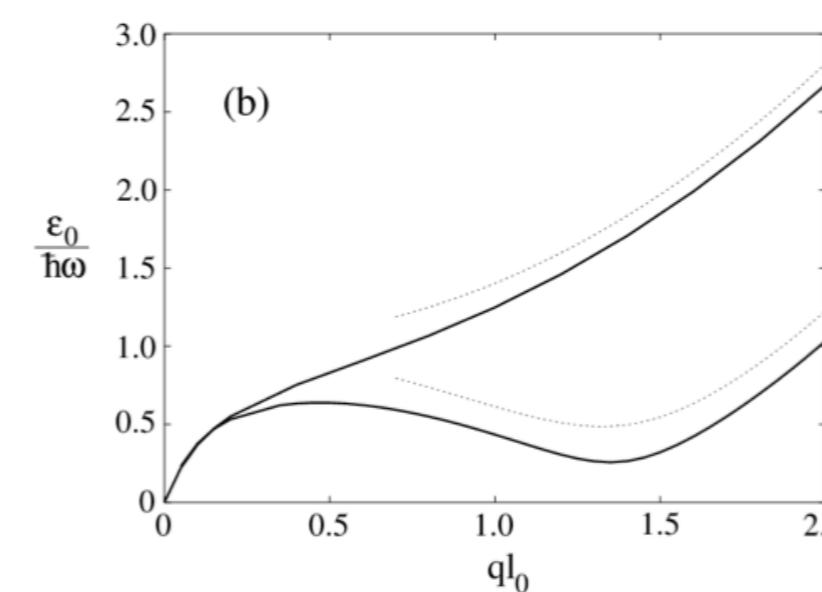
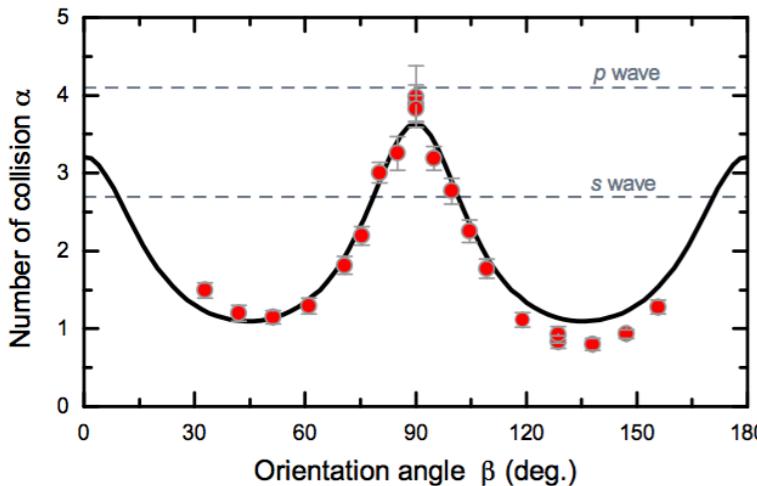
Two-electron atoms
“simple” electronic and nuclear structure ($L=0$, $S=0$ and $I=0$), clock transitions, ...

More laser cooled species: Ho and Tm

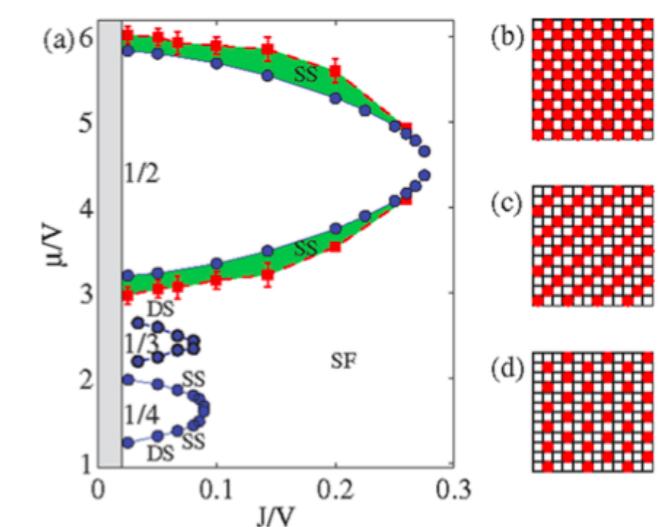
Strongly dipolar systems



Few-body Physics
anisotropic scattering amplitude,
different scattering behavior at low
T, partial wave decomposition...



Many-body Physics
e.g. ground state properties, spectrum
of excitations, novel quantum phases



Outline of the talk



- ◆ Toward non-alkali atoms, the quest for atomic richness and the case of magnetic atoms.
- ◆ Specificity of scattering of ultracold lanthanides (Ln)
- ◆ Random Matrix Theory: Complex systems, dense spectra and chaos
- ◆ Chaos in Feshbach resonances of Lanthanides: First Erbium study and beyond, describing lanthanides chaoticity.
- ◆ Towards a theoretical understanding of the origin of chaos in lanthanides scattering

Specific structure of Ln atoms

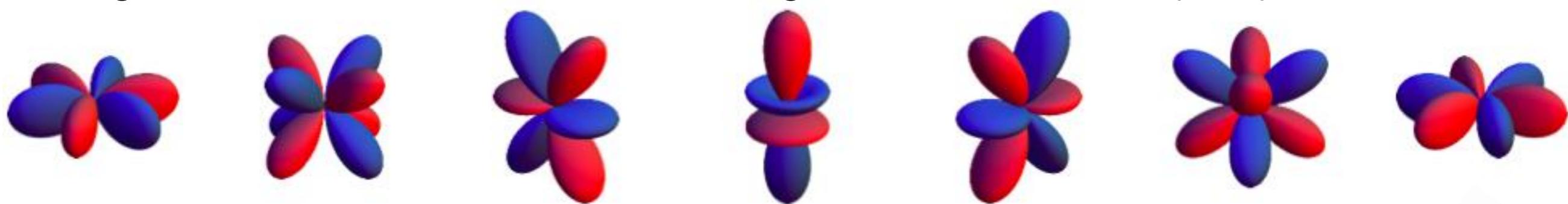


www.erbium.at

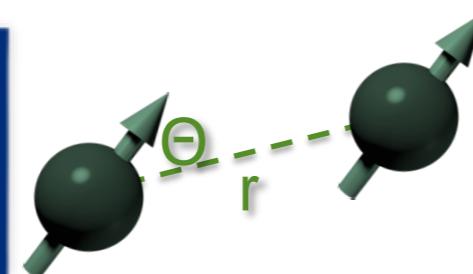
laser-cooled members
Lanthanide (Ln) family

	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	ytterbium 70 Yb 173.04
	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	einsteinium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]

- ◆ partially filled 4f electron shell, submerged below a filled 6s shell.
- ◆ ground state with vacancies of large m_f of the f -shell ($\ell=3$) *f* orbital basis



Large magnetic moment μ !



Magnetic Anisotropy
(long range)

(Erbium $\mu \approx 7\mu_B$, Dysprosium $\mu \approx 10\mu_B$)

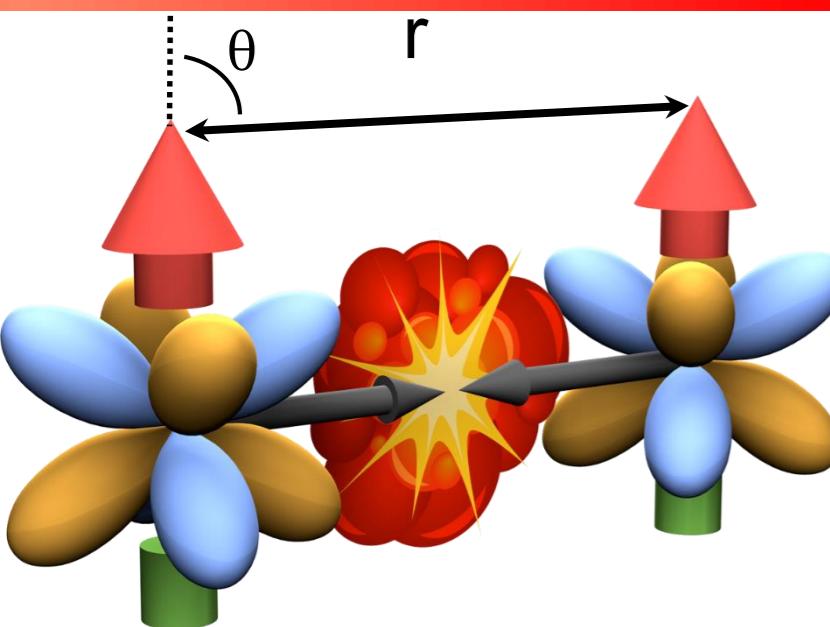
Large total angular momentum j !



Large ground state degeneracy + Orbital Anisotropy (short range)

(Erbium $j=6$, Dysprosium $j=8$)

Interactions of lanthanides atoms



$$\hat{H}_{\text{rel}} = -\frac{\hbar^2}{2\mu_r} \frac{d^2}{d^2\vec{r}} + \hat{V}(\vec{r}) \left(+ \hat{H}_Z(B) \right)$$

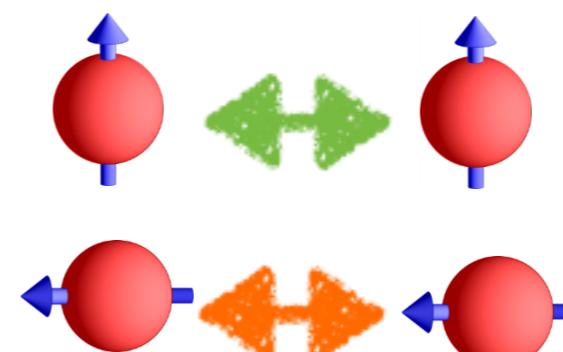
μ_r : reduced mass

Zeeman energy

Which specific interaction potential $\hat{V}(\vec{r})$ for lanthanide atoms?

Dipole-Dipole interaction (DDI):

$$V_{\text{dd}}(\vec{r}) = -\frac{C_3}{|\vec{r}|^3} (3 \cos^2 \theta - 1)$$

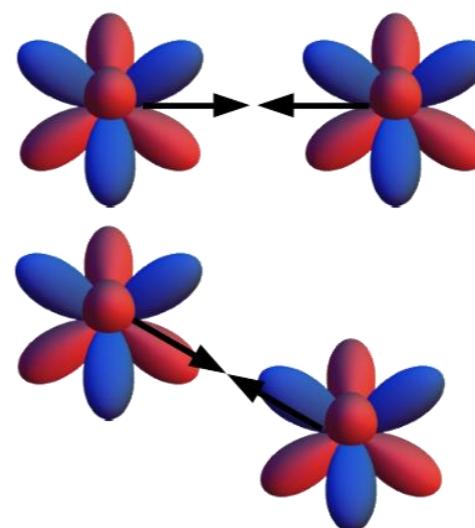


$$C_3 = \frac{\mu_0 \mu^2}{4\pi}$$

Anisotropic van der Waals dispersion:

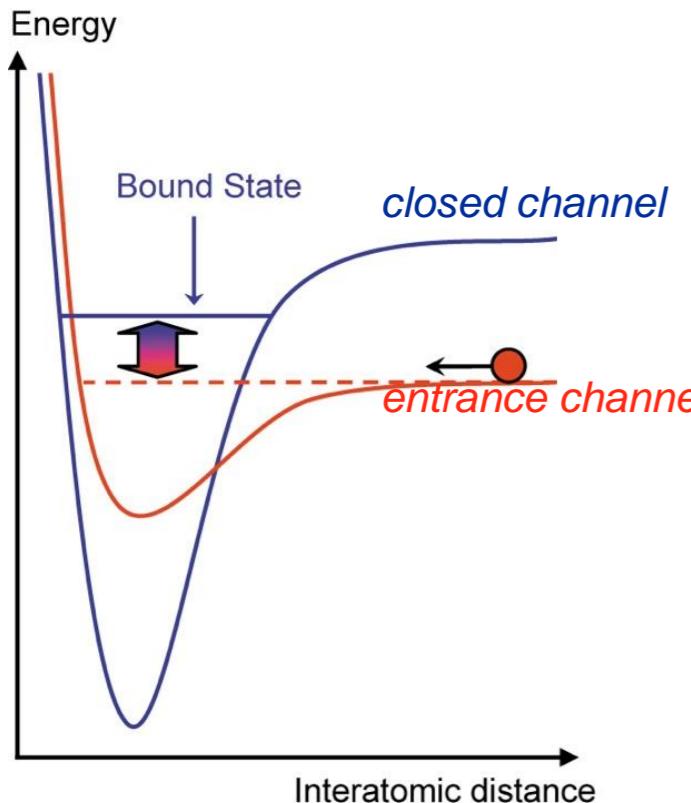
$$V_{\text{vdW}}(\vec{r}) = -\frac{C_6}{|\vec{r}|^6}$$

$$-\frac{C_6^{\text{ani}}}{|\vec{r}|^6} (3 \cos^2 \theta - 1)$$



	C ₆ (u.a)	ΔC ₆ (u.a)
Er	1703	174
Dy	2003	188

Feshbach resonances in Ln



Alkali atoms

→ coupling btw Zeeman states induced by hyperfine coupling btw electron and nuclear spins.

- ★ perturbative, weak coupling
- ★ isotropic
- ★ few channels are coupled

$$\hat{H}_{\text{rel}} = -\frac{\hbar^2}{2\mu_r} \frac{d^2}{d^2\vec{r}} + \hat{V}(\vec{r}) + \hat{H}_Z(B)$$

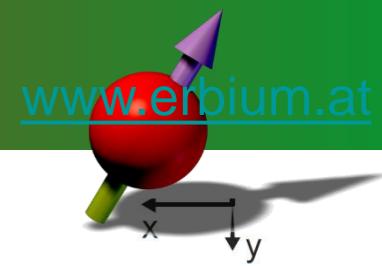
≠
Scattering
scheme!

Lanthanides atoms

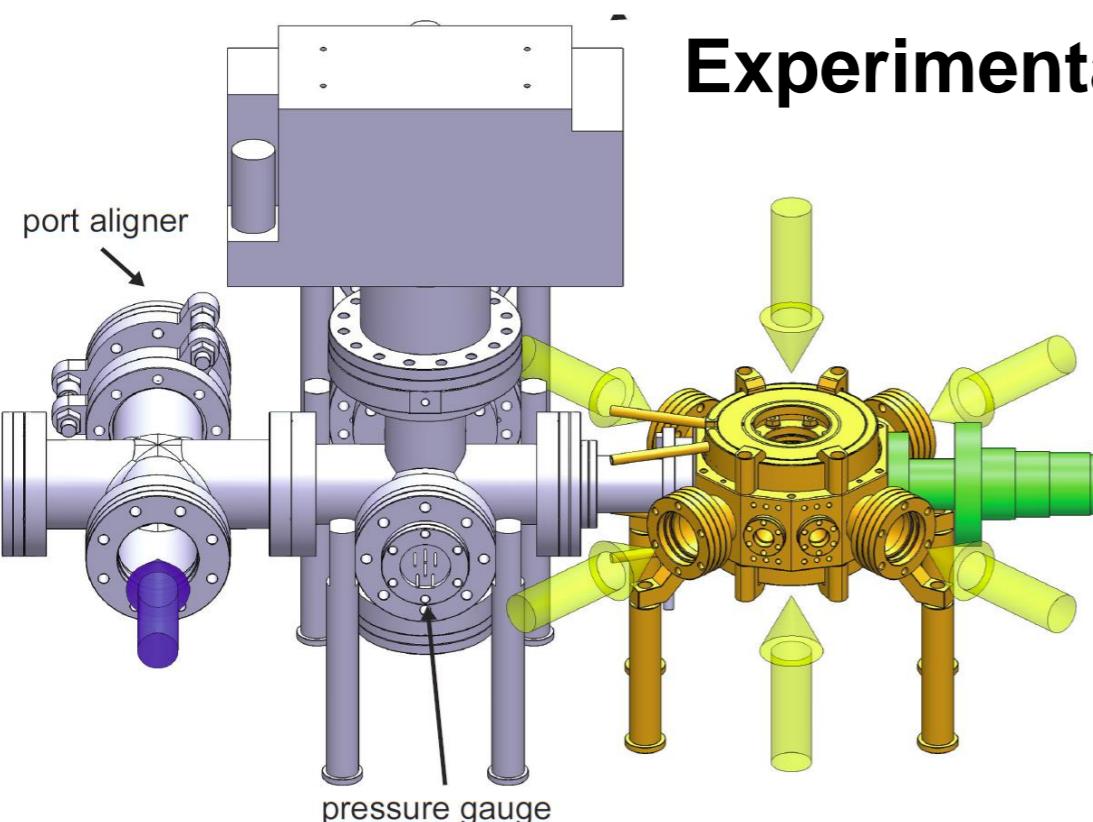
$$\hat{V}(\vec{r}) = \hat{V}_{\text{iso}}(\vec{r}) + \hat{V}_{\text{ani}}(\vec{r})$$

- coupling btw Zeeman states induced by interaction potential itself (V_{ani}).
- ★ typically stronger coupling.
 - ★ anisotropic: bound-states can have $\ell \neq 0$.
 - ★ a large number of channels are coupled (large j).
 - ★ [Partial wave are not a natural basis]

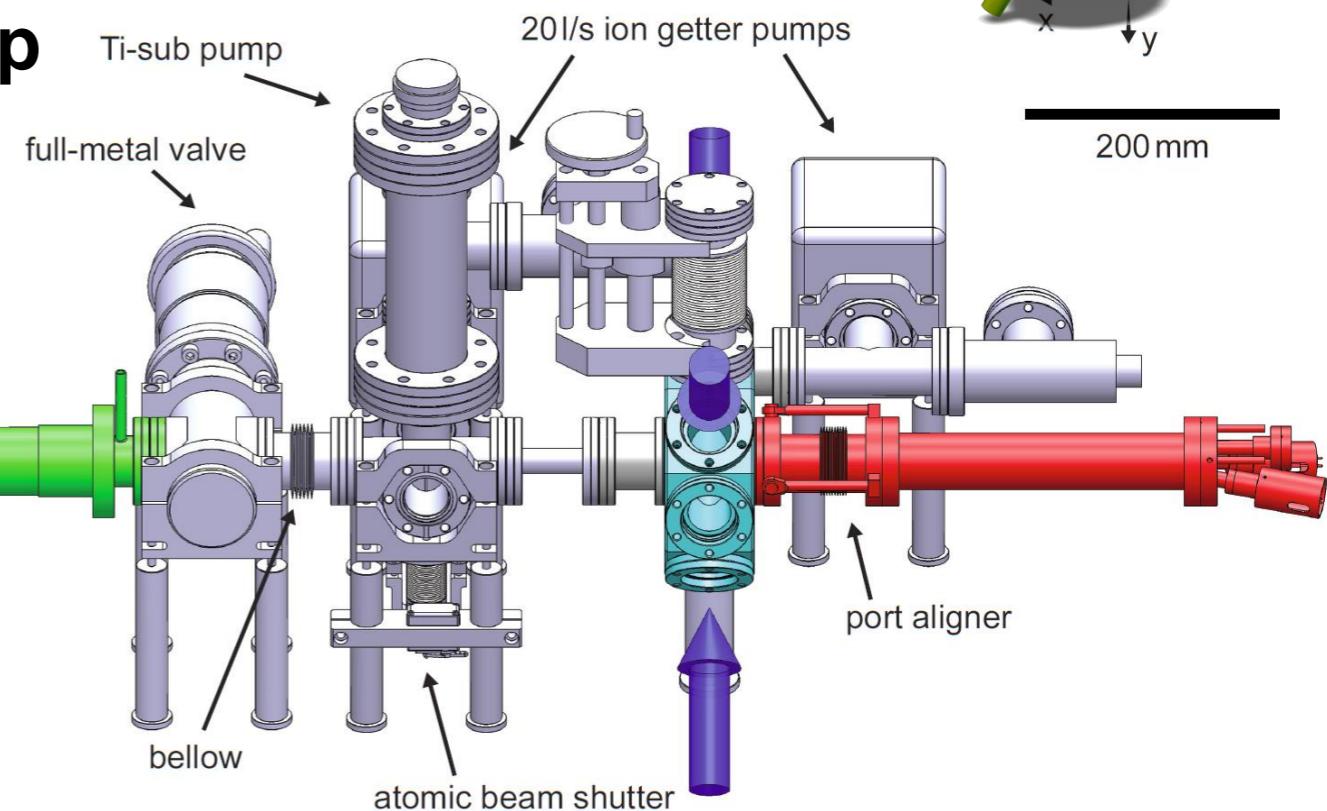
Feshbach Spectroscopy in Ln



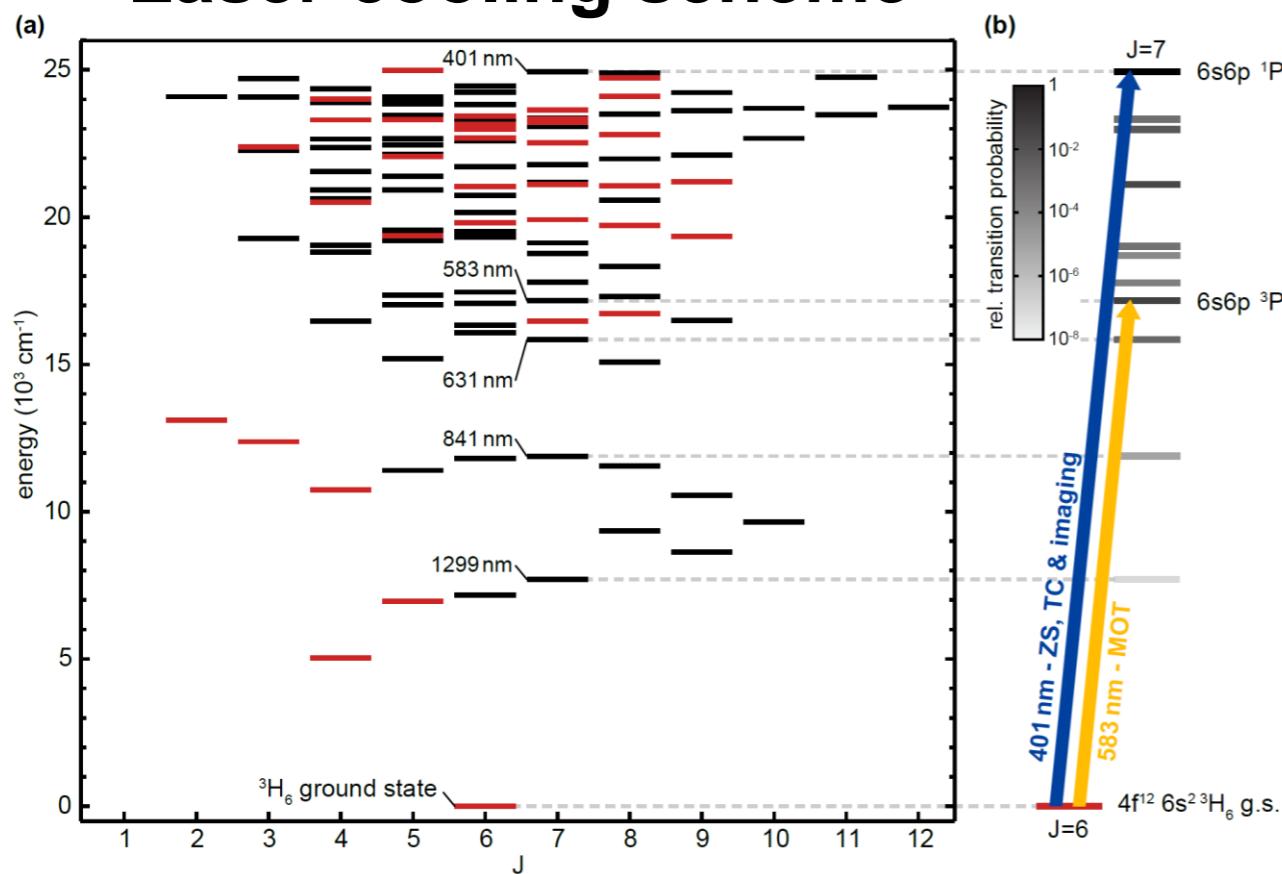
www.erbium.at



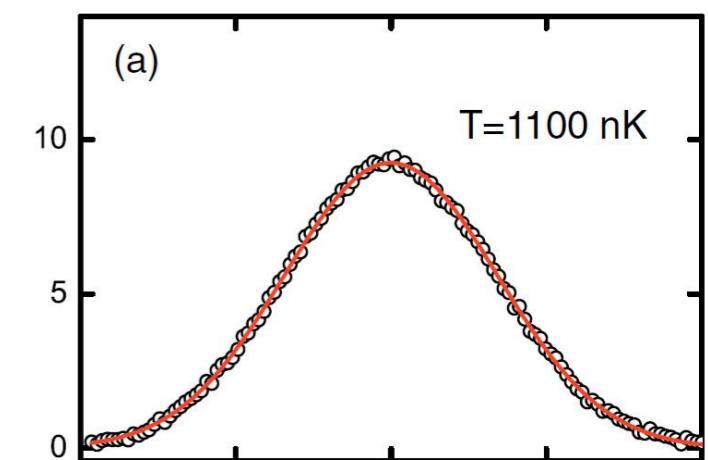
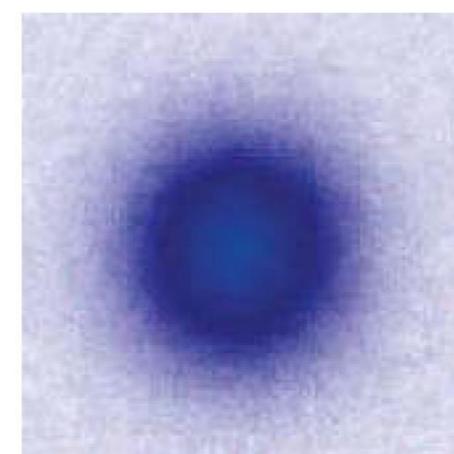
Experimental setup



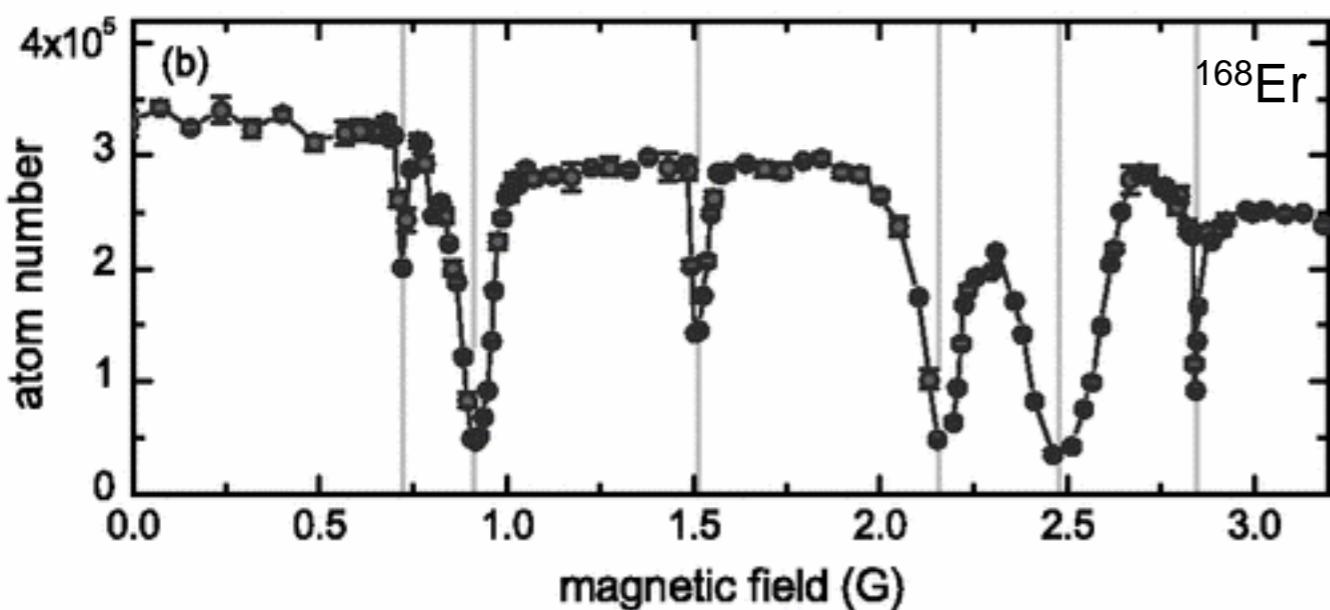
Laser cooling scheme



Detection



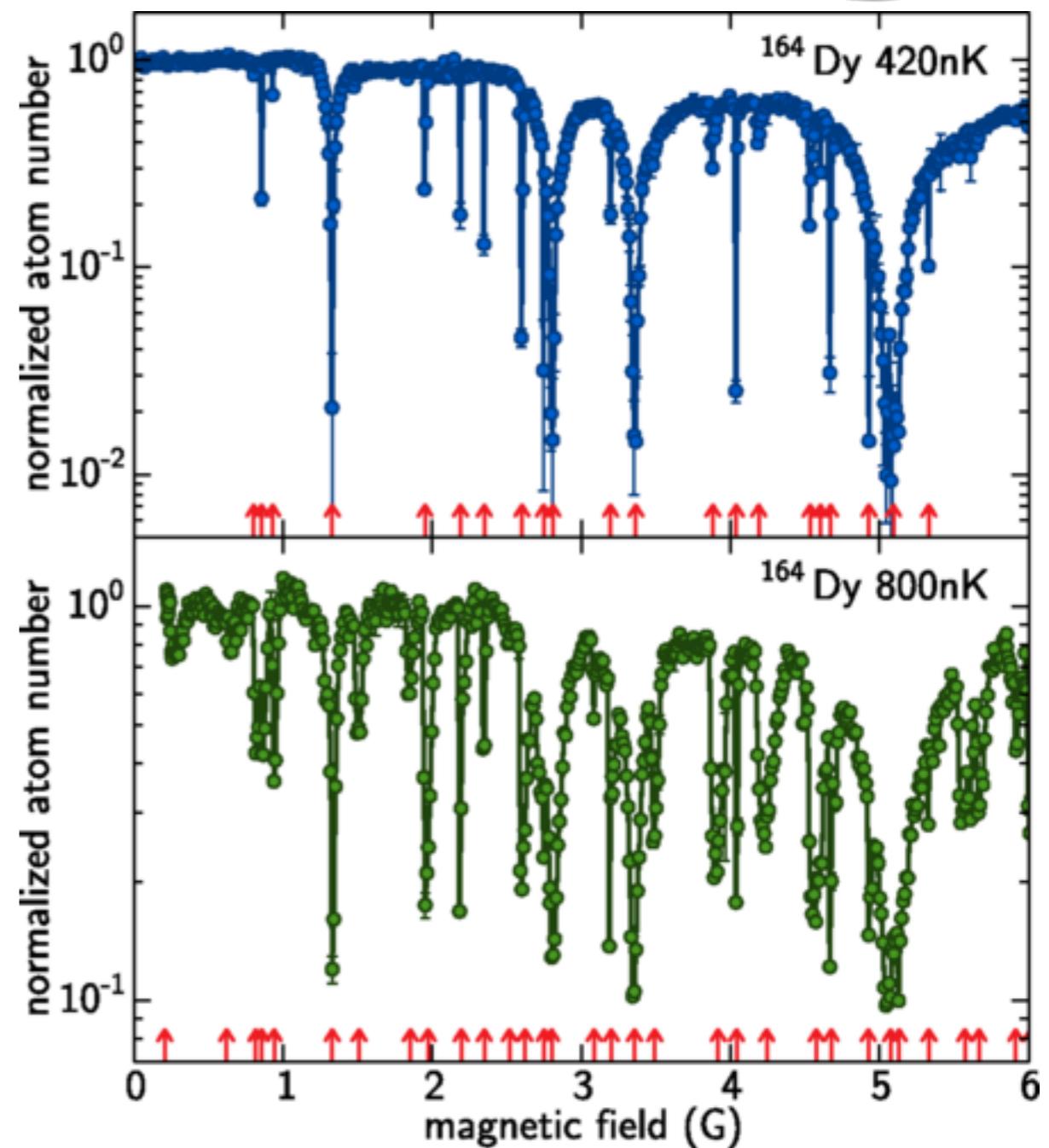
Feshbach Spectroscopy in Ln



Er: K. Aikawa, A. Frisch, M. Mark, S. Baier, A. Rietzler, R. Grimm, and F. Ferlaino, Phys. Rev. Lett. 108, 210401 (2012).

+ Theory works:

A. Petrov, E. Tiesinga, S. Kotochigova, PRL 109 103002 (2012)
for a review, see Svetlana Kotochigova, Report on progress in physics, 77,
093901 (2014)



Dy: K. Baumann, N. Q. Burdick, M. Lu, and B. L. Lev, Phys. Rev. A 89, 020701 (2014)

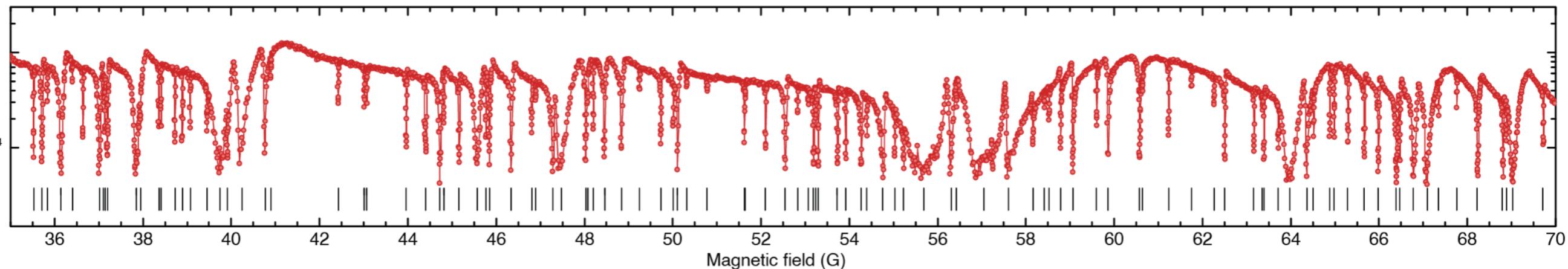
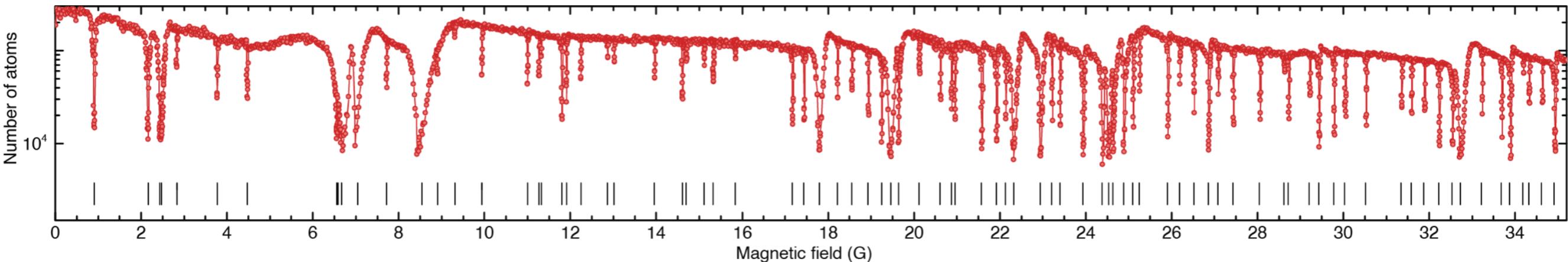
- ◆ high # of resonances compared to alkali: **several per Gauss.**
- ◆ Not easy to encompass from the theory side: **traditional methods fail...**

Feshbach Spectroscopy in Ln



Er: A. Frisch, M. Mark, K. Aikawa, F. Ferlaino, J. L. Bohn, C. Makrides, A. Petrov, and S. Kotchigova, Nature 507, 475 (2014)

Er 168



extensive high-resolution trap loss spectroscopy measurements: 13 200 points

- ◆ Very dense spectra (compare to alkali): **~200 resonances in [0,70]G!!**
- ◆ Not easy to encompass from the theory side: **traditional methods fail...**

Outline of the talk

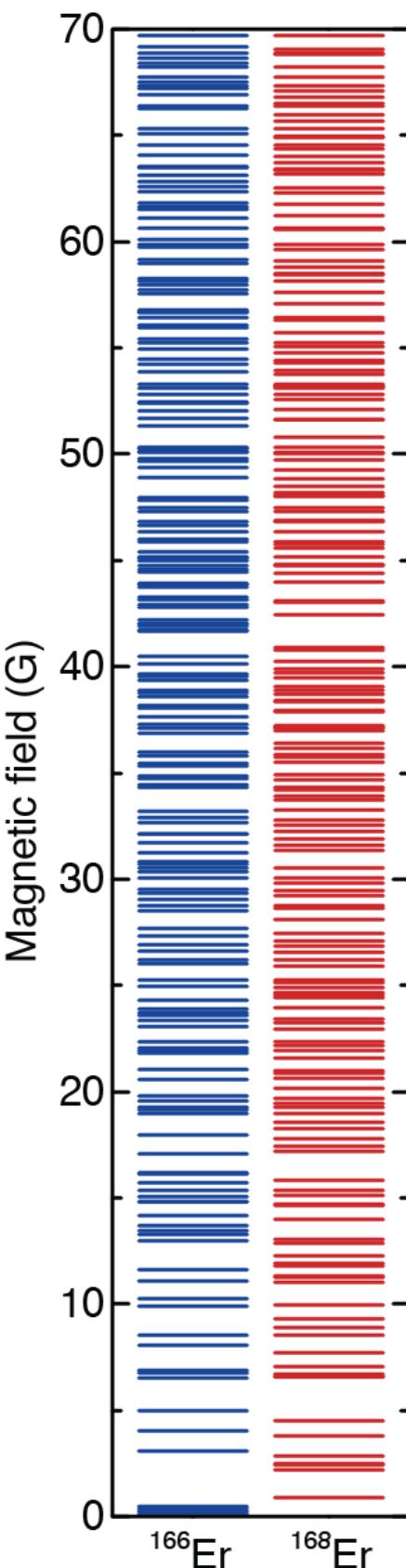


- ◆ Toward non-alkali atoms, the quest for atomic richness and the case of magnetic atoms.
- ◆ Specificity of scattering of ultracold lanthanides
- ◆ Random Matrix Theory: Complex systems, dense spectra and chaos
- ◆ Chaos in Feshbach resonances of Lanthanides: First Erbium study and beyond, describing lanthanides chaoticity.
- ◆ Towards a theoretical understanding the origin of chaos

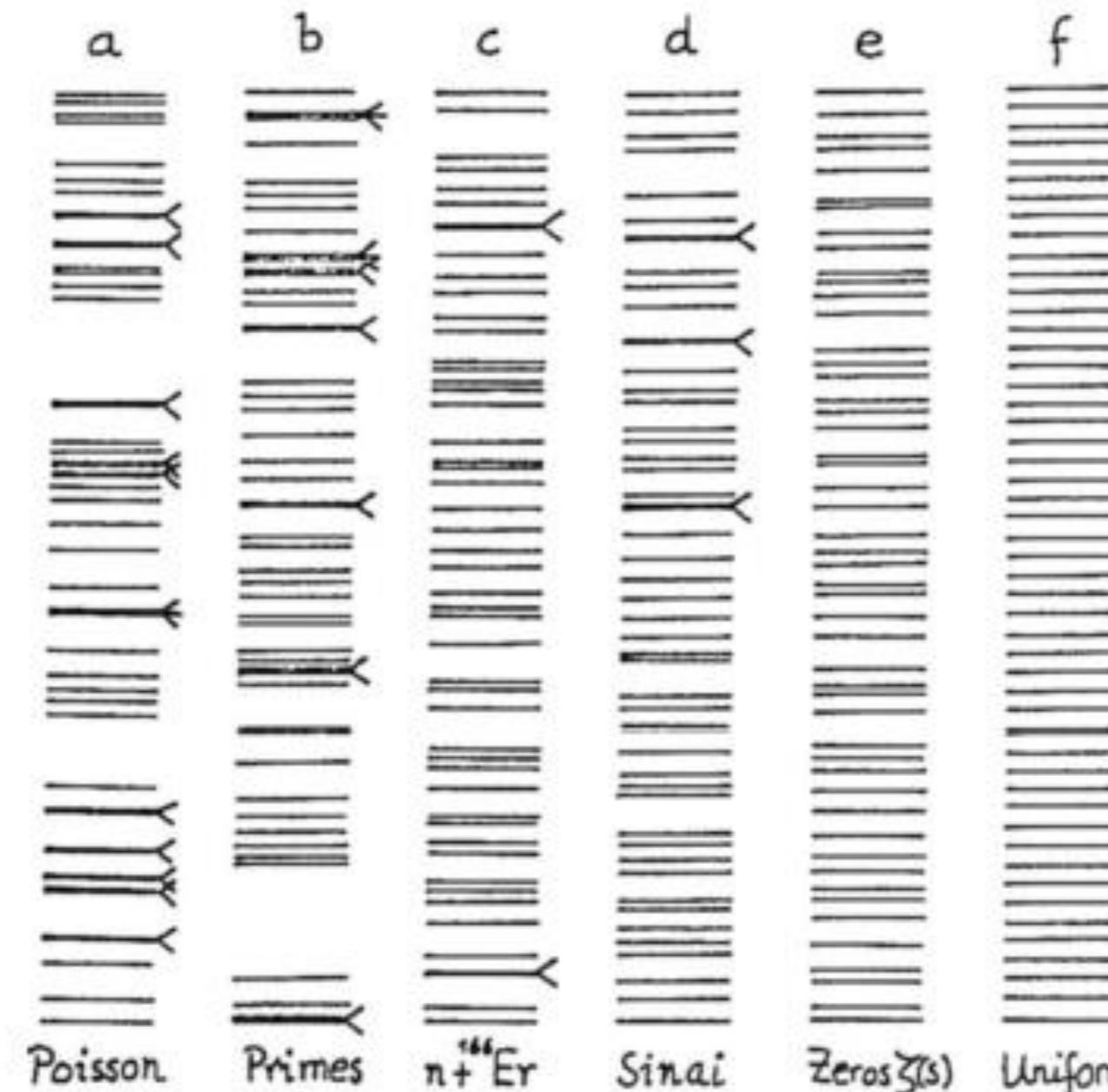
Handling complex spectra



www.erbium.at



Wigner (1950):
Can we identify / forecast **global** spectral properties of a system with complex interactions without integrating the microscopic Hamiltonian ? \Rightarrow statistical approach



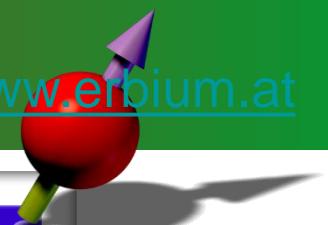
Pseudorandom Matrix

- How to characterize some properties of systems with complex spectra?
Characterised by few statistical properties of the energy spectrum

Look at the global properties of the spectrum
= **correlations**

Bohigas and Giannoni (1984)

Random Matrix Theory



Can predict global spectrum properties:

- Without integrating the real Hamiltonian.
- Statistical analysis of a set of random Hamiltonians.

$$\hat{H}_{\text{real}} \longrightarrow \left\{ \hat{H}_i^{\text{random}} = \begin{pmatrix} H_{1,1} & \cdots & H_{1,n} \\ \vdots & \ddots & \vdots \\ H_{n,1} & \cdots & H_{n,n} \end{pmatrix}_i \right\}_{i \in [1, N]}$$

random coupling terms
Gaussian distributed

Condition on the random matrix:

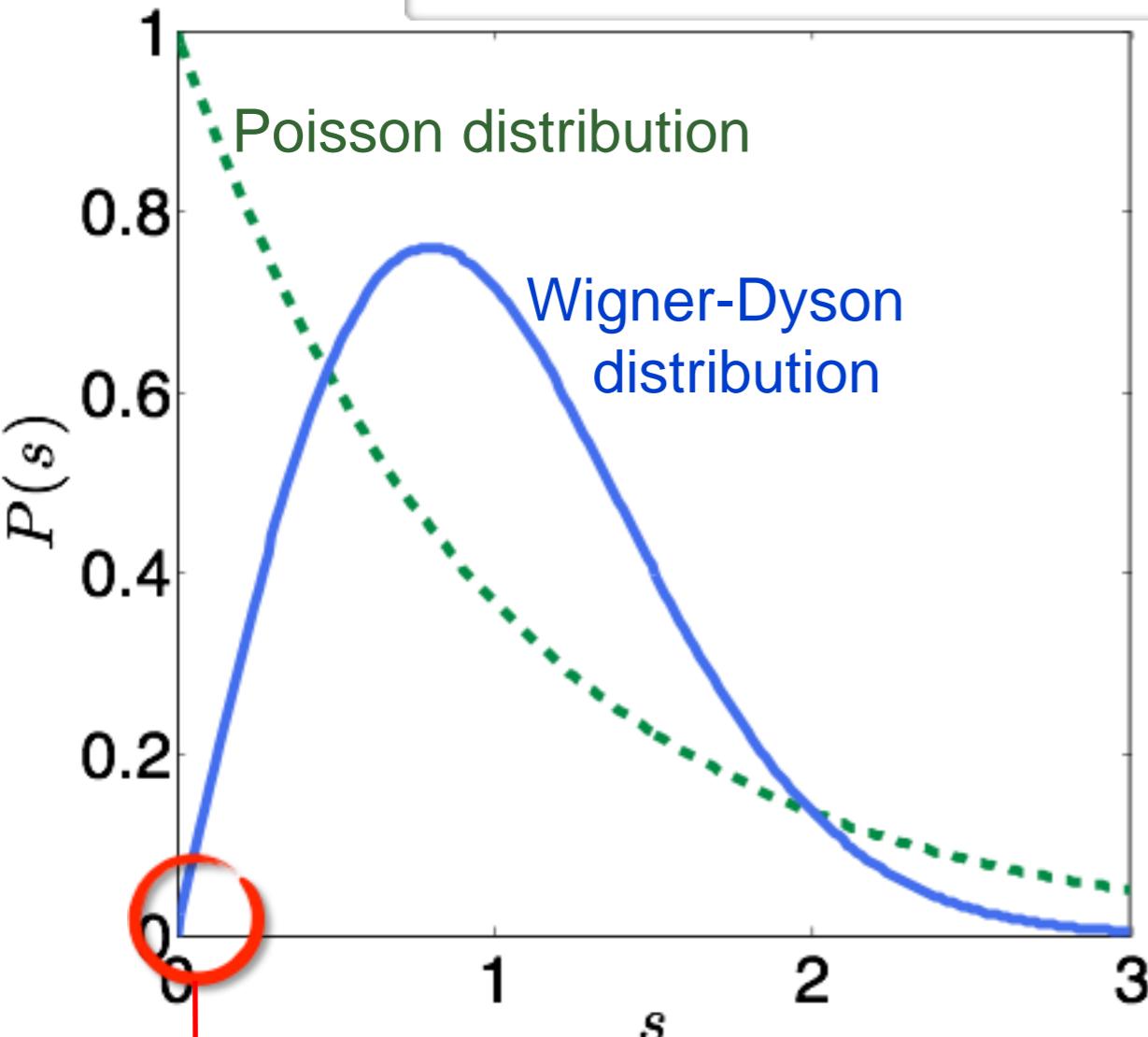
Respect the same **symmetries** as the real H !

Reproduce the correlations of the complex spectrum of a real system !!

Level correlations & RMT



P(s): Nearest-neighbor distribution of energy levels



s = normalized nearest-neighbor level spacing (in units of the mean level spacing)

Wigner surmise excludes degeneracies, $P^{(WD)}(0) = 0$

Poisson law \Leftrightarrow uncorrelated classical dynamics

$$P^{(P)}(s) = \exp(-s)$$

Wigner-Dyson distr. \Leftrightarrow Dynamics of a quantum system with time-reversal and rotational symmetry predicted within **Random Matrix Theory** (Gaussian Orthogonal ensemble)

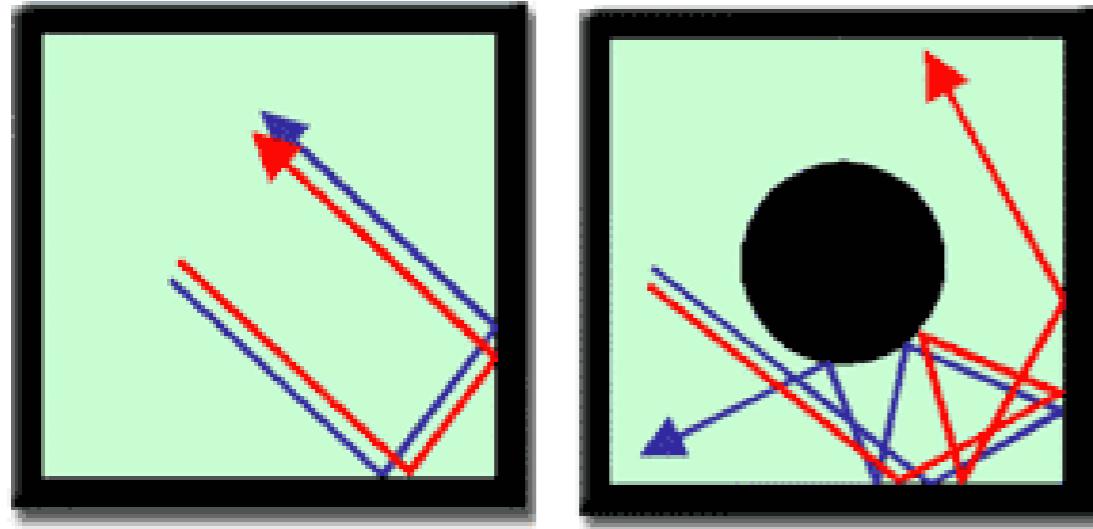
$$P^{(WD)}(s) = \frac{\pi s}{2} \exp\left(-\frac{\pi s^2}{4}\right)$$

Same mean value, different variance.

Wigner-Dyson distr. expresses **level repulsions and spectral rigidity**.

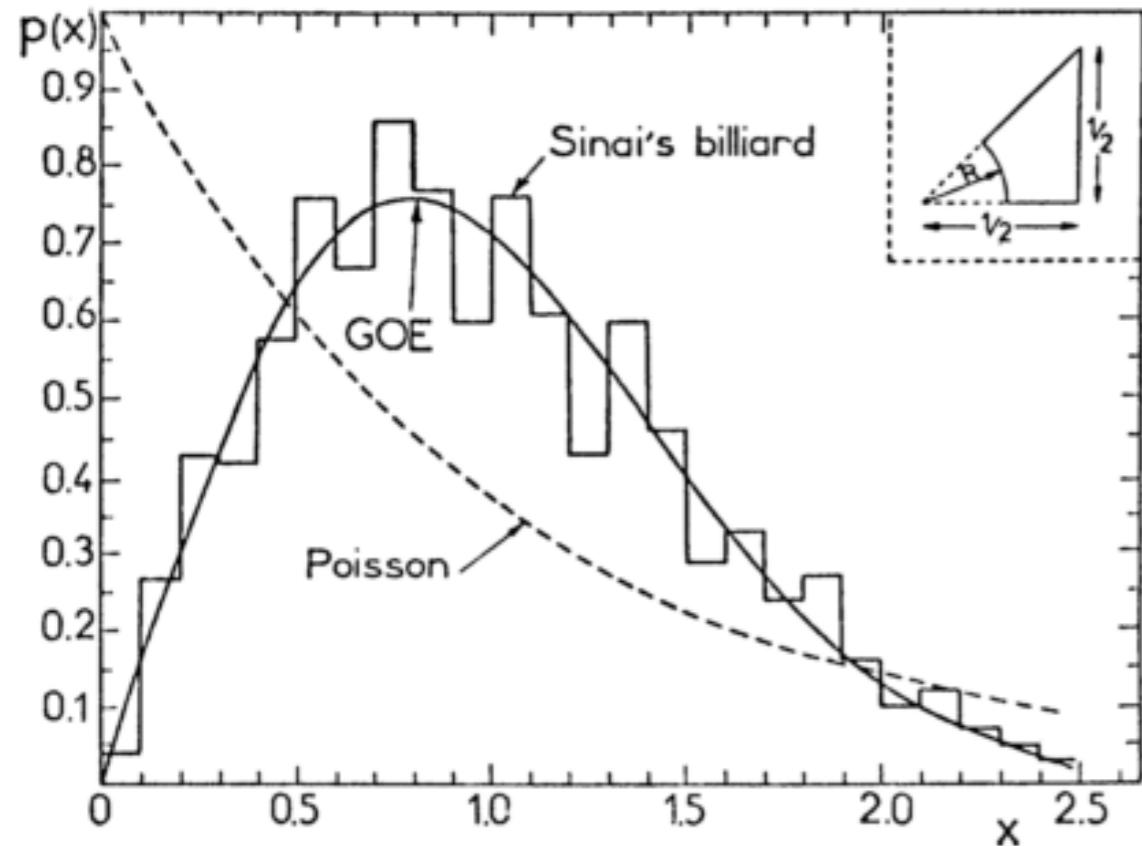
RMT: Parameter-free theory

RMT universality & chaos



BOHIGAS-GIANNONI-SCHMIT CONJECTURE (1984):

The spectral fluctuation properties of a quantum system that is fully chaotic in the classical limit follows the WD distribution



Random Matrix Theory

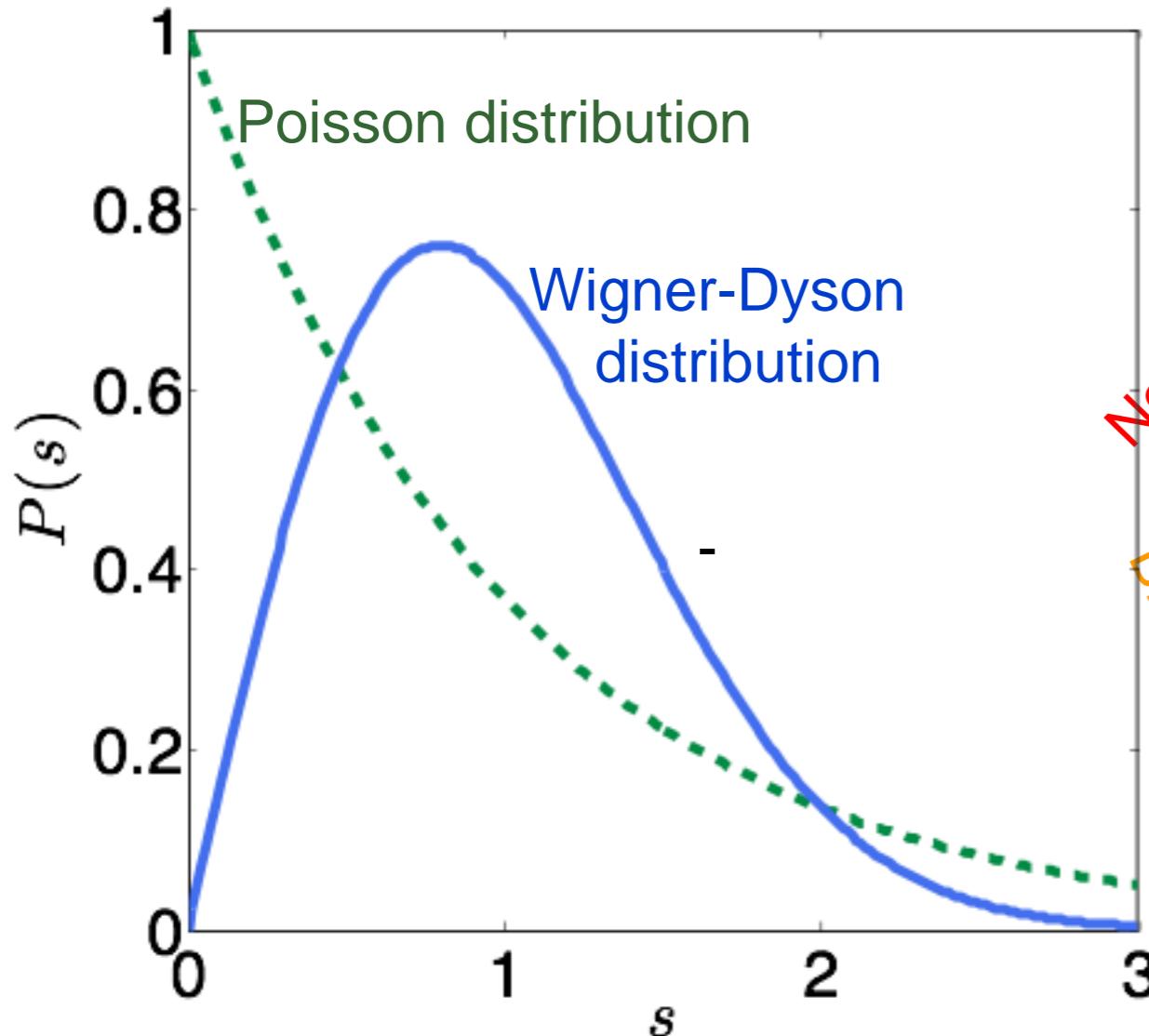


Chaos

⇒ Universality of level correlation functions.

RMT universal applications

$P(s)$: Nearest-neighbor distribution of energy levels



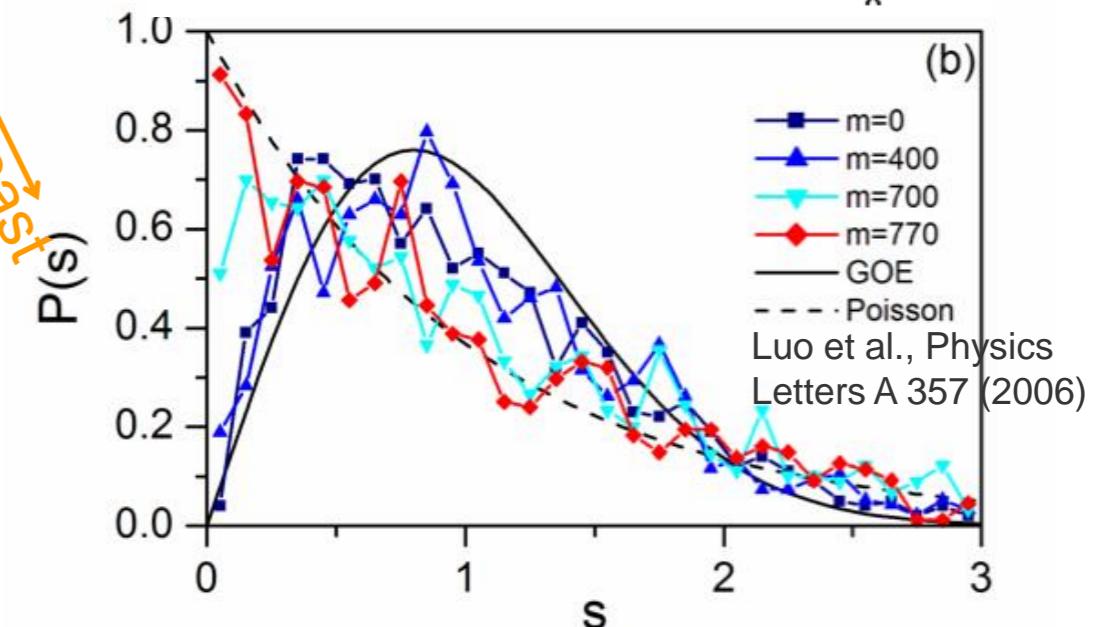
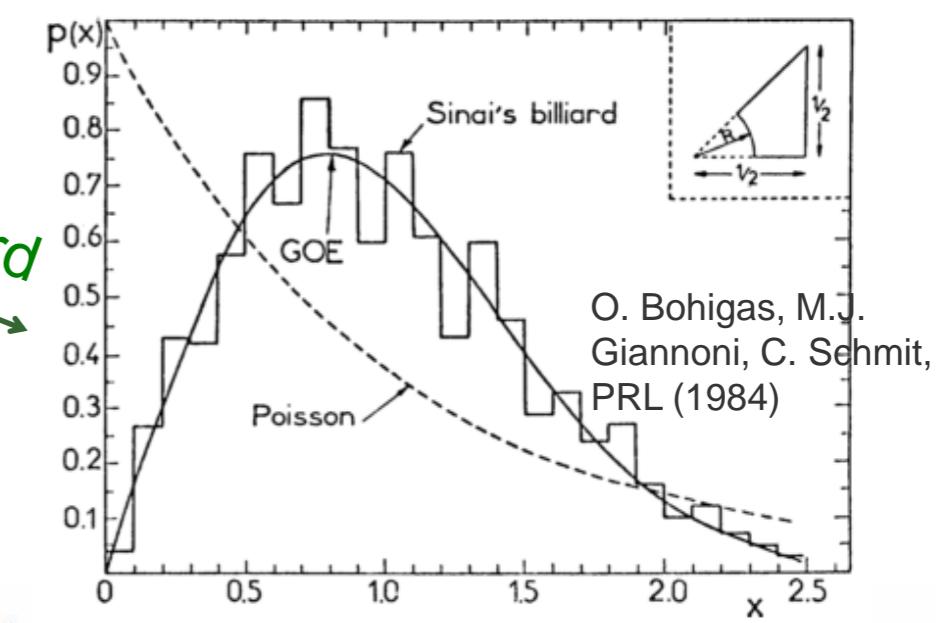
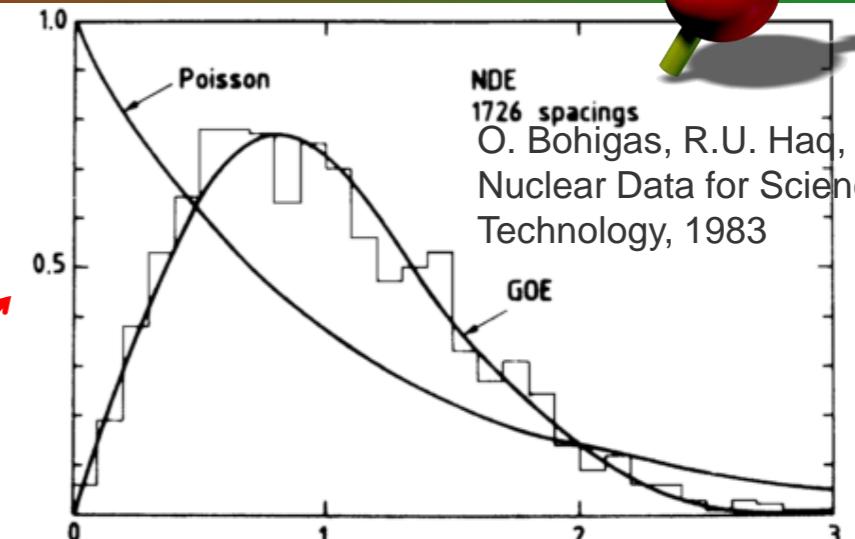
Powerful Tool:

Nuclear physics, Disordered and Mesoscopic Systems, Number theory, Quantum Chromodynamics, Quantum Chaos, Biological systems, Quantum gravity and string theory, risk management in finance, ...

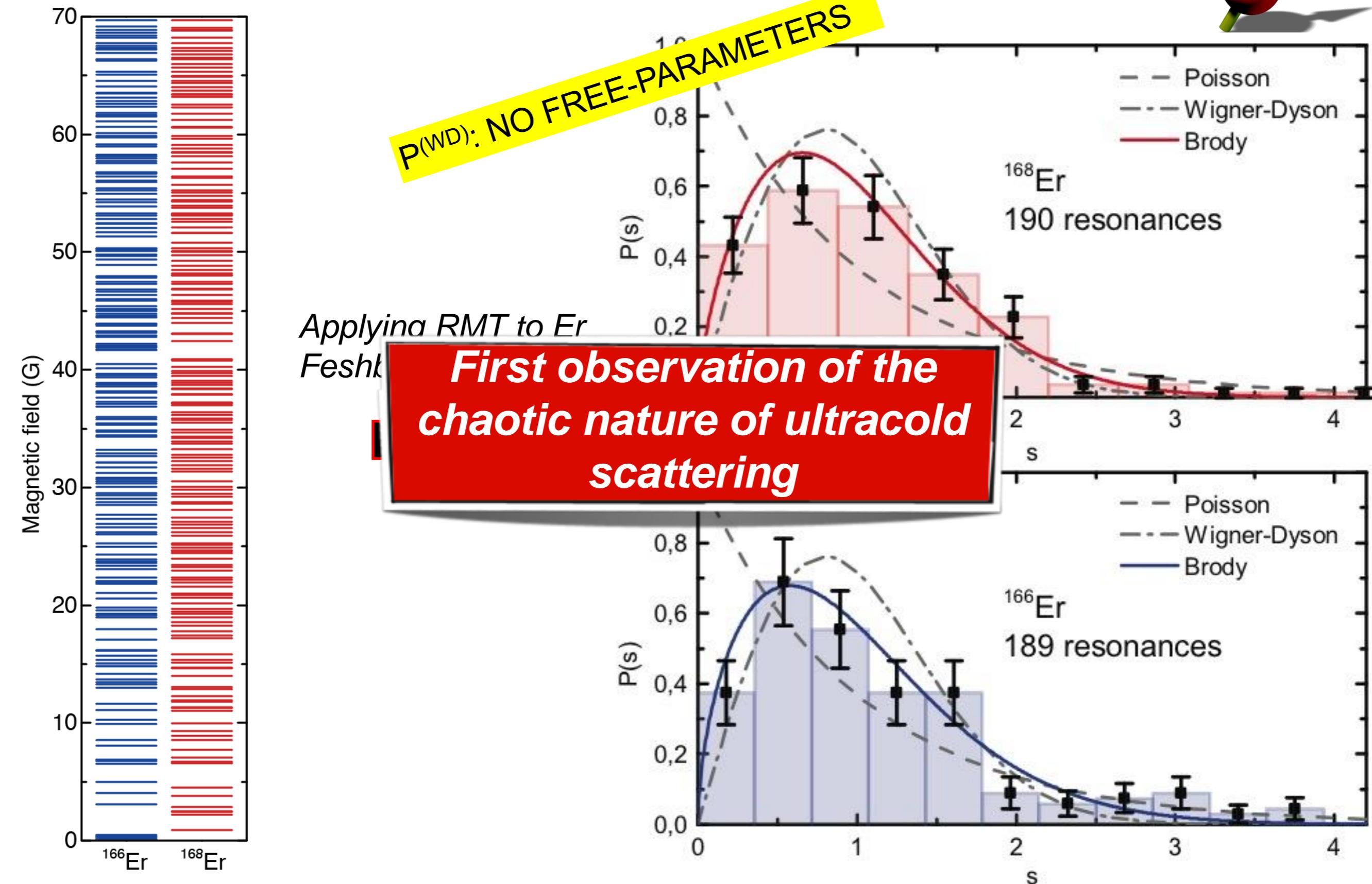
Neutron scattering cross section of ^{238}U

Sinai billiard

Biological networks of yeast



Wigner Surmise in Erbium



Outline of the talk



- ◆ Toward non-alkali atoms, the quest for atomic richness and the case of magnetic atoms.
- ◆ Specificity of scattering of ultracold lanthanides
- ◆ Random Matrix Theory: Complex systems, dense spectra and chaos
- ◆ Chaos in Feshbach resonances of Lanthanides: First Erbium study and beyond, describing lanthanides chaoticity.
- ◆ Towards a theoretical understanding the origin of chaos

Why a new work?



A joint effort to better understand the chaotic scattering of Lanthanide atoms.

Er Group (Ferlaino et al.) + Dy Group (Pfau et al.)
+ Theory Group (Kotochigova/Tiesinga)



Is this generalizable to other atomic species? Thorough comparison of the behavior of 2 Lanthanides:
Er and Dy (+isotopes).

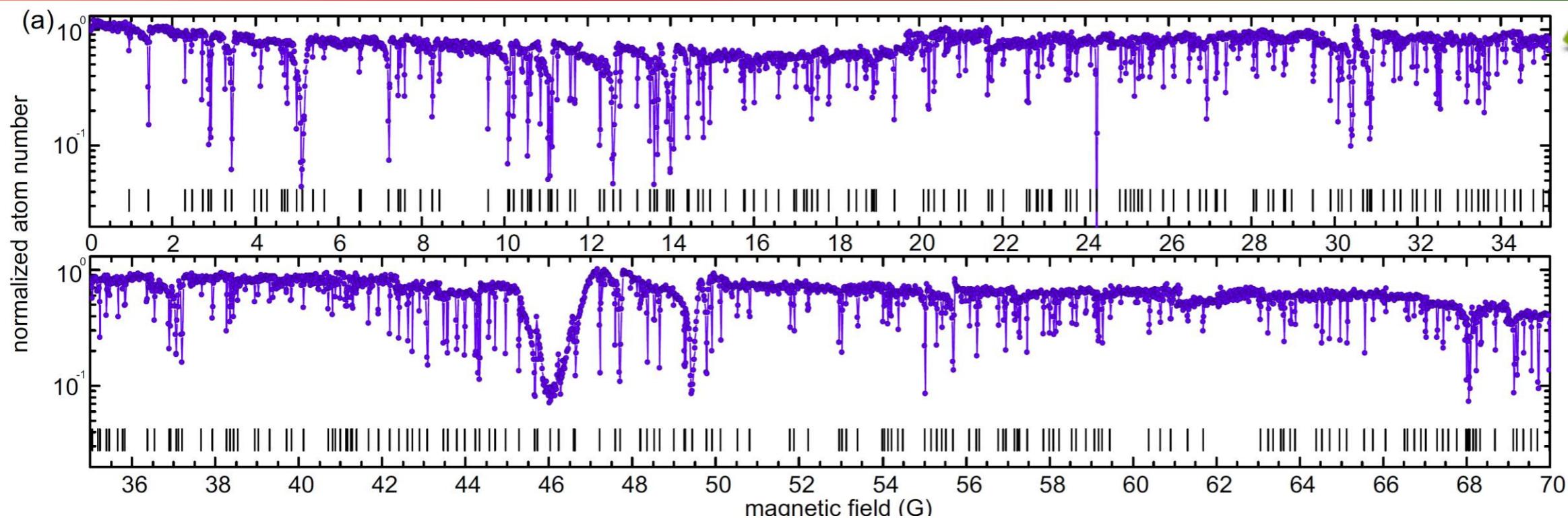
What is the origin of chaotic scattering?
Effort toward a better theoretical understanding.

From where come some specific behavior?

Investigate temperature and magnetic field dependence

Development of more accurate numerical simulations for both species.

New measurements.



Additional extensive high-resolution trap loss spectroscopy measurements:

- ◆ Dy 164 @ 600 nK (Pfau group, Stuttgart)
- ◆ Er 168 @ higher T = 1400 nK.
- ◆ Er 167 @ T = 400 nK.

very dense spectra

N_{res}

¹⁶⁴Dy @ 400 nK

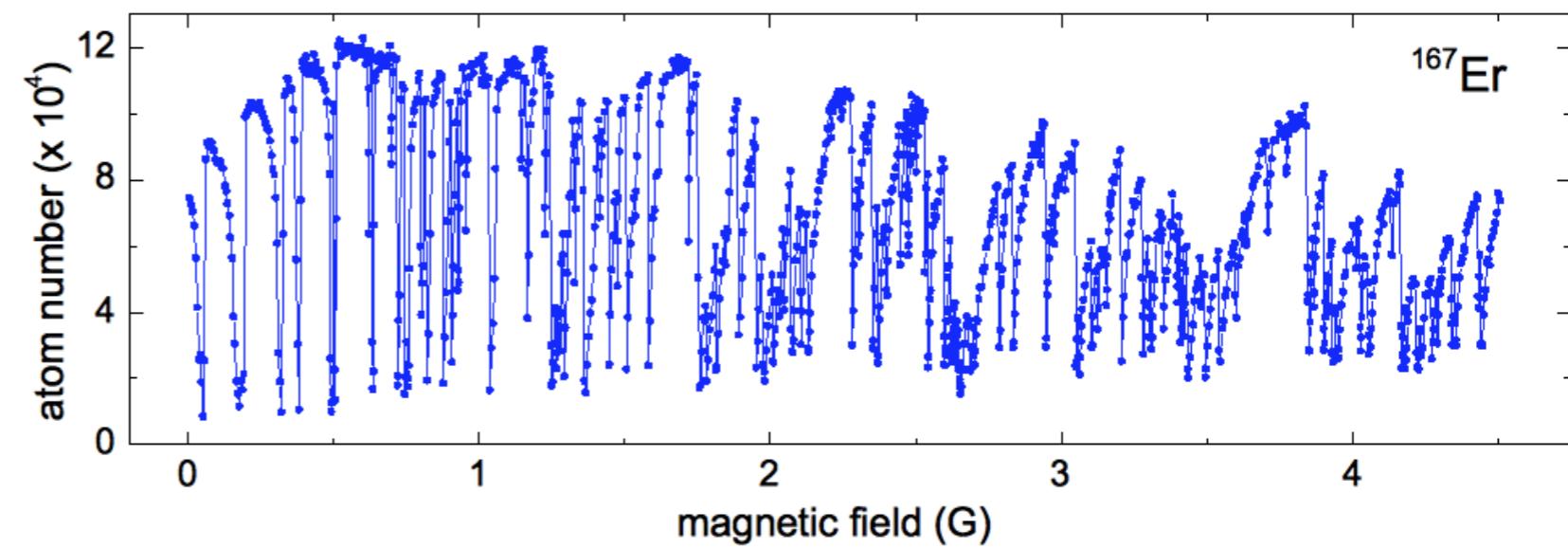
309

¹⁶⁸Er @ 1400
nK

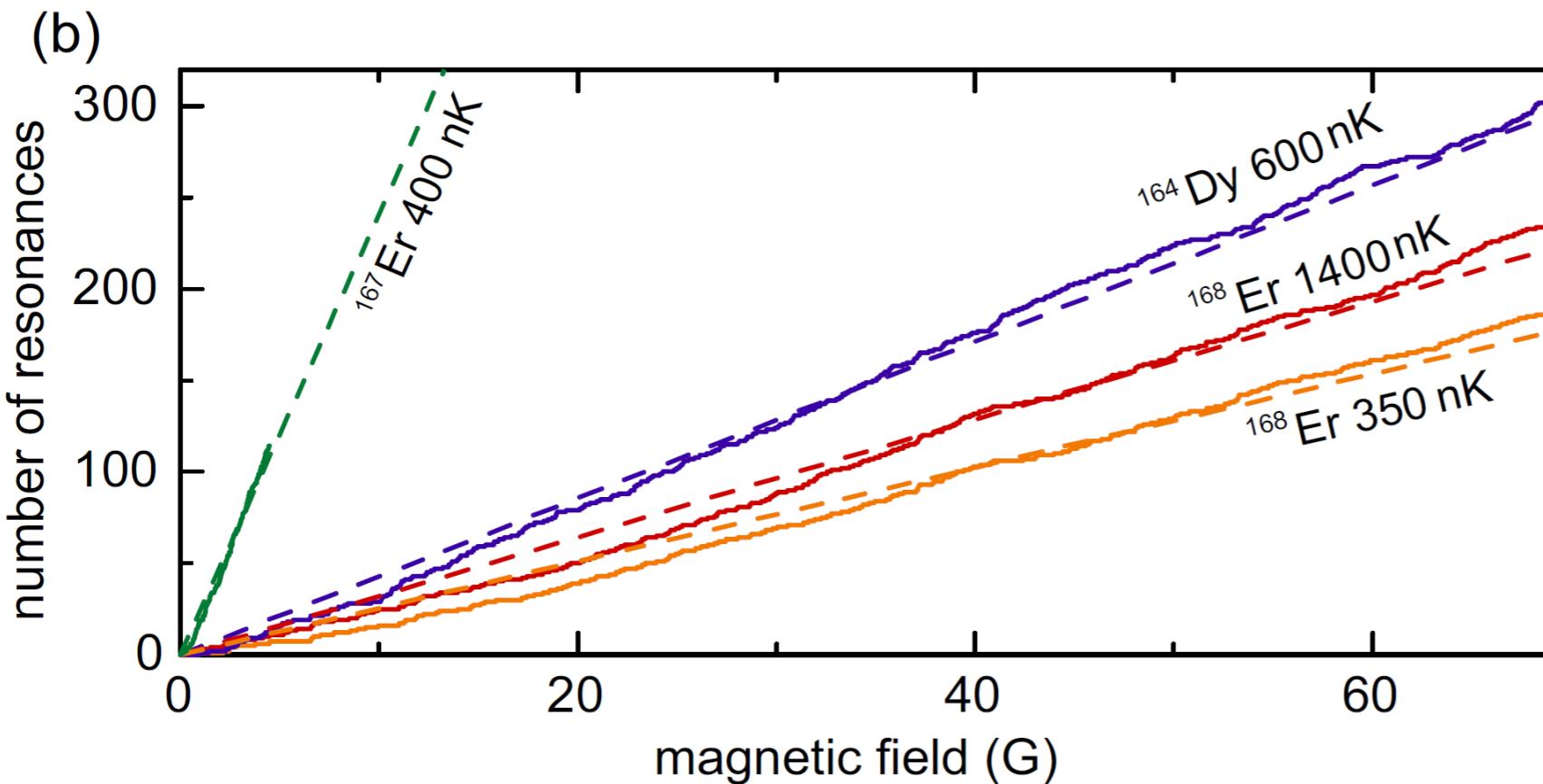
238

¹⁶⁸Er @ 350 nK

189



Density of resonances



$\rho (\text{G}^{-1})$	
$^{168}\text{Er} @ 350 \text{ nK}$	2.7
$^{168}\text{Er} @ 1400 \text{ nK}$	3.4
$^{164}\text{Dy} @ 400 \text{ nK}$	4.3
$^{167}\text{Er} @ 400 \text{ nK}$	25.6

- ◆ Staircase function(B) = number of resonance with $B_{\text{res}} < B$.
- ◆ Derivative: Density of resonances ρ . Deduced from linear fit.

Exact values depend on specific scattering parameters, e.g. **number of channels!**

\Leftarrow # of Zeeman sub-levels in the ground state.

Same order of magnitude:

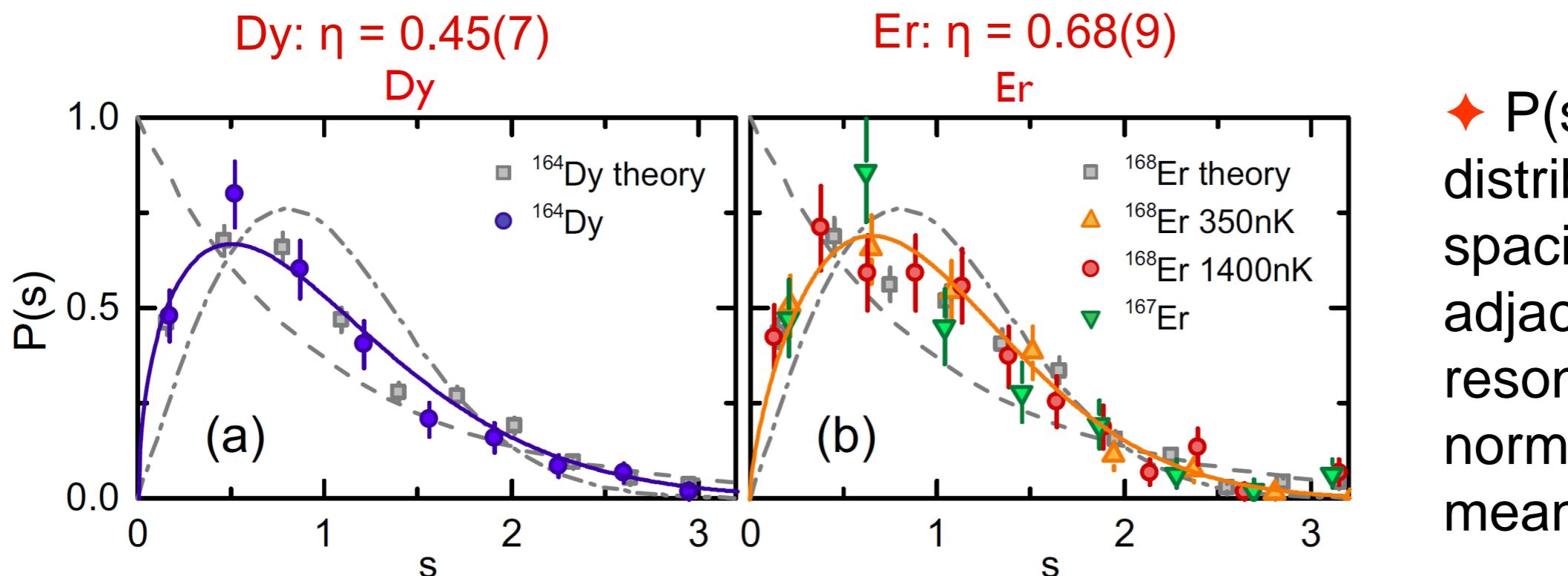
Similar scattering scheme!

Fermionic isotope:
Hyperfine structure

Dy : larger j than Er

Nearest Neighbour spacing distribution

www.erbium.at



◆ $P(s) =$
distribution of the
spacing between
adjacent
resonances,
normalized to the
mean distance $1/\rho$

Extreme cases	$P(s)$
Poisson	$\eta = 0$
Wigner-Dyson	$\frac{\pi s}{2} e^{-\pi s^2/2}$

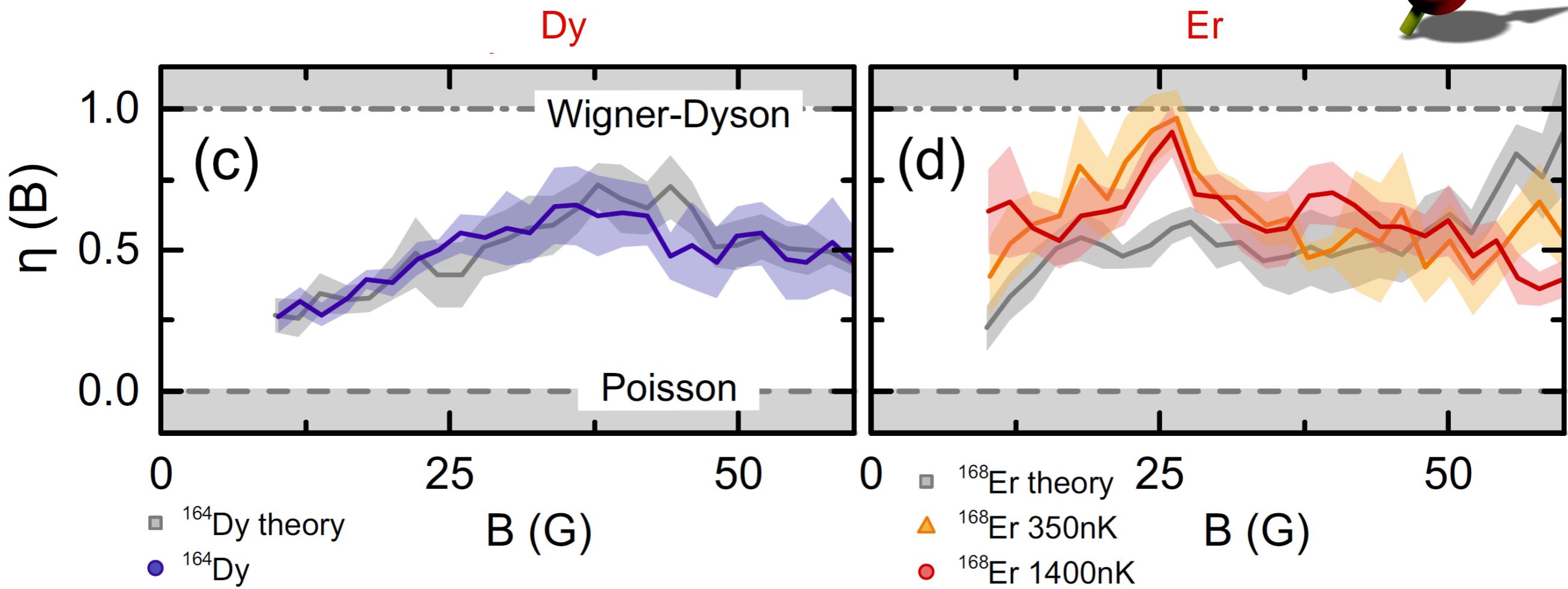
Strong correlation
⇒ Repulsion btw resonances!

Quantify the degree of correlation : interpolate between the 2 distributions.

→ Brody distribution: unique parameter $\eta \in [0,1]$. Empirical

$\eta(\text{Er}) > \eta(\text{Dy})$ even though $j_{\text{Er}} < j_{\text{Dy}}$

Correlation as a function of B



Quantify B and T dependences : fit η of $P(s)$ on sliding B-range $[B - \Delta B/2, B + \Delta B/2]$; $\Delta B = 20\text{G}$

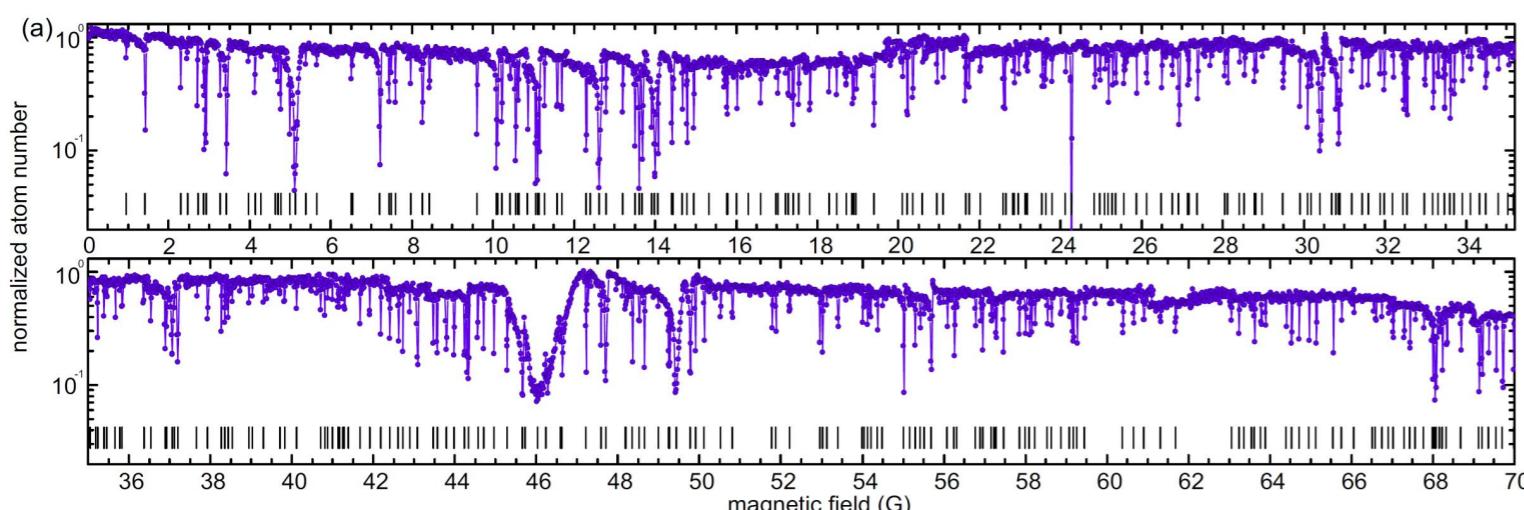
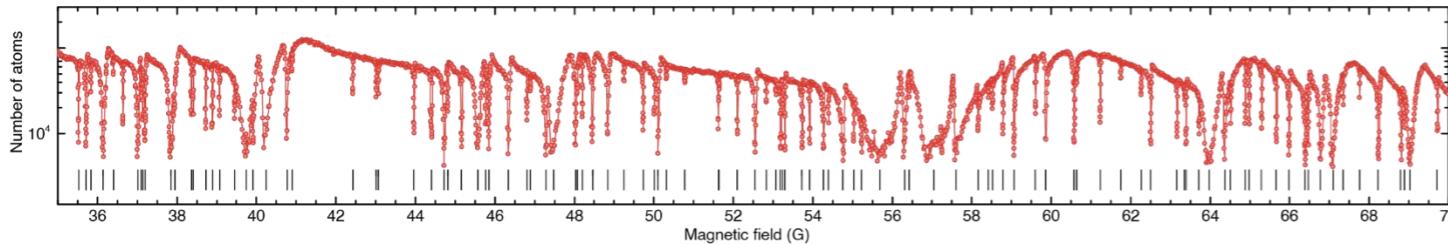
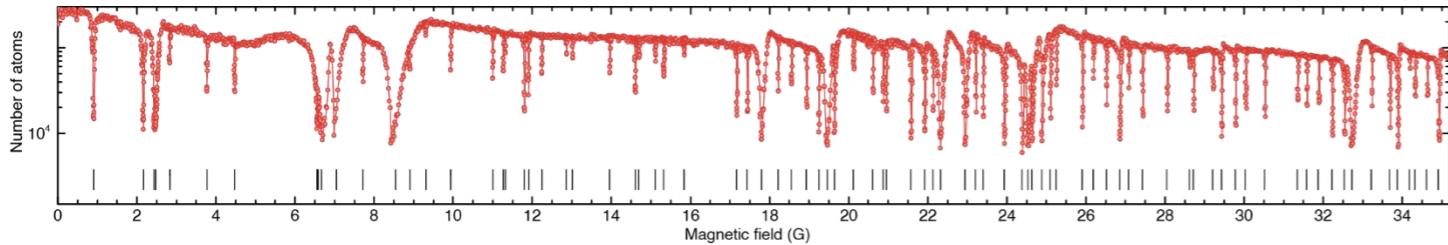
B-dependence: increase of correlation at small B! (Dy)

Never fully correlated
 $\eta \approx 0.5 < 1$

T-dependence : affect mean number but not the correlations! (Er)

Summary of experimental observations

www.erbium.at



The **number of channels** affects the **number of resonances** but no straightforward link:
 $j \rightleftharpoons$ correlation degree

Correlation develops with B

Lanthanides \Rightarrow very dense FR spectra.

RMT analysis of the resonance correlations:

- (partial) levels repulsion
- reduced variance // shot-noise

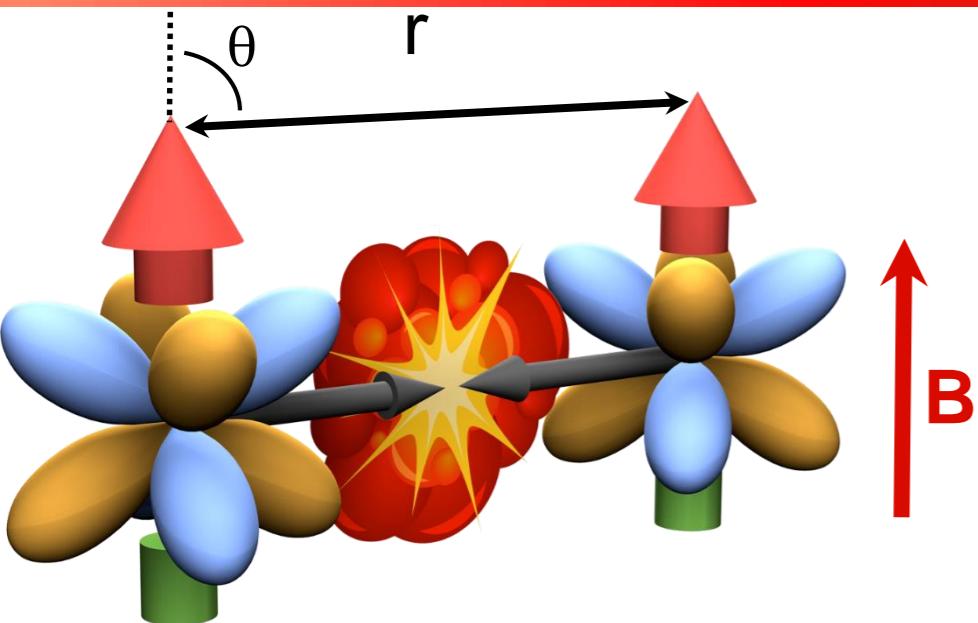
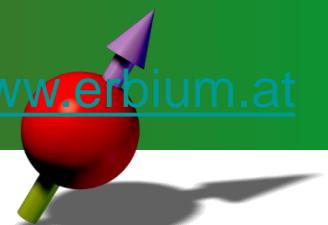
T affects the **number of resonance** but not their **correlations**

Outline of the talk



- ◆ Toward non-alkali atoms, the quest for atomic richness and the case of magnetic atoms.
- ◆ Specificity of scattering of ultracold lanthanides
- ◆ Random Matrix Theory: Complex systems, dense spectra nad chaos
- ◆ Chaos in Feshbach resonances of Lanthanides: First Erbium study and beyond, describing lanthanides chaoticity.
- ◆ Towards a theoretical understanding the origin of chaos

Toy model based on RMT



$$\hat{H}_{\text{rel}} = -\frac{\hbar^2}{2\mu_r} \frac{d^2}{d^2\vec{r}} + \hat{V}(\vec{r}) + \hat{H}_Z(B)$$

Zeeman energy

Anisotropic interaction potential: Coupling of Zeeman sublevels

Difficult to simulate

large j : Large number of Zeeman sublevel in the ground state.

Toy model based on RMT idea



replace by

$$\hat{H}_{\text{RMT}} = \hat{H}_0 + \hat{H}_Z(B)$$

$B=0$ Hamiltonian Zeeman energy

- ◆ Set of random matrices, extract global properties of spectra and average
- ◆ respect symmetry (GOE): $n \times n$ real-symmetric matrix, $n = 500$
- ◆ respect structure (B -dependence)

Toy model based on RMT



$$\hat{H}_{\text{RMT}} = \hat{H}_0 + \hat{H}_Z(B)$$

B=0 Hamiltonian Zeeman energy

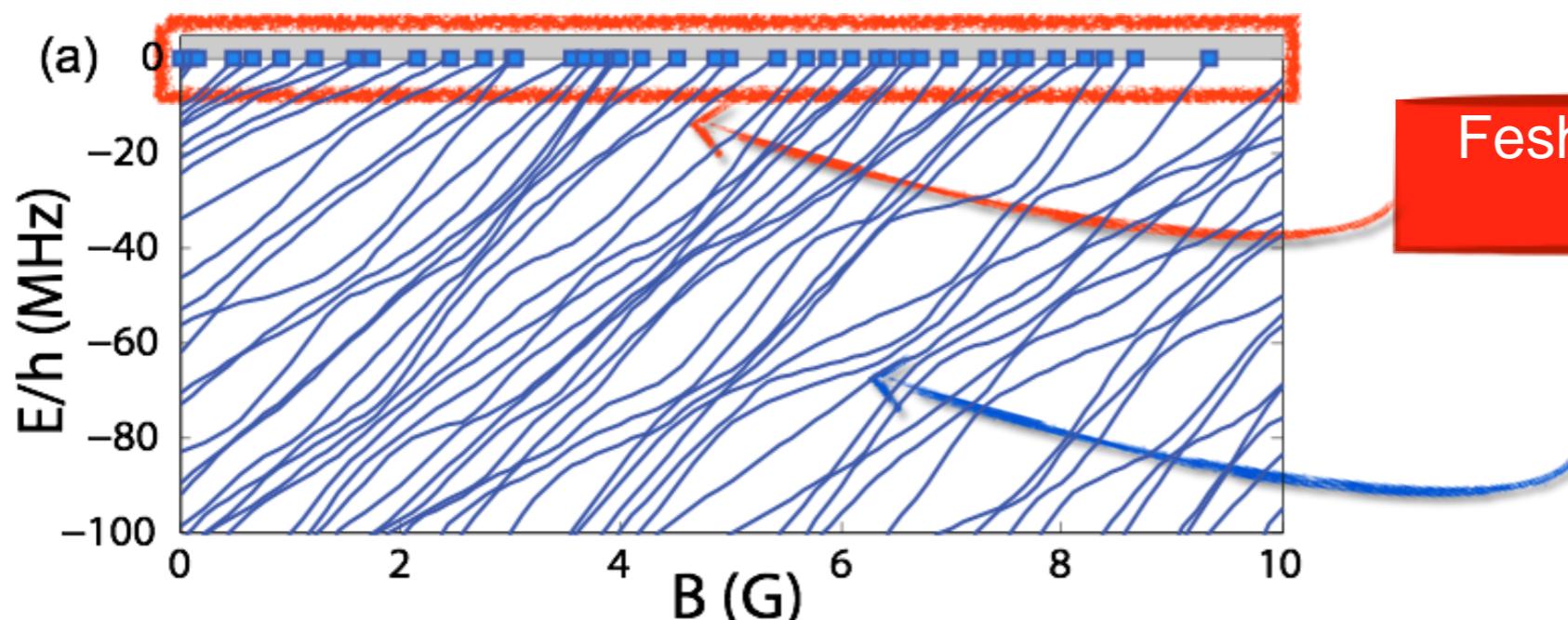
$$\hat{H}_0 = \begin{pmatrix} E_1^{(0)} & & & \\ & \ddots & & 0 \\ & & E_n^{(0)} & \\ 0 & & & \end{pmatrix} + \begin{pmatrix} 0 & & & H_{ij} \\ & \ddots & & \\ H_{ji} & & 0 & \\ & & & \end{pmatrix}$$

$$\hat{H}_Z(B) = g\mu_B B \begin{pmatrix} m_1 & & & 0 \\ & \ddots & & \\ 0 & & m_n & \end{pmatrix}$$

Diagonal ~ «sublevels Energies» distributed with Brody η_d .

Mean spacing ε_d to reproduce

p. Eigenvalues of H_{RMT} :



Feshbach resonances spectrum.
Global properties??

Very dense spectra
=> multiple
(avoided) crossings

Toy model based on RMT



$$\hat{H}_{\text{RMT}} = \hat{H}_0 + \hat{H}_Z(B)$$

B=0 Hamiltonian Zeeman energy

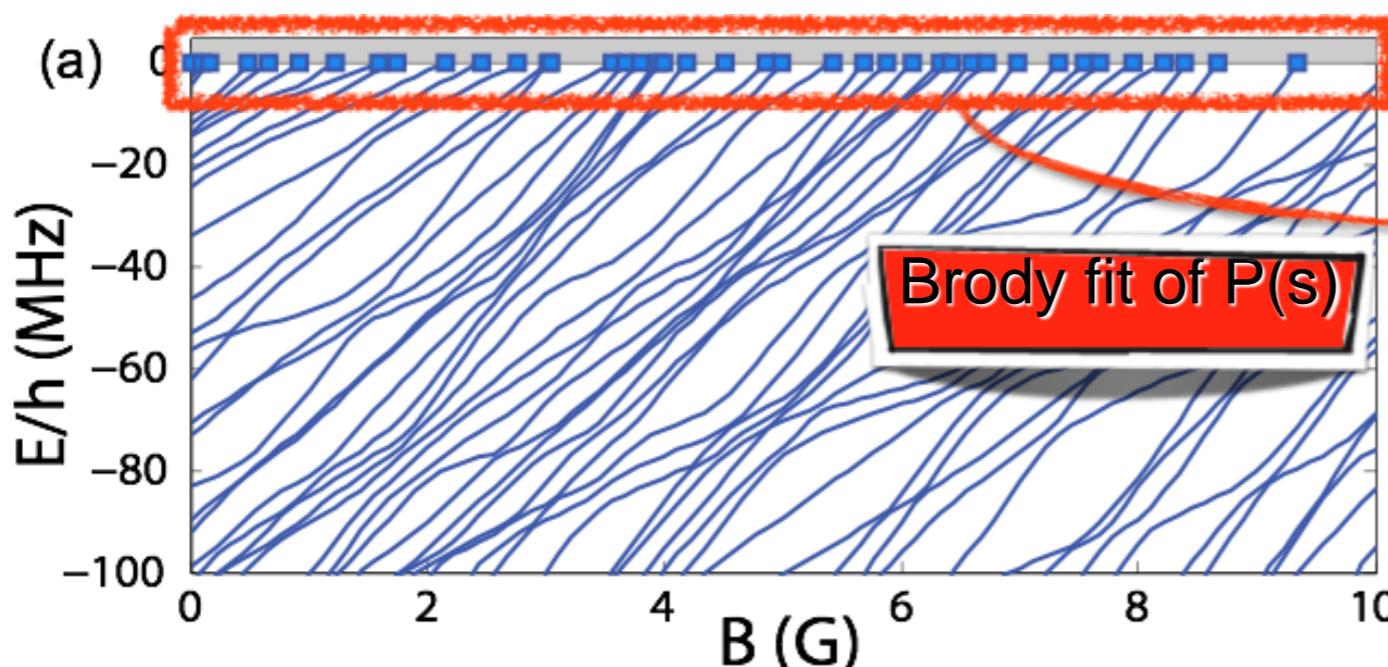
$$\hat{H}_0 = \begin{pmatrix} E_1^{(0)} & & & \\ & \ddots & & 0 \\ & & E_n^{(0)} & \\ 0 & & & \end{pmatrix} + \begin{pmatrix} 0 & & & H_{ij} \\ & \ddots & & \\ H_{ji} & & 0 & \\ & & & \end{pmatrix}$$

Diagonal distributed with
Brody parameter η_d .
Mean spacing ε_d to reproduce

ρ

Coupling between the
sublevels from $V_{\text{ani}}(r)$,
Gaussian-distributed,
strength v_{cpl}

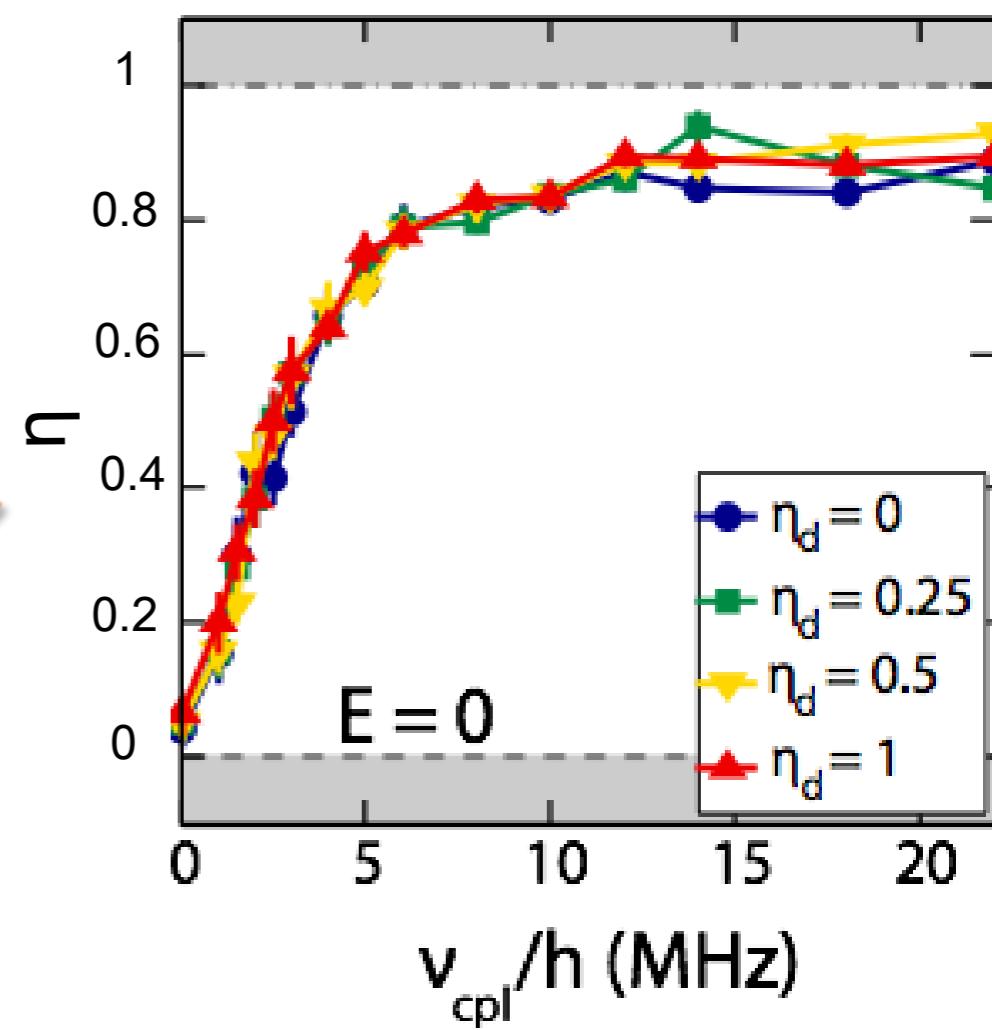
Eigenvalues of H_{RMT} :



mean spacing of $E_i^{(0)}$: $\varepsilon_d/h = 6.4$ MHz

$$\hat{H}_Z(B) = g\mu_B B \begin{pmatrix} m_1 & & & 0 \\ & \ddots & & \\ 0 & & \ddots & \\ & & & m_n \end{pmatrix}$$

Zeeman sublevels
 $m_i \in \{-12, 12\}$



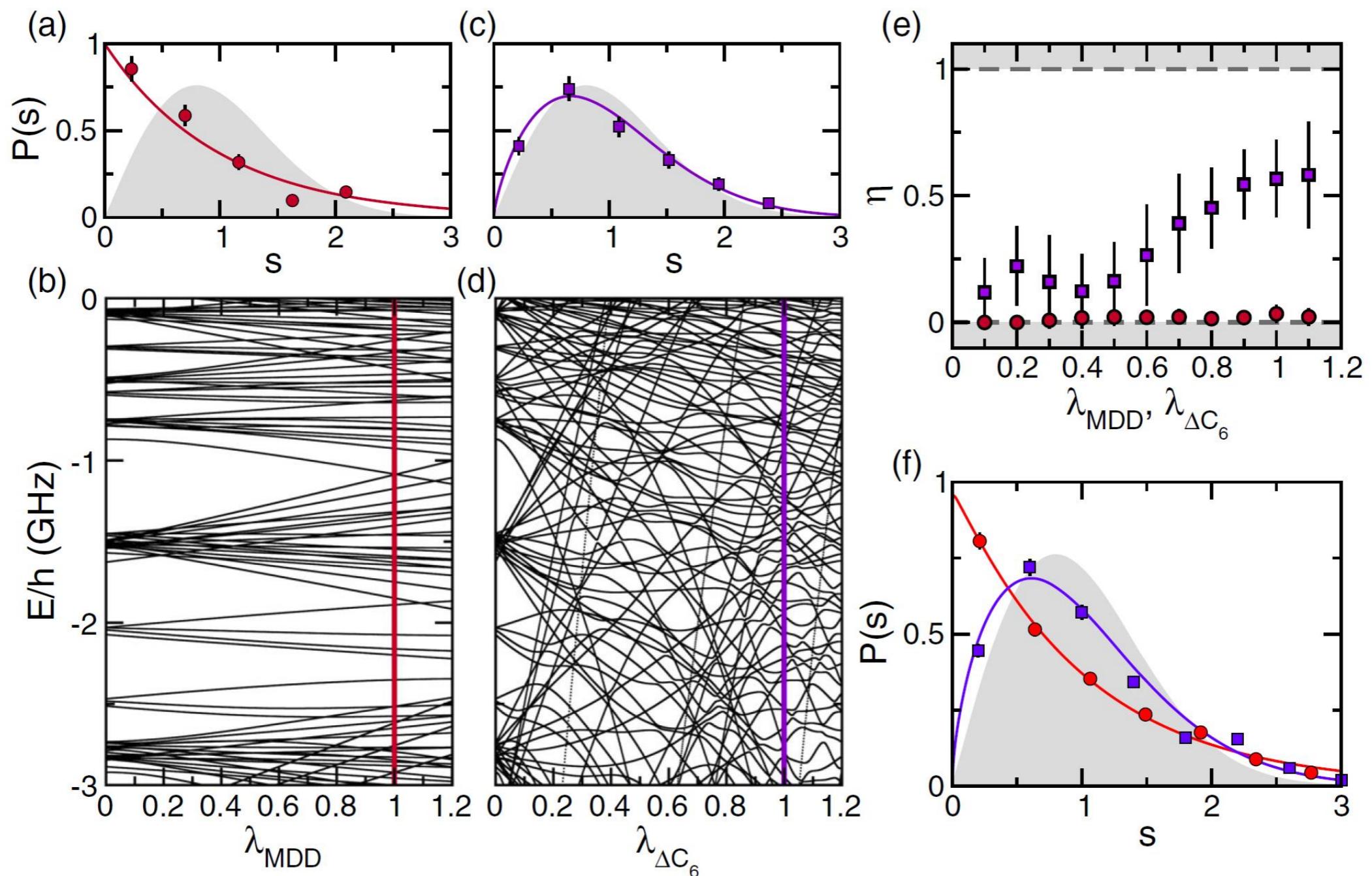
Coupled channel calculations



$$\hat{V}_a(\vec{R}) = \lambda_{\Delta C_6} V_{\Delta C_6}(\vec{R}) + \lambda_{\text{MDD}} V_{\text{MDD}}(\vec{R})$$

$$V_{\Delta C_6}(\vec{R}) = \frac{c_a}{R^6} \sum_{i=1,2} \frac{1}{\sqrt{6}} \{ 3(\hat{R} \cdot \vec{j}_i)(\hat{R} \cdot \vec{j}_i) - \vec{j}_i \cdot \vec{j}_i \} + \dots$$

$$V_{\text{MDD}}(\vec{R}) = -\frac{\mu_0}{4\pi} \frac{(g\mu_B)^2}{R^3} \{ 3(\hat{R} \cdot \vec{j}_1)(\hat{R} \cdot \vec{j}_2) - \vec{j}_1 \cdot \vec{j}_2 \}$$



Coupled channel calculations

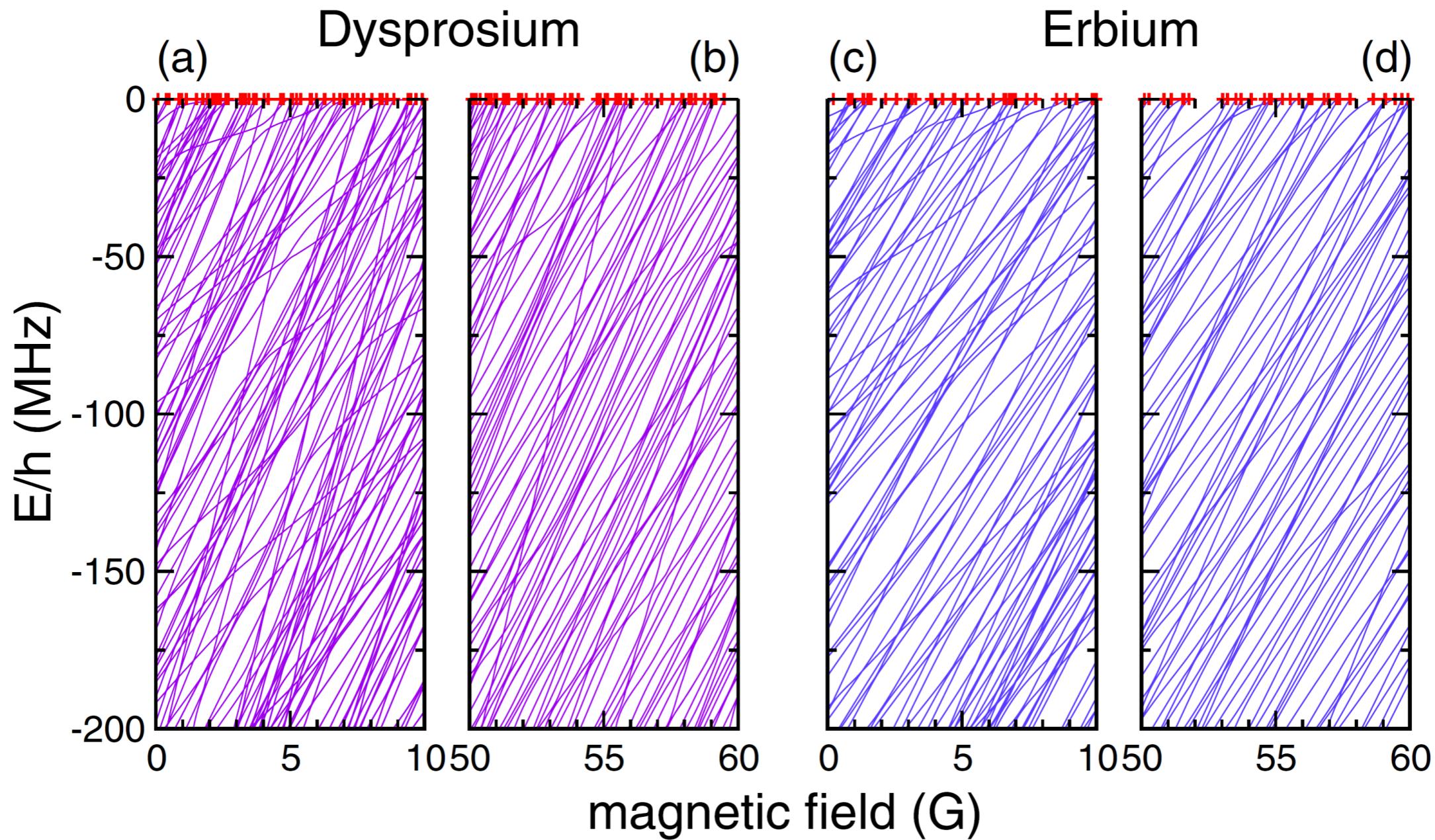


www.erbium.at

$$\hat{V}_a(\vec{R}) = \lambda_{\Delta C_6} V_{\Delta C_6}(\vec{R}) + \lambda_{\text{MDD}} V_{\text{MDD}}(\vec{R})$$

$$V_{\Delta C_6}(\vec{R}) = \frac{c_a}{R^6} \sum_{i=1,2} \frac{1}{\sqrt{6}} \{ 3(\hat{R} \cdot \vec{j}_i)(\hat{R} \cdot \vec{j}_i) - \vec{j}_i \cdot \vec{j}_i \} + \dots$$

$$V_{\text{MDD}}(\vec{R}) = -\frac{\mu_0}{4\pi} \frac{(g\mu_B)^2}{R^3} \{ 3(\hat{R} \cdot \vec{j}_1)(\hat{R} \cdot \vec{j}_2) - \vec{j}_1 \cdot \vec{j}_2 \}$$



Summary of the talk



- ◆ Lanthanides show very rich Feshbach resonance spectra with similar global properties for both Dy and Er isotopes
- ◆ Correlations of the resonances reveal quantum chaos and manifest by spectral rigidity and level repulsion.
- ◆ Explained by anisotropy of the interaction and density stemming from the special electronic structure of Lanthanides



D. Petter



A. Frisch



S. Baier



M. Mark



K. Aikawa



M. Mark



F. Ferlaino



L. Chomaz