KITP, Nov. 9, 2016

Long-range universality in cold two and three body collisions

Paul S. Julienne

Joint Quantum Institute
NIST and The University of Maryland

Thanks to many colleagues in theory and experiment
who have contributed to this work

http://www.jqi.umd.edu/

NIST

Joint
Quantum
Institute

Outline

Long-range universality of bound states and collisions:

1. Two-body (QDT picture)

2. Three-body

3. Molecules and reactive collisions

4. Species with complex or chaotic collisions

What do we mean by “universal”?

Answer: Independent of “short-range” details, characterized by a few simple parameters.

Example: zero-range interaction proportional to
s-wave scattering length a

Only one parameter a depends on the “details”

s-wave scattering phase shift: $\tan \eta(k) \approx -ka$

Bound state energy: $E_b = -\frac{\hbar^2}{2\mu a^2}$

Threshold collision summary

s-wave

$$S(k) = e^{2i\eta(k)} \rightarrow e^{-2ik(a-ib)} \text{ as } k \rightarrow 0$$

Complex scattering length ***a-ib***

Balakrishnan, et al., Chem. Phys. Lett. 280, 5 (1997)
Bohn and PSJ, Phys. Rev. A 56, 1486 (1997)
J. Hutson, New J. Phys. 9, 152 (2007)

E-dependent $\alpha(k) = a(k) - ib(k) = -\frac{\tan \eta(k)}{k} = \frac{1}{ik}\frac{1-S(k)}{1+S(k)}$

mean field	$\frac{4\pi\hbar}{\mu}a(0)n$
loss rate	$\frac{4\pi\hbar}{\mu}b(0)n$

Need variation with E away from E=0

- precision binding energy measurements
- lattice zero point energy $a(E_n)$
- few-body beyond "scattering length universality"
- finite temperature QDGs

Effective range expansion

$$k \cot \eta(E) = -\frac{1}{a} + \frac{1}{2} r_0 k^2$$

Flambaum, Gribakin, and Harabati, Phys. Rev. A 59, 1998 (1999)
Gao, Phys. Rev. A 62, 050702 (2000)

$$r_0 = 2.918 \bar{a} \frac{\bar{a}^2 + (a - \bar{a})^2}{a^2}$$

$$\bar{a} = \frac{2\pi}{\Gamma(\frac{1}{4})^2} \left(\frac{2\mu C_6}{\hbar^2} \right)^{\frac{1}{4}}$$

Bound state corrections

$$E_b = -\frac{\hbar^2}{2\mu(a - \bar{a})^2}$$

Gribakin, Flambaum, Phys. Rev. A 48, 446 (1993)
or improved formula of
Gao, J. Phys. B 37, 4273 (2004)

Still not good enough—we can do much better

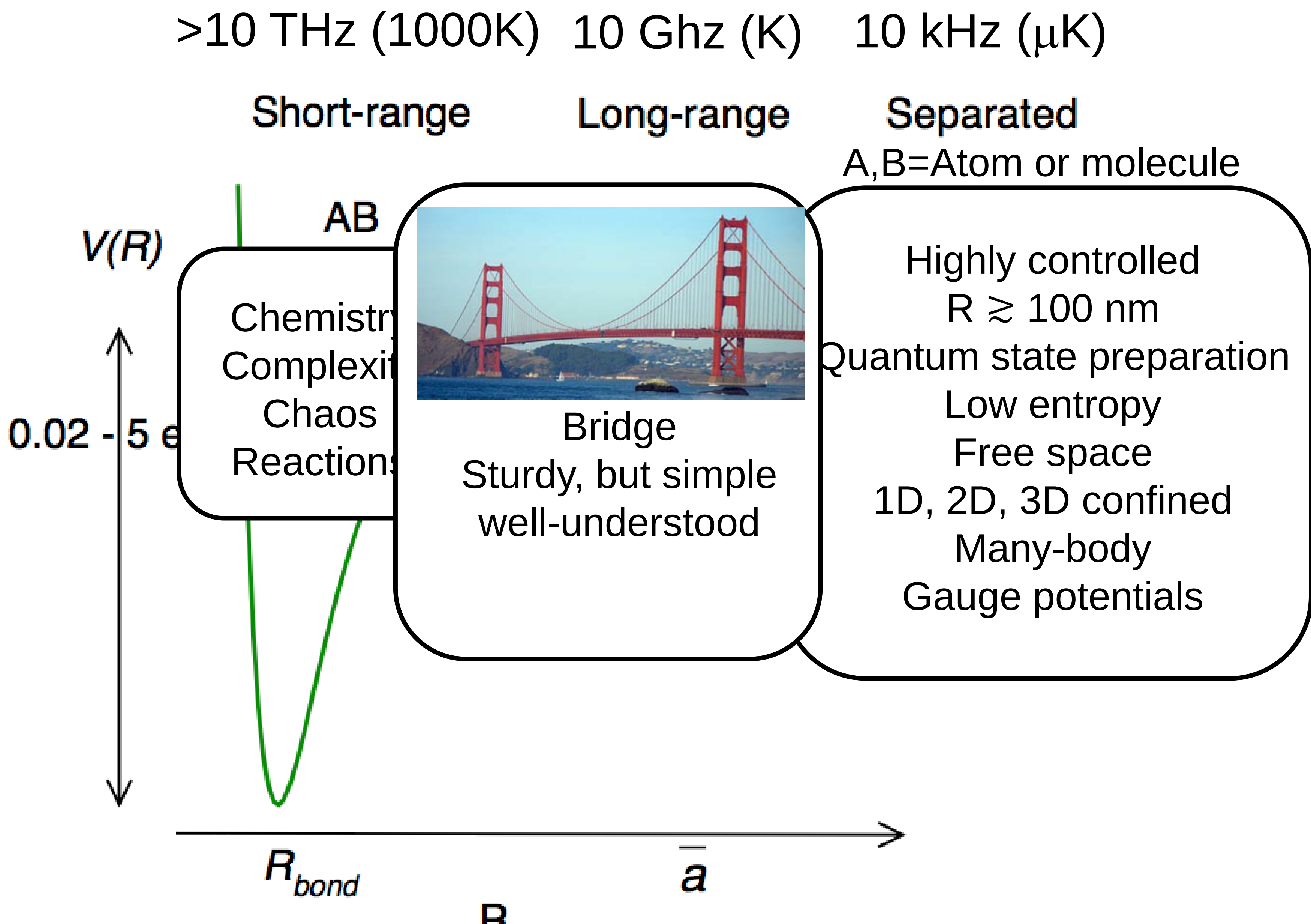


Fig. 2, PSJ Faraday Disc 142, 361 (2009)

>10 THz (1000K) 10 Ghz (K) 10 kHz (μK)

Short-range **Long-range** **Separated**

A,B=Atom or molecule

A few
Parameters (QDT)

Phase (a_{bg})
Feshbach strength (s_{res})
Reactivity (y)

Chemistry
Complexity
Chaos
Reactions

Not unique
More than one way
To build a bridge
(Mies/PSJ/Hutson
Greene/Bohn, Gao)
Analytic
Numerical

Highly controlled
R $\gtrsim$ 100 nm
Quantum state preparation
Low entropy
Free space
1D, 2D, 3D confined
Many-body
Gauge potentials

R_{bond} $\bar{a}$

R

Fig. 2, PSJ Faraday Disc 142, 361 (2009)

Quantum defect theory

1. Pick a reference problem we can solve

   Classic example: Coulomb potential, H-like atom
   or p = 6 or p = 4 potential

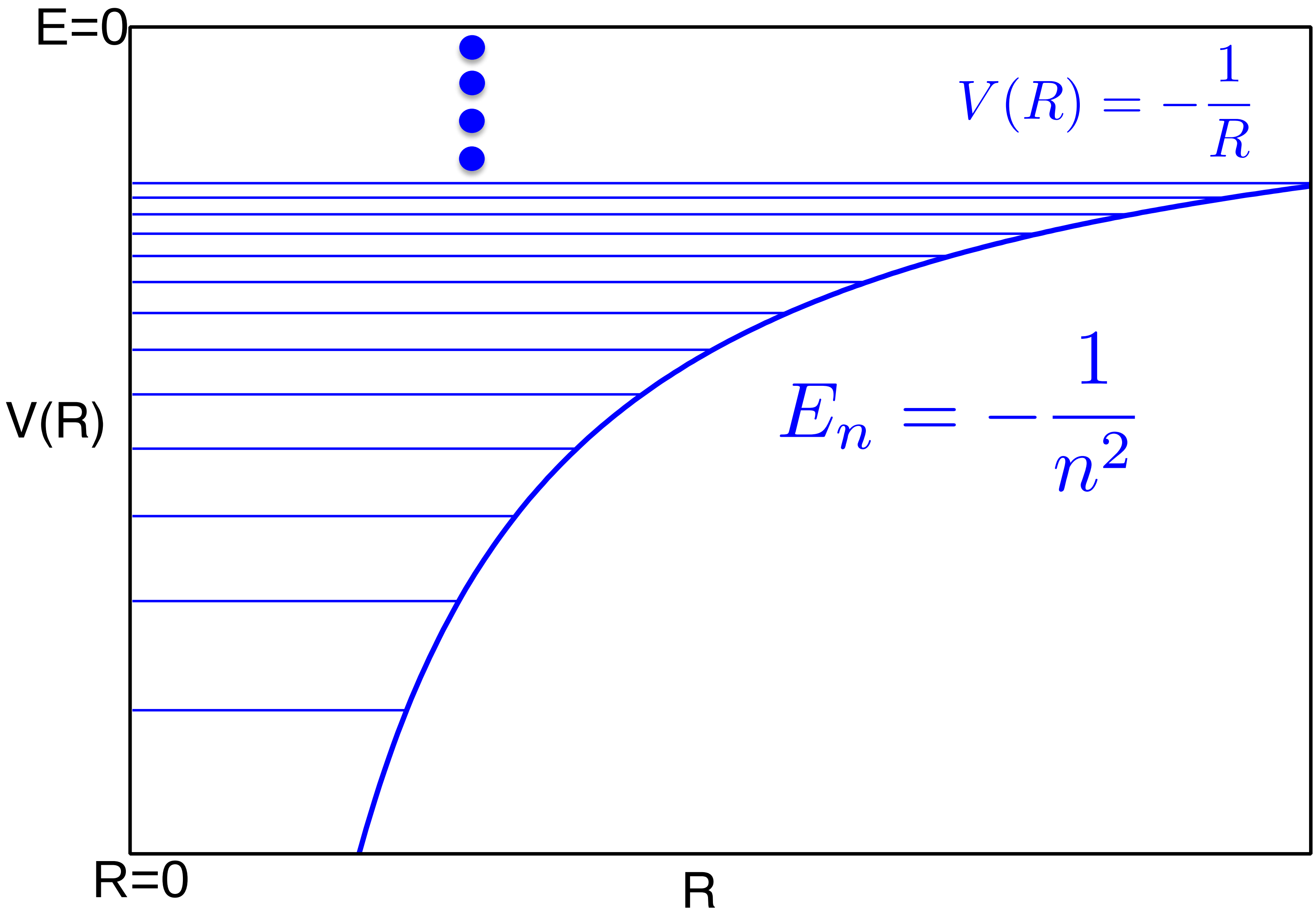
   Independent solutions f(R,E), g(R,E)

2. Parameterize dynamics by a few "physical" QDT parameters
   subject to experimental fitting
   and theoretical interpretation
   phase (diagonal, scattering length)
   interactions (non-diagonal, multichannel)

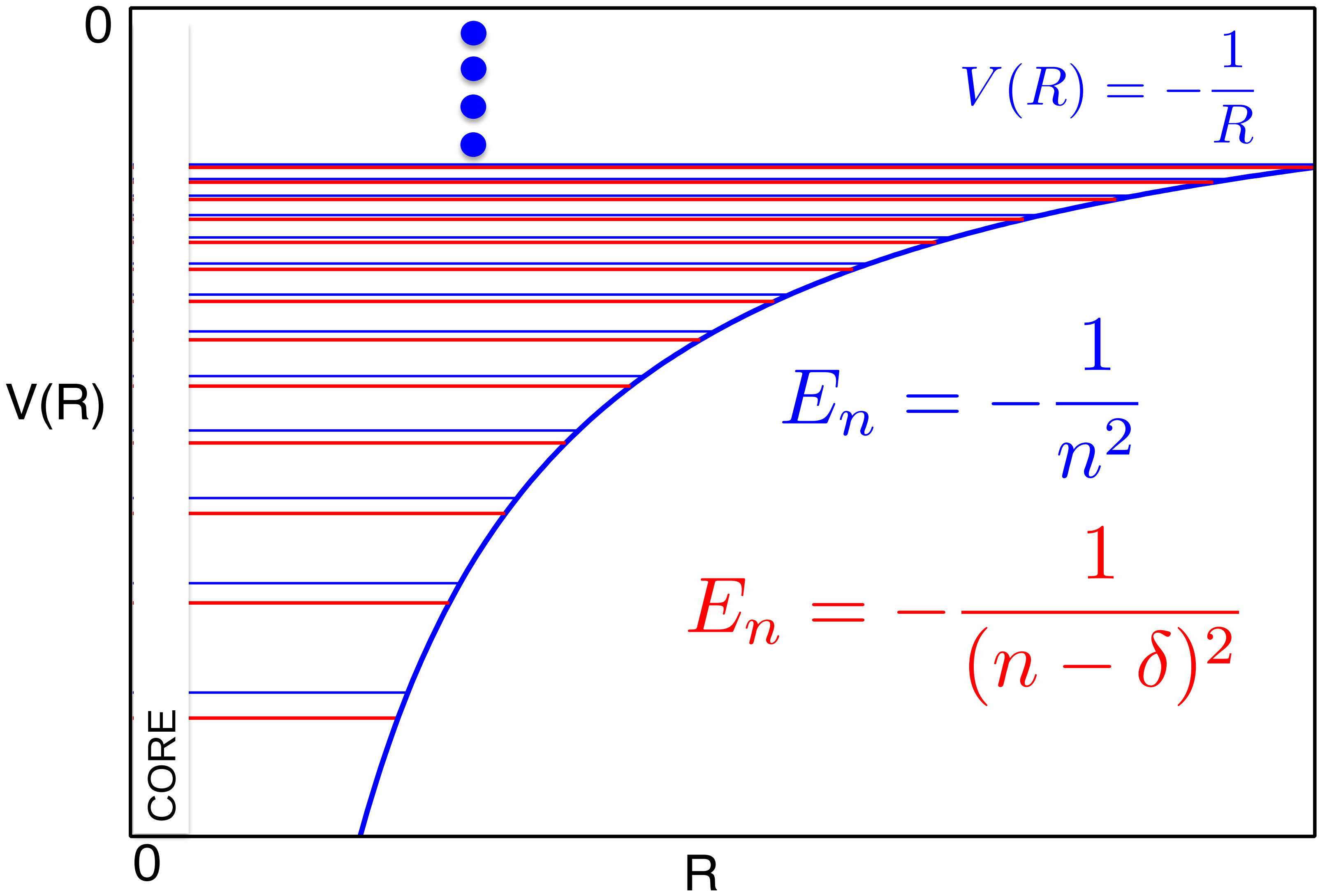
3. Use methods of QDT to calculate
   bound and scattering states, resonances, cross sections, etc.

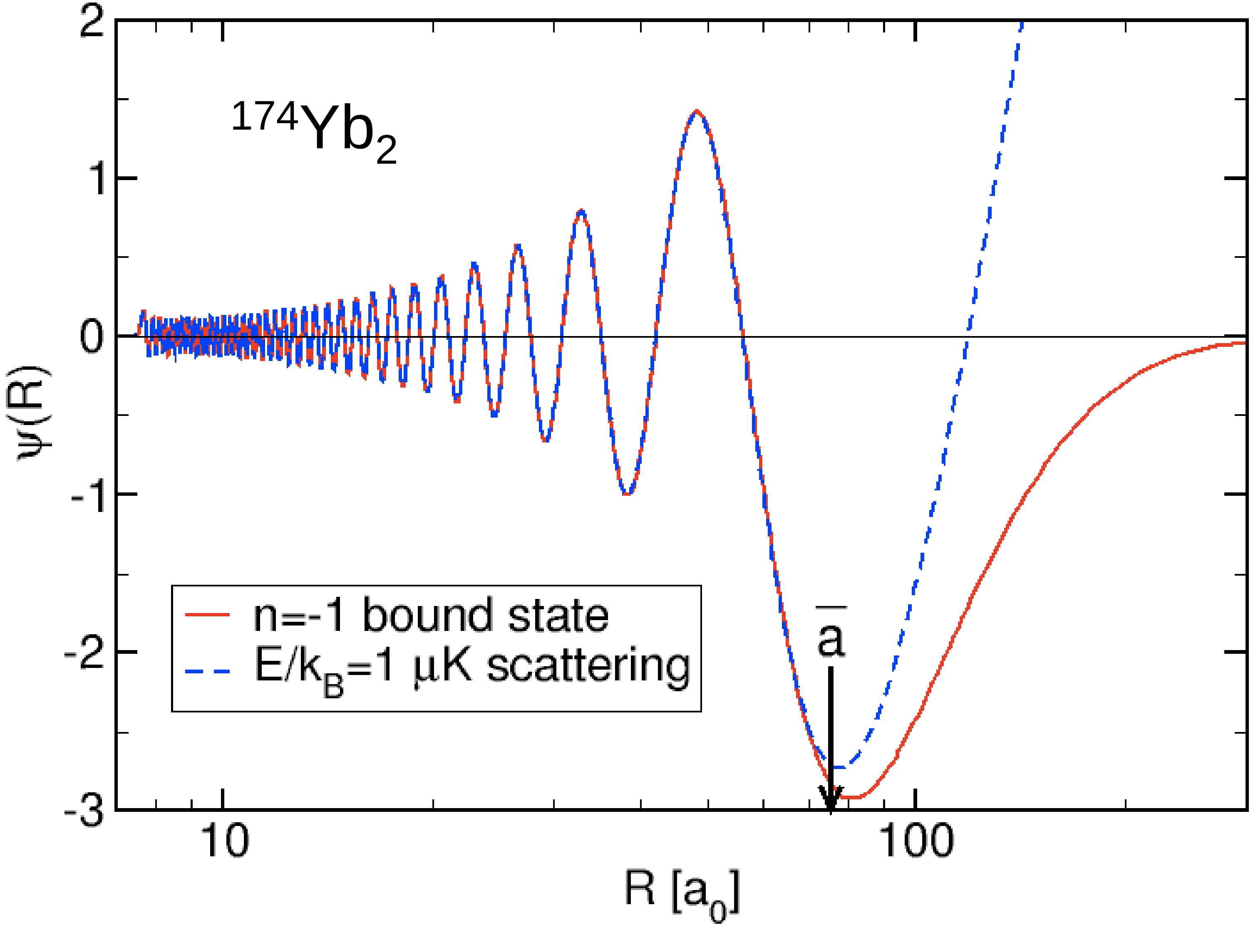
$$\Psi(R,E) = [f(R,E) + g(R,E)\, K]\, A$$

H atom



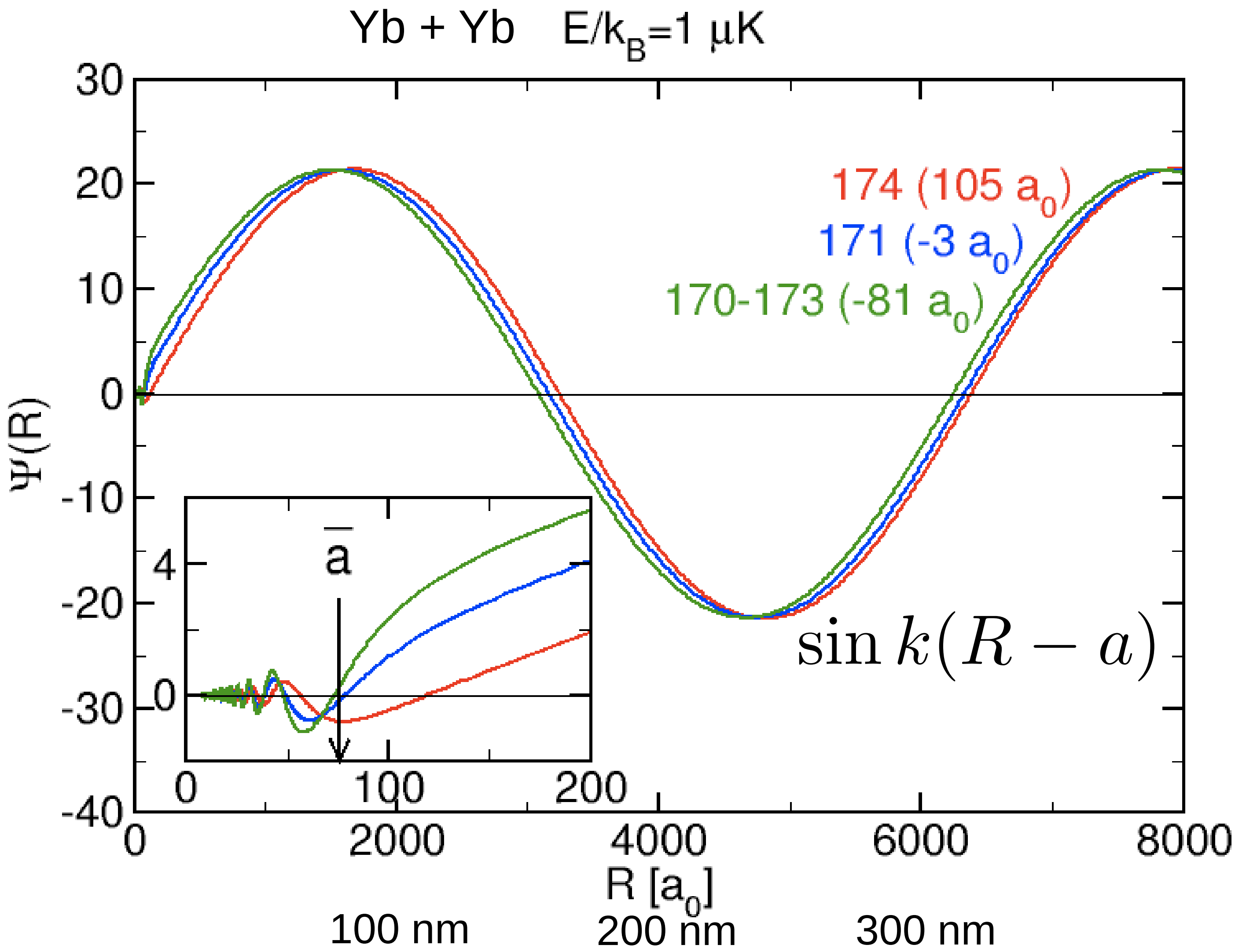
Multi-electron atom





From Krems et al, Cold Molecules, PSJ Chapter 6, arXiv:0902.1727

QDT: The s-wave scattering length + long range potential determine the scattering and bound state properties (of all partial waves) near threshold.



From Krems et al, Cold Molecules, PSJ Chapter 6, arXiv:0902.1727

Van der Waals potential

Write the Schrödinger equation in length and energy units of

$$R_{\rm vdw} = \frac{1}{2}\left(\frac{2\mu C_6}{\hbar^2}\right)^{\frac{1}{4}}$$

or

$$\bar{a} = \frac{\Gamma(3/4)}{\Gamma(5/4)} R_{\rm vdW} = 0.956 R_{\rm vdW}$$

Gribakin and Flambaum, Phys. Rev. A 48, 546 (1993)

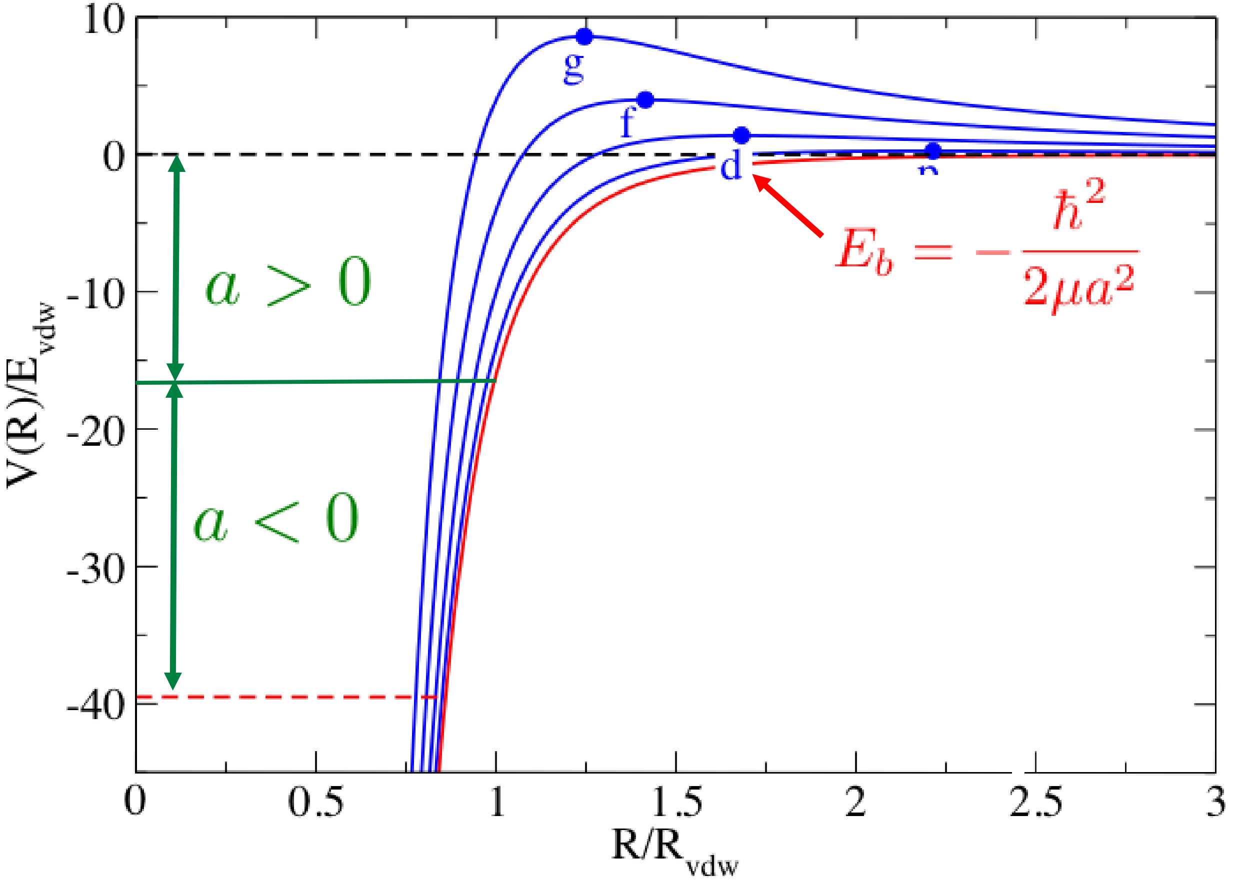
$$E_{\rm vdw} = \frac{\hbar^2}{2\mu R_{\rm vdw}^2}$$

The potential becomes $-\frac{16}{r^6} + \frac{\ell(\ell+1)}{r^2}$ vdw units.

This potential has exact analytic solutions and many useful properties.

B. Gao, Phys. Rev. A 58, 1728, 4222 (1998) + series of papers.
See Jones, et al., Rev. Mod. Phys. 78, 483 (2006) Photoassociation
and Chin et al., Rev. Mod. Phys. 82, 1225 (2010) Feshbach resonances

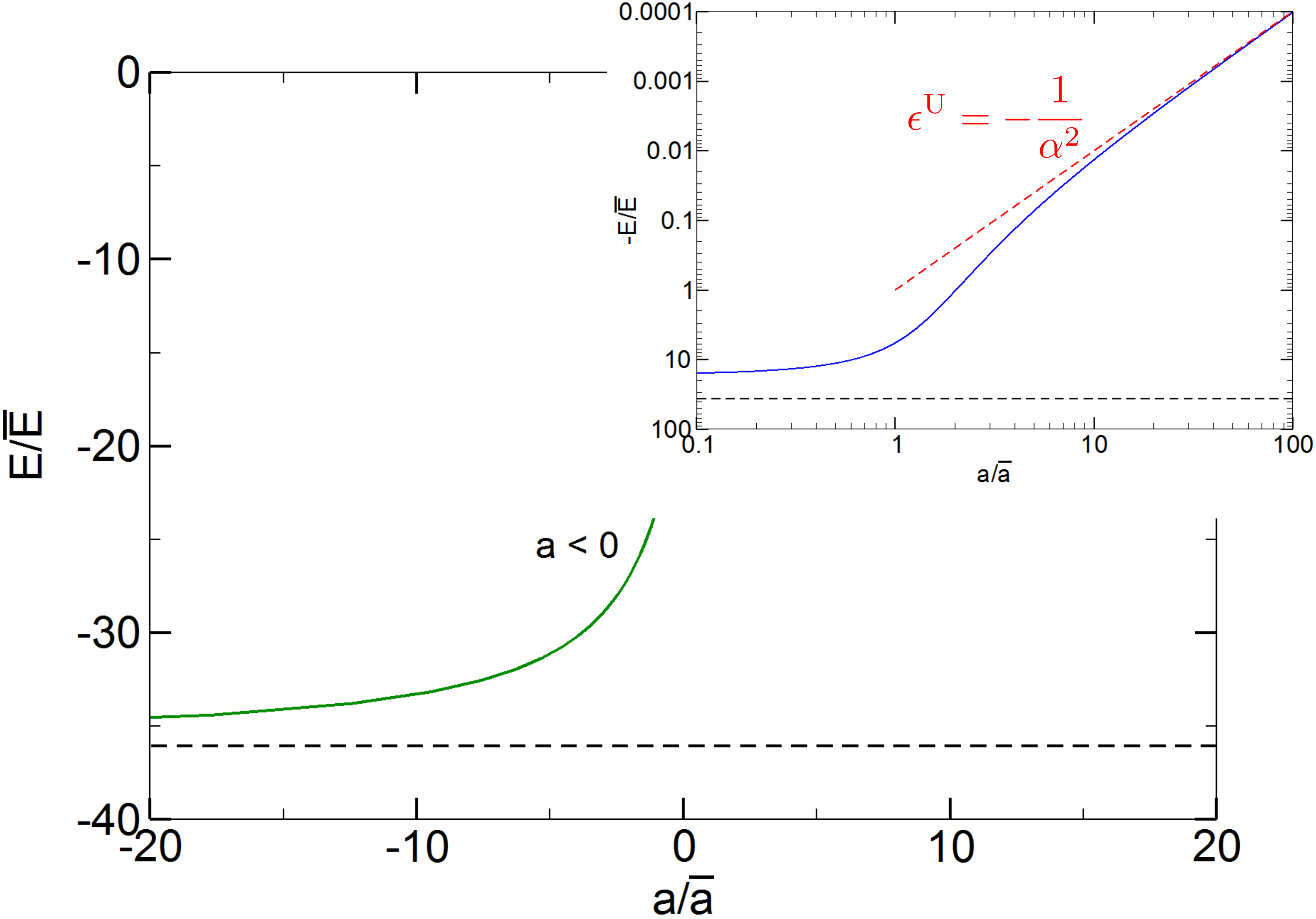
“Size” of vdW potential



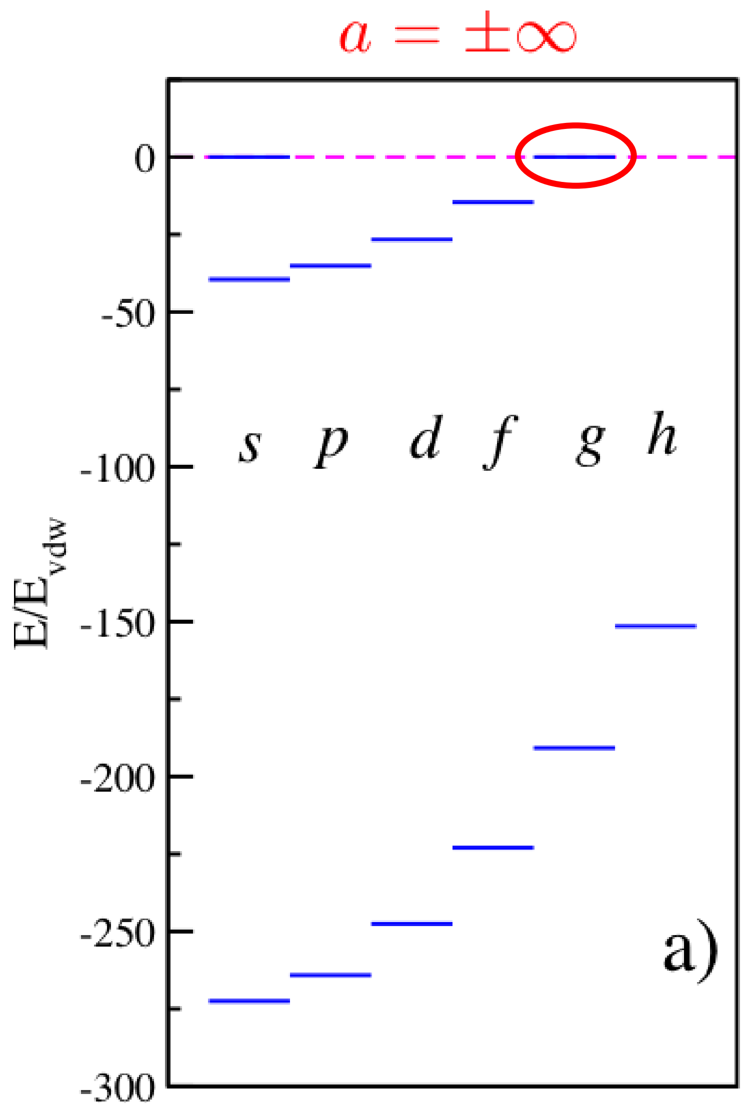
Universal

Jones, et al., Rev. Mod. Phys. 78, 483 (2006)

Universal energy of last (-1) bound state of vdW potential



Universal vdW bound state spectrum: depends on a



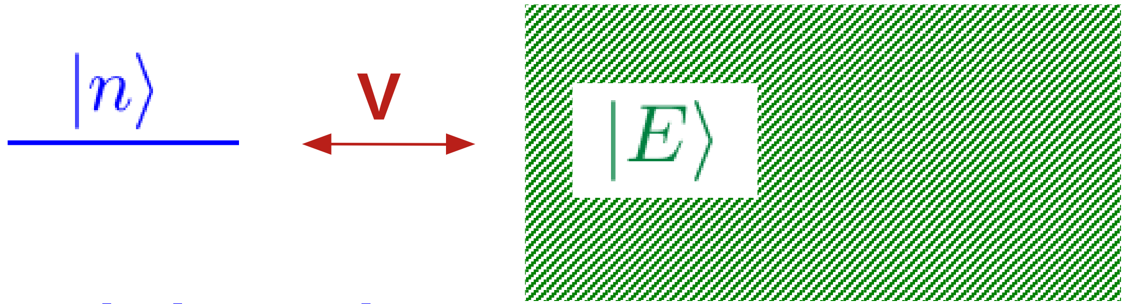
Gao, Phys. Rev. A 62, 050702 (2000); Chin et al, Rev. Mod. Phys. 82, 1225 (2010)

Resonant Scattering Picture

following U. Fano, Phys. Rev. 124, 1866 (1961); see Chin et al, RMP (2010)

Bound state

Continuum



Closed channel (Resonance)

Open channel (Background)

$$\eta(E) = \eta_{\mathrm{bg}} + \eta_{\mathrm{res}}(E)$$

width

$$\Gamma_n = 2\pi |\langle n|V|E\rangle|^2$$

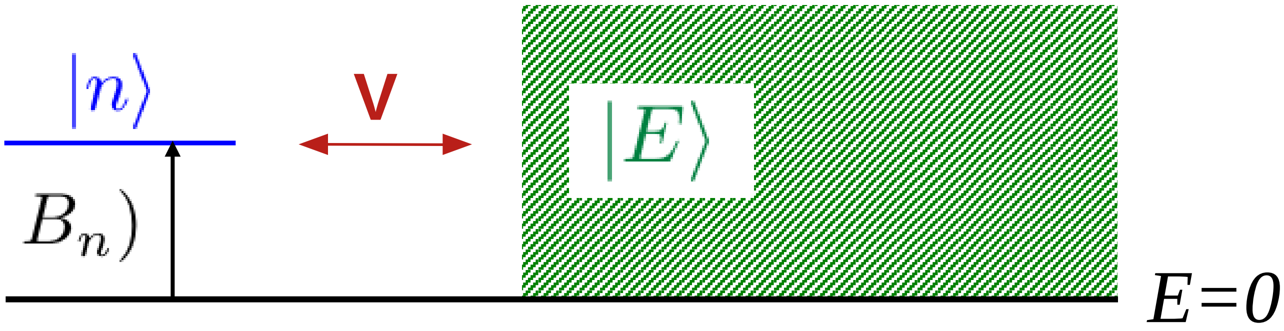
$$\eta_{\mathrm{res}} = -\tan^{-1} \frac{\frac{1}{2}\Gamma_n}{E - E_n - \delta E_n}$$

$$\delta E_n = \int \frac{|\langle n|V|E'\rangle|^2}{E_n - E'} dE'$$

shift

Threshold Resonant Scattering

$$E_n = \delta\mu(B - B_n)$$



$$\eta(E,B) = \eta_{\mathrm{bg}}(E) - \tan^{-1}\frac{\frac{1}{2}\Gamma(E)}{E - E_n - \delta E_n(E)}$$

As E → 0 $\quad \eta_{\mathrm{bg}} = -k a_{\mathrm{bg}} \quad\quad \frac{1}{2}\Gamma_n(E) = (k a_{\mathrm{bg}})\,\delta\mu\,\Delta_n$

$$a(B) = a_{bg}\left(1 - \frac{\Delta_n}{B - B_0}\right)$$

$$s_{\mathrm{res}} = \frac{a_{\mathrm{bg}}}{\bar{a}}\frac{\Delta\mu_{\mathrm{diff}}}{\bar{E}}$$

Shifted $\quad B_0 = B_n + \delta B_n$

Universal form of vdW threshold Feshbach scattering

Strength

$$\eta(\epsilon, B) = \eta_{\rm bg}(\epsilon) - \tan^{-1}\left(\frac{\kappa s_{\rm res}}{\epsilon - m_{\rm dif}(B - B_0)}\right)$$

$$\epsilon = E/\bar{E} \qquad \eta_{\rm bg} = -\kappa\alpha_{\rm bg} \qquad \kappa = k\bar{a} \qquad m_{\rm dif} = \frac{\mu_{\rm dif}}{\bar{E}}$$

"background" scattering length

$\eta_{\rm bg}(\epsilon),\ s_{\rm res}(\epsilon),\ B_0(\epsilon)$ are UNIVERSAL functions of ϵ, $\alpha_{\rm bg}$

PSJ & Gao, Atomic Physics 20 (ICAP 2006), ed. by C. Roos, H. Haffner, and R. Blatt
(available at arxiv:0609013).

More accurate than the effective range expansion:
Blackley, Hutson, PSJ, PRA 89, 042701 (2014)

Extension to multiple overlapping resonances:
Jachymski & PSJ, PRA 88, 052701 (2013)

Universal three-body properties

Universal few-body physics

Universality of the Three-Body Parameter for Efimov States in Ultracold Cesium

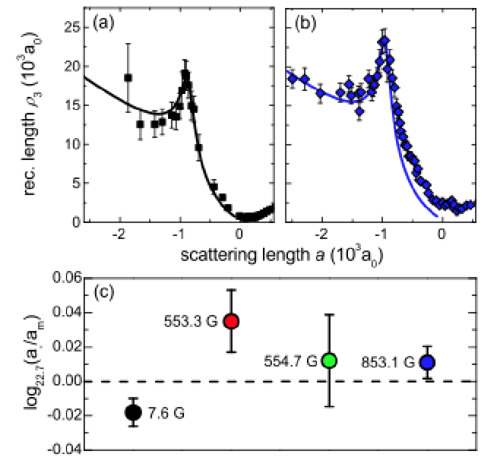
M. Berninger,[1] A. Zenesini,[1] B. Huang,[1] W. Harm,[1] H.-C. Nägerl,[1] F. Ferlaino,[1] R. Grimm,[1,2] P. S. Julienne,[3] and J. M. Hutson[4]

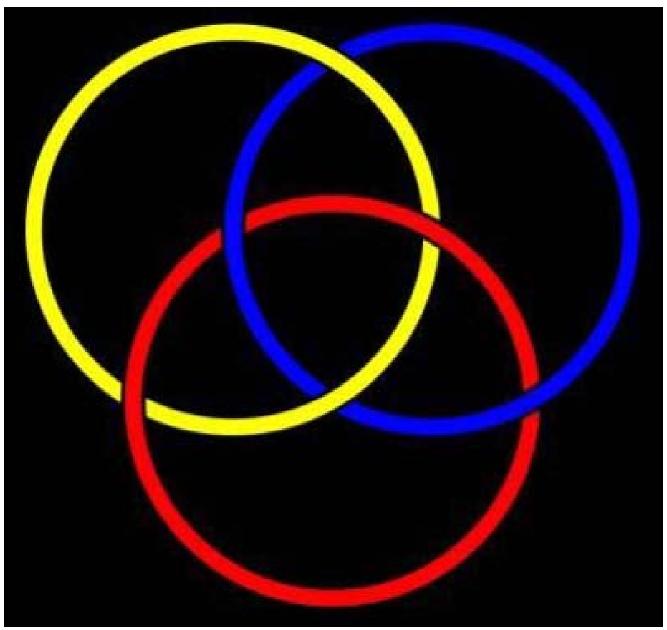
[1] *Institut für Experimentalphysik and Zentrum für Quantenphysik, Universität Innsbruck, 6020 Innsbruck, Austria*
[2] *Institut für Quantenoptik und Quanteninformation, Österreichische Akademie der Wissenschaften, 6020 Innsbruck, Austria*
[3] *Joint Quantum Institute, NIST and the University of Maryland, Gaithersburg, Maryland 20899-8423, USA*
[4] *Department of Chemistry, Durham University, South Road, Durham, DH1 3LE, United Kingdom*

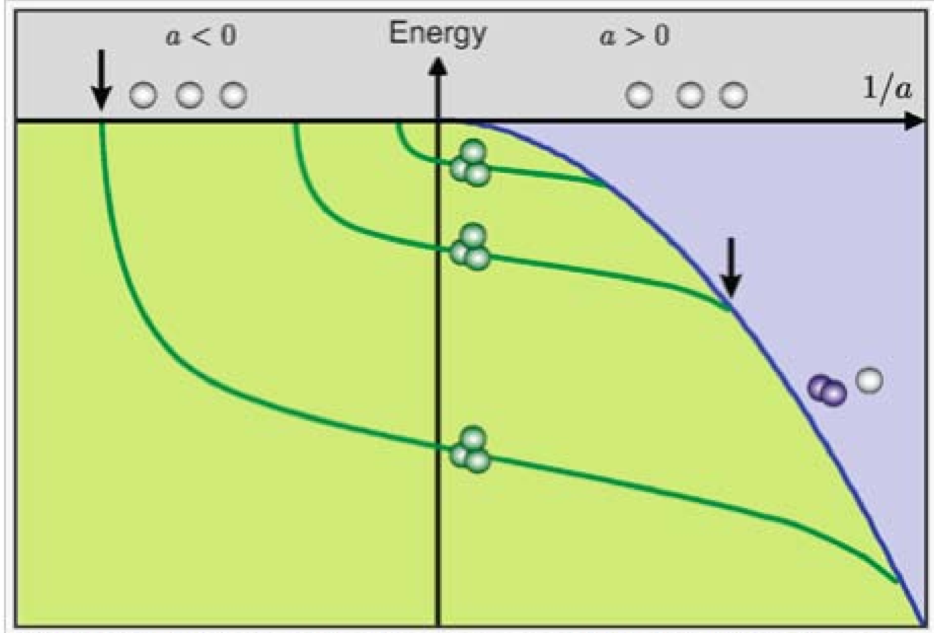
(Dated: July 27, 2011)

Phys. Rev. Lett. 107, 120401 (2011)
Original Cs experiment: T. Kraemer et al., Nature 440, 315 (2006)

Theory: J. Wang et al, Phys. Rev. Lett. 108**,** 263001 (2012)
Naidon et al, Phys. Rev. Lett*.* 112**,** 105301 (2014)







Picture, courtesy of the University of Innsbruck, shows a graph of Efimov triplet states as a function of the scattering length, a, and the binding energy. Outside the green area the three atoms exist singly or as a pair plus a lone atom.

3-Body recombination of 3 alkali-metal atoms

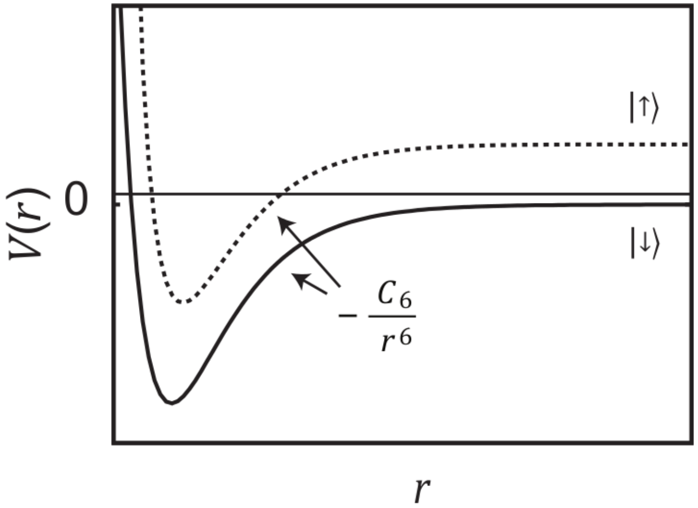
Universal van der Waals physics

Use only known 2-body physics + additive pairwise van der Waals potentials for 3 atoms

Y. Wang & PSJ, Nat. Phys. 10, 768 (2014)

Cs + Cs + Cs → Cs_2 + Cs

Two-channel Cs + Cs interaction: "Exact" 2-body Feshbach model



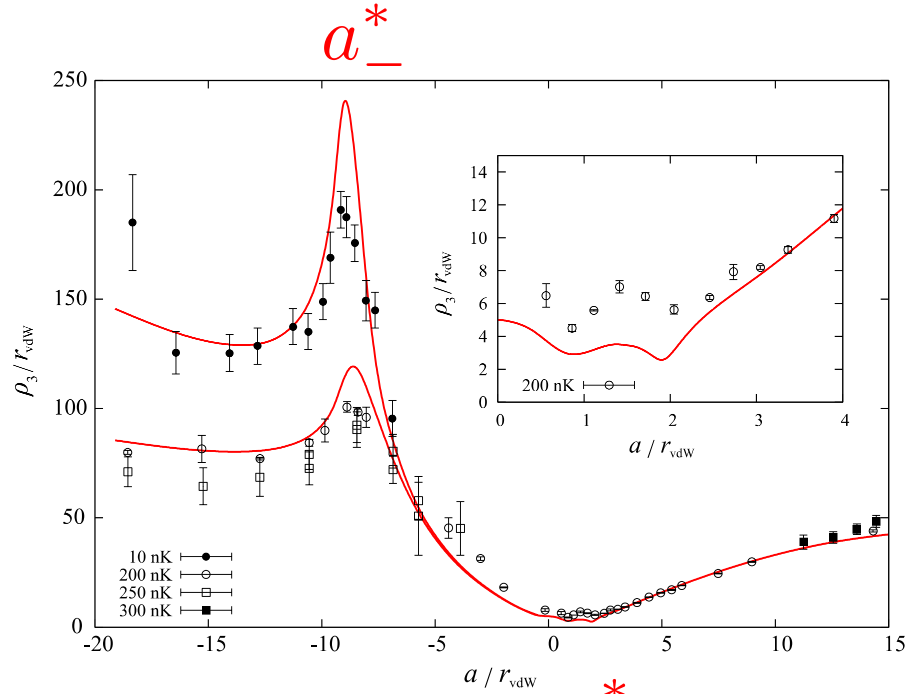
2-channel numerical model

Using $s_{\rm res}, \alpha_{\rm bg}, n_{\rm dif}$ for Cs-Cs

6-12 Lennard-Jones potentials
+ short-range coupling
Mies (2000), PSJ(2006)

Number of bound states can be varied, N = 2 to 4.

Numerically solve 3B equations in hyperspherical basis

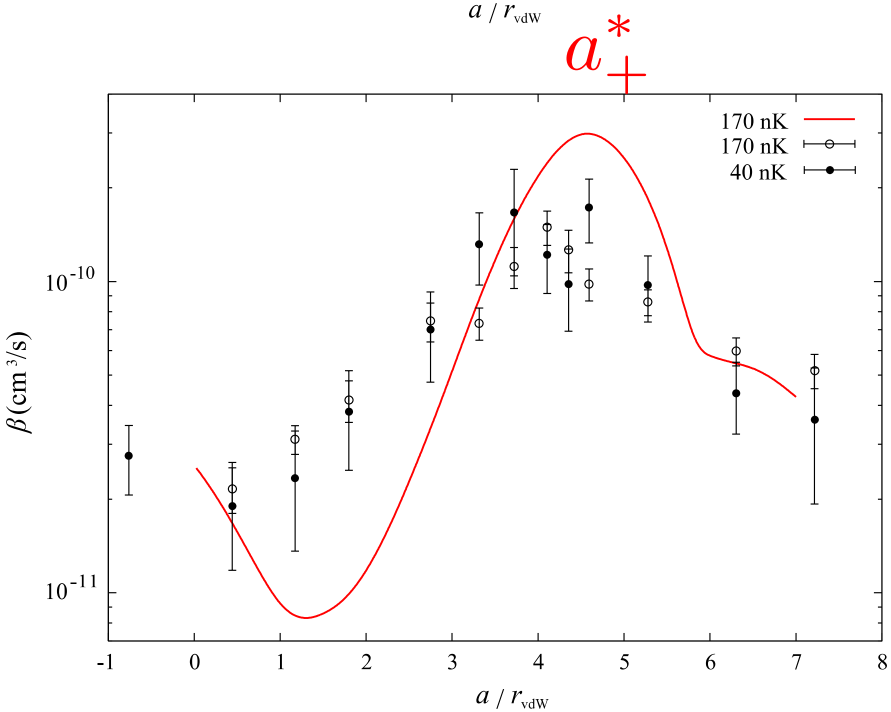


3-body recombination Cs+Cs+Cs near B=0

Points: Innsbruck data

Line: Theory—numerical
<u>No adjustable parameters</u>
Nat. Phys. 10, 768 (2014)

T. Kraemer et al., Nature 440, 315 (2006)



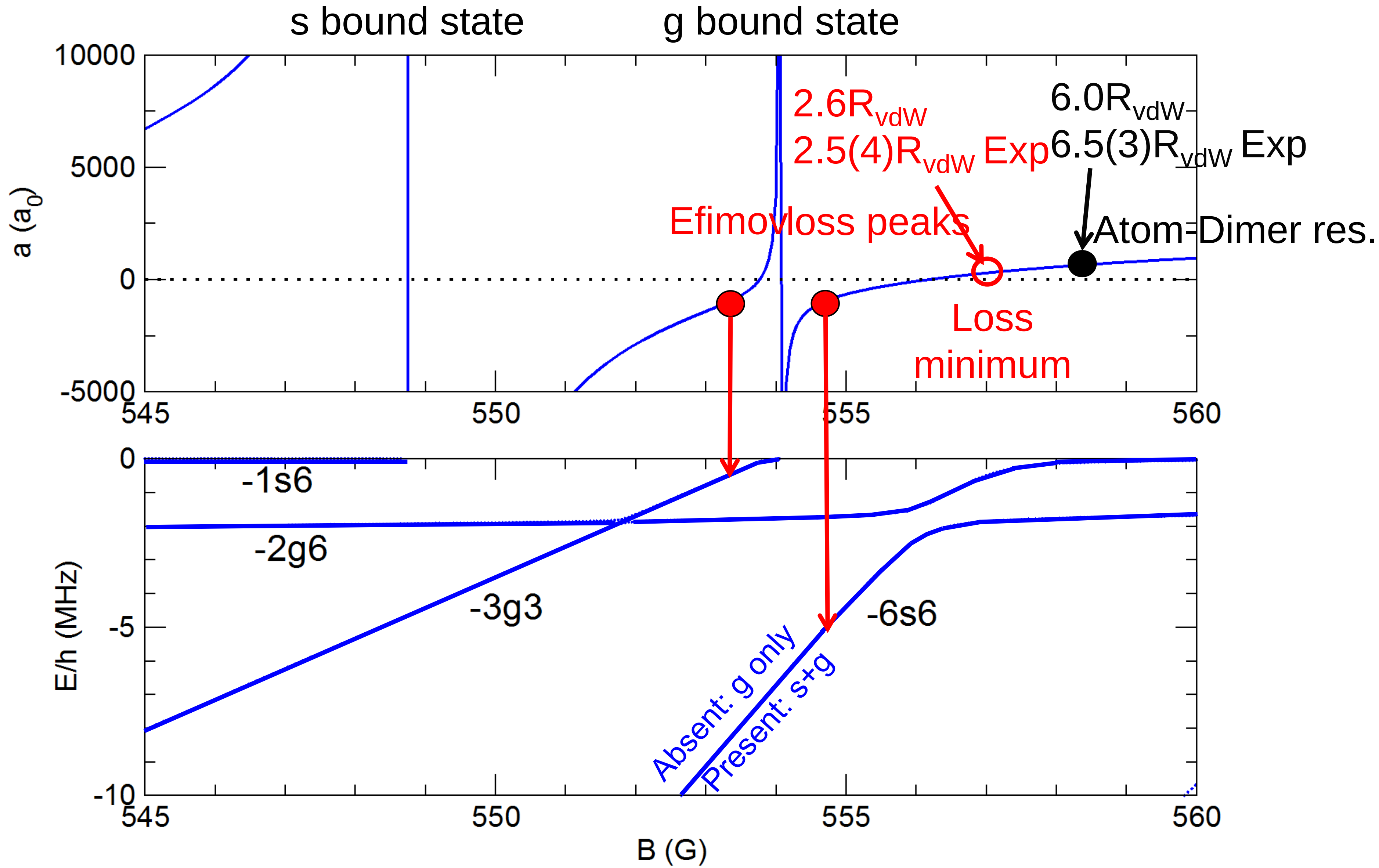
Atom-dimer relaxation Cs + Cs_2

$$a_+^* / |a_-^*| =$$ 0.53 calculated

0.47(3) exp.

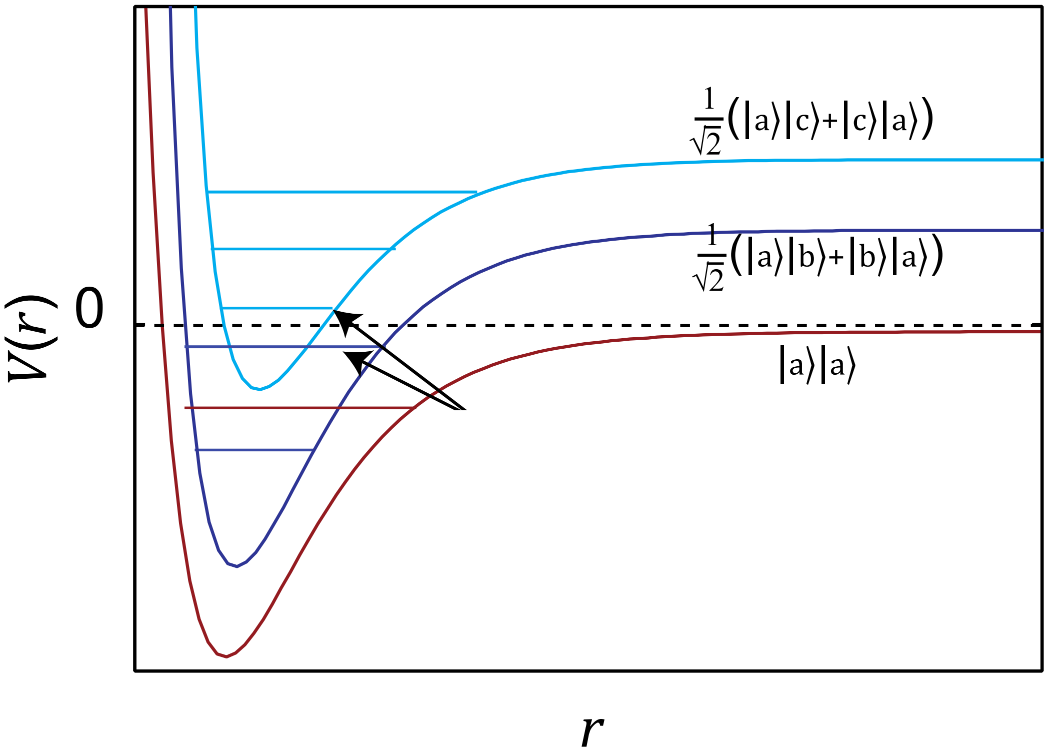
1.06 universal
(s-wave unitarity)

S. Knoop et al., Nature Phys. 5, 227 (2009)



Cs coupled channels model from Berninger, et al, Phys. Rev. A 87, 032517 (2013)
Cs overlapping resonances (multiple s_{res}): Jachymski, PSJ, PRA 88, 052701(2013)
Efimov measurements: Innsbruck, Phys. Rev. Lett. 107**,** 120401 (2011);
Few-Body Syst. 51**,** 113–133 (2011); Phys. Rev. A 90, 022704(2014)
3-body theory: Wang and PSJ, Nat. Phys. 10, 768(2014)

3-channel 2-resonance model for universal van der Waals 3-body physics



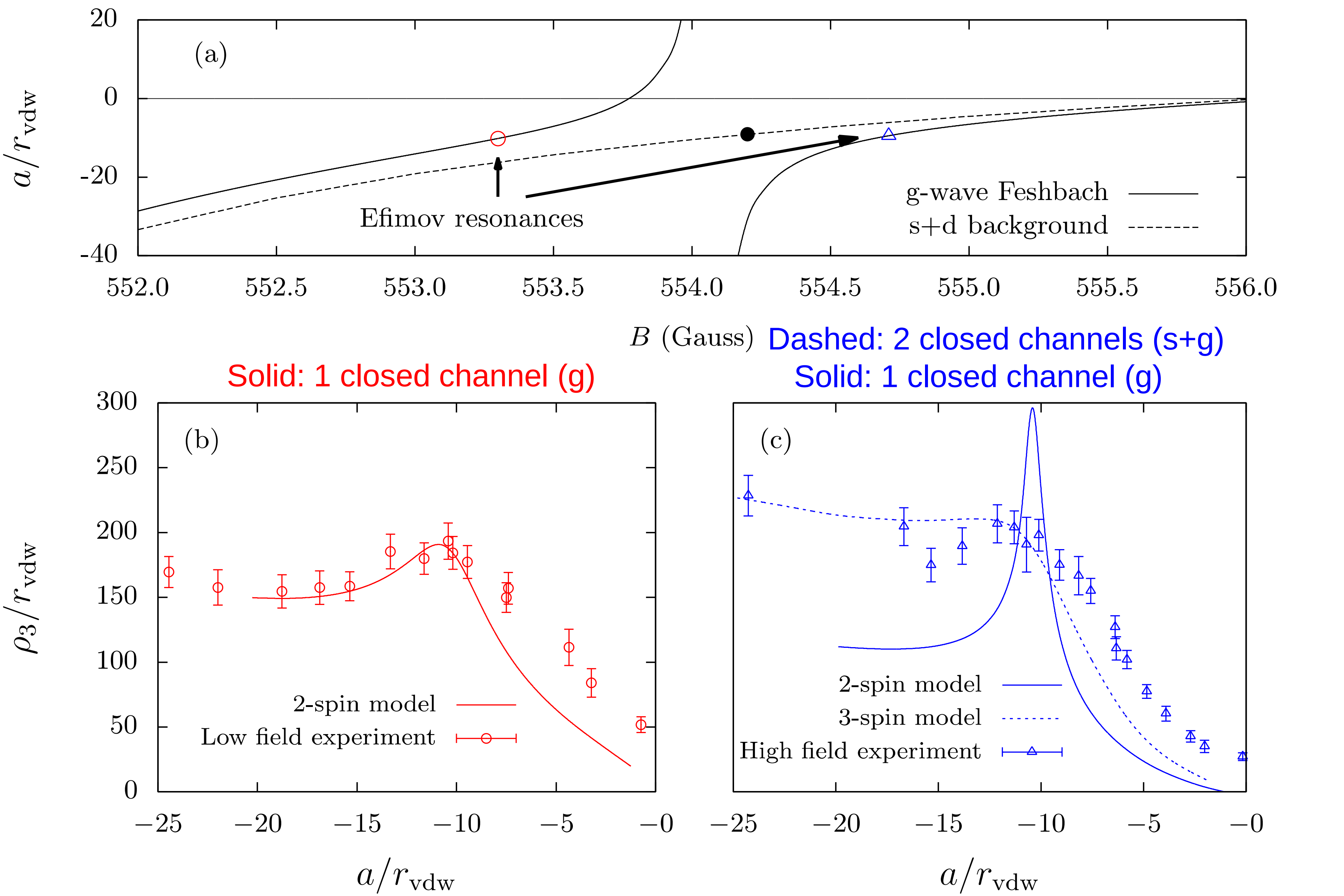
Simultaneously describes two closed channels with overlapping resonances

States of recombination come from BOTH channels.

Necessary for universal van der Waals physics near 554G Cs resonance

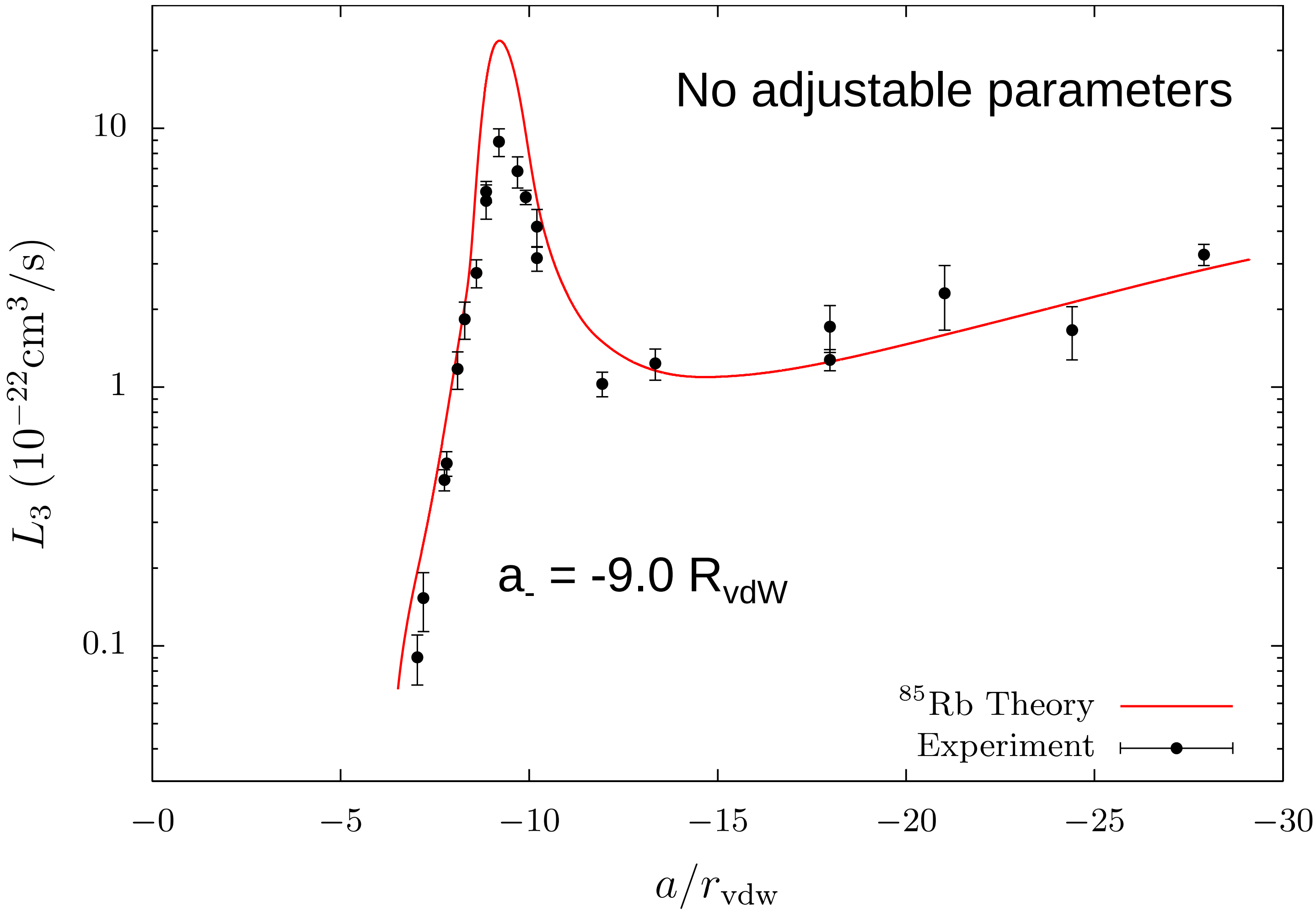
$$a(B) = a_{\mathrm{bg}}\left(1-\frac{\Delta_1}{B-B_1}\right)\left(1-\frac{\Delta_2}{B-B_2}\right)$$

Jachymski, PSJ, PRA 88, 052701(2013)
Y. Wang & PSJ, Nat. Phys. 10, 768 (2014)



Calculations: no adjustable parameters

2-spin model, ^{85}Rb, s_{res} = 28, α_{bg} = -5.4



JILA data: Wild, et al., Phys. Rev. Lett. 108, 145305 (2012)

Universality
in complex or chaotic collisions

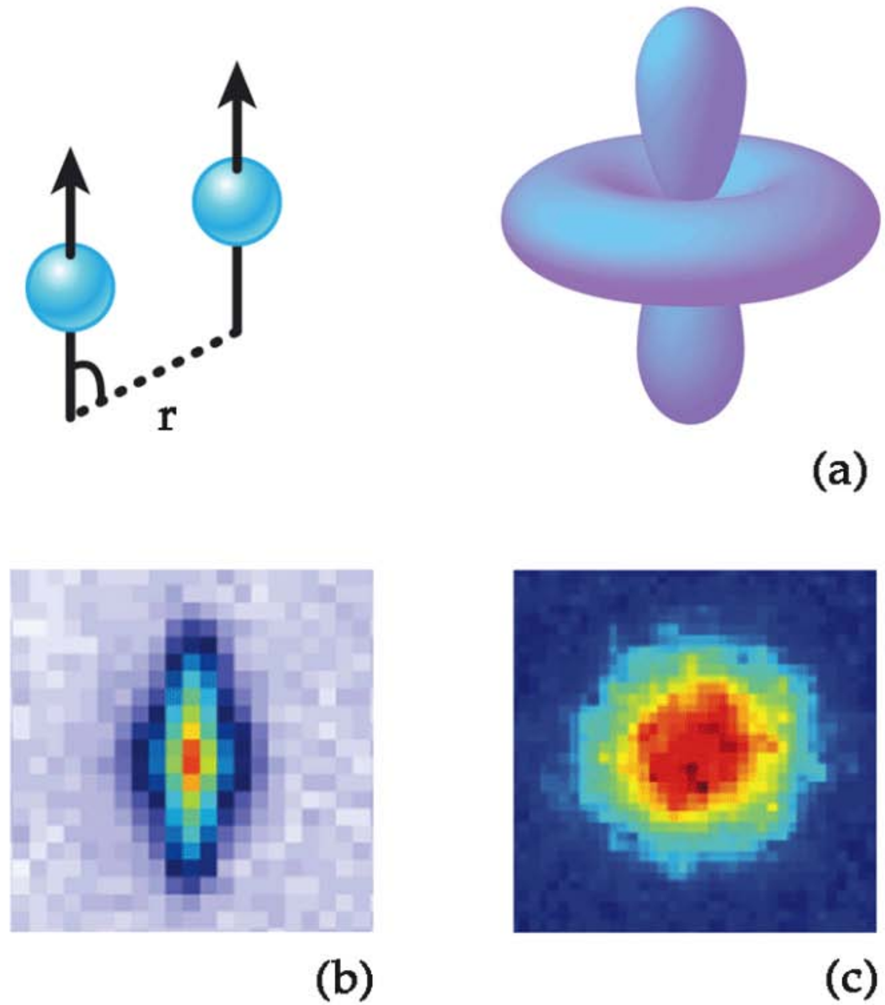
Physics

B. Laburthe-Tolra, Physics 5, 58 (2012)
"Quantum Dipolar Gases in Boson or Fermion Flavor"

$4f^{12}6s^{2}\ {}^{3}H_{6}$

$7\mu_B$

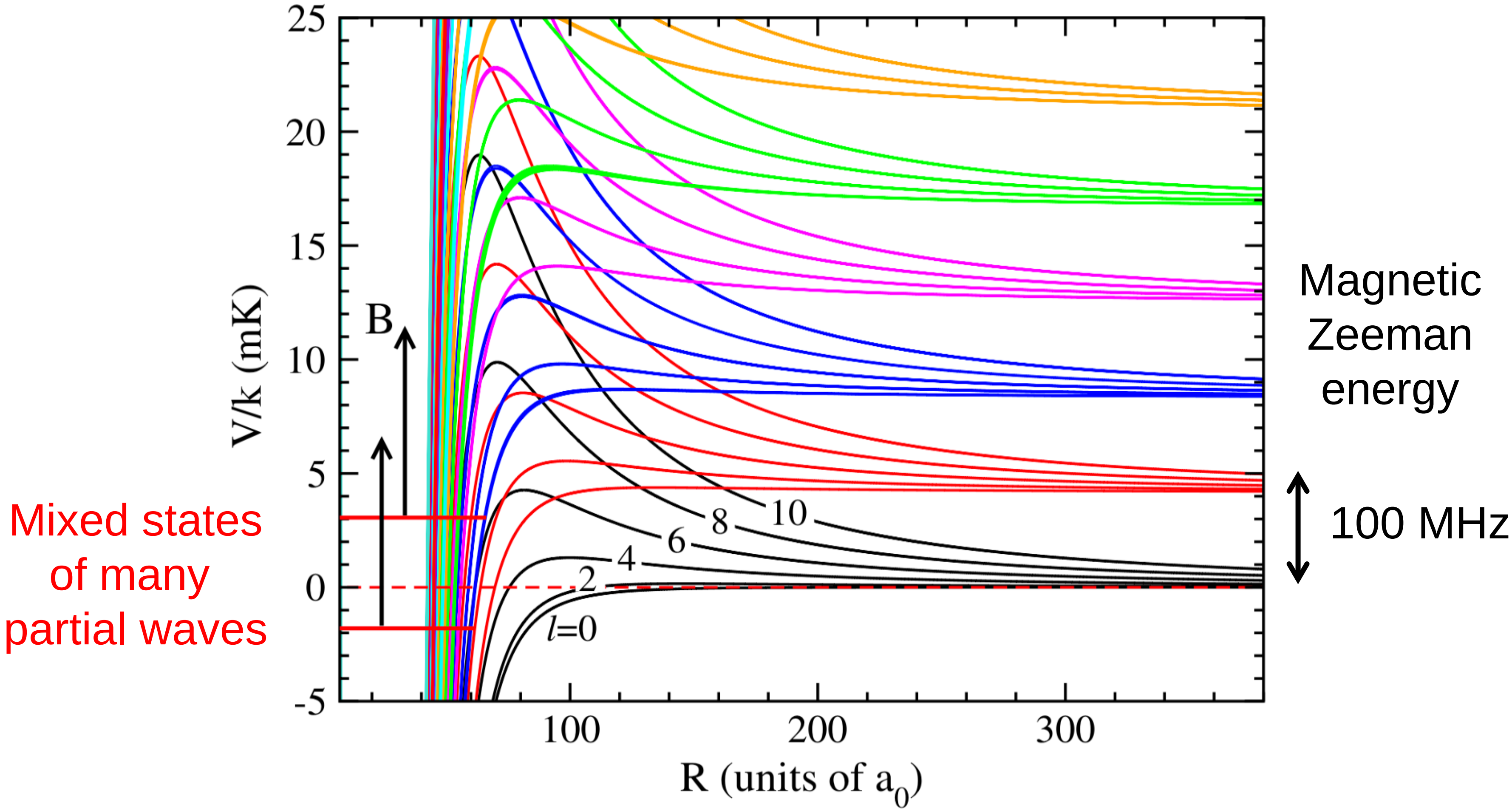
Ferlaino group
Innsbruck
^{168}Er
30000 atoms
order 100nK



$4f^{10}6s^{2}\ {}^{5}I_{8}$

$10\mu_B$

Lev group
Stanford
^{161}Dy
6000 atoms
64nK $T/T_F=0.2$



Diagonal potential energy curves for ^{164}Dy + ^{164}Dy at B = 50G

Asymptotic $|(j_1 j_2) j m_j, l m_l\rangle$ channels, $m_j + m_l = -16$, $0 \leq l \leq 10$

From Petrov, Tiesinga, Kotochigova, PRL 109, 103002 (2012)

LETTER

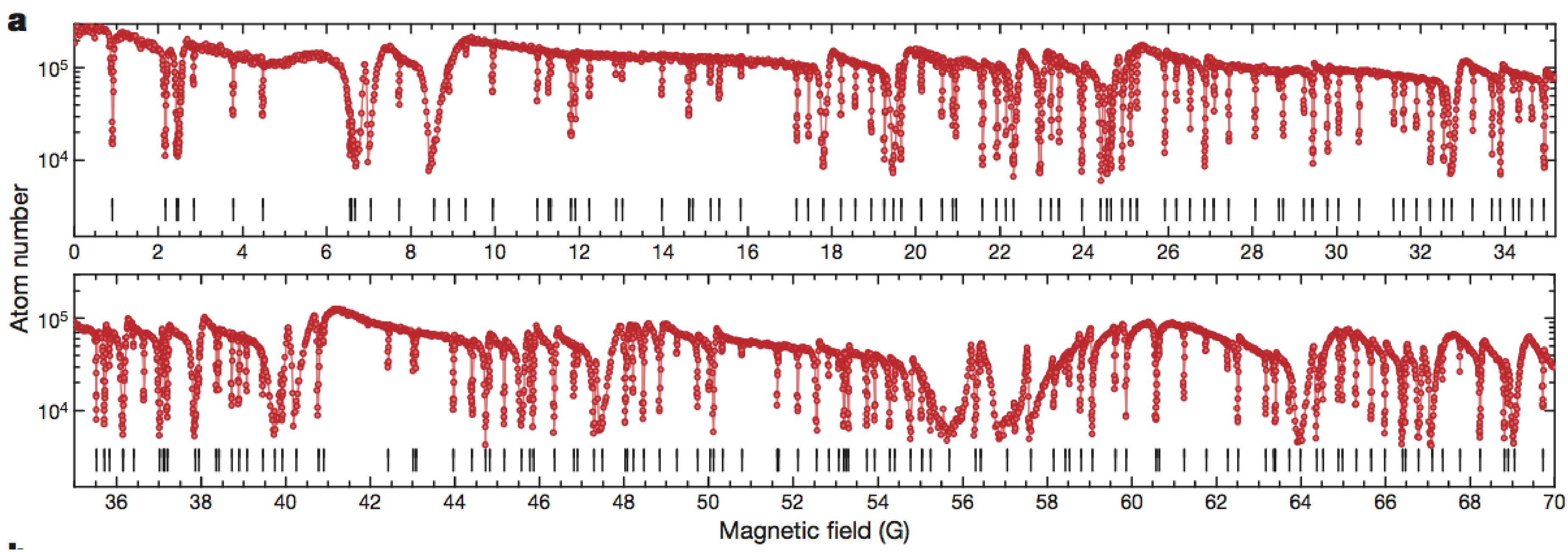
Nature online, March 12, 2014

doi:10.1038/nature13137

Quantum chaos in ultracold collisions of gas-phase erbium atoms

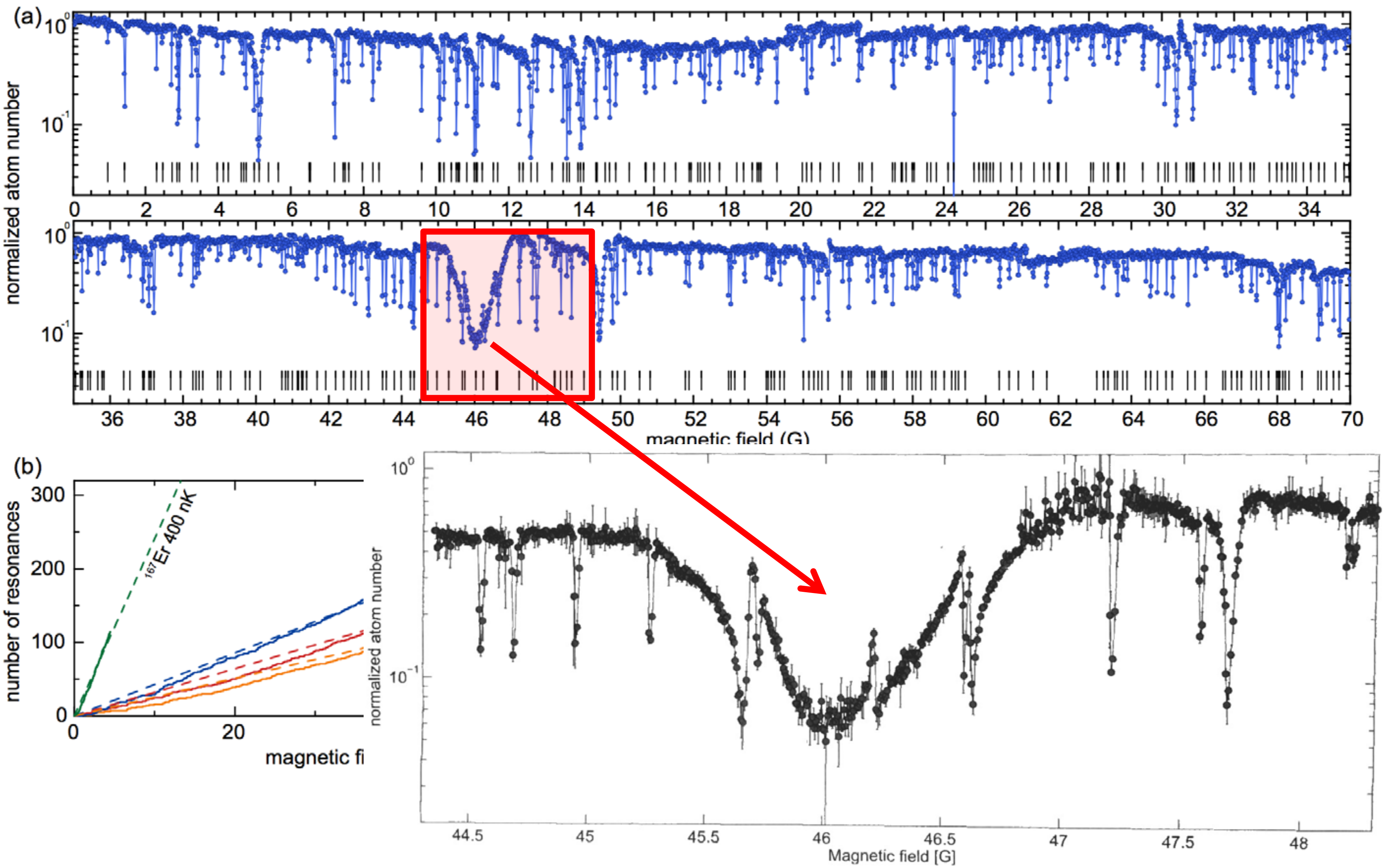
$$\dot{n} = -L_3 n^3$$

Albert Frisch[1], Michael Mark[1], Kiyotaka Aikawa[1], Francesca Ferlaino[1], John L. Bohn[2], Constantinos Makrides[3], Alexander Petrov[3,4,5] & Svetlana Kotochigova[3]



^{168}Er in ground state $^3H_6$(m=-6)

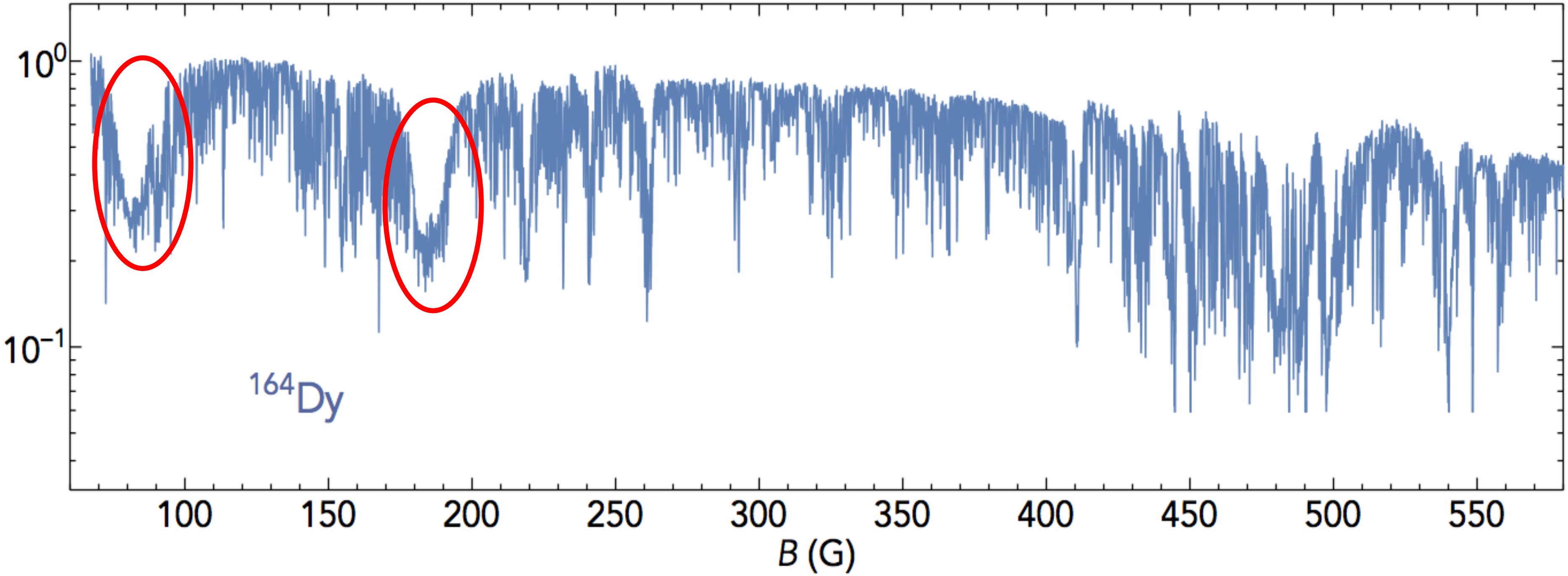
^{164}Dy M=-8



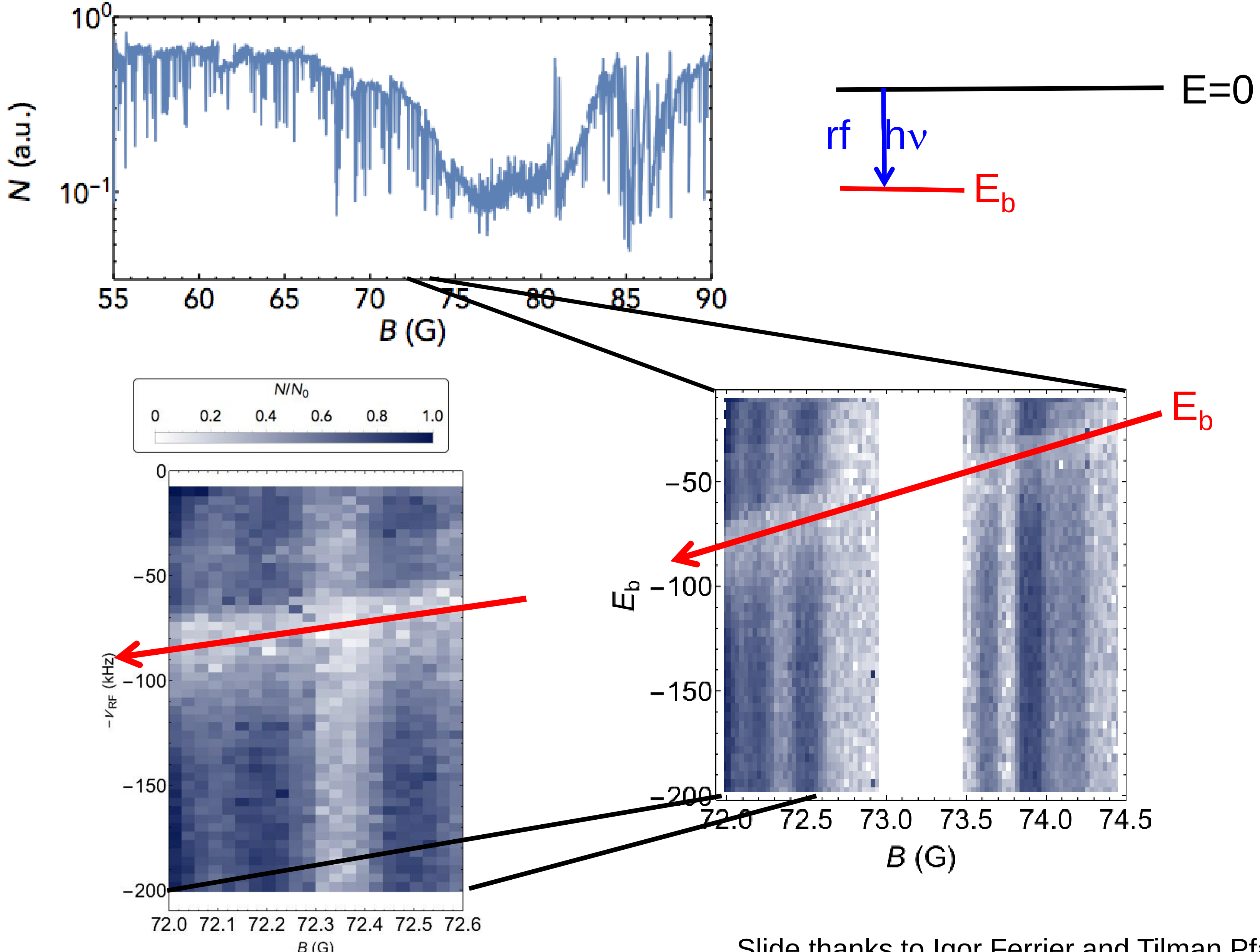
Pfau/Ferlaino/Kotochigova collaboration, arxiv:1506.05221

Feshbach resonances in Dysprosium

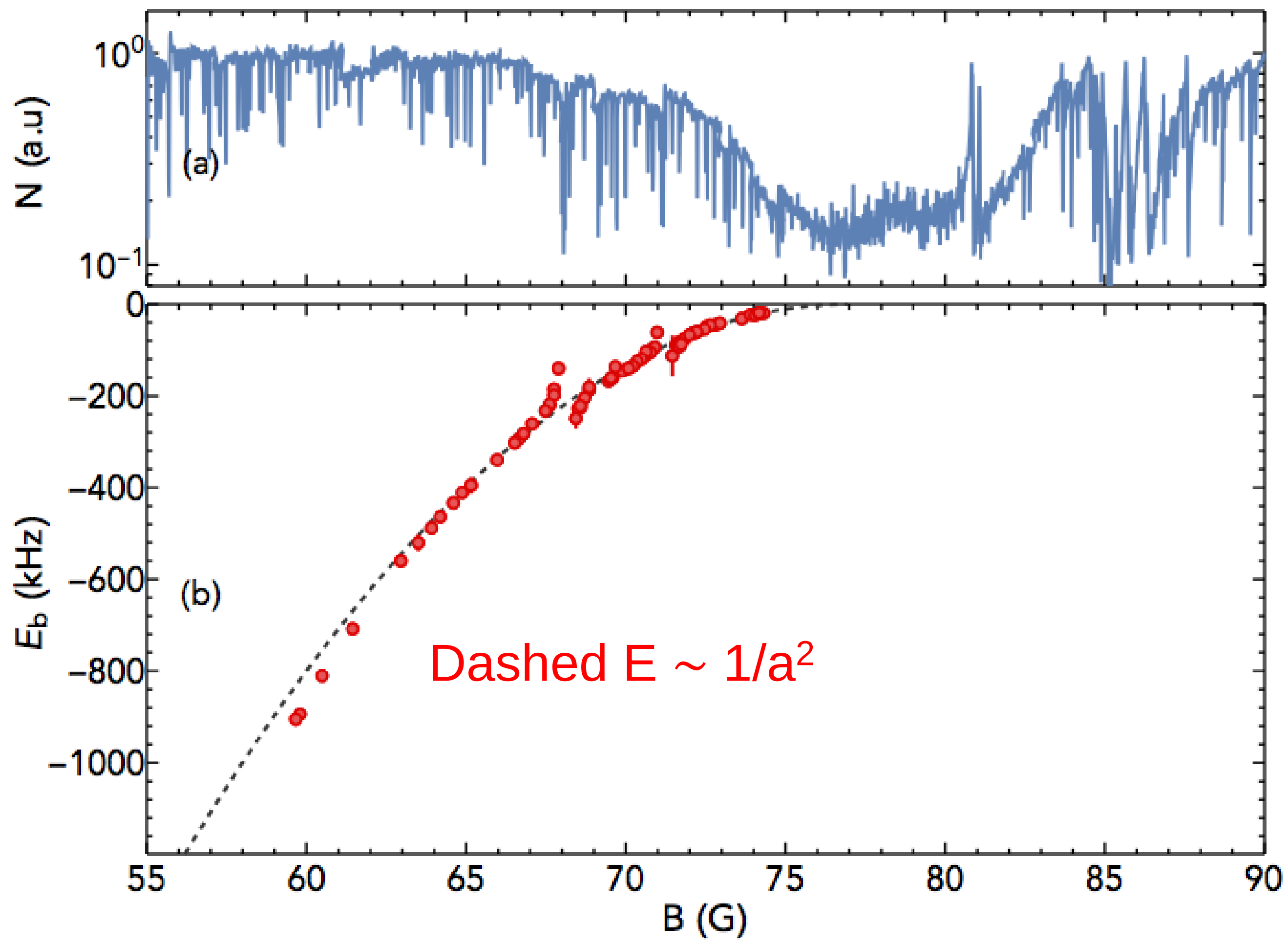
Atom-loss spectroscopy of ^{164}Dy at high field, observation of several broad features



T. Maier, I. Ferrier-Barbut, H. Kadau, M. Schmitt, M. Wenzel, C. Wink, T. Pfau, K. Jachymski, and PSJ, Phys. Rev. A, 92, 060702 (2015).

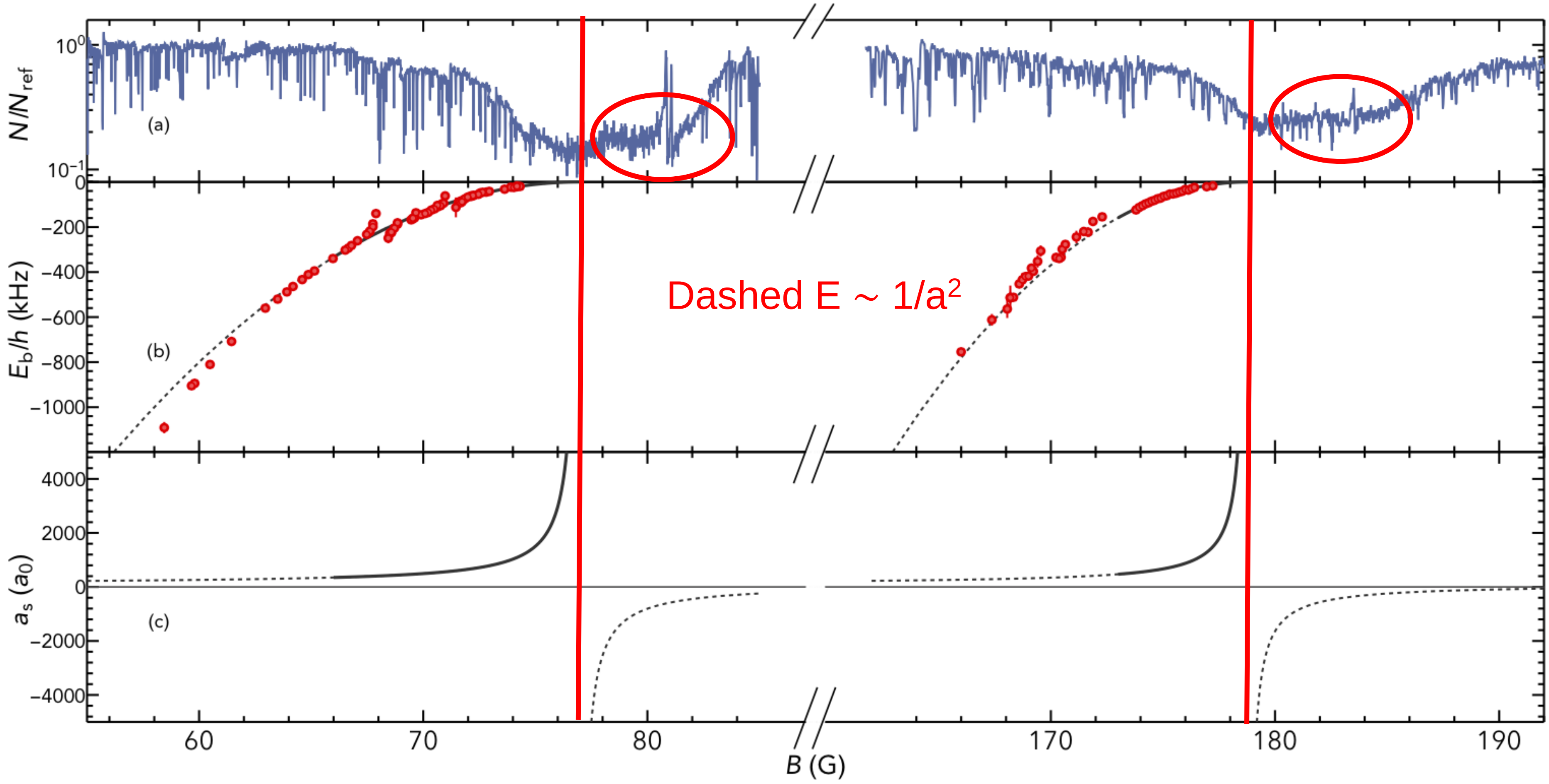


Slide thanks to Igor Ferrier and Tilman Pfau



Signature of “universal” s-wave halo state

Slide thanks to Igor Ferrier and Tilman Pfau



Signature of “universal” s-wave state

Scattering of two structureless dipoles

Bohn, Cavagnero, Ticknor, New. J. Phys. *11,* 055039 (2009)

s-wave: p=6 van der Waals
d-wave: p=3 dipolar + p=6 van der Waals

s-d off-diagonal coupling ➔ adiabatic s-wave p=4 term

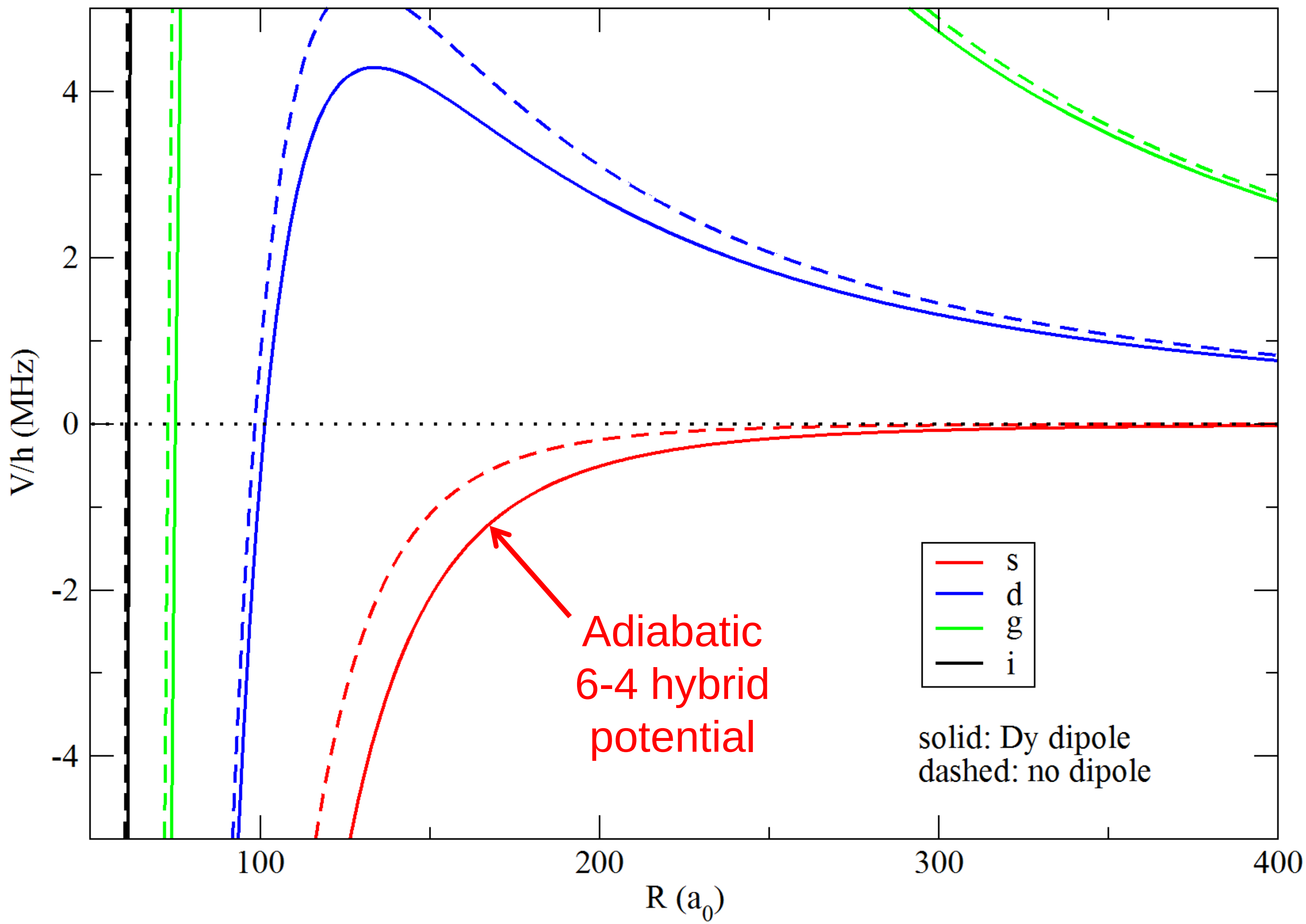
Dy+Dy: R_6 = 154 a_0 E_6/h = 0.93 MHz or ≈ 50 μK

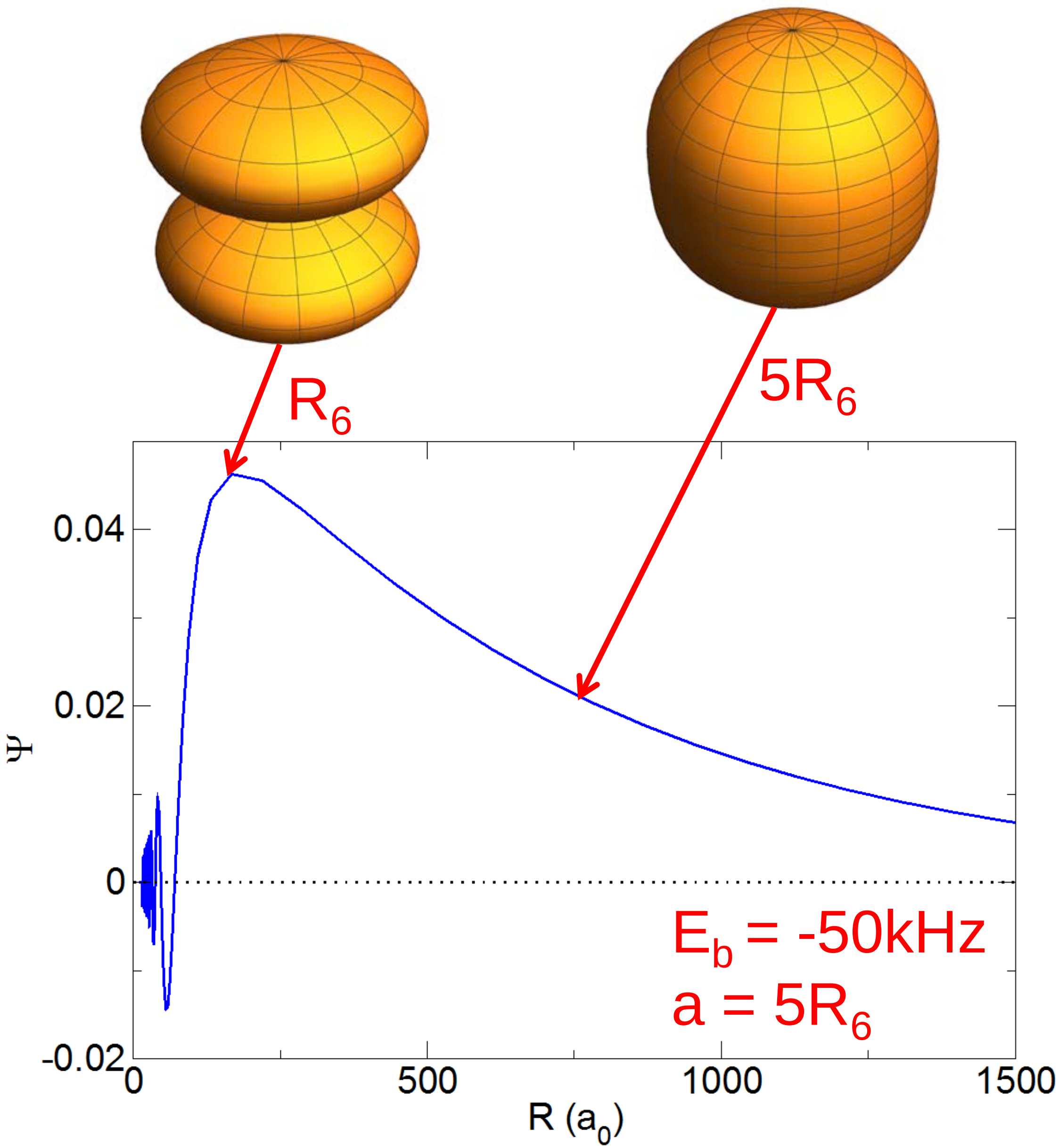
R_3 = 194 a_0 (Bohn definition)
R_4 = 143 a_0

Solve s-wave (1-channel) scattering for a single potential to get "universal" E(a) function in reduced units of E/E_p and a/R_p.

Do this for a p=6 potential, or a p=3 potential or a p=6 + p=4 "hybrid" potential (scale with E_6, a_6).

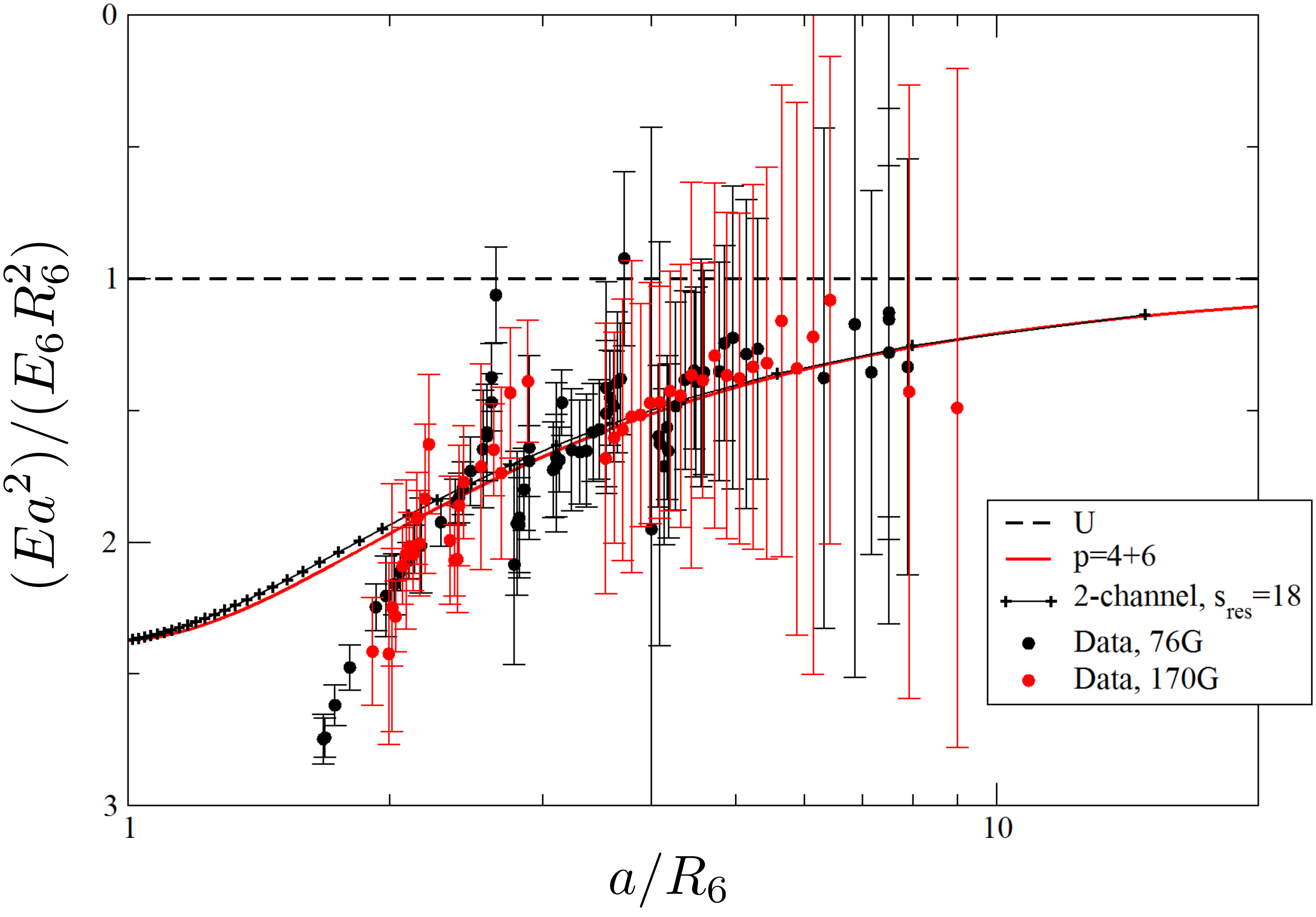
Dy$_2$ adiabatic potentials

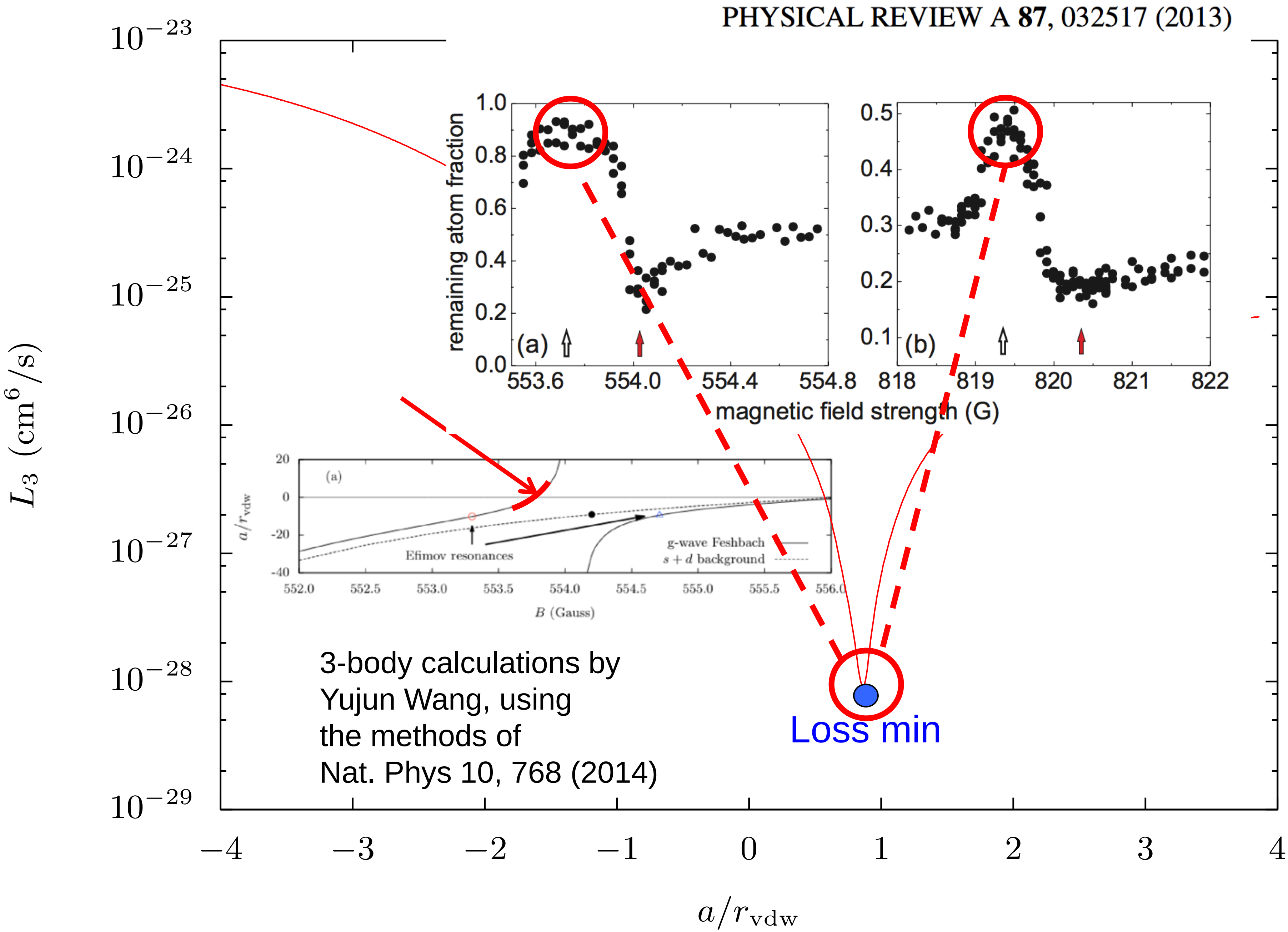


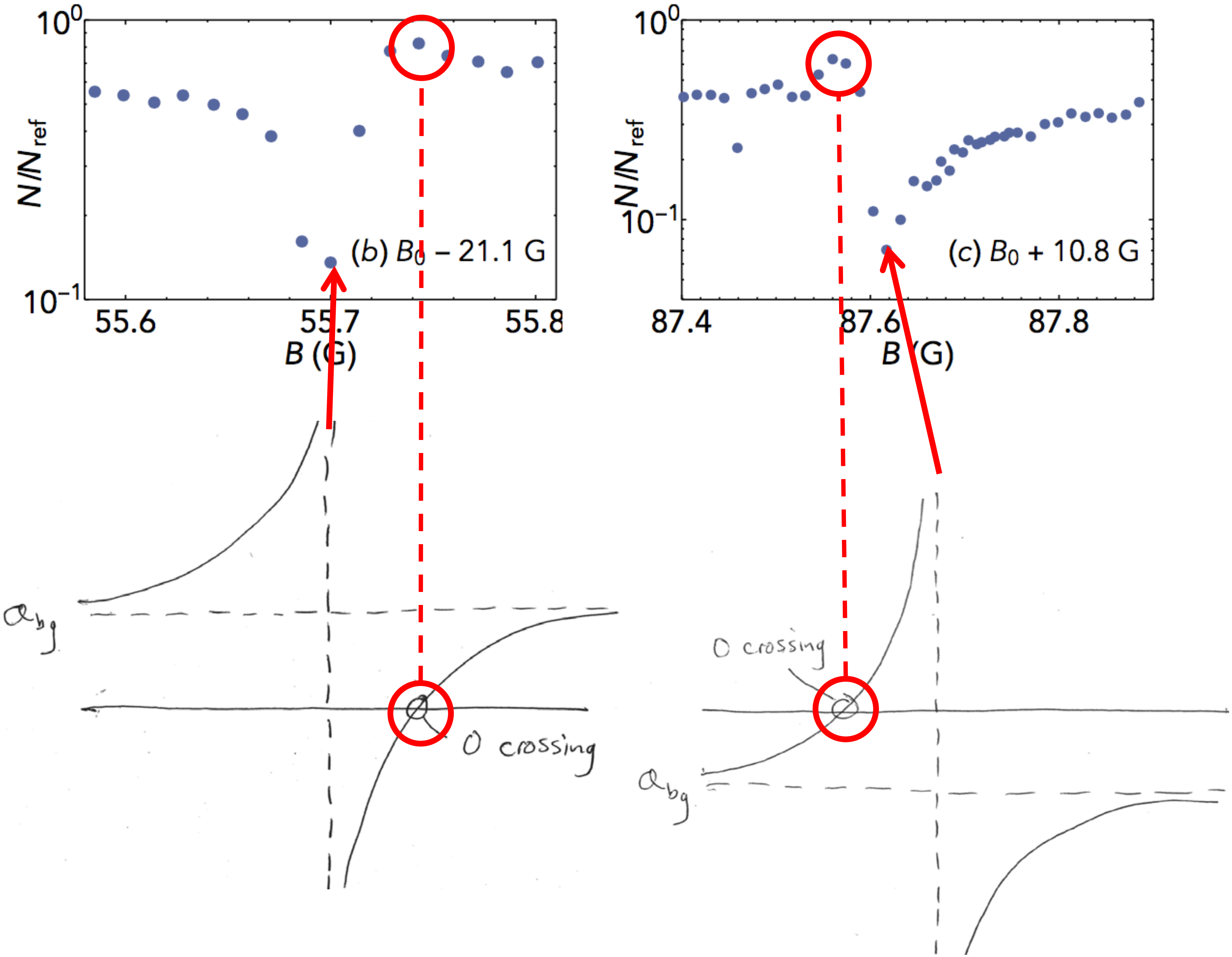


R6
5R6
0.04
0.02
0
-0.02
Ψ
0
500
1000
1500
R (a0)
Eb = -50kHz
a = 5R6

Ea^2 versus a in scaled units



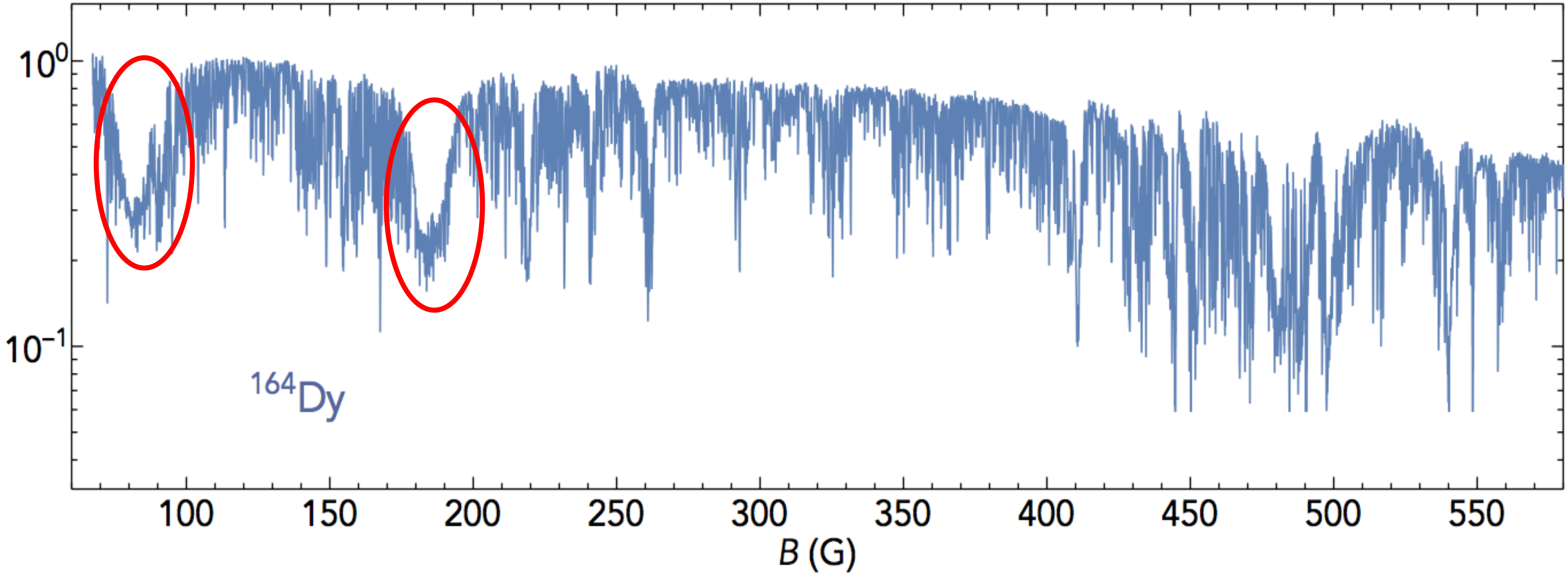

PHYSICAL REVIEW A 87, 032517 (2013)
remaining atom fraction
1.0
0.8
0.6
0.4
0.2
0.0
(a)
553.6
554.0
554.4
554.8
0.5
0.4
0.3
0.2
0.1
(b)
818
819
820
821
822
magnetic field strength (G)
20
0
-20
-40
(a)
a/r_vdw
Efimov resonances
g-wave Feshbach
s + d background
552.0
552.5
553.0
553.5
554.0
554.5
555.0
555.5
556.0
B (Gauss)
3-body calculations by
Yujun Wang, using
the methods of
Nat. Phys 10, 768 (2014)
Loss min
L_3 (cm^6/s)
10^{-23}
10^{-24}
10^{-25}
10^{-26}
10^{-27}
10^{-28}
10^{-29}
−4
−3
−2
−1
0
1
2
3
4
a/r_{vdw}



10^0
10^{-1}
N/N_{ref}
(b) B_0 – 21.1 G
55.6
55.7
55.8
B (G)
10^0
10^{-1}
N/N_{ref}
(c) B_0 + 10.8 G
87.4
87.6
87.8
B (G)
a_{bg}
0 crossing
0 crossing
a_{bg}

Feshbach resonances in Dysprosium

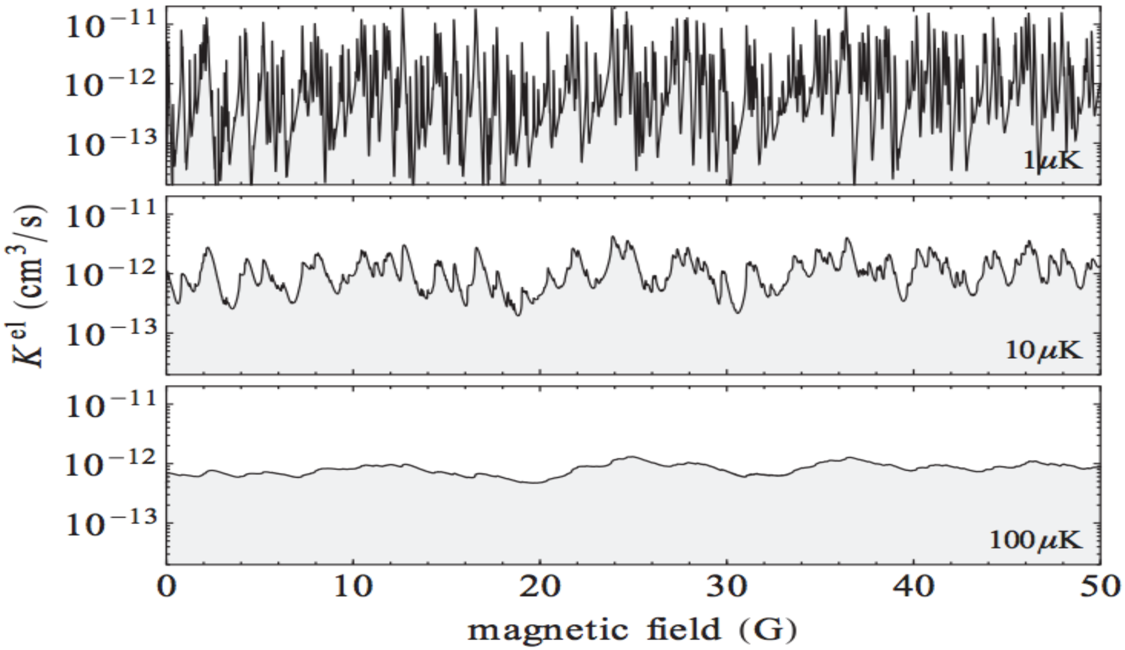
Atom-loss spectroscopy of ^{164}Dy at high field, observation of several broad features



Patterned complexity

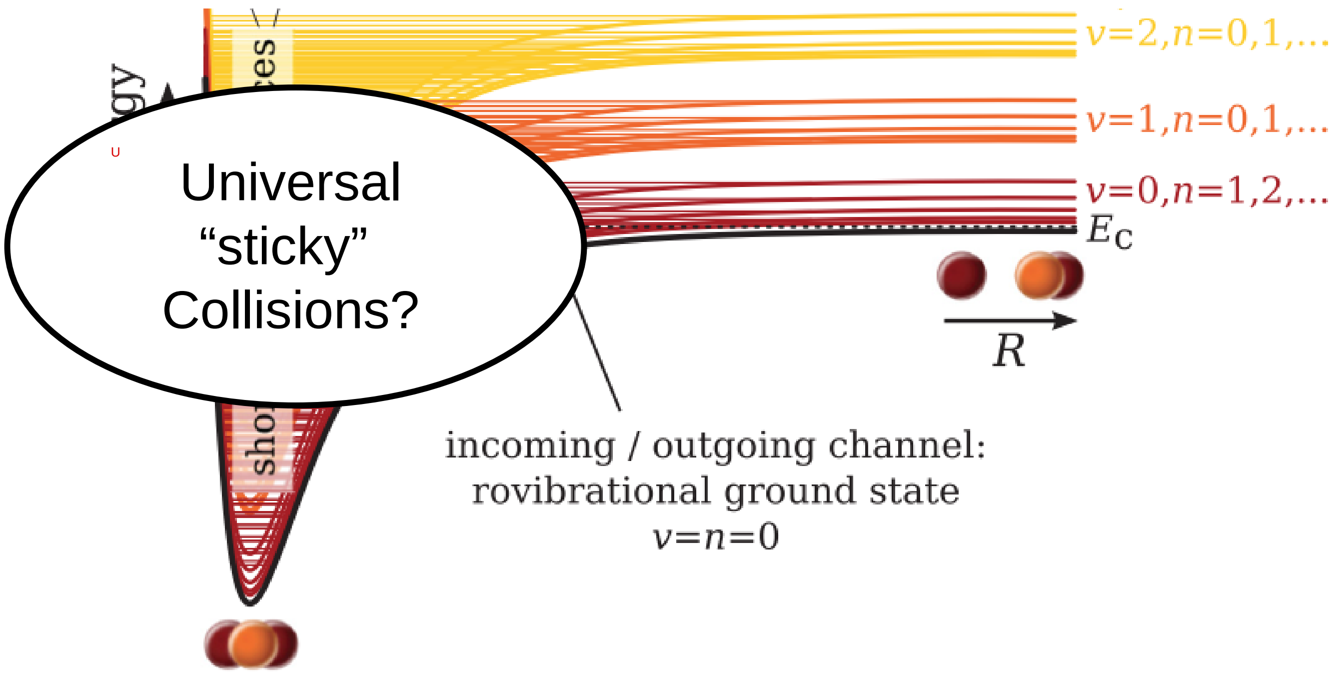
T. Maier, I. Ferrier-Barbut, H. Kadau, M. Schmitt, M. Wenzel, C. Wink, T. Pfau, K. Jachymski, and PSJ, Phys. Rev. A, 92, 060702 (2015).

From Mayle, Ruzic, Bohn, Phys. Rev. A 85, 062712 (2012)

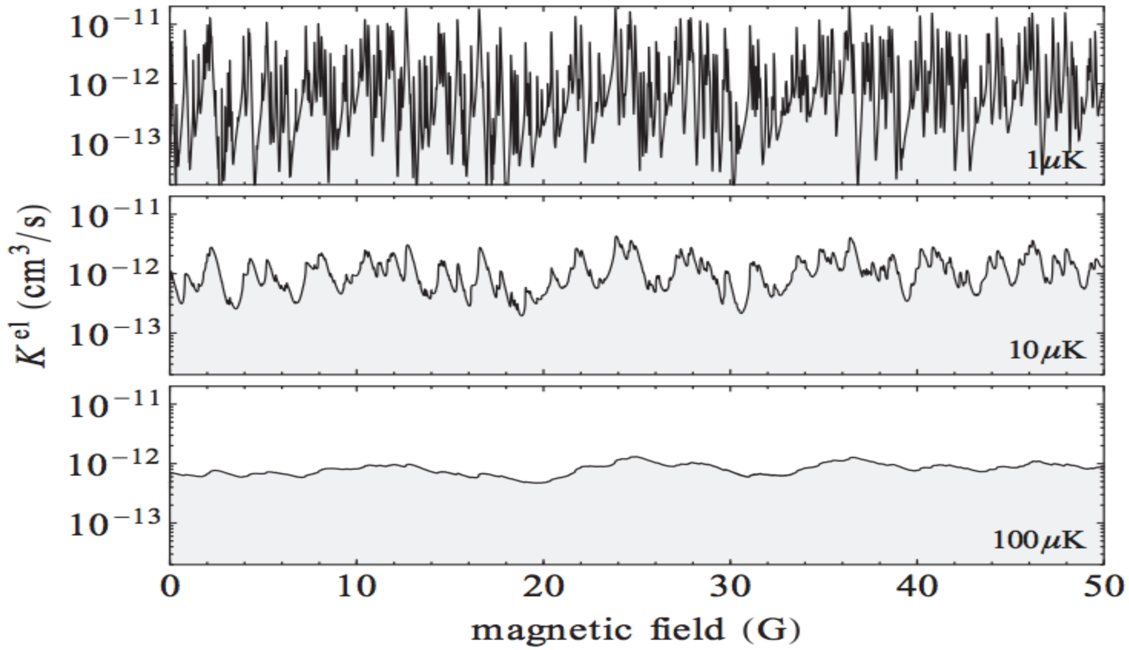


Toy Statistical model

Rb + KRb

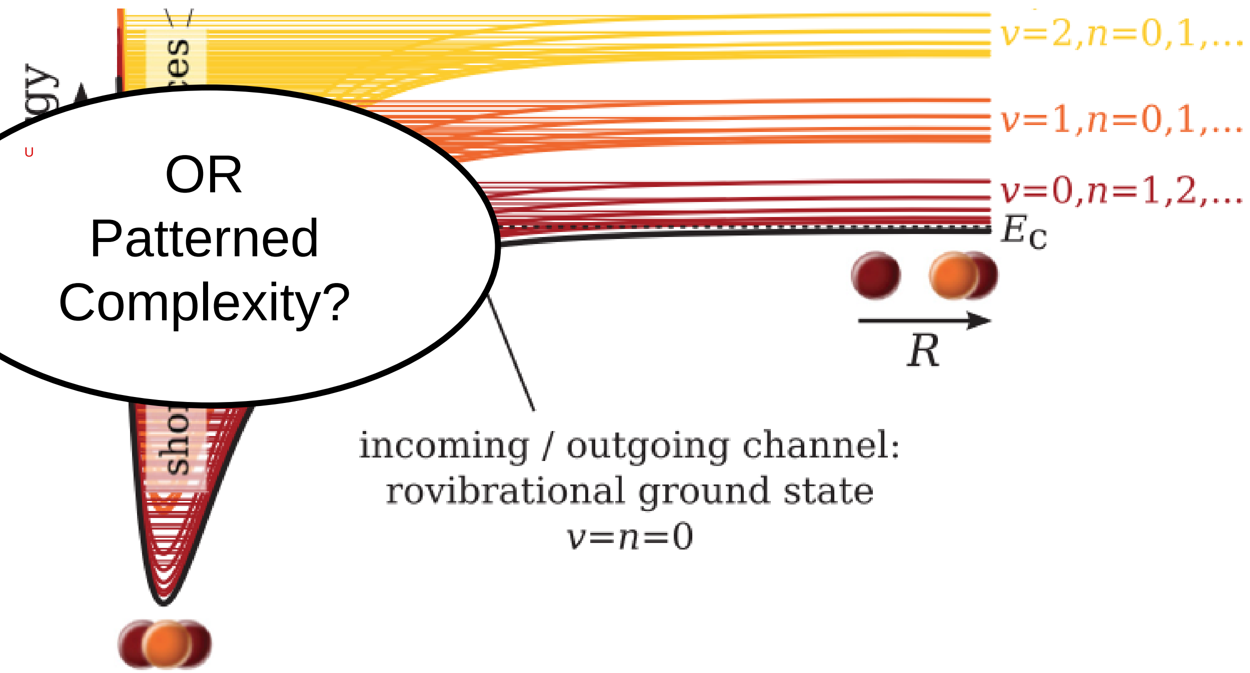


From Mayle, Ruzic, Bohn, Phys. Rev. A 85, 062712 (2012)



Toy Statistical model

Rb + KRb



OR
Patterned
Complexity?

The End