INT program on universality in few-body systems, May 5, 2014, Seattle

Van der Waals Universality in cold atomic and molecular systems

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,
especially to Yujun Wang and Rudi Grimm and colleagues at Innsbruck

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

Supported by an AFOSR MURI

Outline

What do we mean by "universal"
in cold atomic and molecular collisions?

Focus on explaining "van der Waals universality"

Tutorial: Properties of vdW potential & "Quantum Defect" viewpoint

Illustrate by examples:

Bound states & precision measurements for $^7Li_2$ and $^6Li_2$

Cs 3-body numerical model (Yujun Wang)

Realistic, no-adjustable parameter, 2-body physics

→ L_3 at all scattering lengths, including Efimov

→ Atom-dimer resonances

Universal molecular inelastic and reactive 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: $E_b = -\frac{\hbar^2}{2\mu a^2}$

Everybody uses it in ultracold work

bosons or fermions

2-body, few-body, many-body, lattices, etc.

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"
- thermodynamics and equations of state of 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)

Still not good enough

REVIEWS OF MODERN PHYSICS, VOLUME 82, APRIL–JUNE 2010

Feshbach resonances in ultracold gases

Cheng Chin

Department of Physics and James Franck Institute, University of Chicago, Chicago, Illinois 60637, USA

Rudolf Grimm

Center for Quantum Physics and Institute of Experimental Physics, University of Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria and Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, Otto-Hittmair-Platz 1, 6020 Innsbruck, Austria

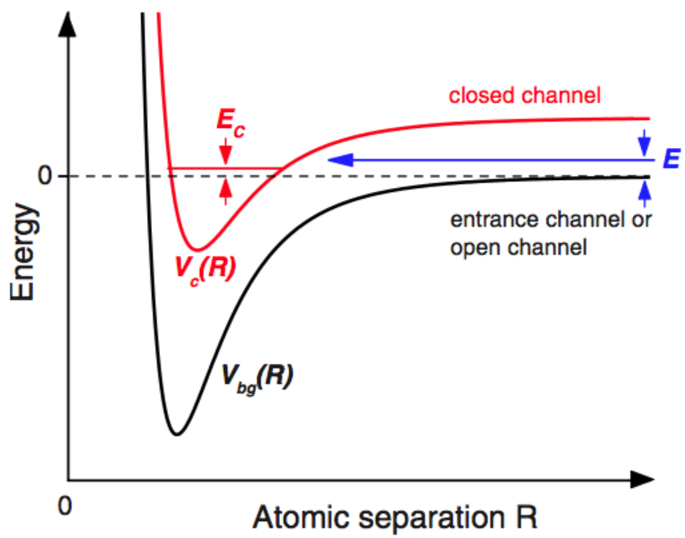
Paul Julienne and Eite Tiesinga

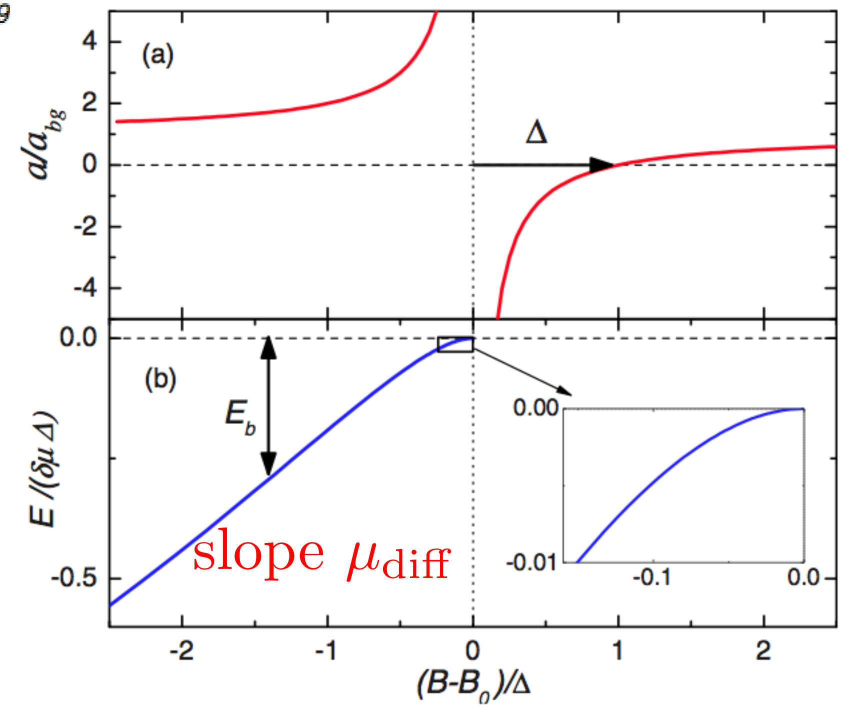
Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, 100 Bureau Drive, Gaithersburg, Maryland 20899

Resonance strength

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

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





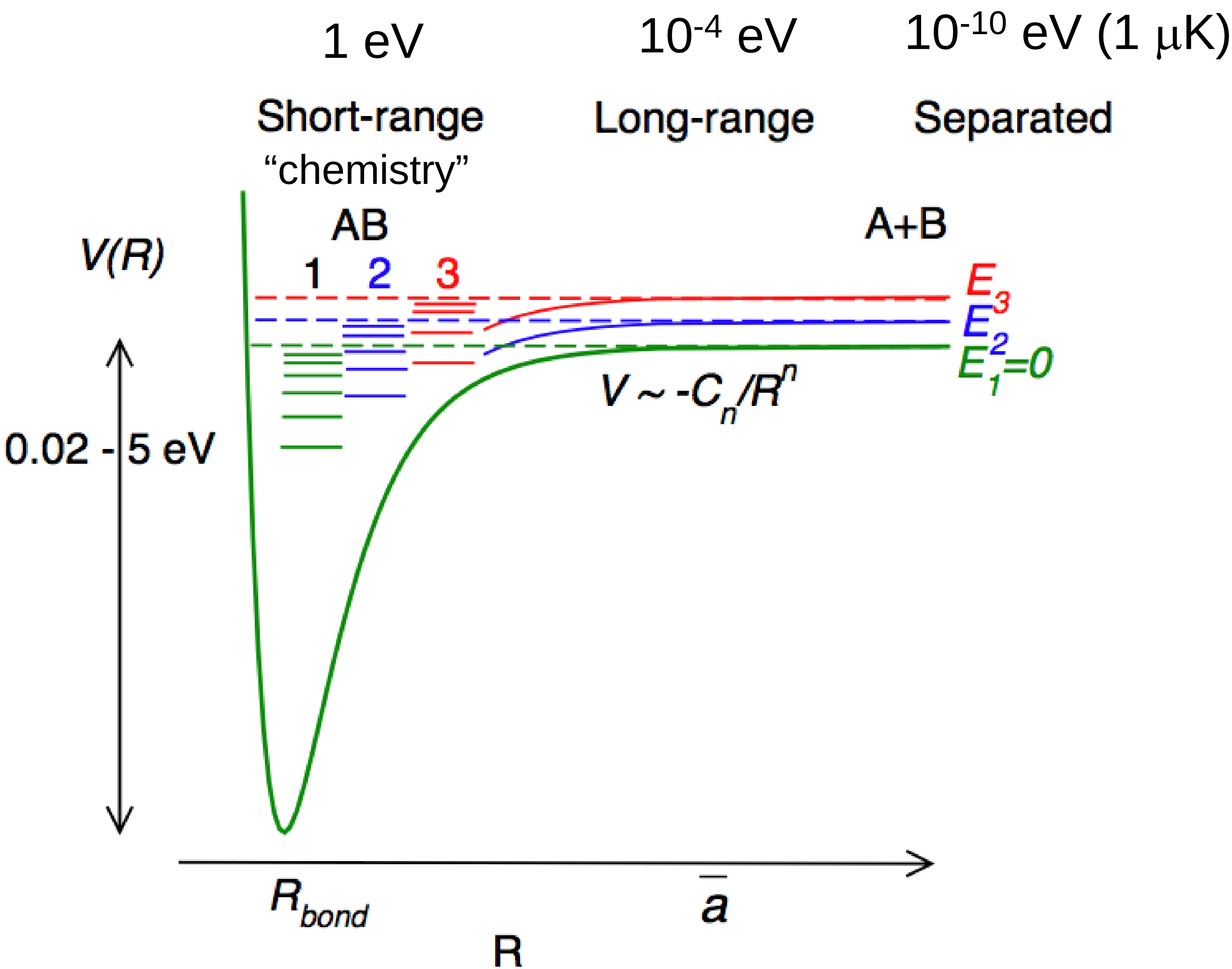


Fig. 2, PSJ Faraday Disc 142, 361 (2009)

Van der Waals universality

Universal Van de Waals (long-range) physics
underlies the 2-body physics
determining the few-body and many-body physics
realized with cold atoms and molecules
on an energy scale >> E_{vdW}

Feshbach resonances

$\eta(E,B)$, $E_b(B)$ depends on only 3 "quantum defect" parameters

a_{bg} (background), s_{res}(pole strength), μ_{diff}(tune with B)

(e.g., Gao & PSJ (2006); Jachymski & PSJ, PRA 88, 052701 (2013))

Three-body physics near tunable Feshbach

depends on same 3 parameters + pairwise vdW forces

(Numerical implementation: Y. Wang & PSJ, arxiv:1404.0483)

Atomic and molecular collisions

"Universal" reaction rates (Idziaszek & PSJ, PRL 104, 113202(2010))

Generalized (Jachymski, Krych, Idziaszek, PSJ (2013); also Gao)

Long-range potential

$$V(R) = -\frac{C_p}{R^p} + \frac{\hbar^2 \ell(\ell+1)}{2\mu R^2}$$

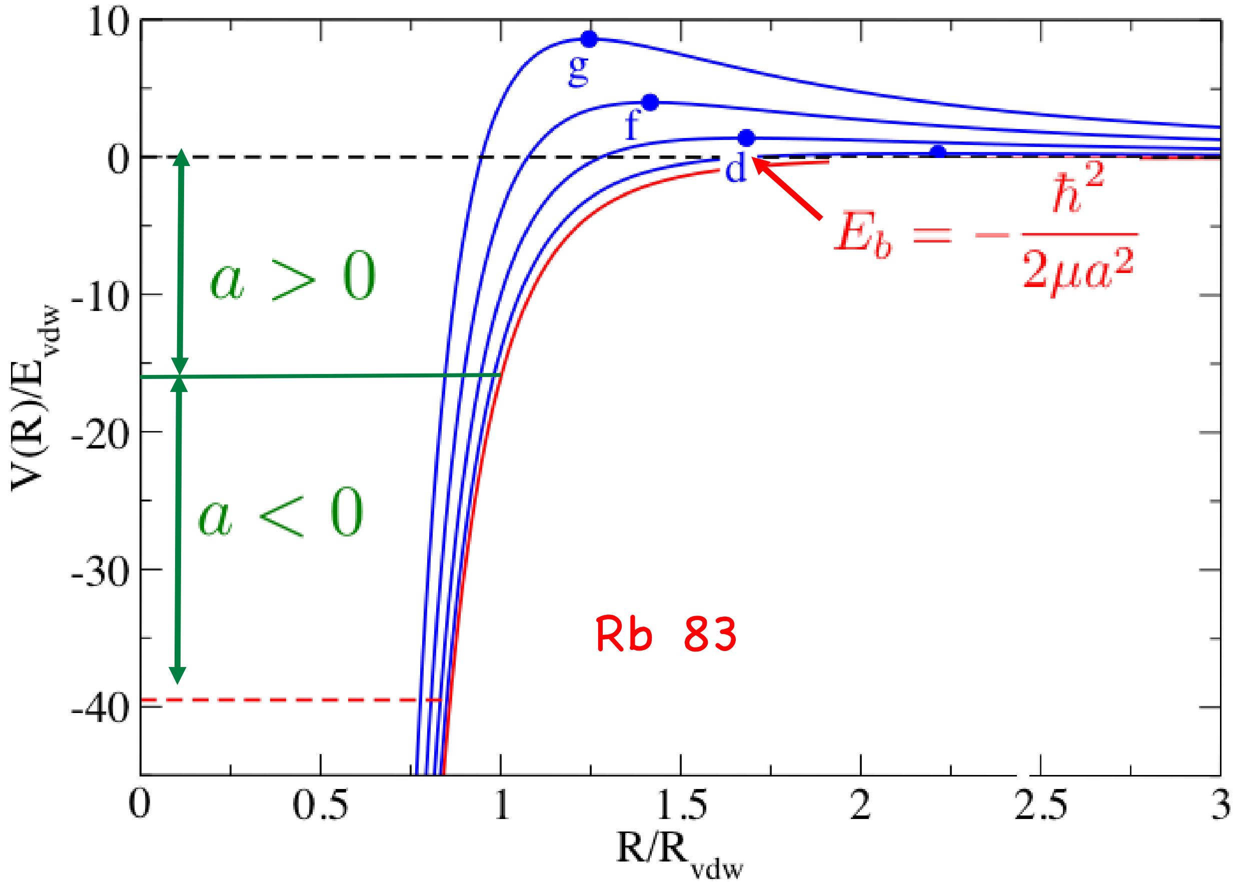
Characteristic length $$R_p = \left(\frac{2\mu C_p}{\hbar^2}\right)^{\frac{1}{p-2}}$$

energy $$E_p = \frac{\hbar^2}{2\mu R_p^2}$$

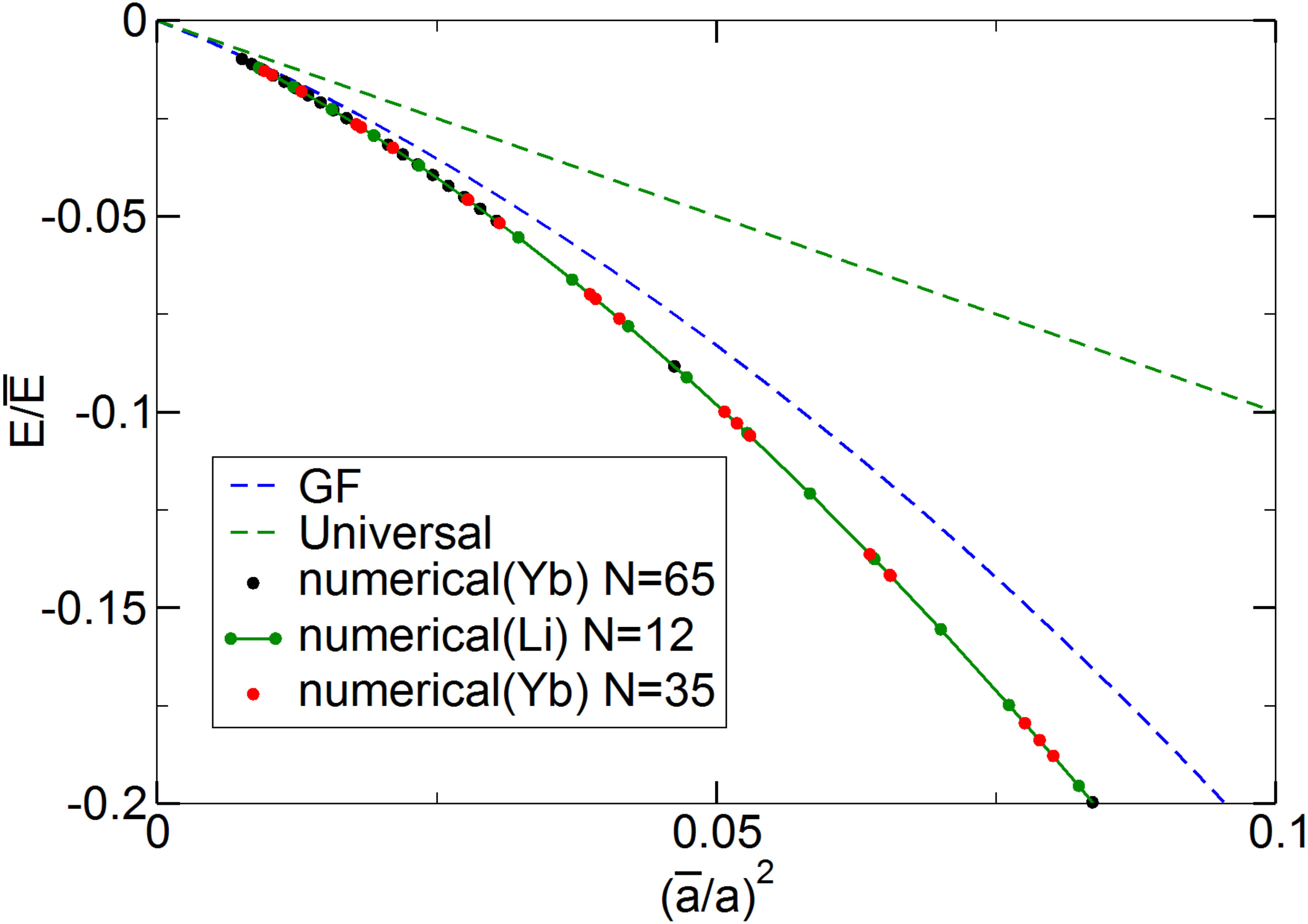
"Universal"potential in E_p, R_p units $$v(r) = -\frac{1}{r^p} + \frac{\ell(\ell+1)}{r^2}$$

Sometimes we use $R_{\mathrm{vdW}} = \frac{1}{2} R_6$ or $\bar{a} = 0.478\ldots R_6$

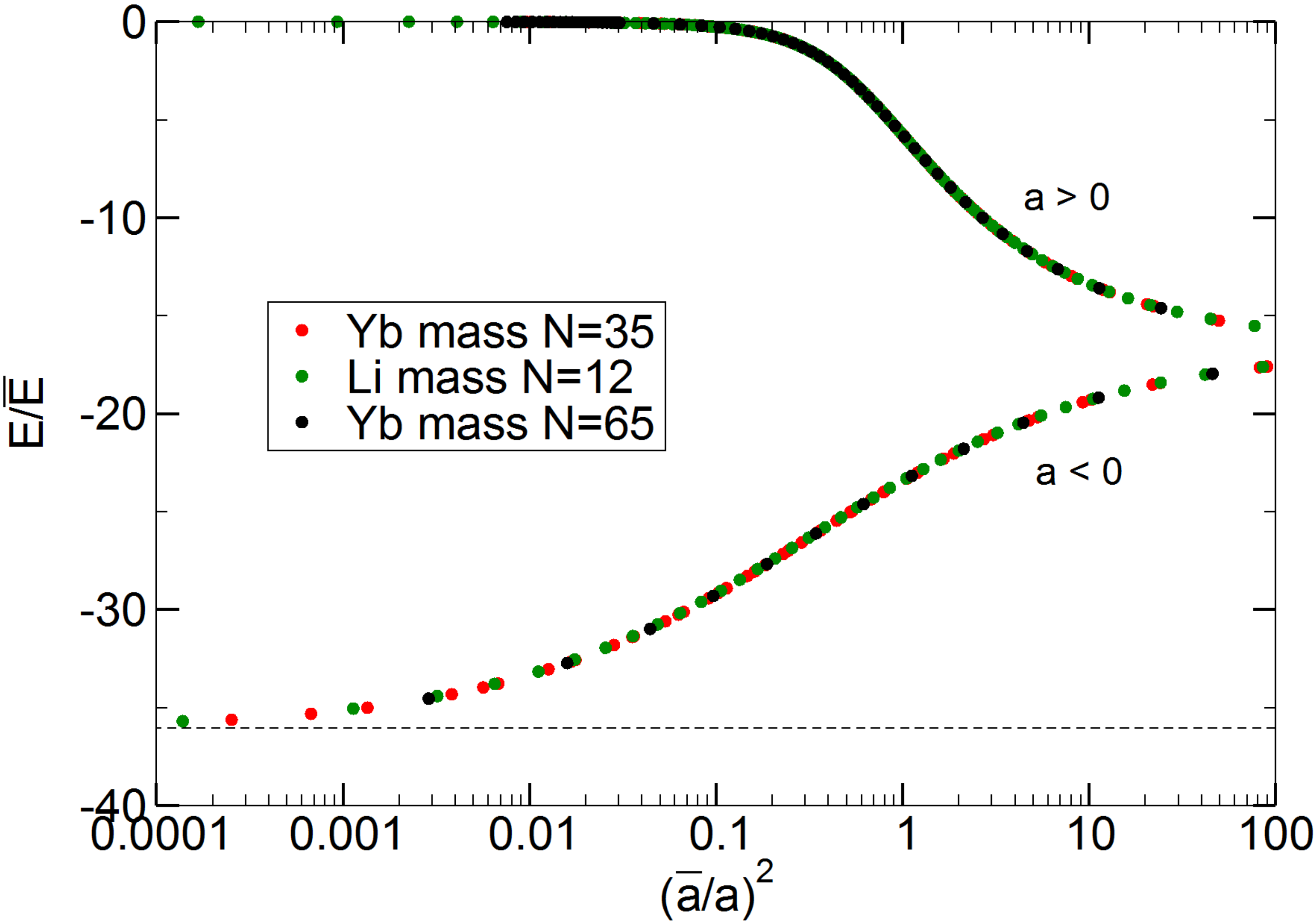
“Size” of vdW potential



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



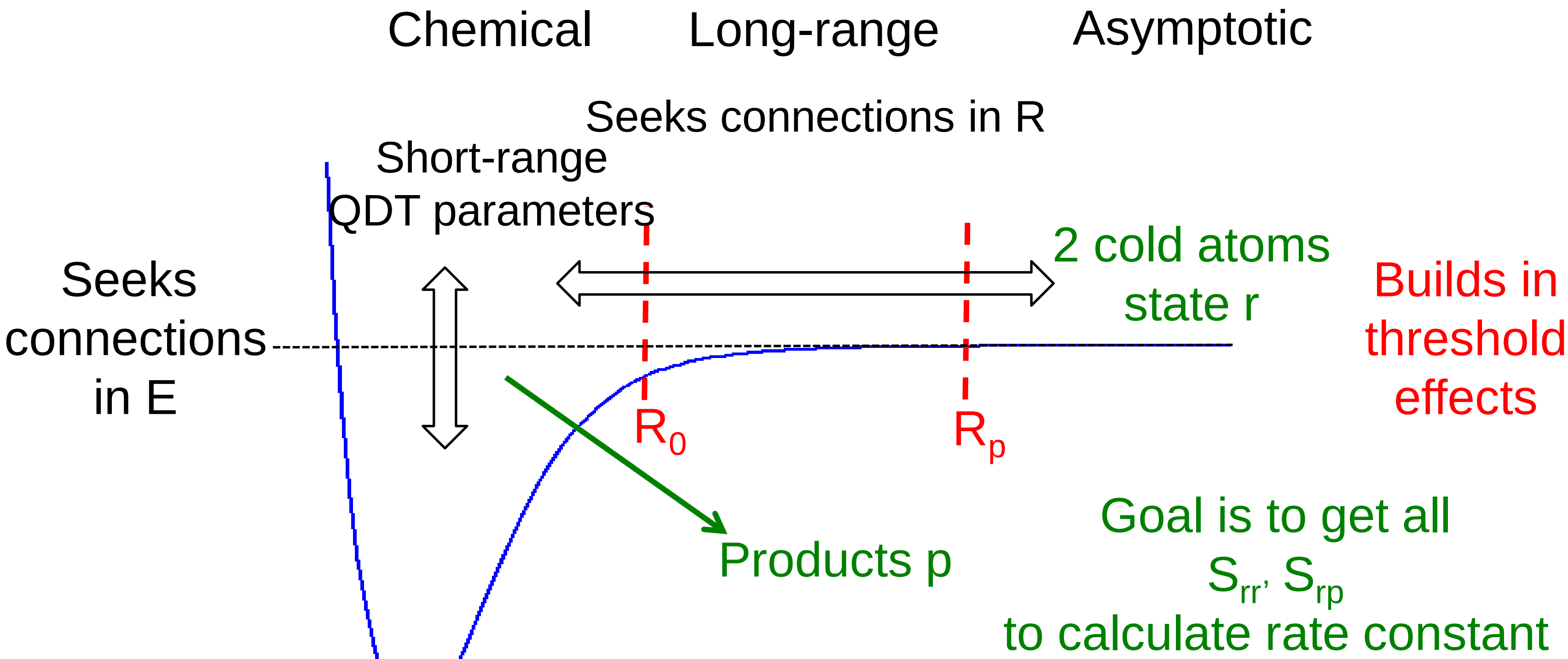
0
-0.05
-0.1
-0.15
-0.2
0
0.05
0.1
E/Ē
(ā/a)^2
GF
Universal
numerical(Yb) N=65
numerical(Li) N=12
numerical(Yb) N=35



E/$\bar{E}$
($\bar{a}$/a)^2
0
-10
-20
-30
-40
0.0001
0.001
0.01
0.1
1
10
100
a > 0
a < 0
Yb mass N=35
Li mass N=12
Yb mass N=65

QDT model

Fano, Seaton, Greene/Bohn, Mies, PSJ, Gao, Hutson, Idziaszek



MQDT takes advantage of the specific analytic structure of ¨ (R,E) with semiclassical insights

Follow Mies, J. Chem. Phys. 80, 2514(1984), PSJ & Mies, JOSA B6, 2257 (1989)

Quantum defect theory

1. Pick a reference problem we can solve

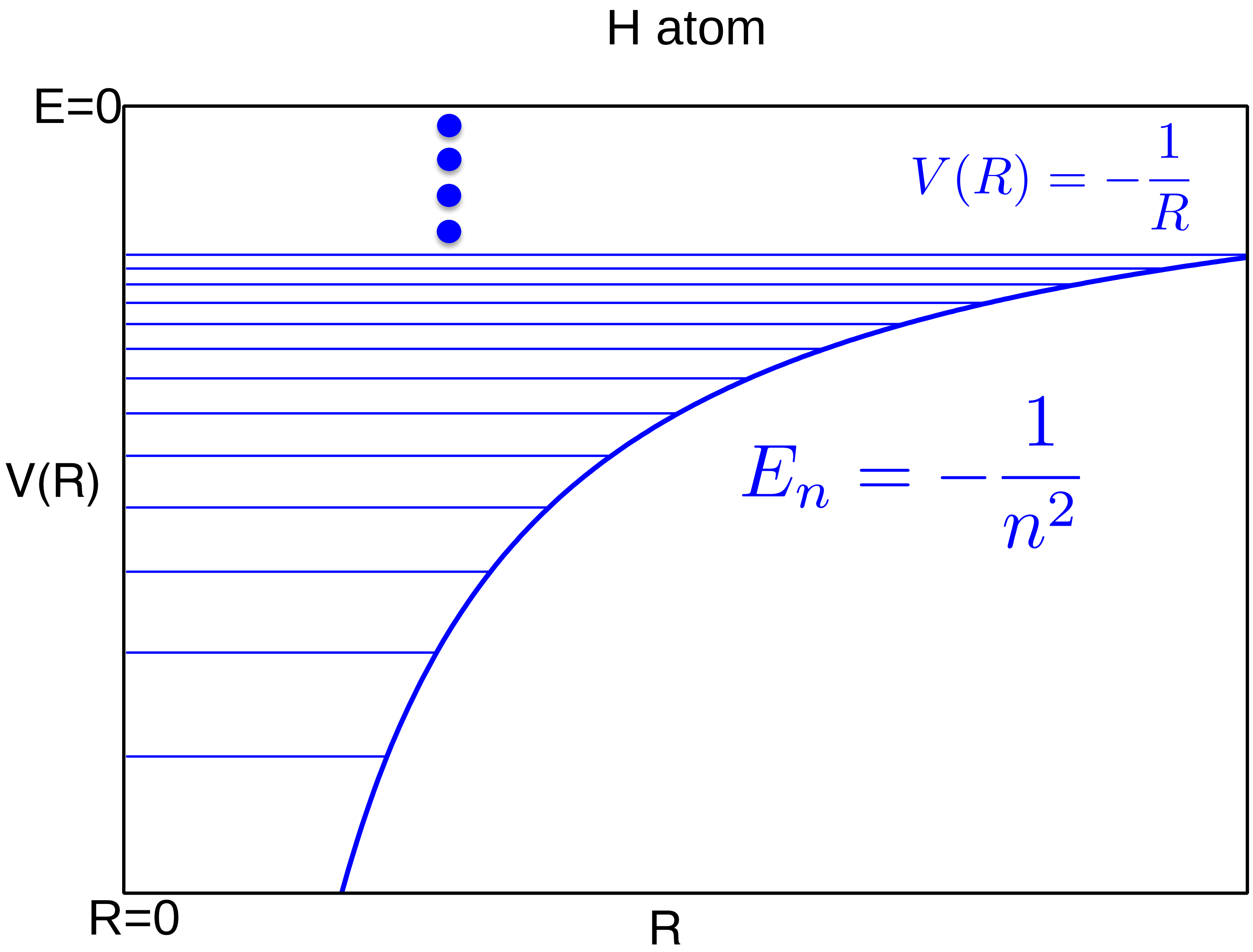
   Classic example: Coulomb potential, H-like atom
   or $p = 6$ or $p = 4$ potential

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

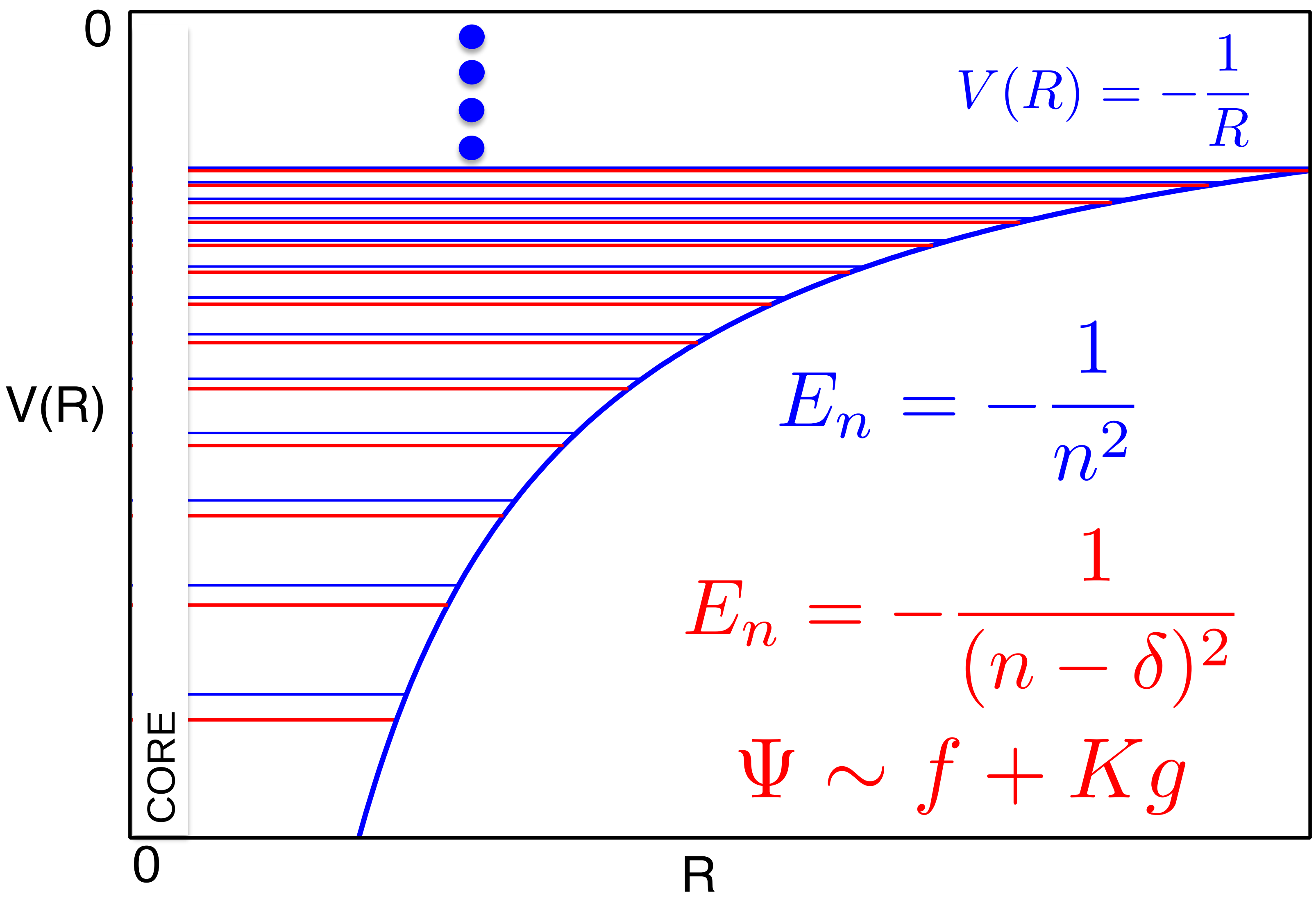
2. Parameterize dynamics by a few "physical" QDT parameters
   subject to experimental fitting
   and theoretical interpretation
   phase (diagonal, scattering length)
   interactions (non-diagonal, inelastic events)

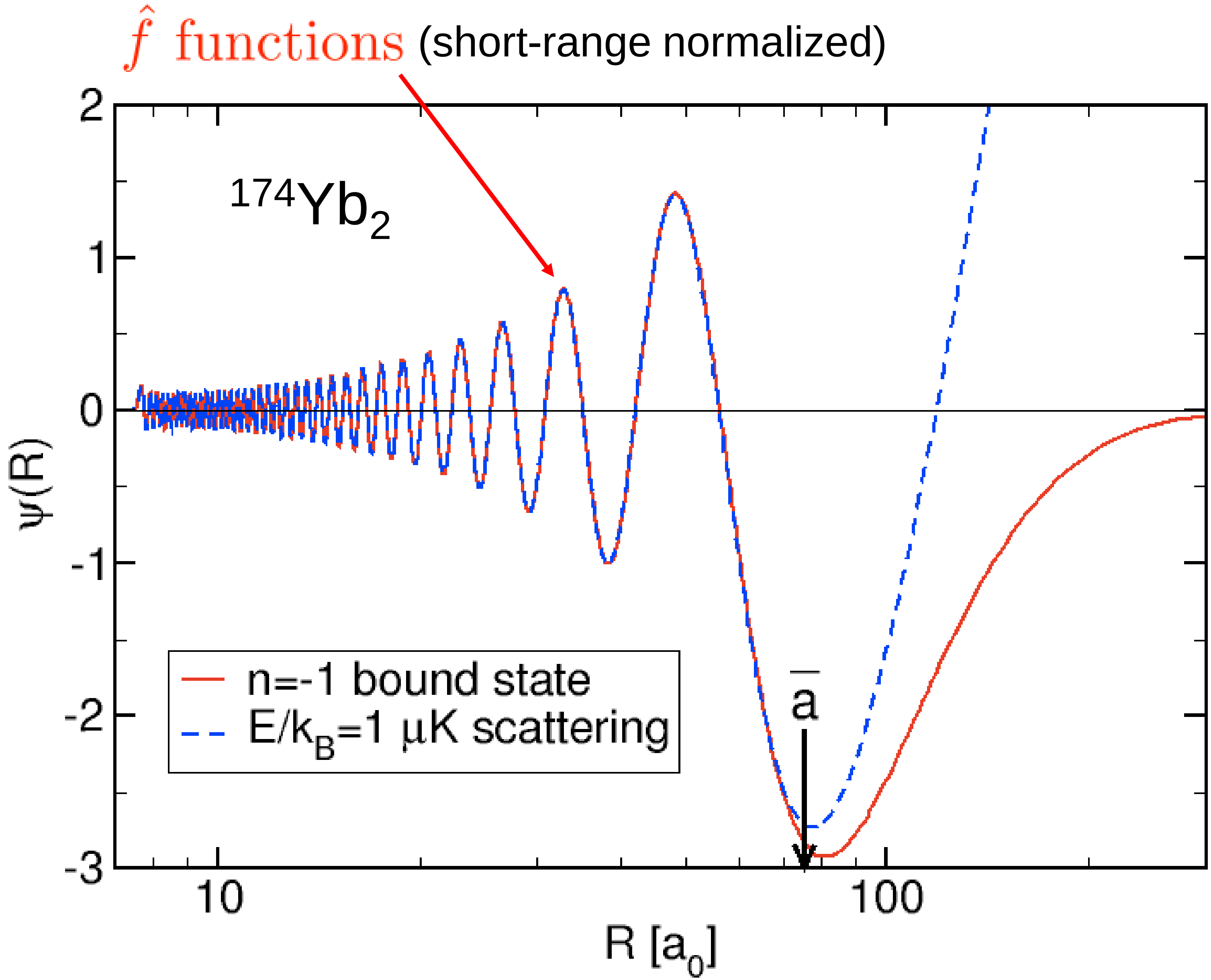
3. Use methods of QDT to calculate
   bound and scattering states, resonances, cross sections, etc.

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


H atom
E=0
$V(R) = -\frac{1}{R}$
V(R)
$E_n = -\frac{1}{n^2}$
R=0
R

Multi-electron atom

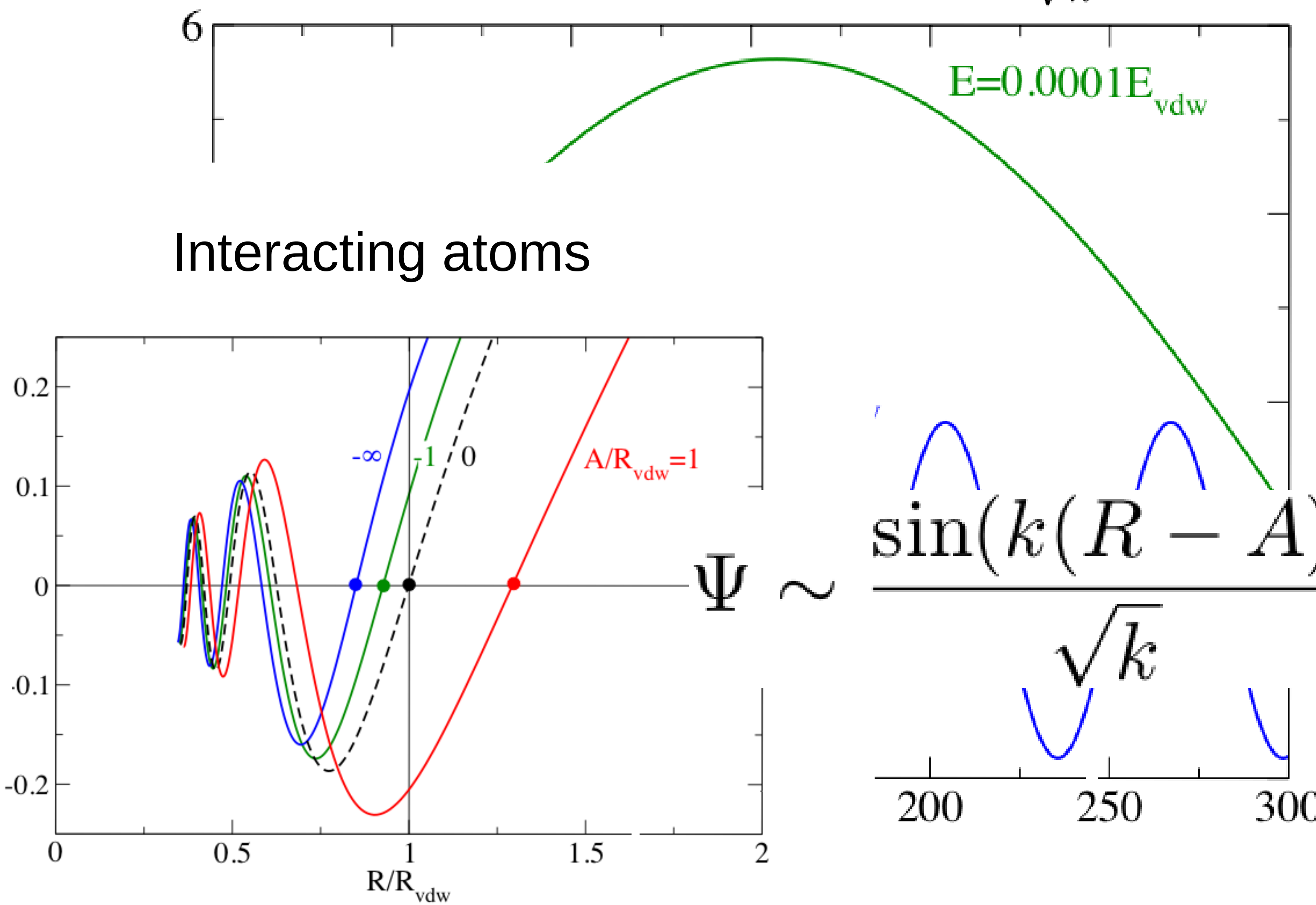




PSJ, arXiv:0902.1727 Chapter 6, *Cold Molecules*, ed. by R. Krems et al.

Noninteracting atoms $\Psi \sim \frac{\sin(kR)}{\sqrt{k}}$

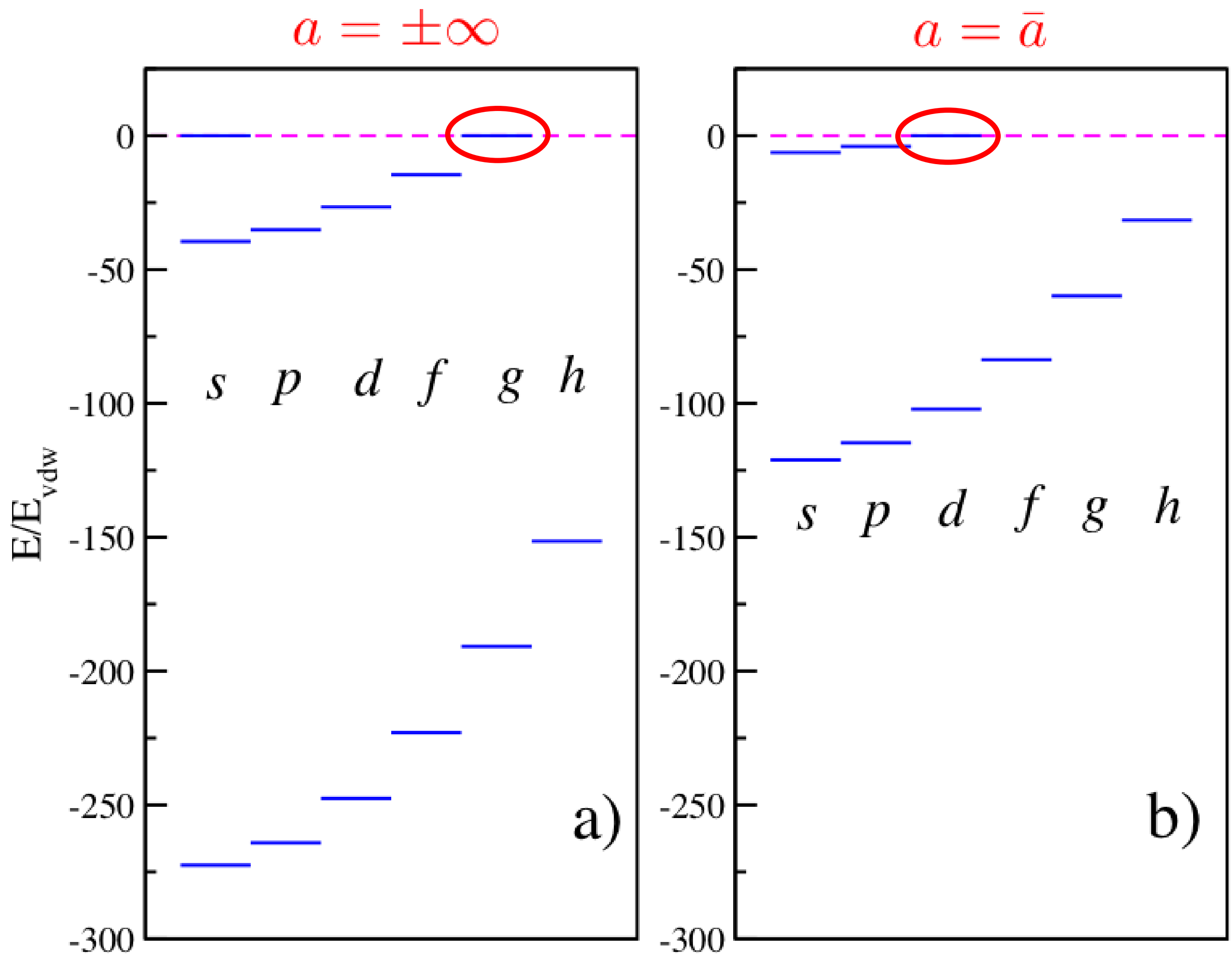
Interacting atoms



$$\Psi \sim \frac{\sin(k(R-A))}{\sqrt{k}}$$

See Jones et al, Rev. Mod. Phys. 78, 483 (2006), Fig. 16

Universal vdW bound state spectrum: depends on a



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

Van der Waals Quantum Defect Theory (QDT)

PSJ and B. Gao, in Vol 869 AIP Conf. Proc., 261–268 (2006), arXiv:physics/0609013v1
Chin et al RMP(2010); Jachymski, PSJ, PRA 88, 052701(2013); Blackley et al PRA 89, 042701(2014)

vdW QDT

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

$$\eta_{\mathrm{res}}(E,B) = -\tan^{-1}\frac{\frac{1}{2}\Gamma(E)}{E - \mu_{\mathrm{diff}}(B - B_{\mathrm{c}}) + \delta E_{\mathrm{c}}(E)}$$

$$\Gamma(E) = \frac{1}{2}\bar{\Gamma} C(E)^{-2}$$

$$\delta E_{\mathrm{c}}(E) = \frac{1}{2}\bar{\Gamma}\tan\lambda(E)$$

$\bar{\Gamma}$ = short range strength independent of E, B

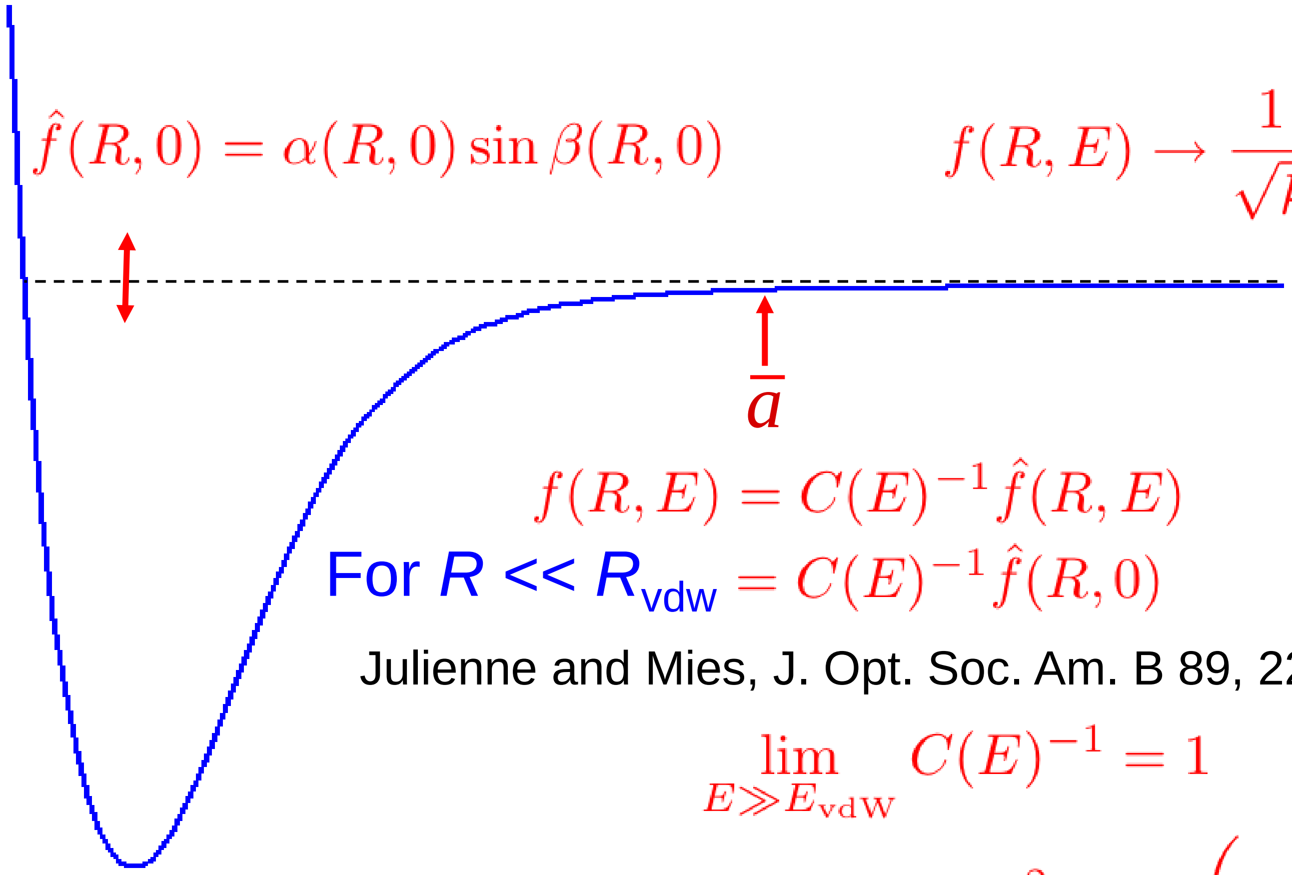
η_{bg}(E), C(E)$^{-2}$, tan λ(E) are analytic QDT functions of the background channel, given C_6 and a_{bg}

$$\lim_{E\to 0}\eta(E) = -k a_{\mathrm{bg}}$$

$$\lim_{E\to 0} C(E)^{-2} = k\bar{a}\left(1 + \left(1 - \frac{a_{\mathrm{bg}}}{\bar{a}}\right)^2\right)$$

$$\lim_{E\to 0}\tan\lambda(E) = 1 - \frac{a_{\mathrm{bg}}}{\bar{a}}$$

Semiclassical interpretation (Mies 1984)



$$\hat{f}(R,0) = \alpha(R,0)\sin\beta(R,0)$$

$$f(R,E) \rightarrow \frac{1}{\sqrt{k}}\sin(kR+\eta(E))$$

$$f(R,E) = C(E)^{-1}\hat{f}(R,E)$$

For R << R_{vdw} $= C(E)^{-1}\hat{f}(R,0)$

Julienne and Mies, J. Opt. Soc. Am. B 89, 2257 (1989)

$$\lim_{E \gg E_{\mathrm{vdW}}} C(E)^{-1} = 1$$

$$\lim_{E\rightarrow 0} C(E)^{-2} = k\bar{a}\left(1+\left(\frac{a}{\bar{a}}-1\right)^2\right)$$

$$\alpha(R,E) = \frac{1}{k(R,E)^{\frac{1}{2}}}$$

$$\beta(R,E) = \int_{R_t}^{R} k(R',E)dR' + \frac{\pi}{4}$$

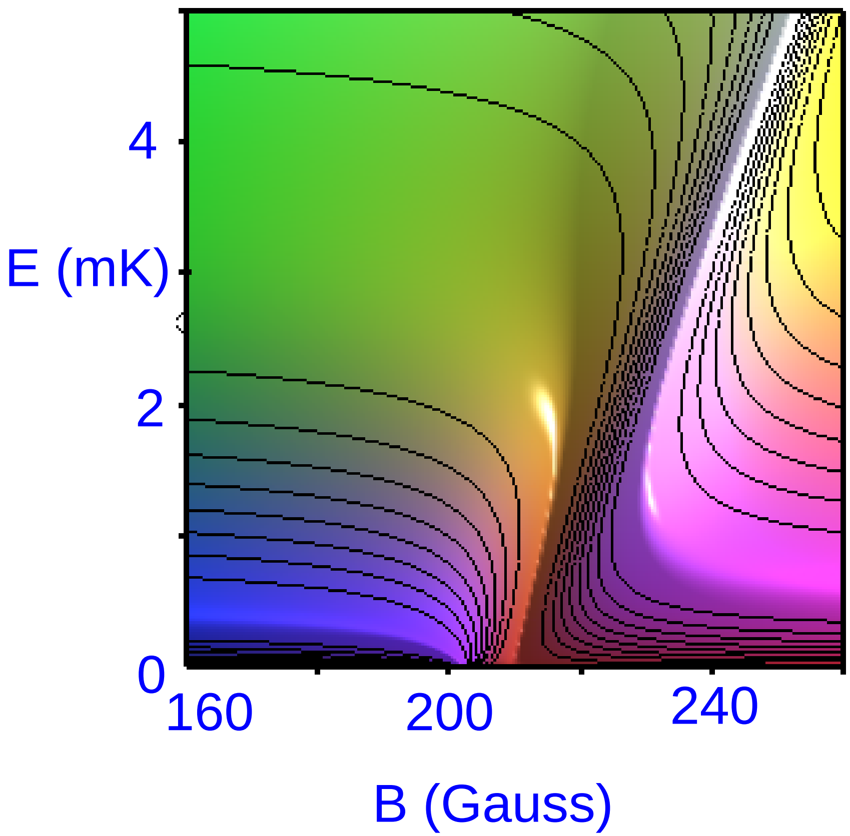
PSJ, arXiv:0902.1727 Chapter 6 of *Cold Molecules*, ed. by R. Krems et al.

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

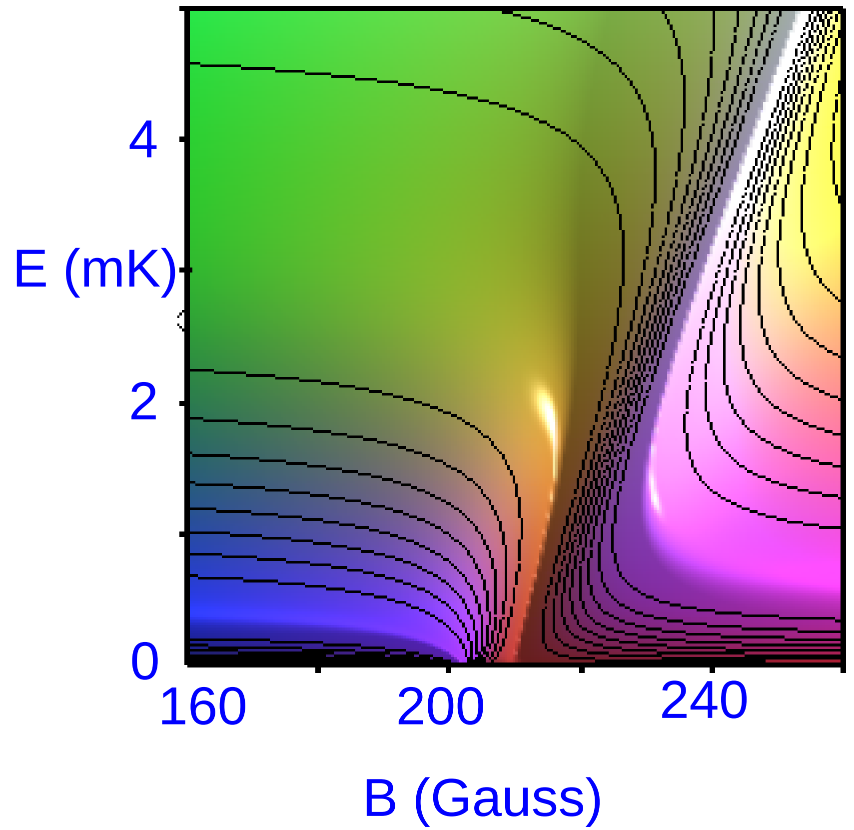
$$\sin^2 \eta(E,B)$$

$^{40}K(a+b)$

Coupled channels
Numerical



Van der Waals MQDT theory



From 2006 ICAP; see Blackley et al, PRA 89, 042701(2014)

$s_{\text{res}} = 59$

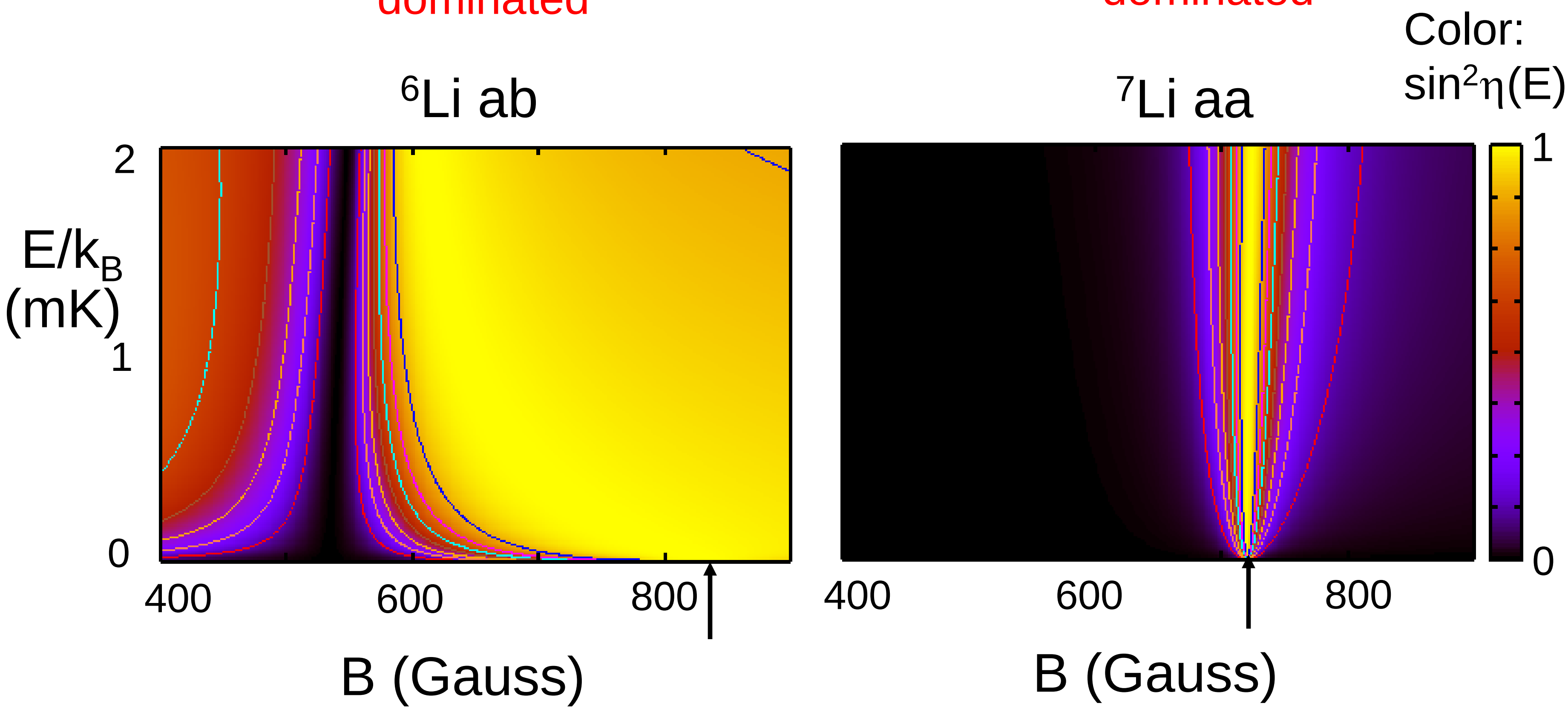
$\Delta = 300\,\text{G}$

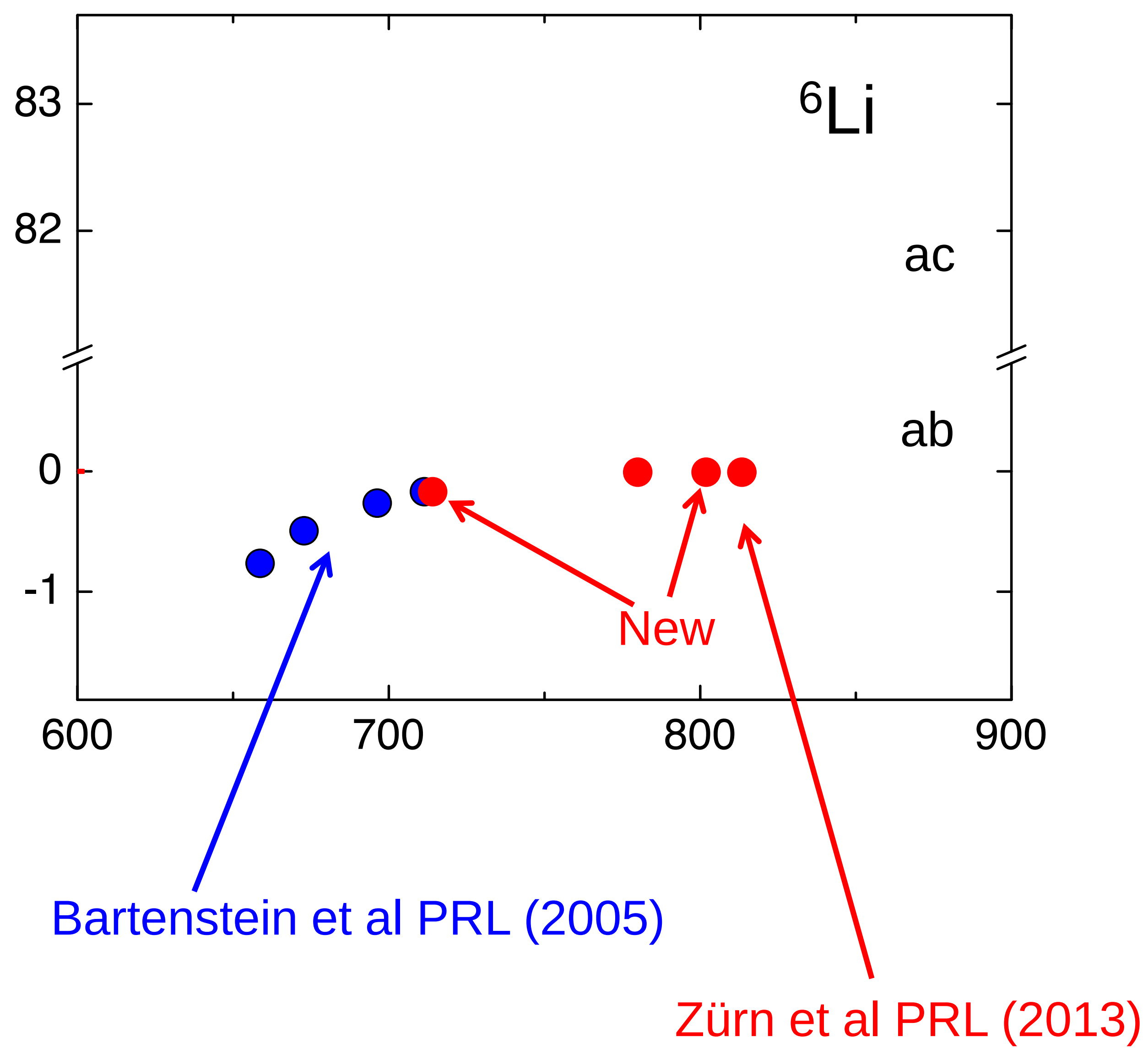
Entrance channel dominated

$s_{\text{res}} = 0.61$

$\Delta = 180\,\text{G}$

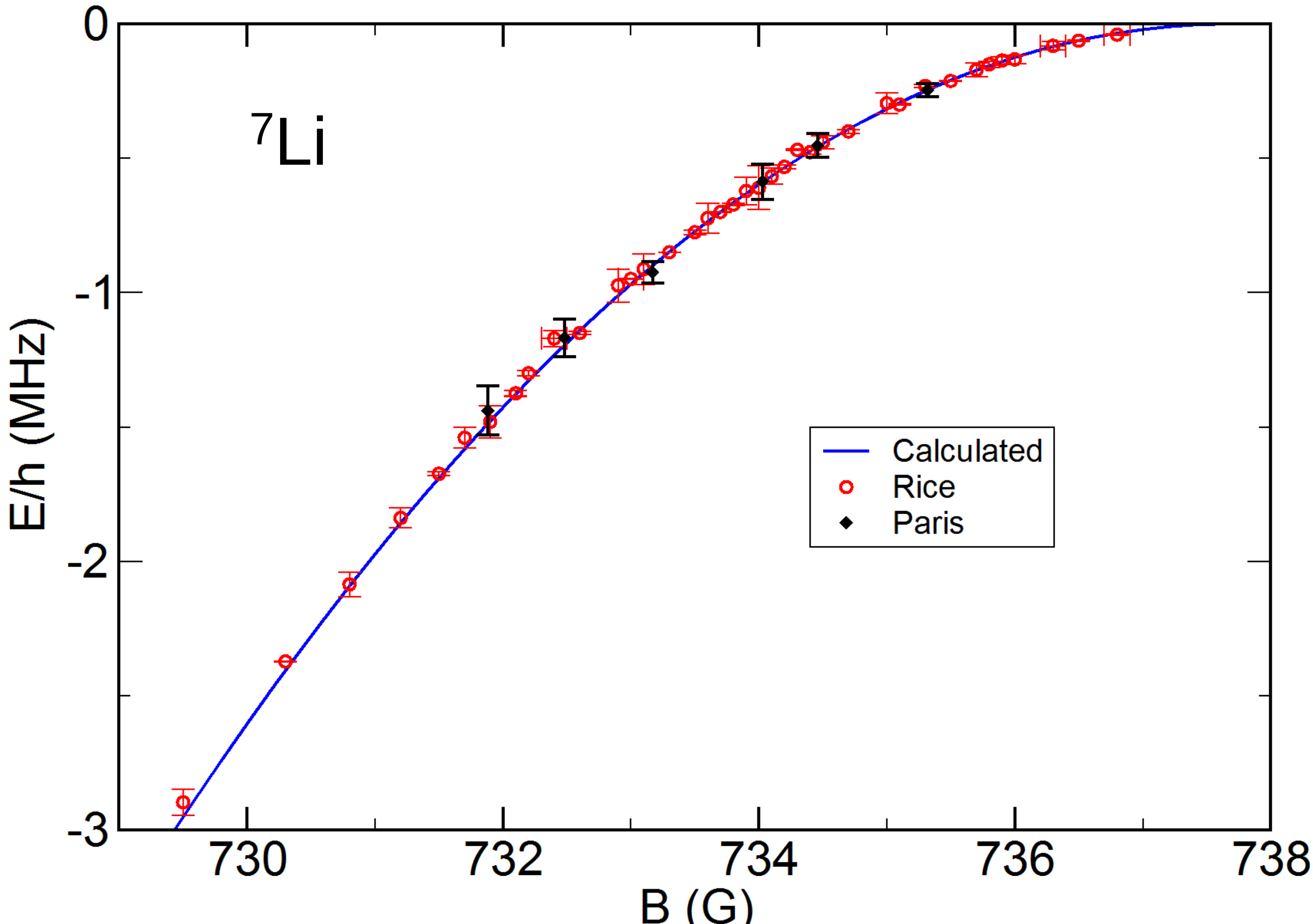
Closed channel dominated





^{6}Li
83
82
ac
ab
0
-1
New
600
700
800
900
Bartenstein et al PRL (2005)
Zürn et al PRL (2013)

Coupled channels fit, PSJ & J. Hutson, arxiv:1404.2623
(full Hamiltonian)



Universal energy: $E^{\mathrm{U}} = -\frac{\hbar^2}{2\mu a^2}$

Reduced E and length: $\epsilon = E/\bar{E}$ and $r = a/\bar{a}$

$$\epsilon^{\mathrm{U}} = -\frac{1}{r^2}$$

$$\epsilon^{\mathrm{U}} r^2 = -1$$

$$\epsilon^{\mathrm{U}} = -\frac{1}{r^2}$$

Universal

$$\epsilon^{\mathrm{GF}} = -\frac{1}{(r-1)^2}$$

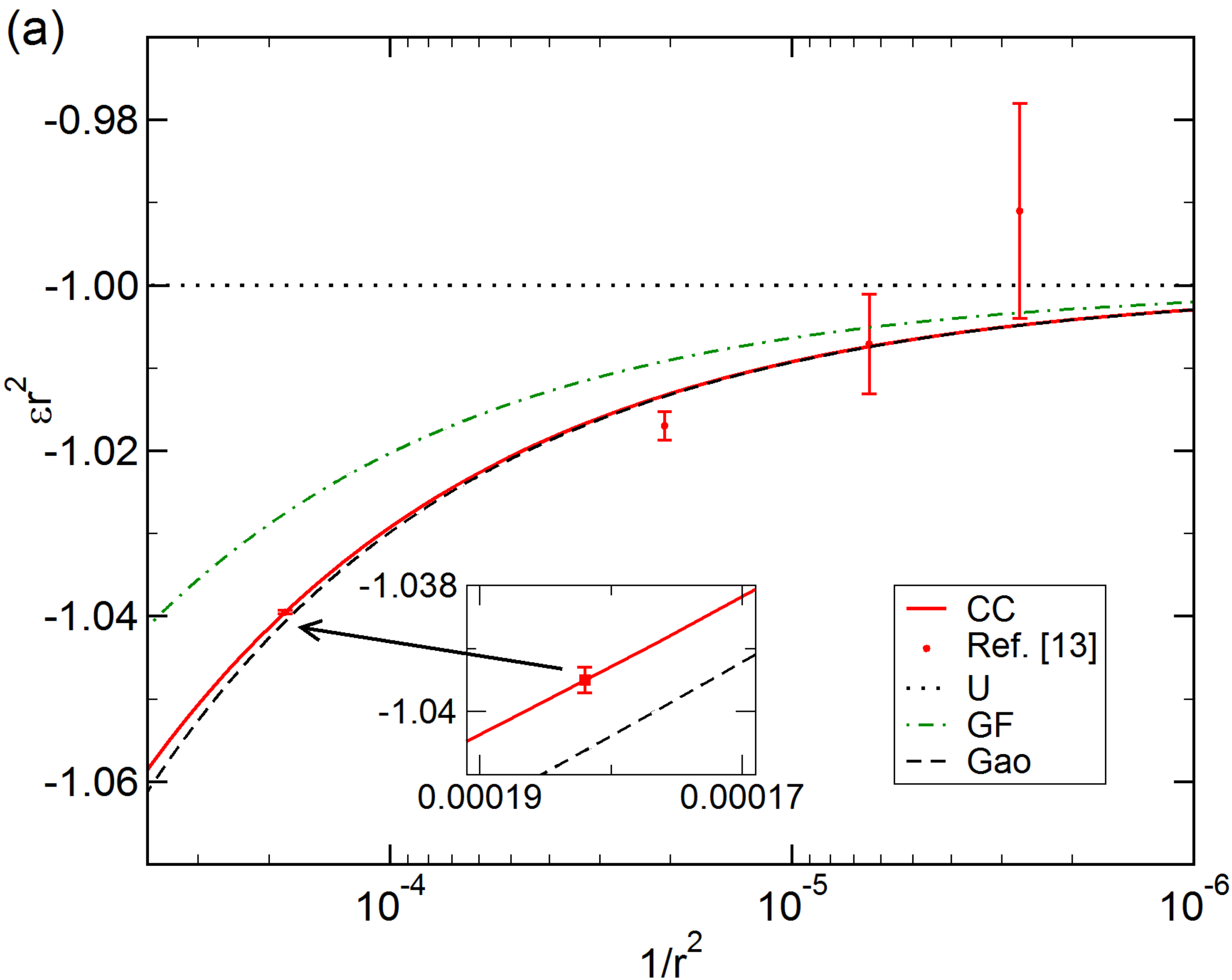
Gribakin and Flambaum, PRA 48, 546 (1993)

$$\epsilon^{\mathrm{G}} = \epsilon^{\mathrm{GF}} \left(1 + \frac{g_1}{r-1} + \frac{g_2}{(r-1)^2}\right)$$

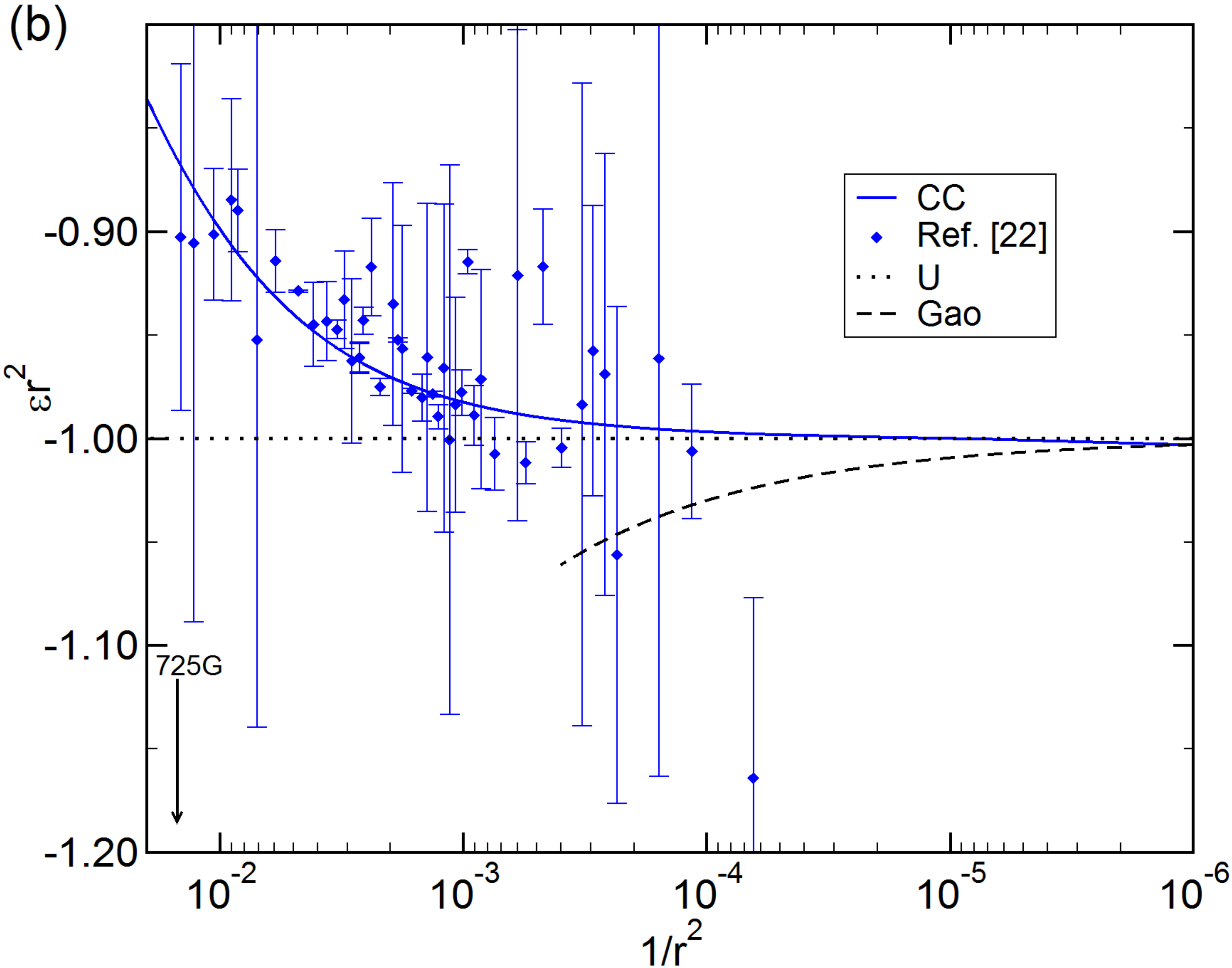
$$g_1 = \Gamma(\frac{1}{4})^4/(6\pi^2) - 2 \approx 0.9179$$

$$g_2 = (5/4)g_1^2 - 2 \approx -0.9468$$

Gao, J. Phys. B 37, 4273 (2004)

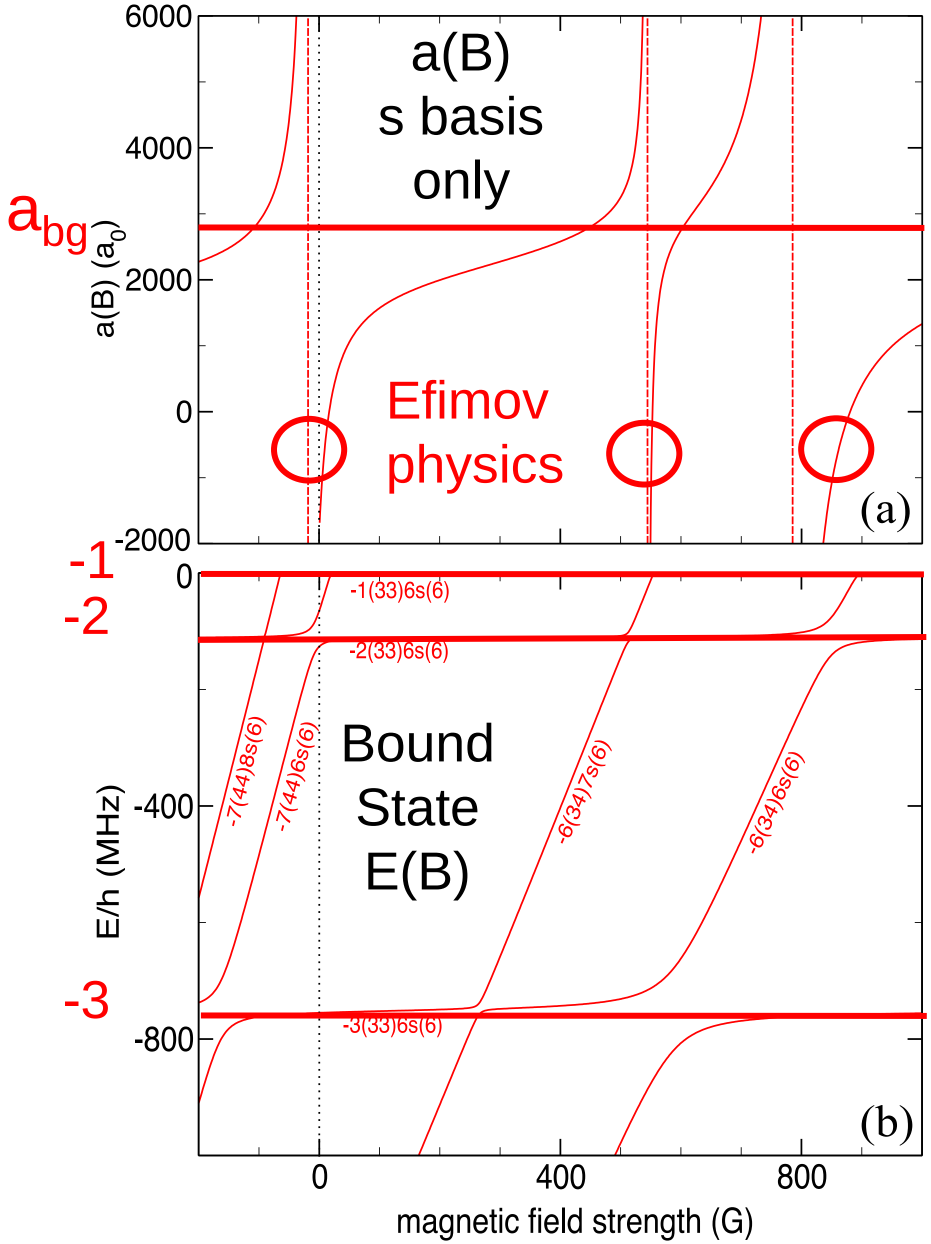


PSJ & J. Hutson, arxiv:1404.2623



PSJ & J. Hutson, arxiv:1404.2623

Cs+Cs Innsbruck/Hutson/PSJ Phys. Rev. A 87, 032517 (2013)

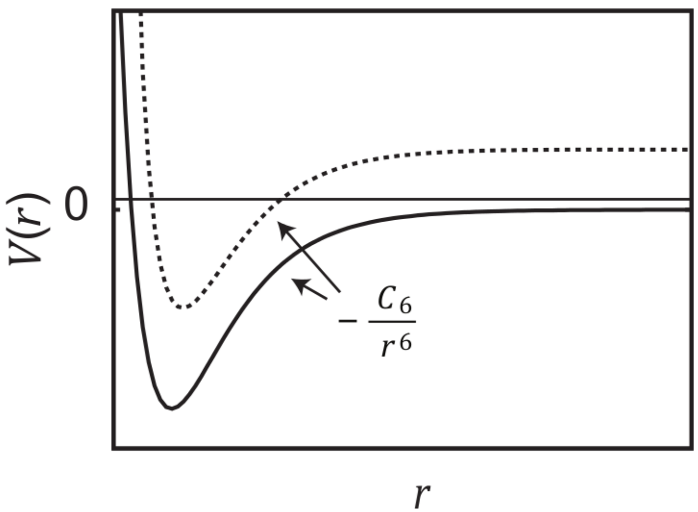


3-Body recombination of 3 alkali-metal atoms

Computer codes and calculations by Yujun Wang
Methods of Chris Greene group

Cs + Cs + Cs

Two-channel Cs + Cs interaction



Set up 2-channel numerical model to give s_{res}, a_{bg} and a(B) for Cs-Cs

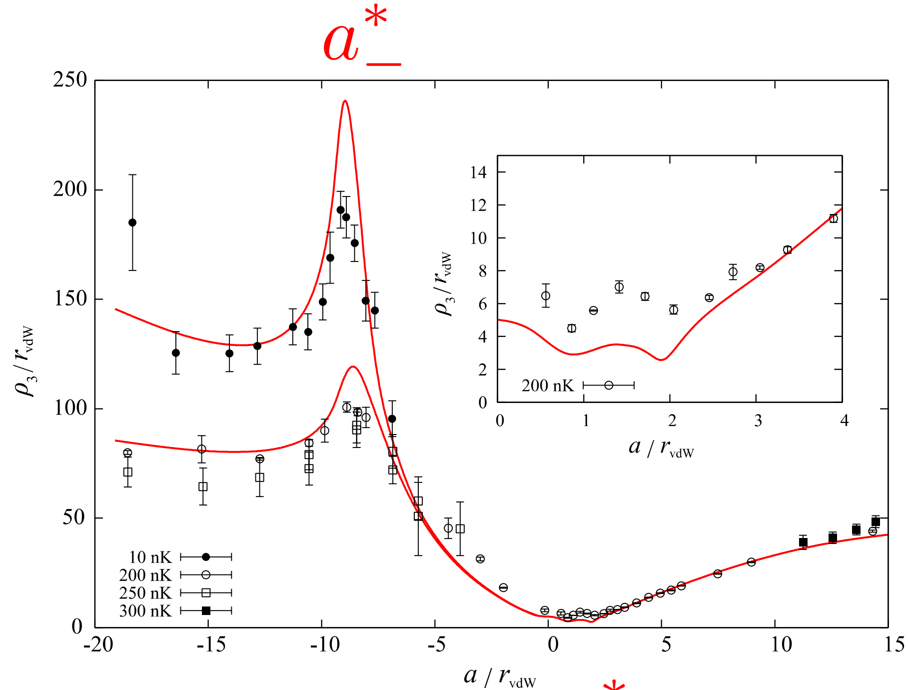
"Exact" 2-body Feshbach model

s_{res} = 560, r_{bg} = 16.8

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



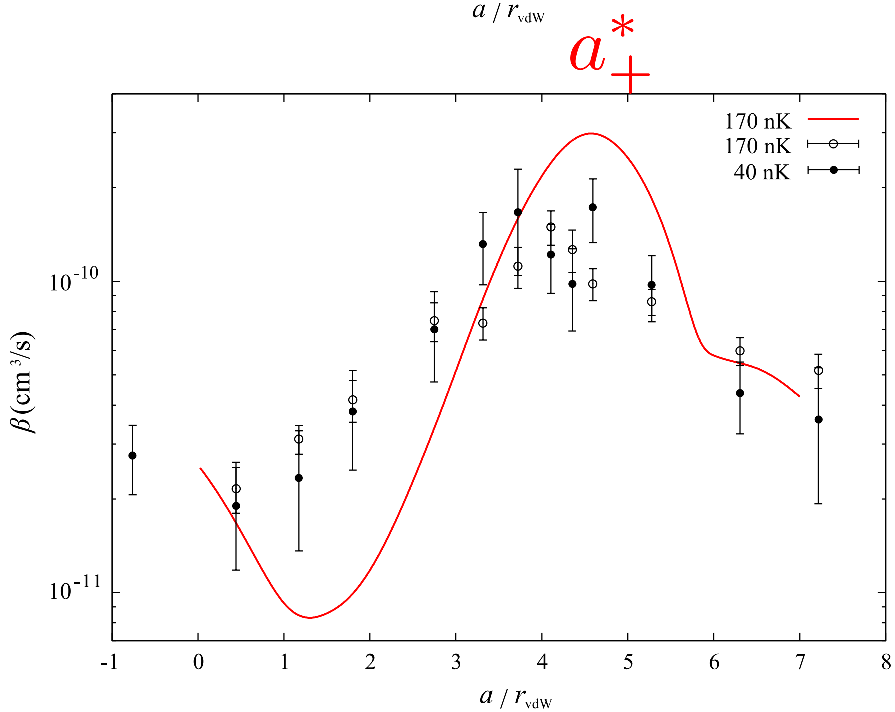
3-body recombination Cs+Cs+Cs

Points: Innsbruck data

Line: Theory—numerical

No adjustable parameters

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



Atom-dimer relaxation Cs + Cs_2

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

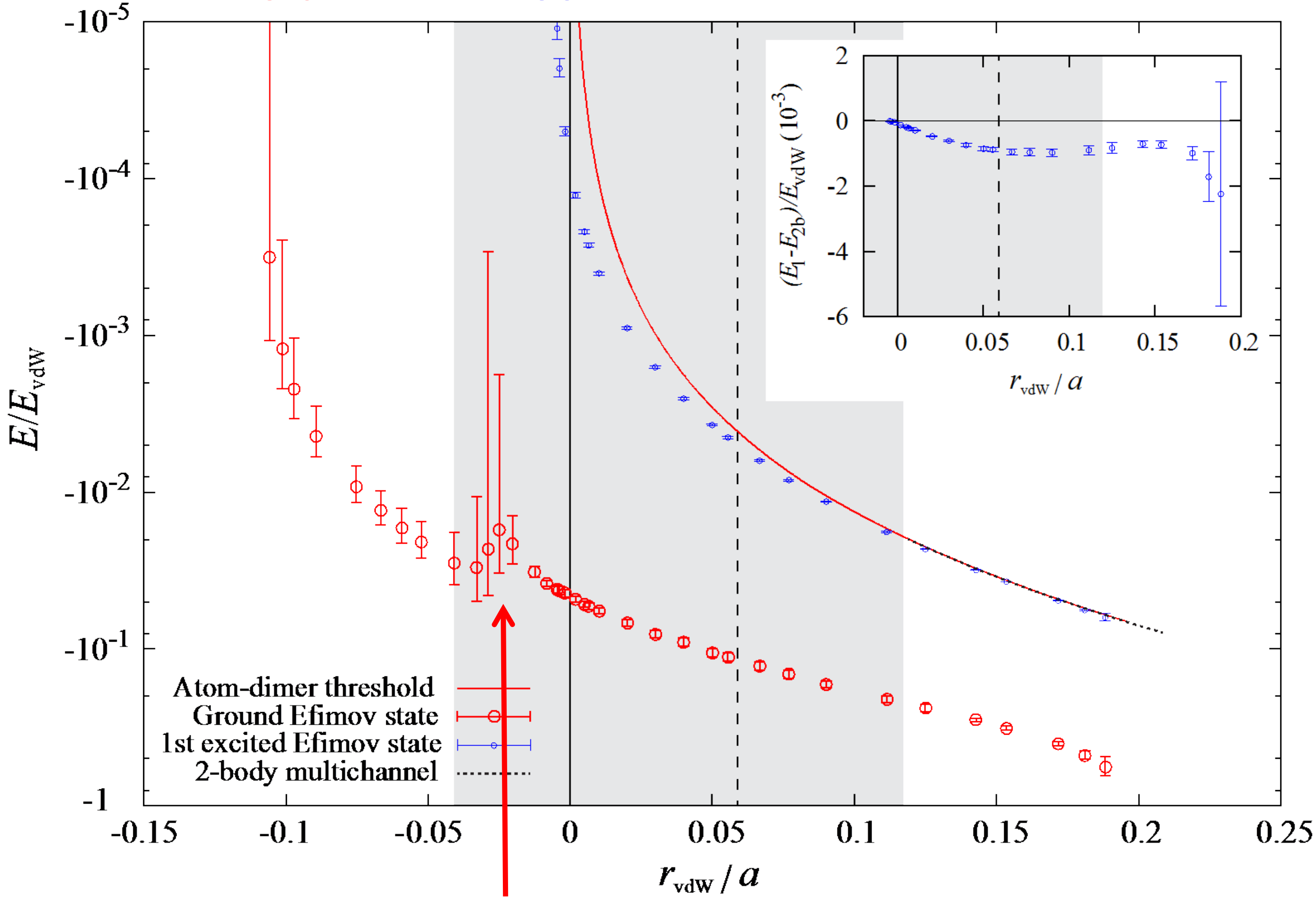
0.47(3) exp.

1.06 universal
(s-wave unitarity)

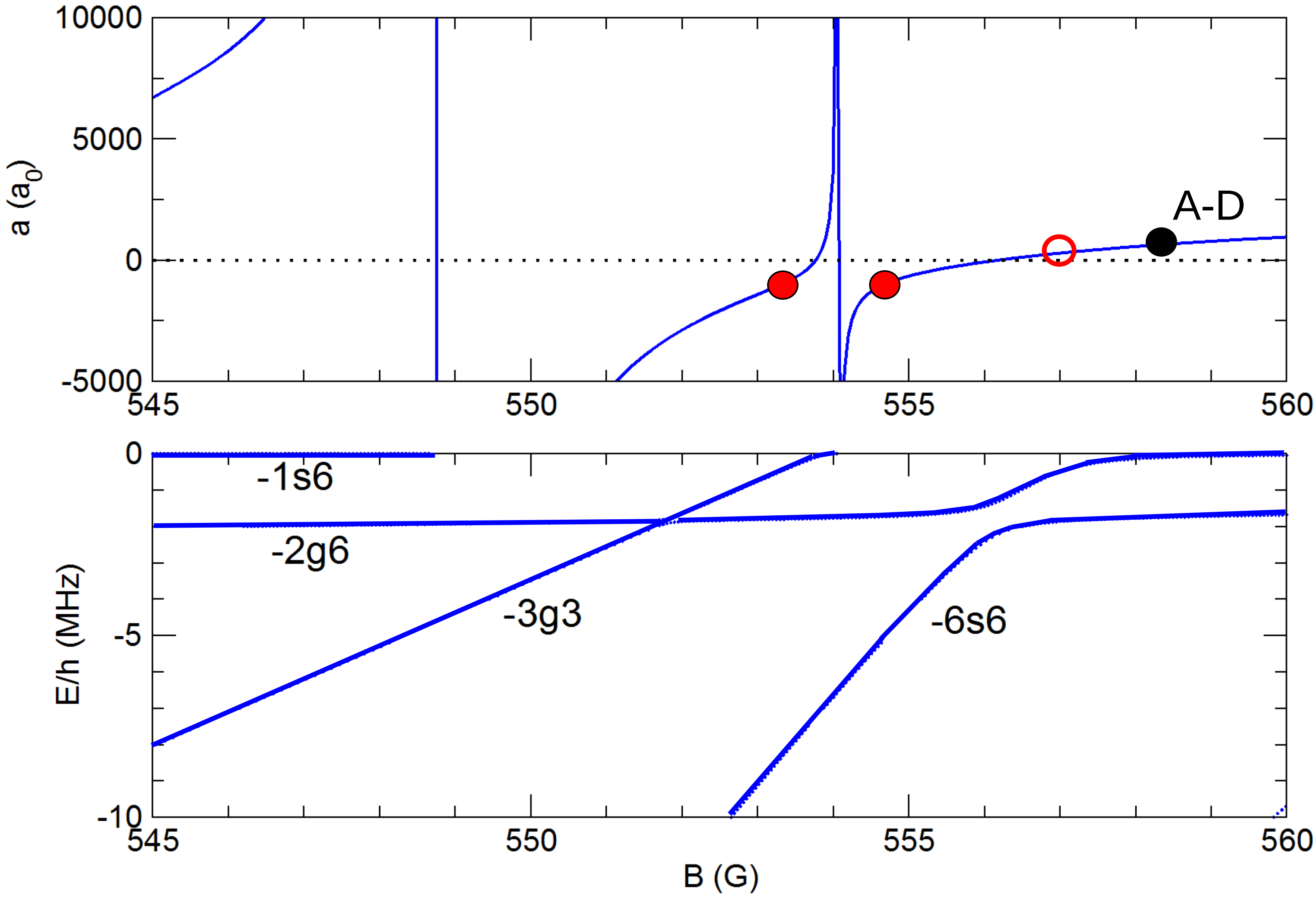
S. Knoop et al., Nature Phys. 5, 227 (2009)

a_-^* Ratio = 20.7 vs 22.7

-8.9 -185

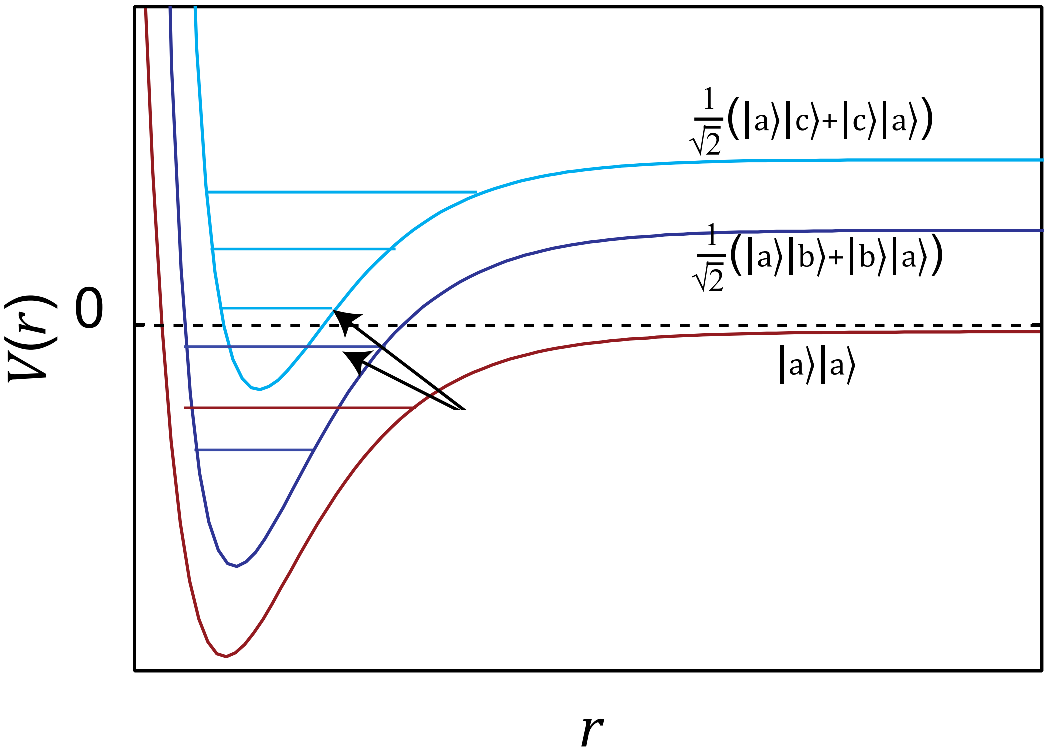


“Non-universal” d-wave resonance
Depends on N



Berninger, et al, Phys. Rev. A 87, 032517 (2013)
Jachymski, PSJ, PRA 88, 052701(2013)

3-channel 2-body model



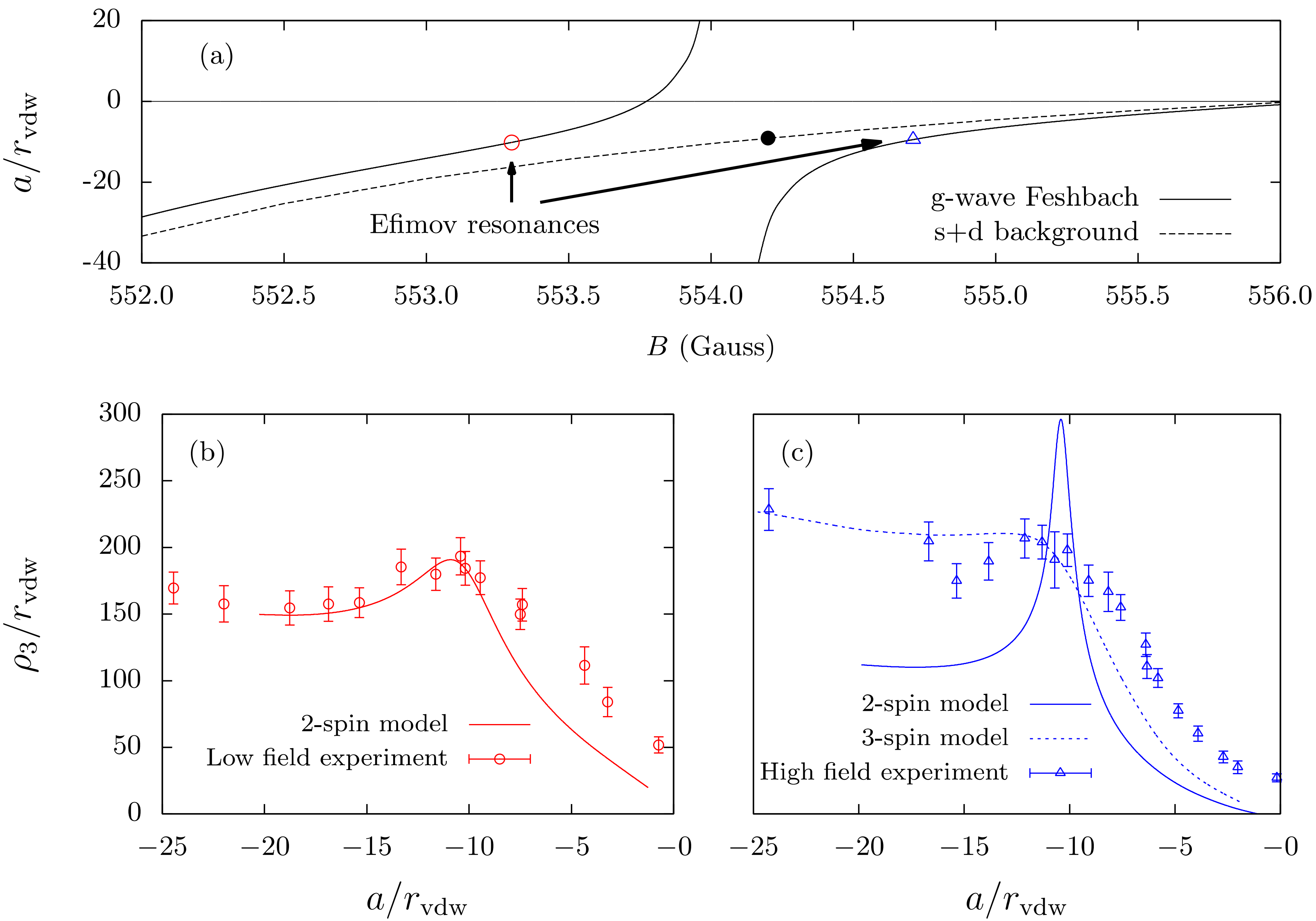
Simultaneously describes two closed channels with overlapping resonances

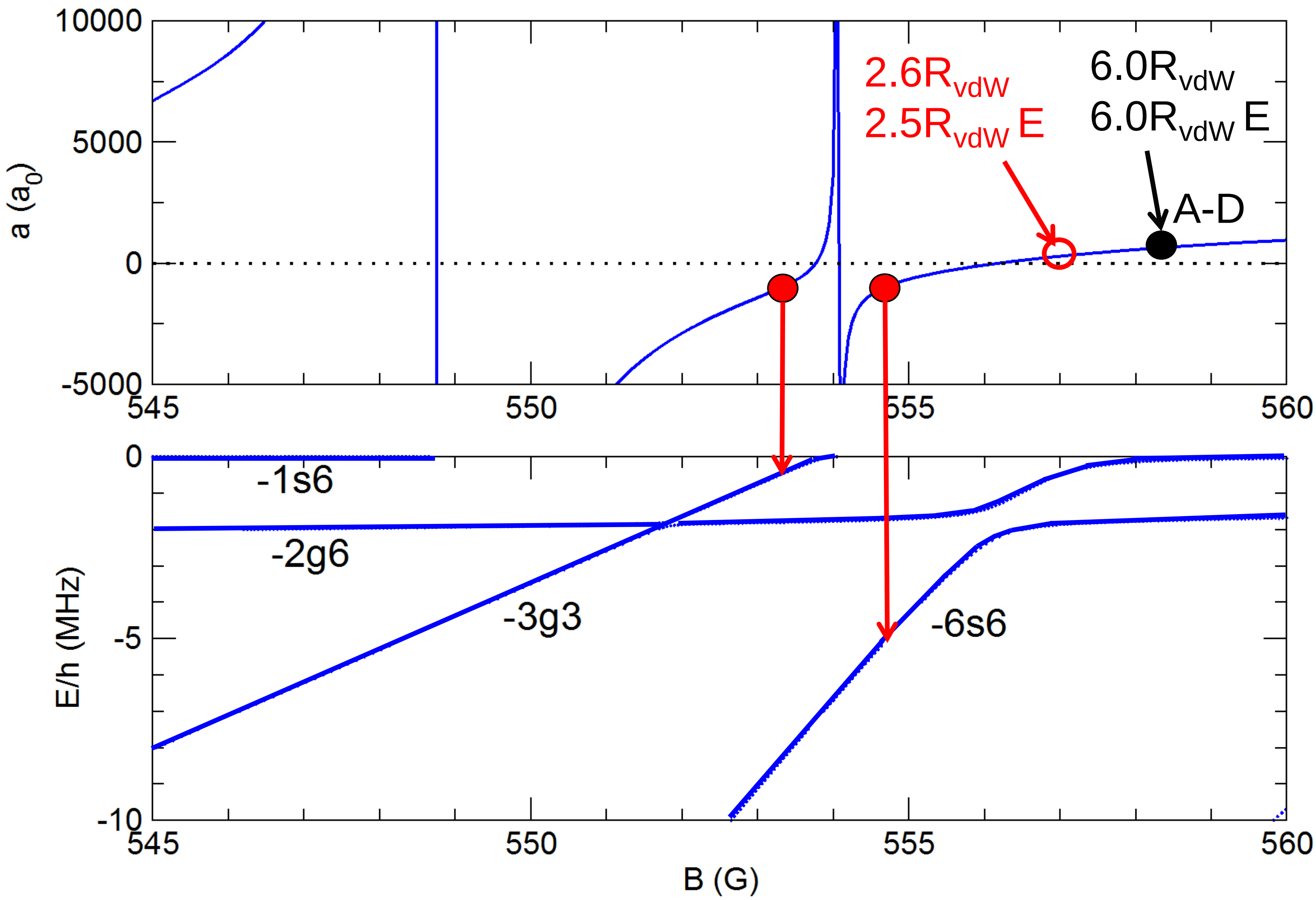
States of recombination come from BOTH channels.

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

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

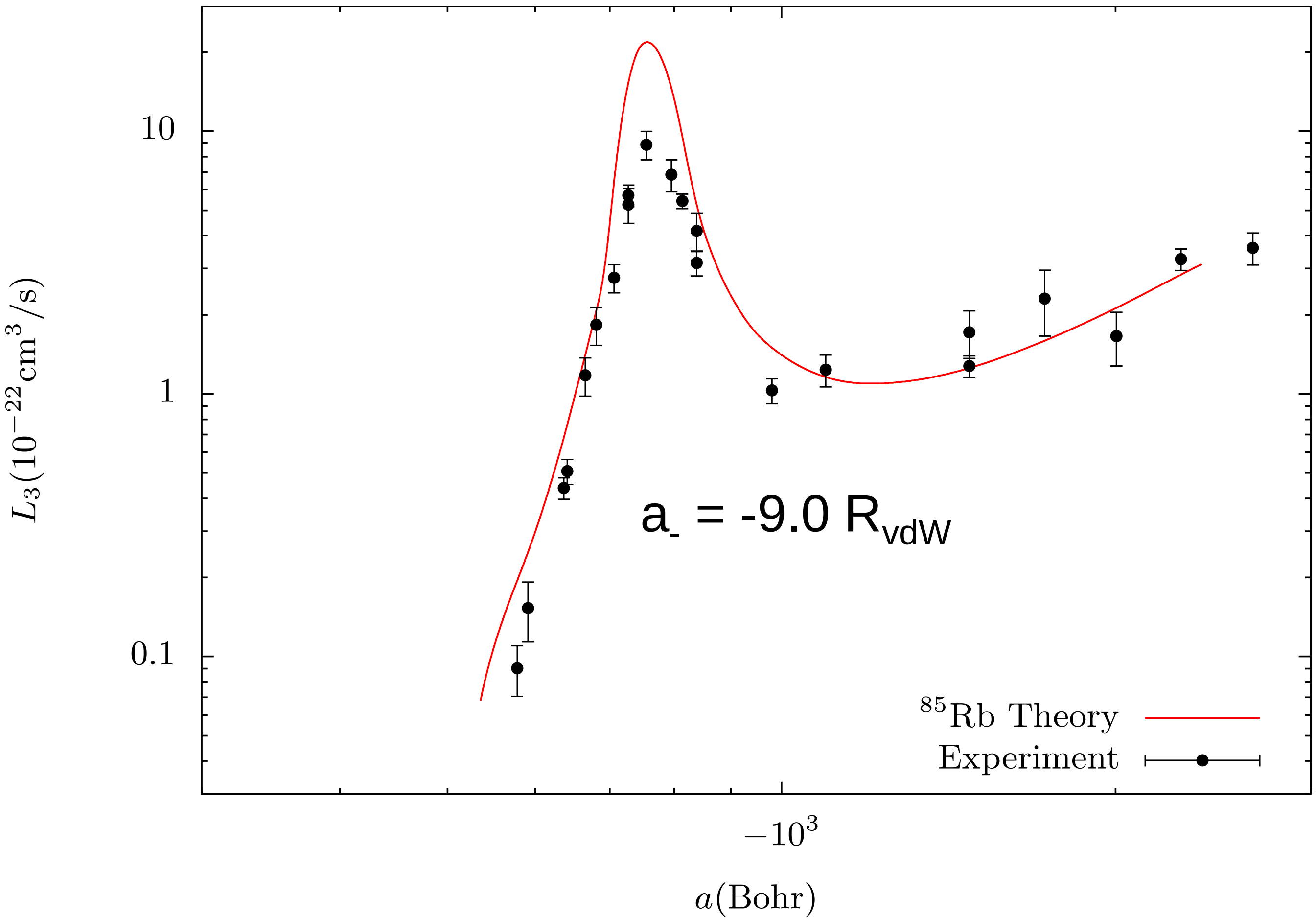
Jachymski, PSJ, PRA 88, 052701(2013)


(a)
Efimov resonances
g-wave Feshbach
s+d background
$a/r_{\rm vdw}$
B (Gauss)
20
0
-20
-40
552.0
552.5
553.0
553.5
554.0
554.5
555.0
555.5
556.0
(b)
2-spin model
Low field experiment
$\rho_3/r_{\rm vdw}$
$a/r_{\rm vdw}$
300
250
200
150
100
50
0
−25
−20
−15
−10
−5
−0
(c)
2-spin model
3-spin model
High field experiment
$a/r_{\rm vdw}$
−25
−20
−15
−10
−5
−0



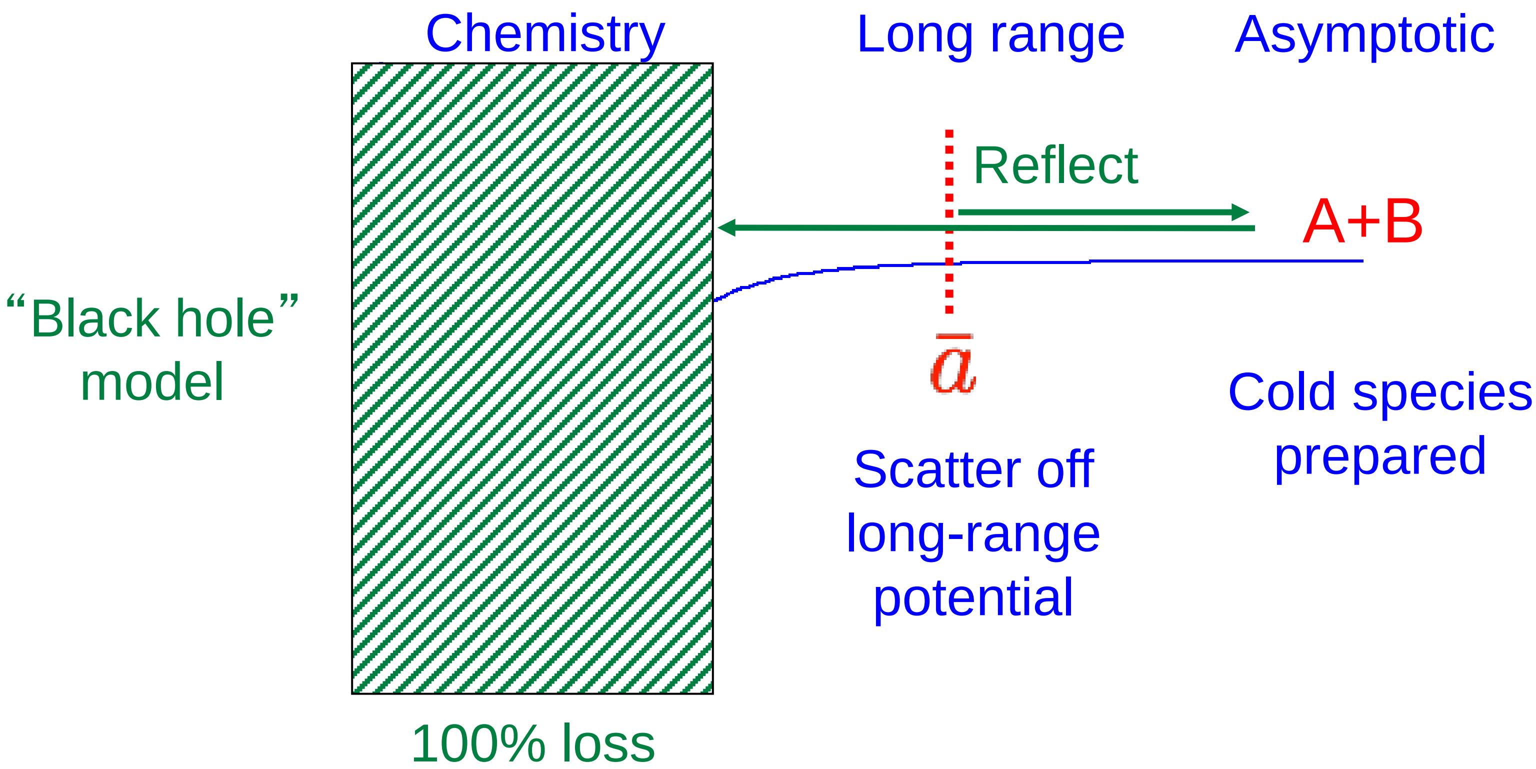
Berninger, et al, Phys. Rev. A 87, 032517 (2013)
Jachymski, PSJ, PRA 88, 052701(2013)

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



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

“Universal” van der Waals rate constants



$$\tilde{a}_0 = \bar{a}(1-i) \qquad K^{\rm loss}_{\ell=0}(E) = 2\frac{h}{\mu}\,\bar{a}$$

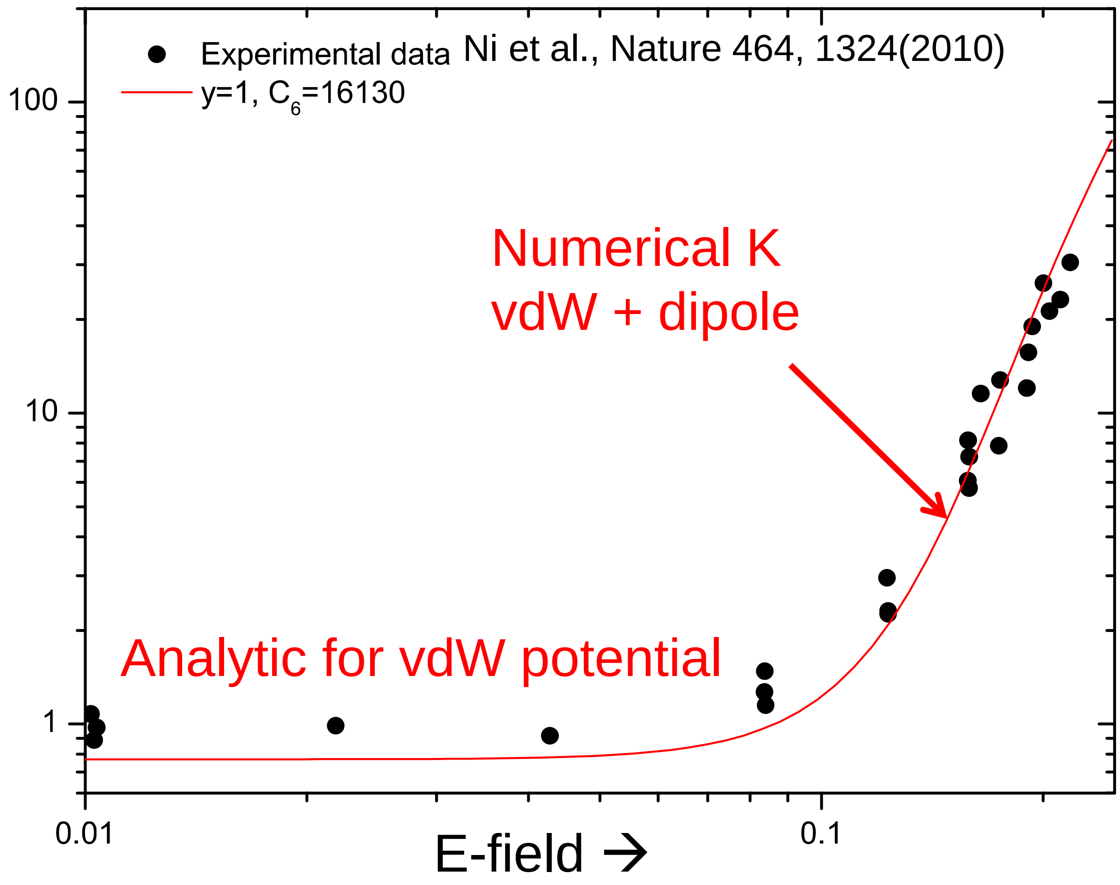
$$\tilde{a}_1 = \bar{a}_1(k\bar{a})^2(-1-i) \qquad K^{\rm loss}_{\ell=1}(E) = 12\frac{h}{\mu}\,\bar{a}_1(k\bar{a})^2$$

$$\bar{a}_1 = 1.064\bar{a}$$

Reaction rate for identical ultracold $^{40}K^{87}Rb$ fermions

$^{40}K^{87}Rb$ has Universal "chemistry"

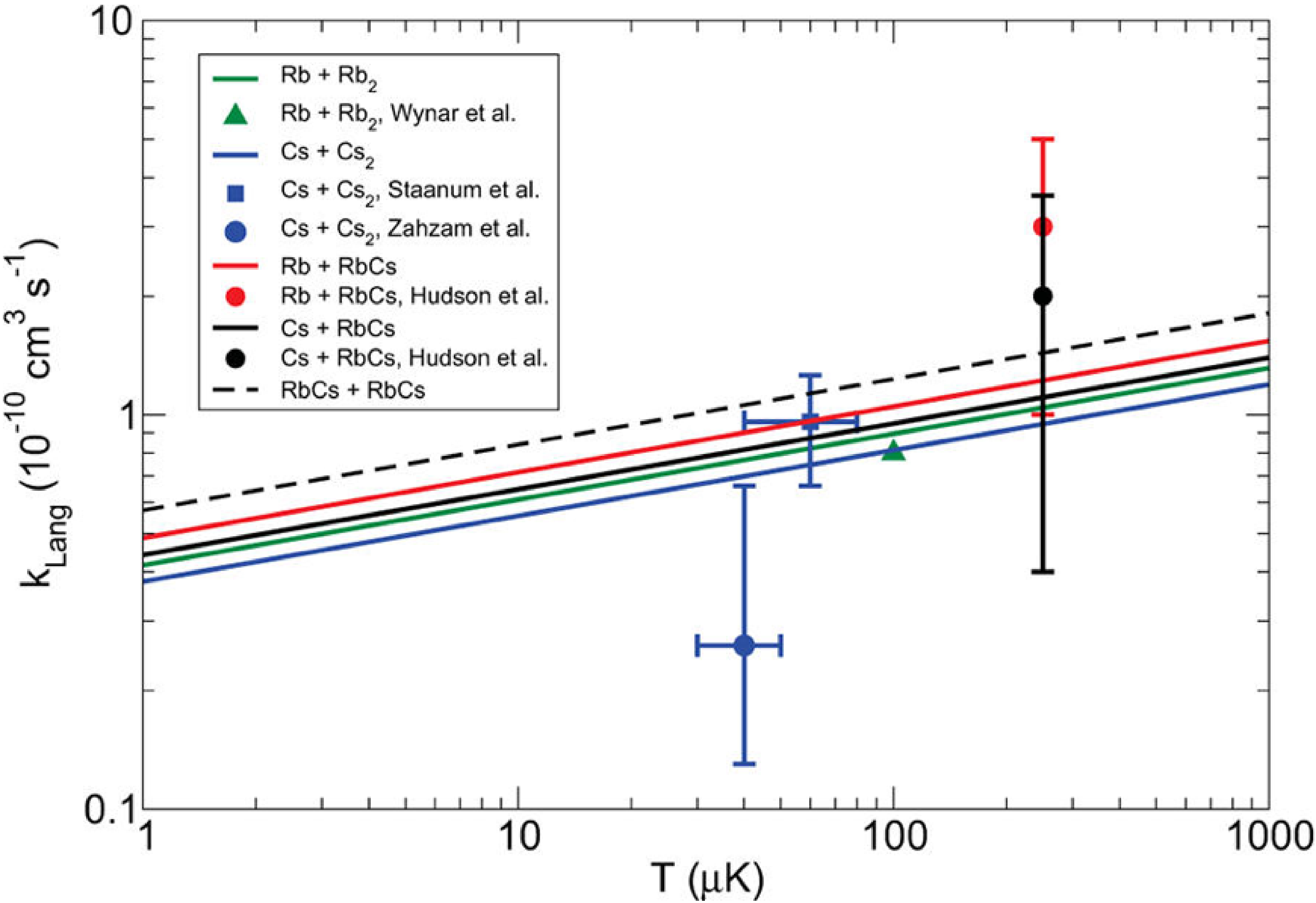
$KRb + KRb \rightarrow K_2 + Rb_2$



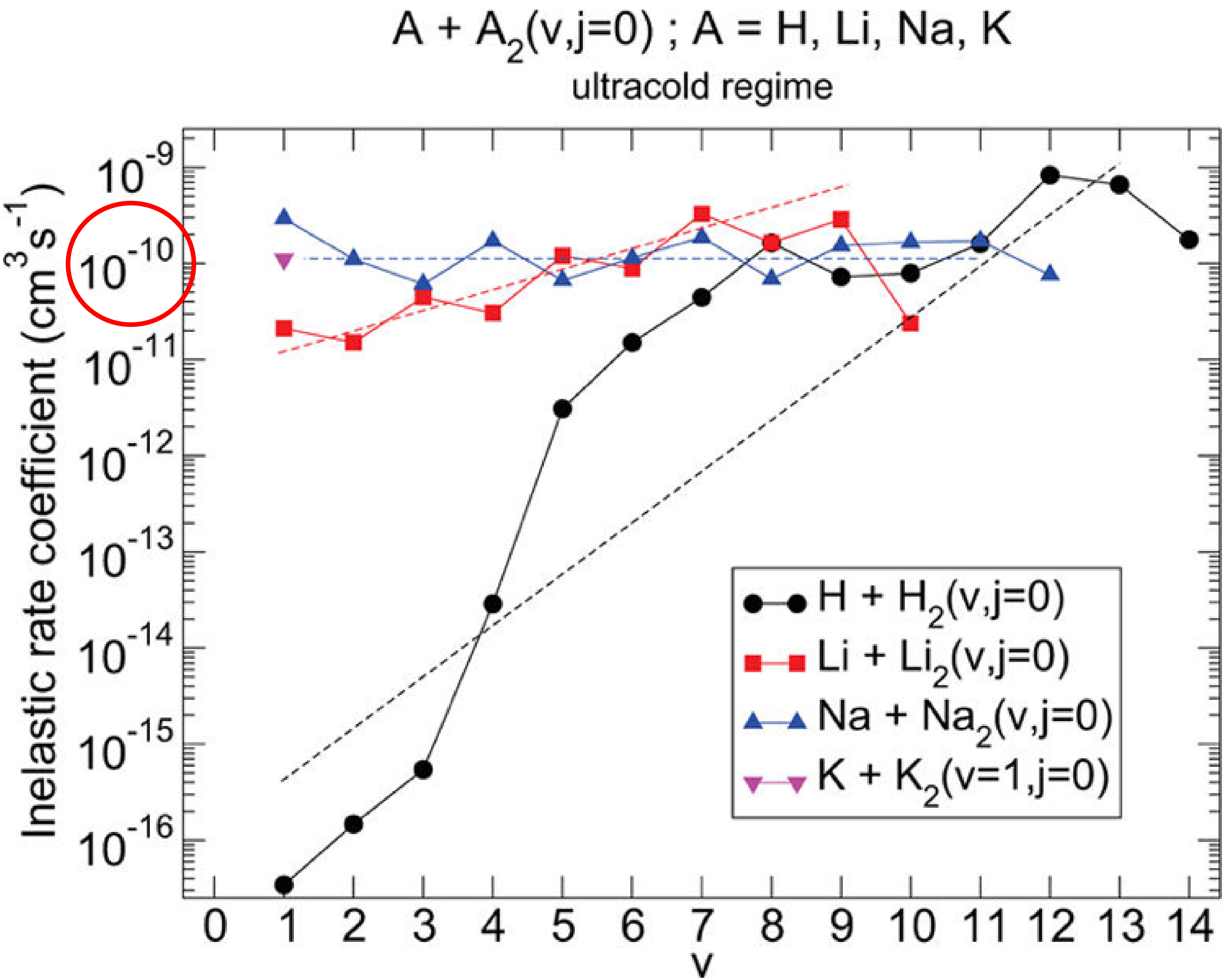
Numerical HΨ=EΨ for dipole +vdW potential

Z. Idziaszek, G. Quéméner, J.L. Bohn, P.S. Julienne, Phys. Rev. A 82, 020703R (2010)

Similar QT theory of G. Quéméner, J.L. Bohn, Phys. Rev. A81, 022702(2010)



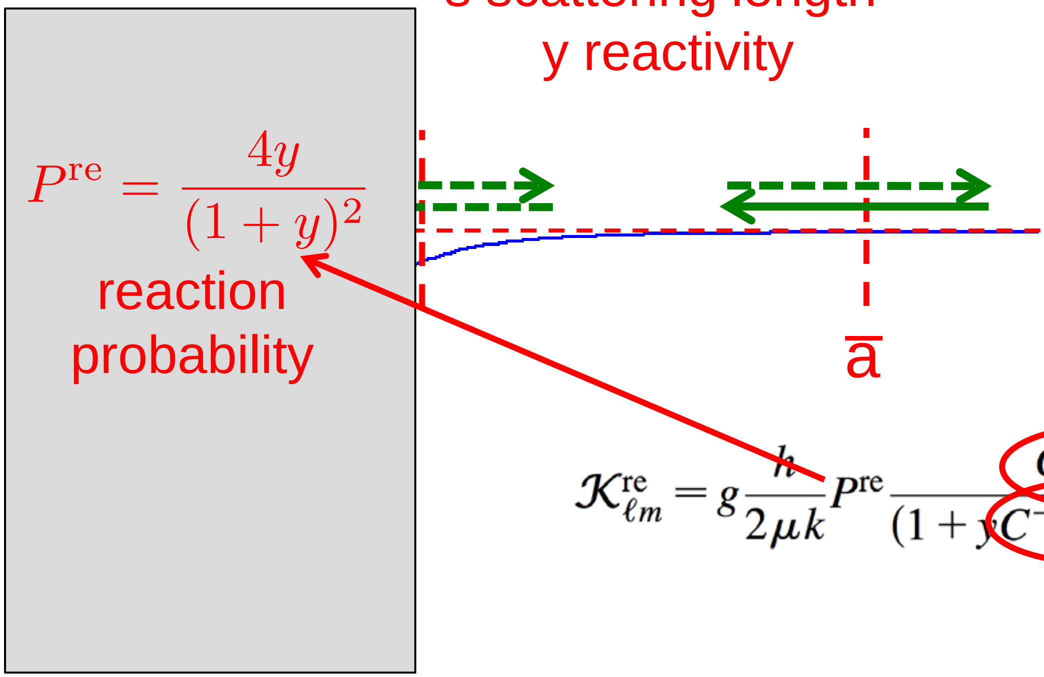
From Quéméner and PSJ, Chem. Rev. (2012)



From Quéméner and PSJ, Chem. Rev. (2012)

Universal “grey hole” reaction rate theory

2 vdW QDT parameters:
s scattering length
y reactivity



Determined by s

$$\mathcal{K}^{\mathrm{re}}_{\ell m} = g\frac{h}{2\mu k} P^{\mathrm{re}} \frac{C^{-2}(E,\ell)(1+y)^2}{(1+yC^{-2}(E,\ell))^2 + y^2\tan^2\lambda(E,\ell)}$$

“chemistry”

y=1 special case, “black hole,” Langevin theory

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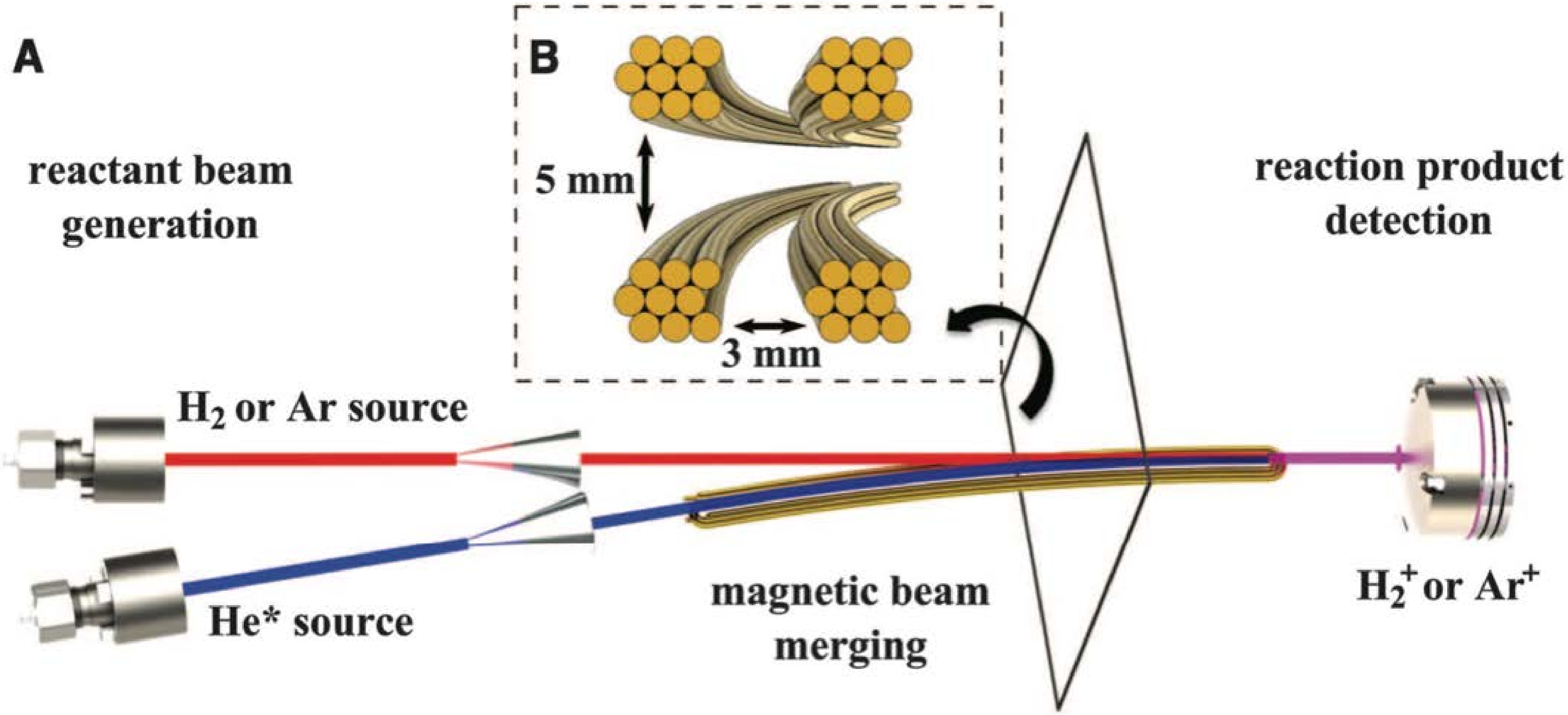
Jachymski, Krych, Idziaszek, PSJ, Phys. Rev. Lett. 110, 213202 (2013)

Penning ionization in cold merged beam collisions



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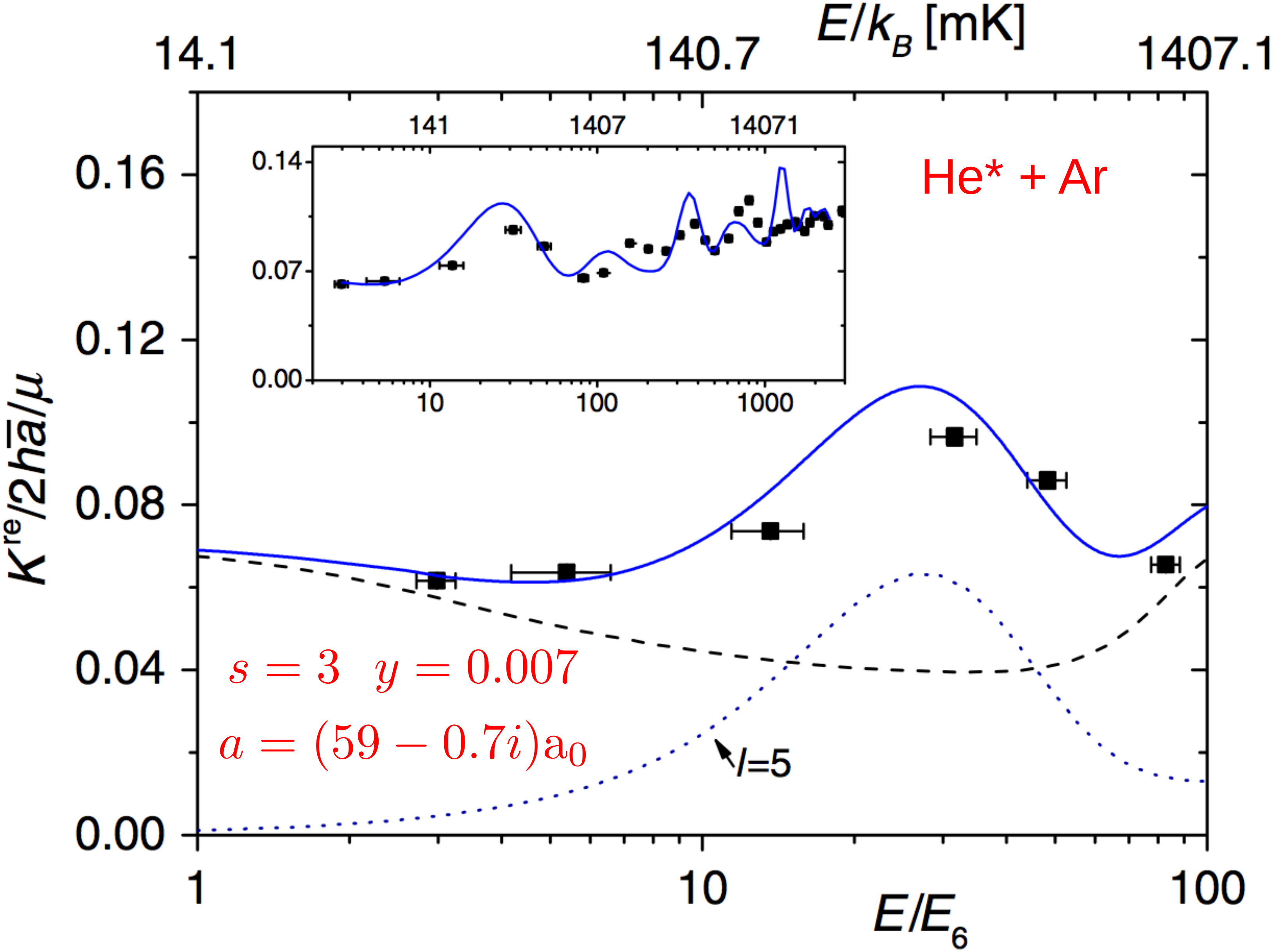

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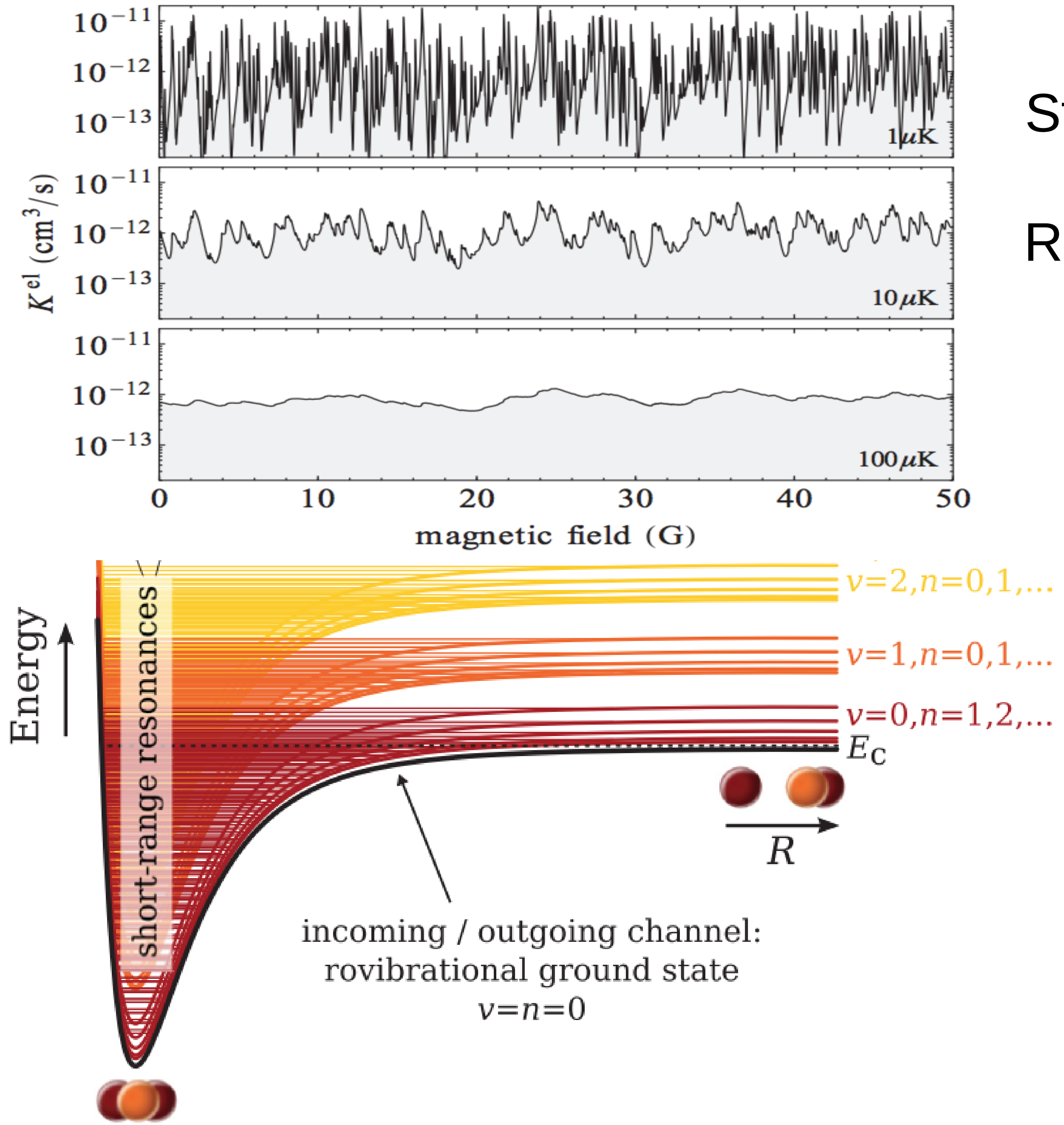


"Toy"
Statistical
model
Rb + KRb

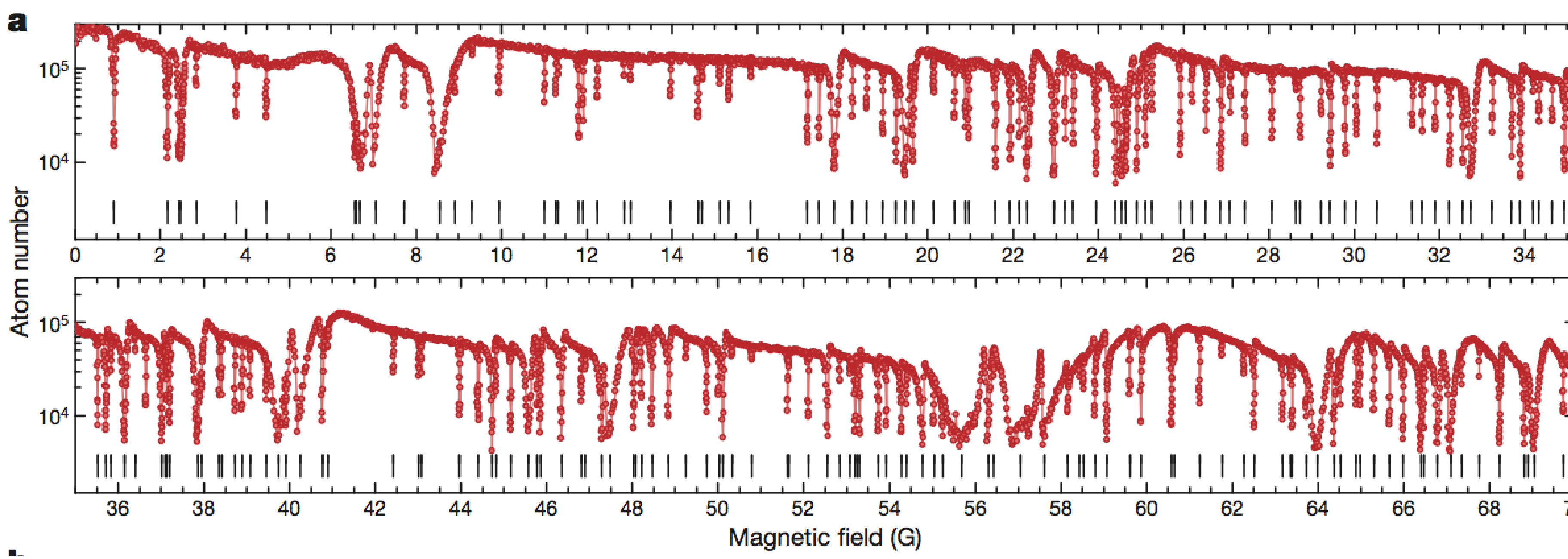
LETTER

Nature online, March 12, 2014

arXiv:1312.1972v1
doi:10.1038/nature13137

Quantum chaos in ultracold collisions of gas-phase erbium atoms

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 ground state ^{3}H (91 potential energy curves)

The End