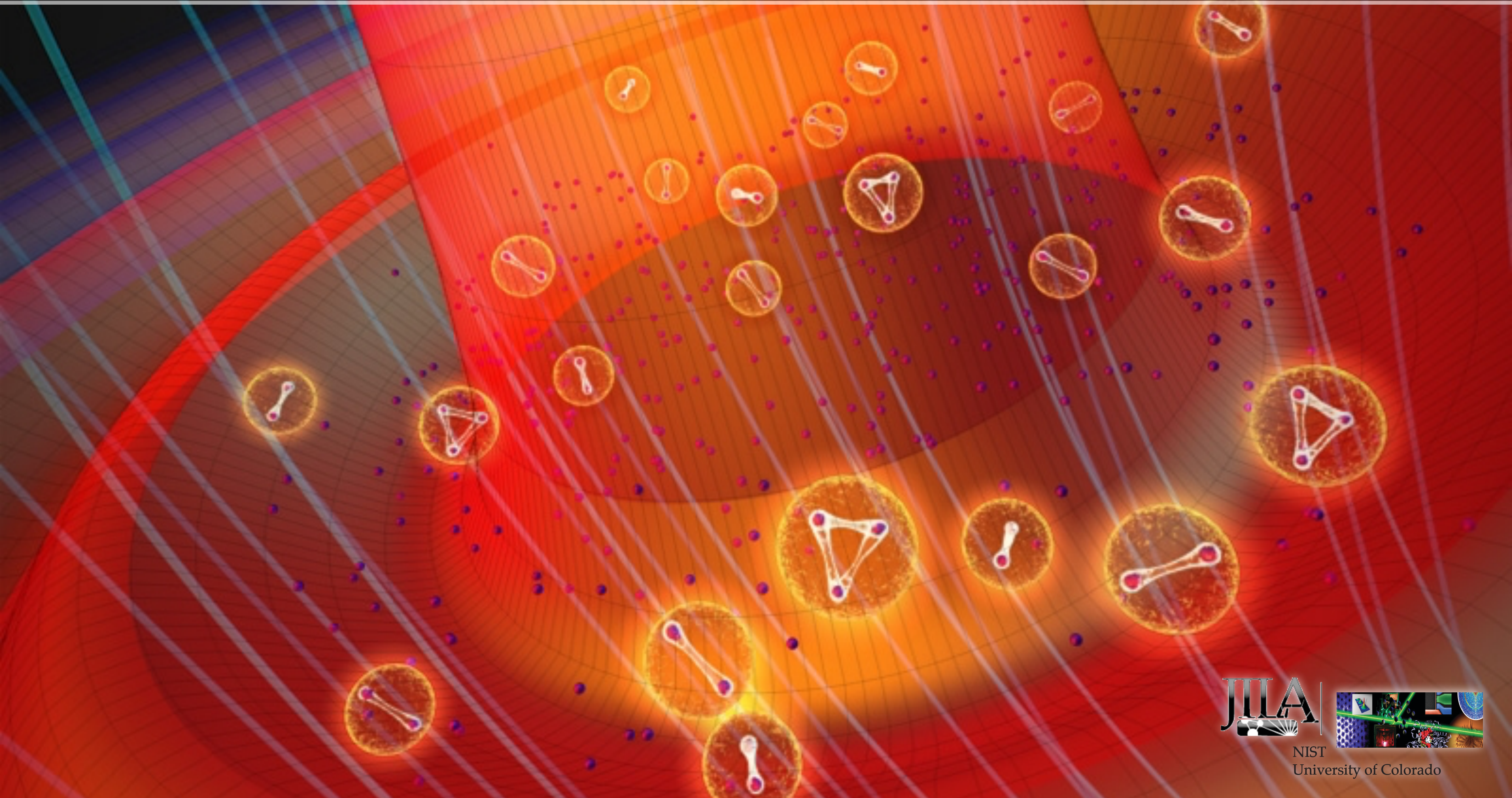
Multichannel nature of few-body interactions in ultracold atomic systems and chemical reactions

Jose P. D'Incao

JILA, NIST, and Department of Physics, University of Colorado at Boulder, Boulder, CO



NIST
University of Colorado

This talk…

The Story of Three Experiments and one Quest

…building more realistic models for few-body atomic physics (predictive power)

Eric Cornell (JILA/NIST)

NASA ($)

Jun Ye (JILA/NIST)

Paul Julienne (NIST/JQI)

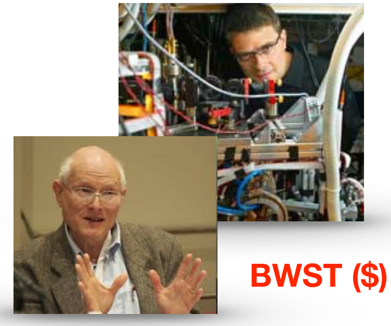
$^{39}\mathrm{K}$

Long-range physics…
(> r_vdW)

Short-range physics…
(< r_vdW)

$^{87}\mathrm{Rb}$ $^{85}\mathrm{Rb}$

Johannes Denschlag (Ulm/GE)



BWST ($)

Paul Julienne (NIST/JQI)

Both!?

$^{7}\mathrm{Li}$ ....

Lev Khaykovich (Bar-Ilan)

NSF ($)

Paul Julienne (NIST/JQI)

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Multichannel aspects of Efimov Universality

Ultracold chemical reactions (propensity rules, lifetimes, …)

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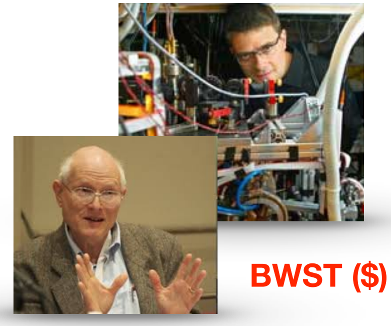

BWST ($)

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All of the above, challenges, puzzles…

$^{7}\mathrm{Li}$ ■ ■ ■ ■ ■

Lev Khaykovich (Bar-Ilan)

NSF ($)

Paul Julienne (NIST/JQI)

A new universal picture…

A new universal picture

van der Waals Universality

Refers to the Efimov physics obtained using (single channel) vdW interactions, -C6/r^6, leading to a three-body parameter depending only on rvdW.

Theory:

Wang, D'Incao, Esry, Greene, PRL 108, 263001 (2012)
Naidon, Endo, Ueda, PRA 90, 022106 (2014)
Schmidt, Rath, Zwerger, EPJB 85, 386 (2012)

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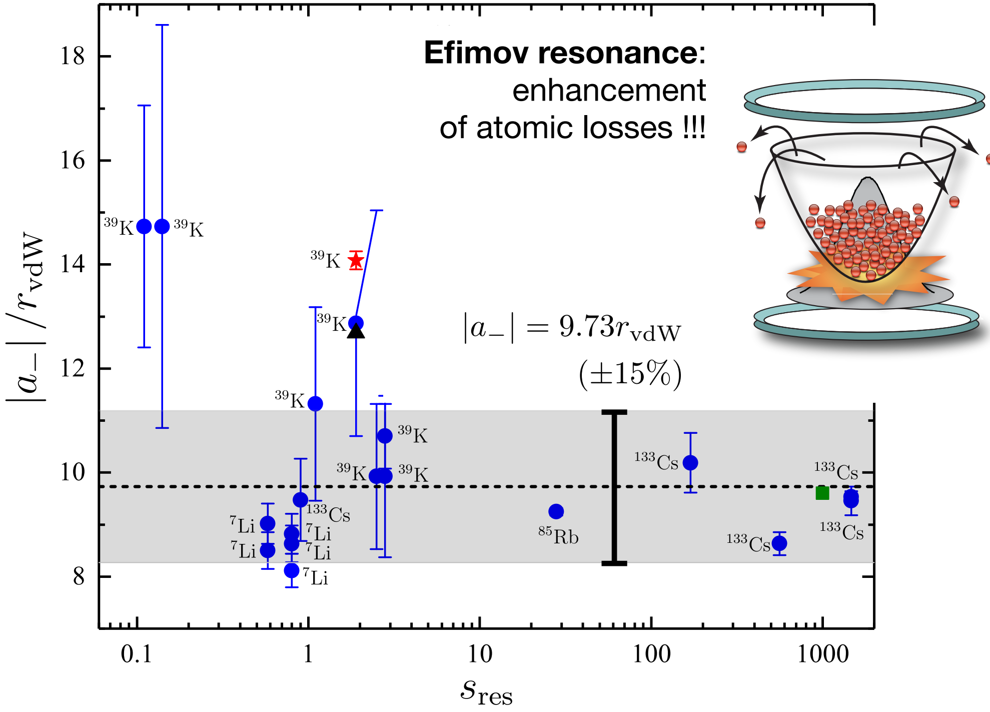
Ultracold Gases Experiments

$\boxed{s_{\mathrm{res}}}$ **Resonance Strength**

$s_{\mathrm{res}} \gg 1$: strong (broad)

$s_{\mathrm{res}} \ll 1$: weak (narrow)

Innsbruck, Bar-Ilan, Rice, LENS, Aarhus, JILA, Chicago,…



Efimov resonance: enhancement of atomic losses !!!

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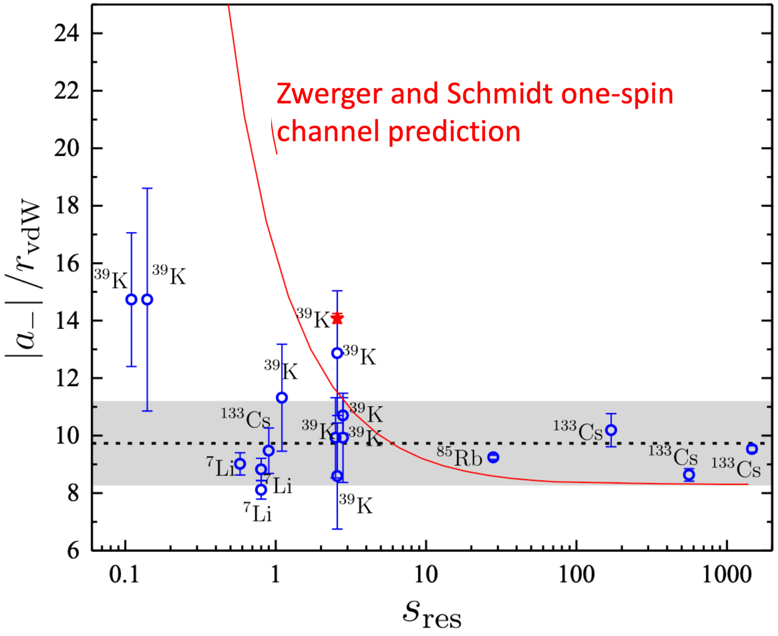
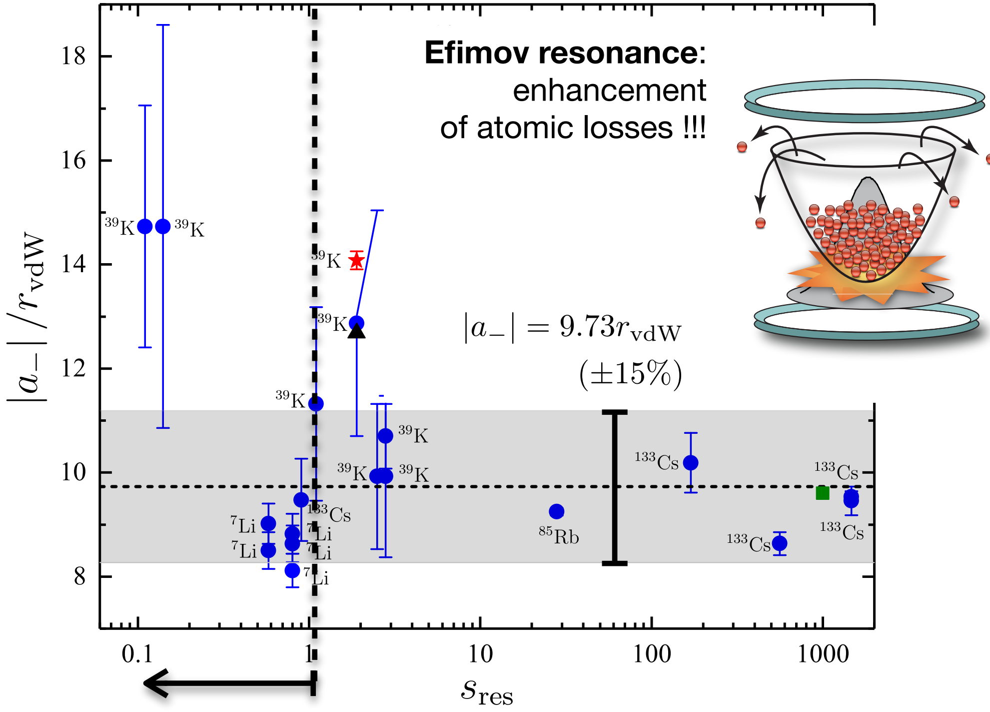


Zwerger and Schmidt one-spin channel prediction



Efimov resonance: enhancement of atomic losses !!!

$|a_-| = 9.73 r_{\text{vdW}}$ $(\pm 15\%)$

Narrow Resonances Alters Efimov Physics

Petrov, PRL 93, 143201 (2004)
Wang, D'Incao, Esry, PRA 83, 042710 (2011)
Schmidt, Rath, Zwerger, EPJB 85, 386 (2012)

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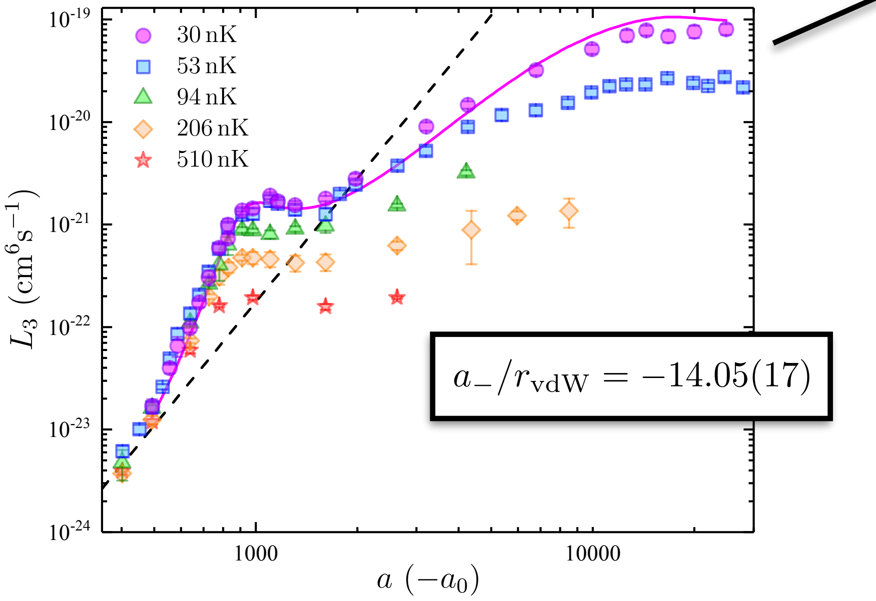
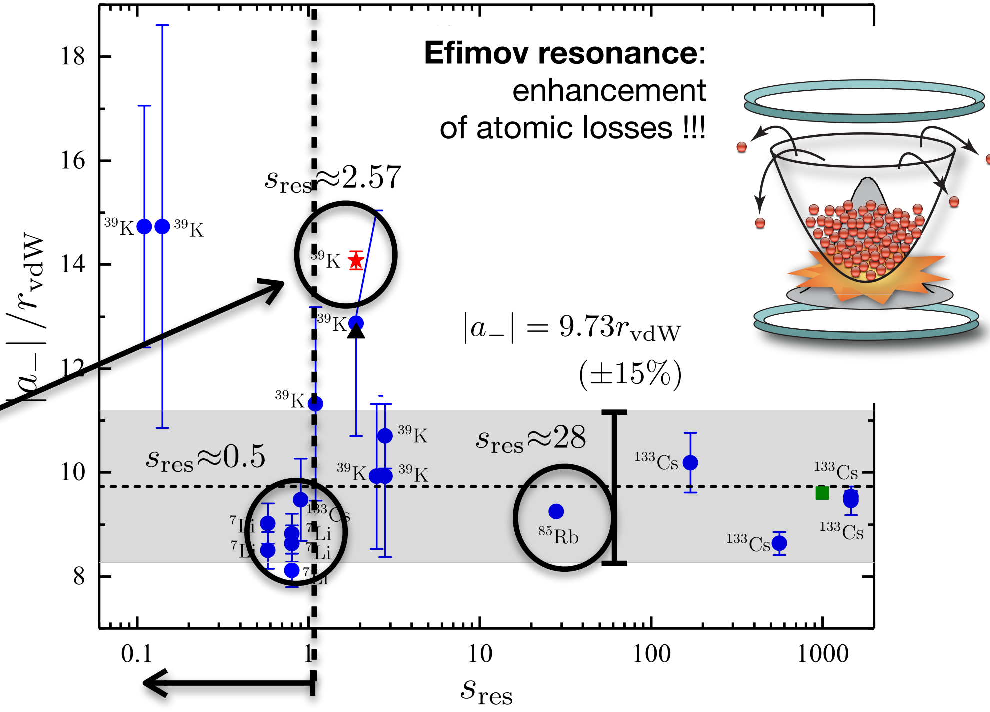
39K recombination @JILA (sres=2.57)



$$a_-/r_{\rm vdW} = -14.05(17)$$

Ultracold Gases Experiments



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Few-body Physics for 39K Atoms

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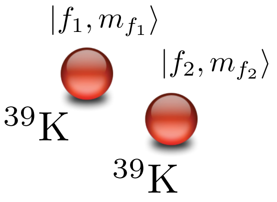
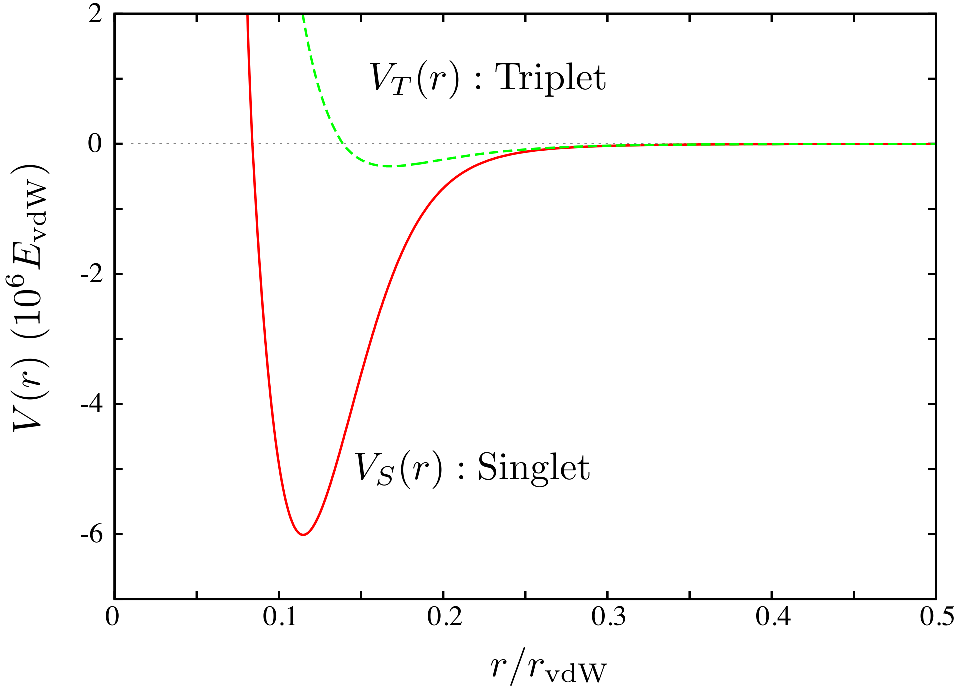
Atom-Atom Interaction



$$\boxed{\hat{V}(r) = \sum_{SM_S} |SM_S\rangle V_S(r) \langle SM_S|}$$

[Singlet: $V_{S=0}(r) \equiv V_S(r)$, Triplet: $V_{S=1}(r) \equiv V_T(r)$]

Falke, et al., PRA 78, 012503 (2008)



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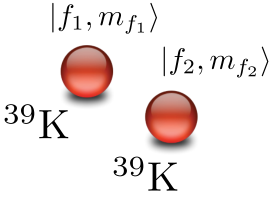

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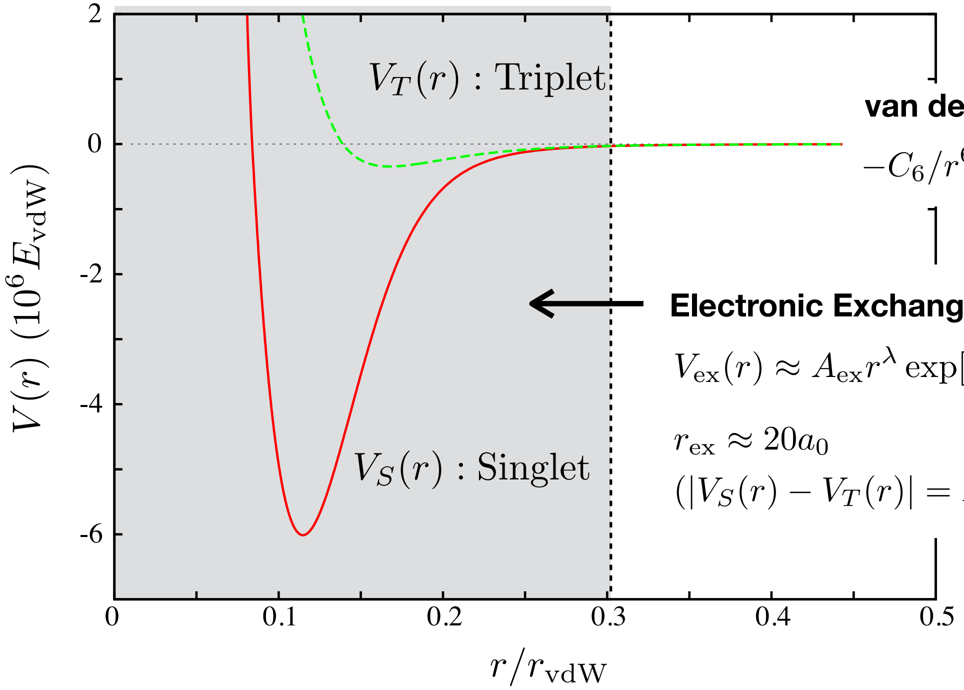

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van der Waals

$-C_6/r^6$

Electronic Exchange

$V_{\mathrm{ex}}(r) \approx A_{\mathrm{ex}} r^{\lambda} \exp[-r/\beta]$

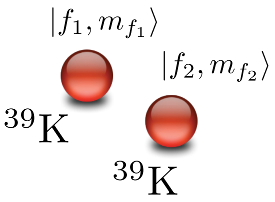
$r_{\mathrm{ex}} \approx 20a_0$

$(|V_S(r) - V_T(r)| = E_{\mathrm{vdW}})$

PS.: rvdW is not the only short-range length scale. In general r_vdW>>r_ex, (no V3B) but **not always!**

Few-Body Physics for 39K Atoms

Atom-Atom Interaction



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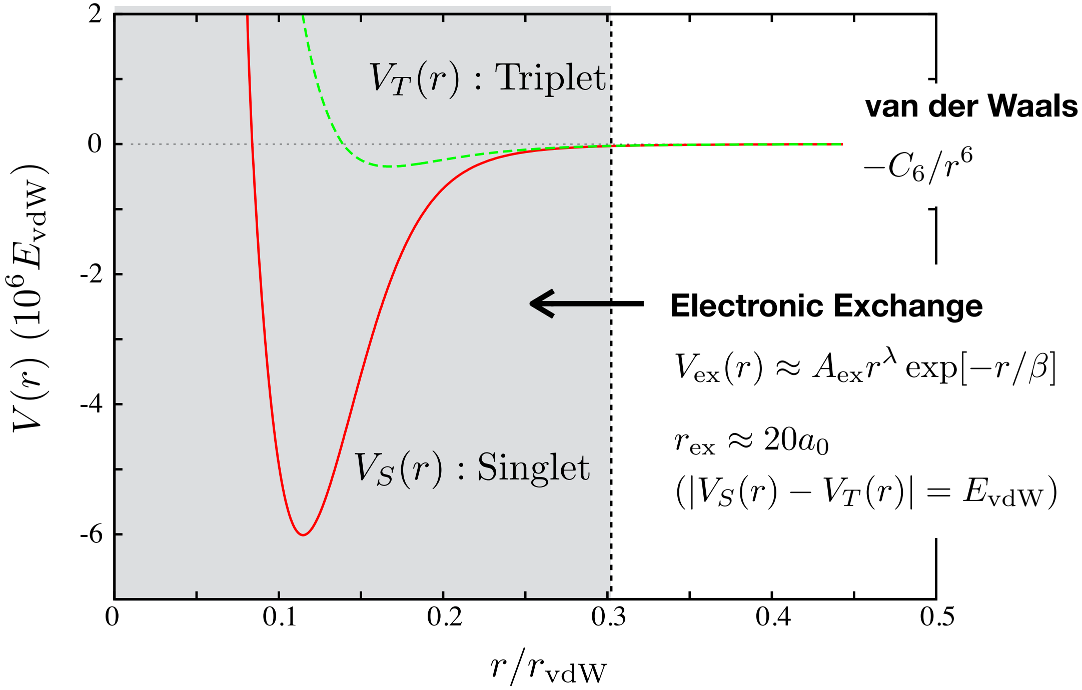

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"Reduced" Atom-Atom Interaction

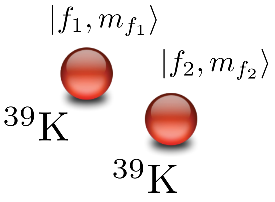
Reduced Model (1st generation)

$$\boxed{V_{S/T}(r) = -\frac{C_6}{r^6}\left(1 - \frac{\lambda_{S/T}^6}{r^6}\right)}$$

$\{\lambda_S, \lambda_T\} \rightarrow \{a_S, a_T\}$

Few-Body Physics for 39K Atoms

Atom-Atom Interaction



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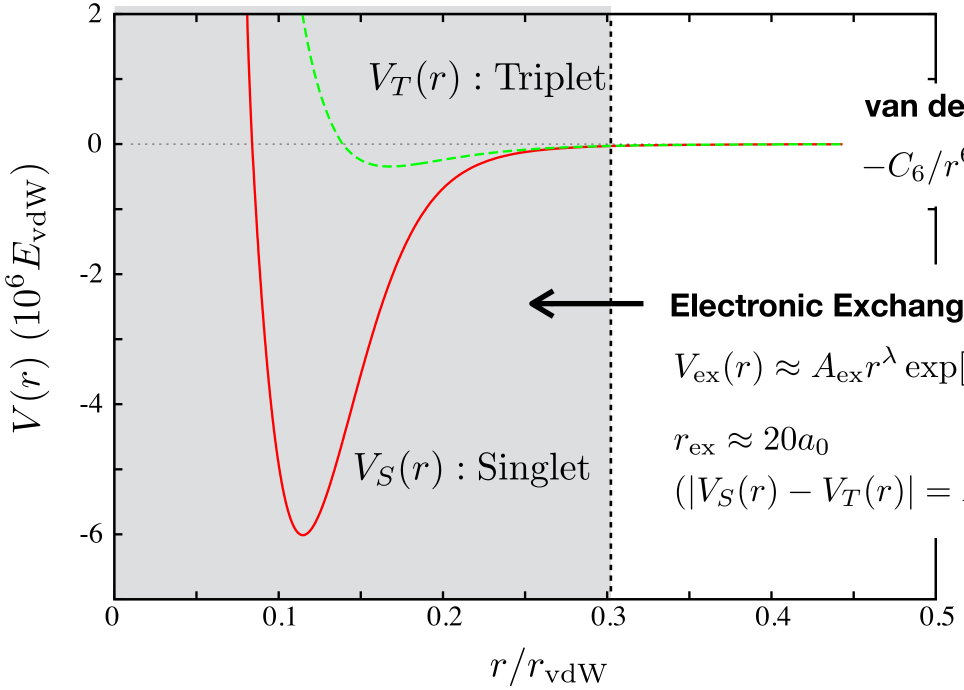

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$\{\lambda_S, \lambda_T\} \rightarrow \{a_S, a_T\}$

…has some limitations (spin physics)

Reduced Model (2nd generation)

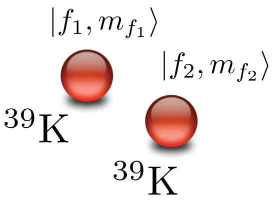
$$\boxed{V_{S/T}(r) = V_{S/T}^{*}(r) + \frac{\lambda_{S/T}^6}{r^{12}}}$$

$V_{S/T}^{*}$: ab initio

$\{\lambda_S, \lambda_T\} \rightarrow \{a_S, a_T\}$

Few-Body Physics for 39K Atoms

Atom-Atom Interaction



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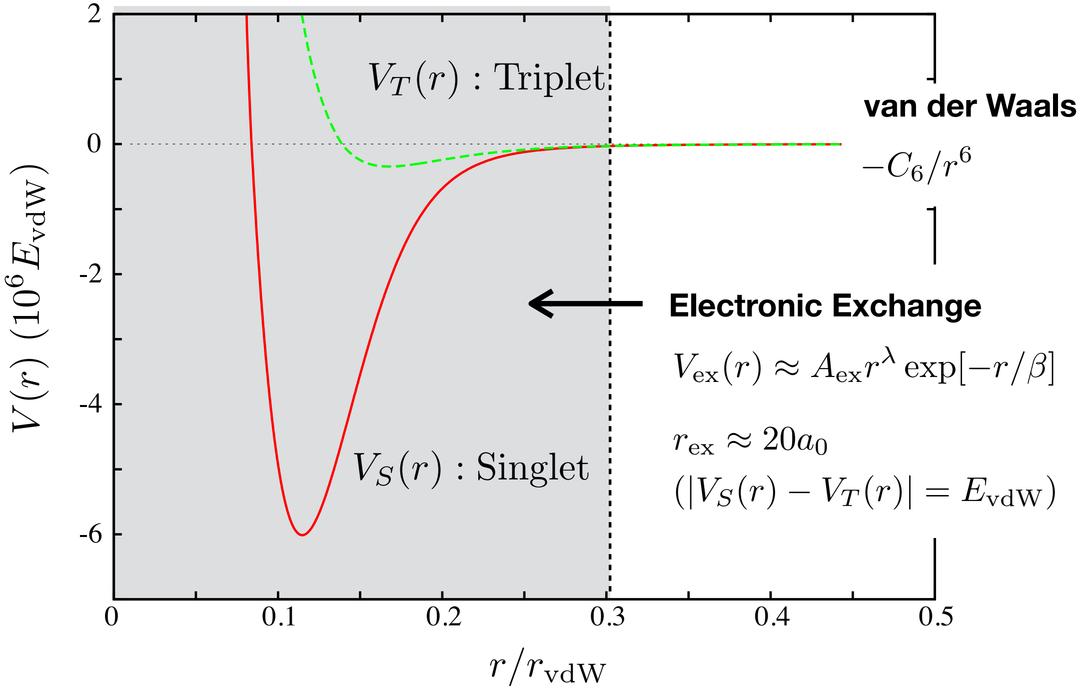

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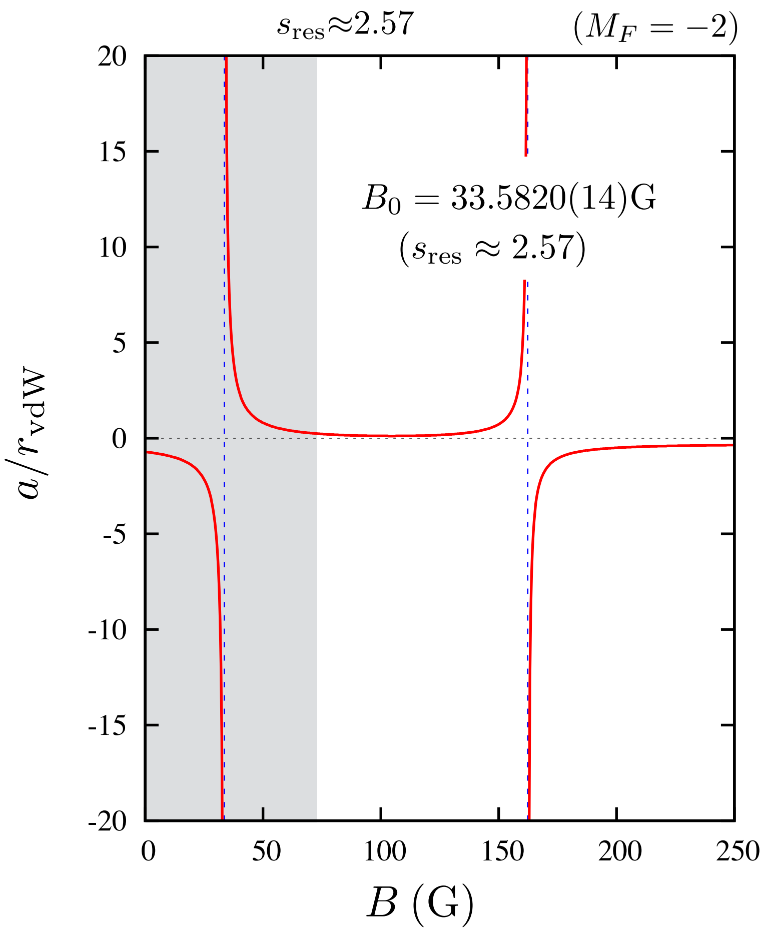
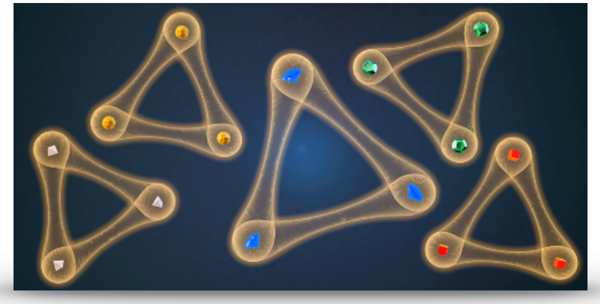
39K Feshbach Resonance



Efimov Physics for 39K atoms at JILA

39K3 Efimov states are “anomalous”



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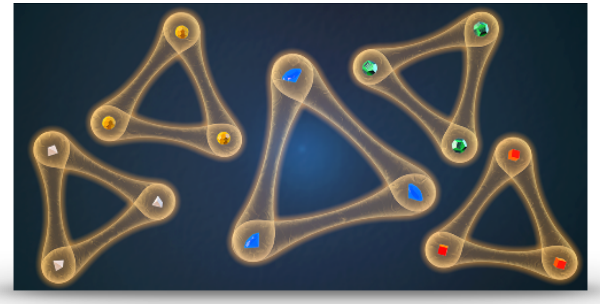

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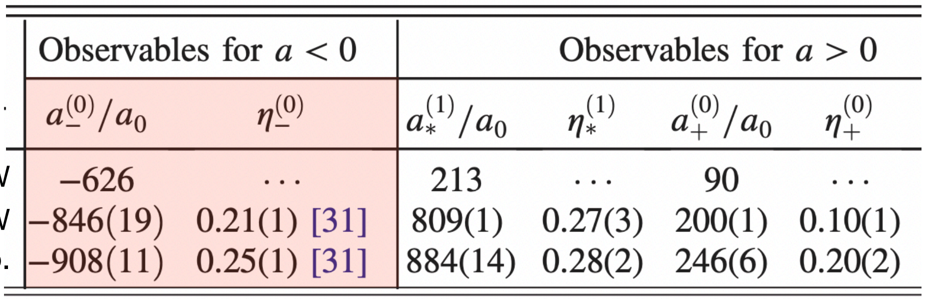

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vdW	−626	···	213	···	90	···
MC-vdW	−846(19)	0.21(1) [31]	809(1)	0.27(3)	200(1)	0.10(1)
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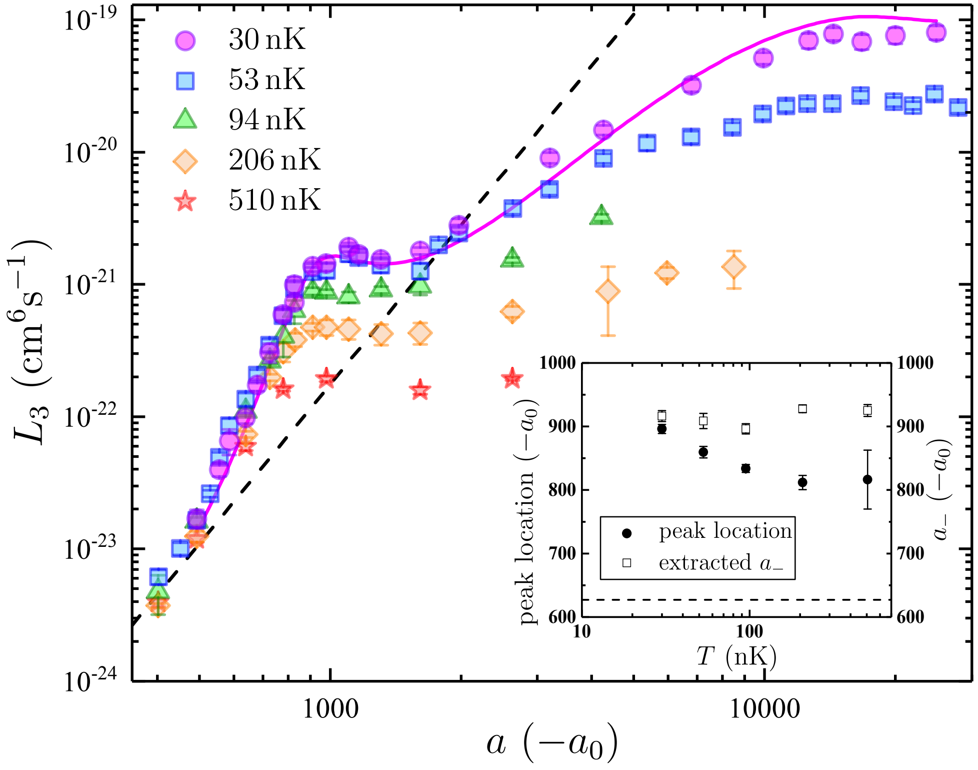
Three-body Recombination (a<0)



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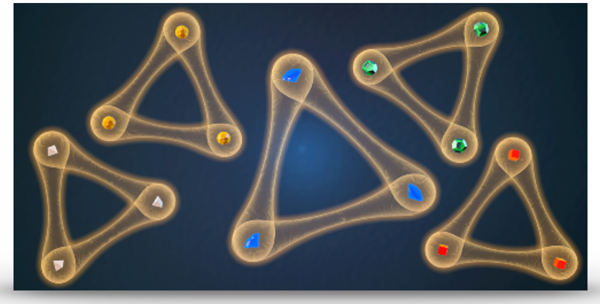

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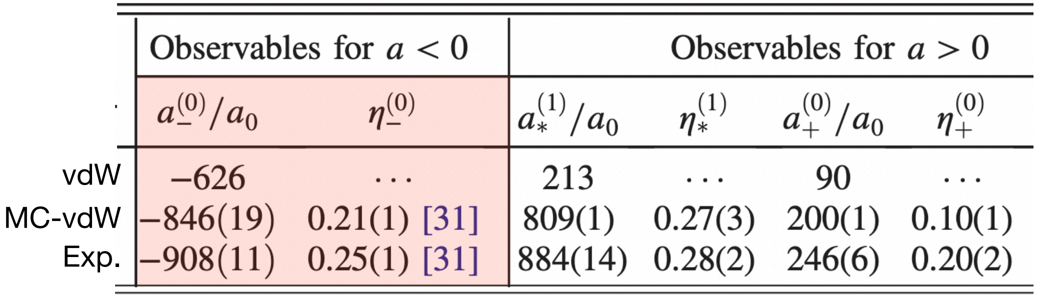

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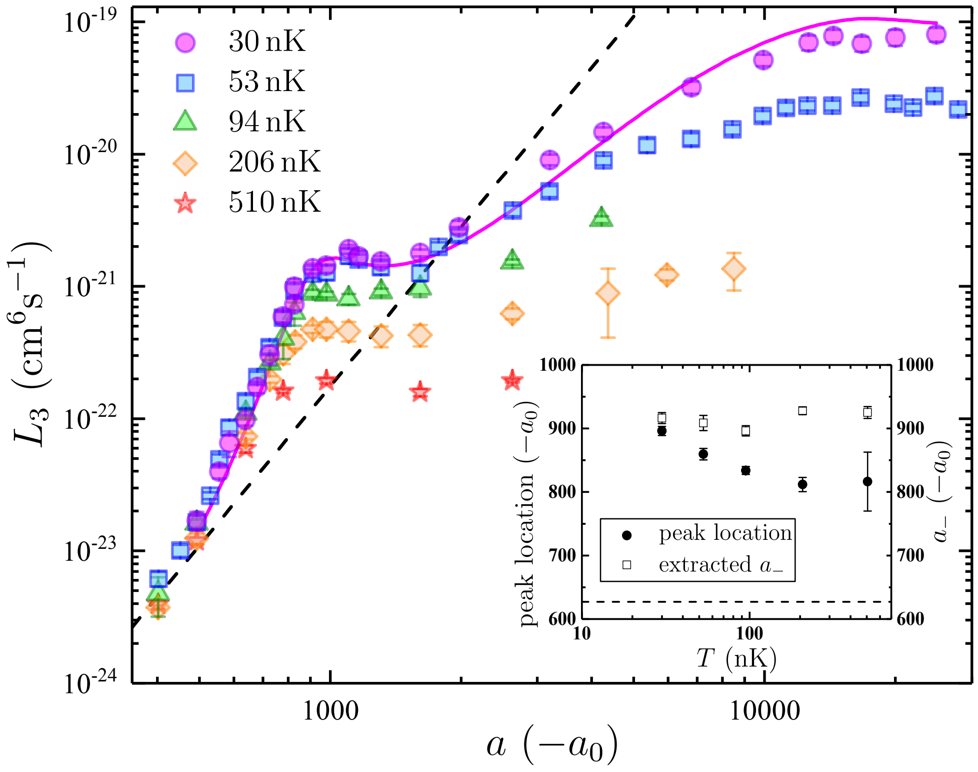

Inelasticity Parameter
(short-range physics)
Hyperfine Structure is important!

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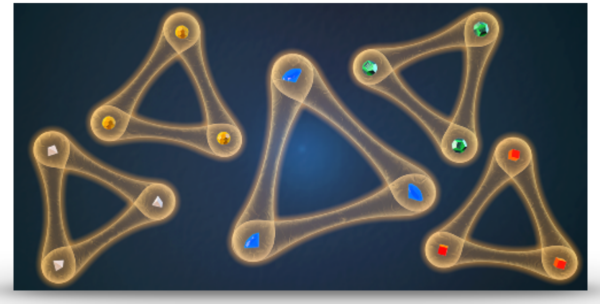

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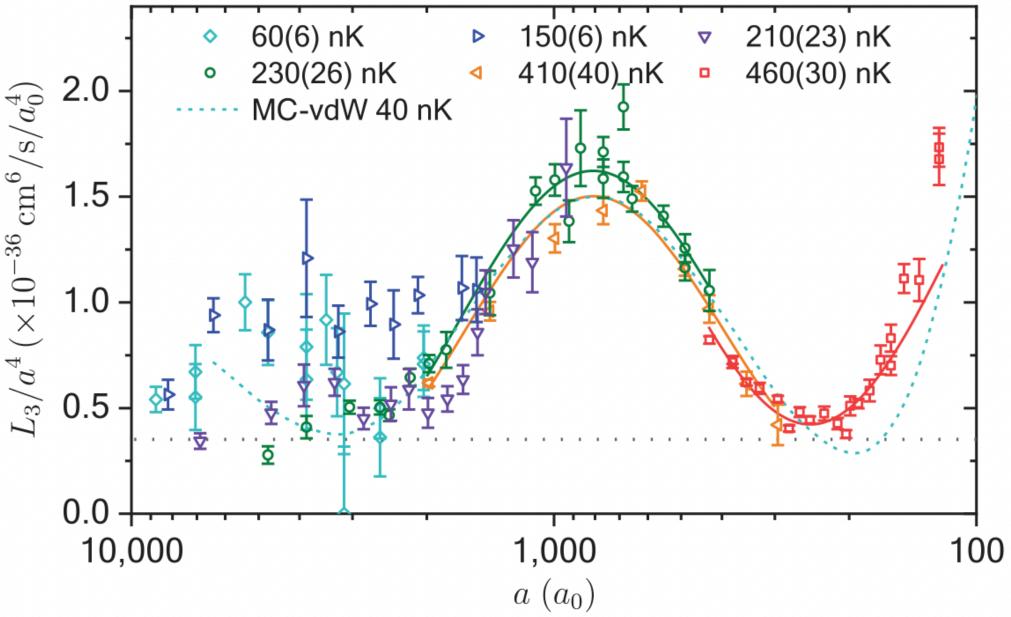

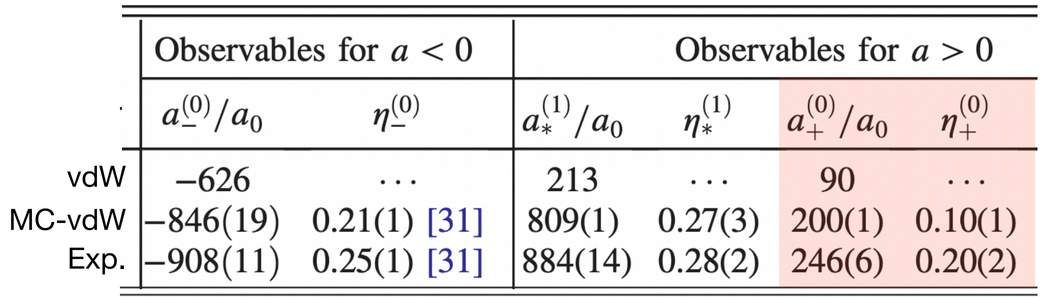

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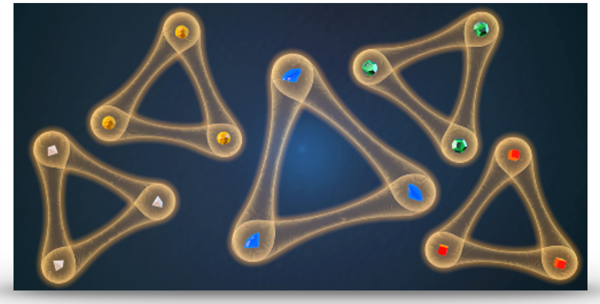

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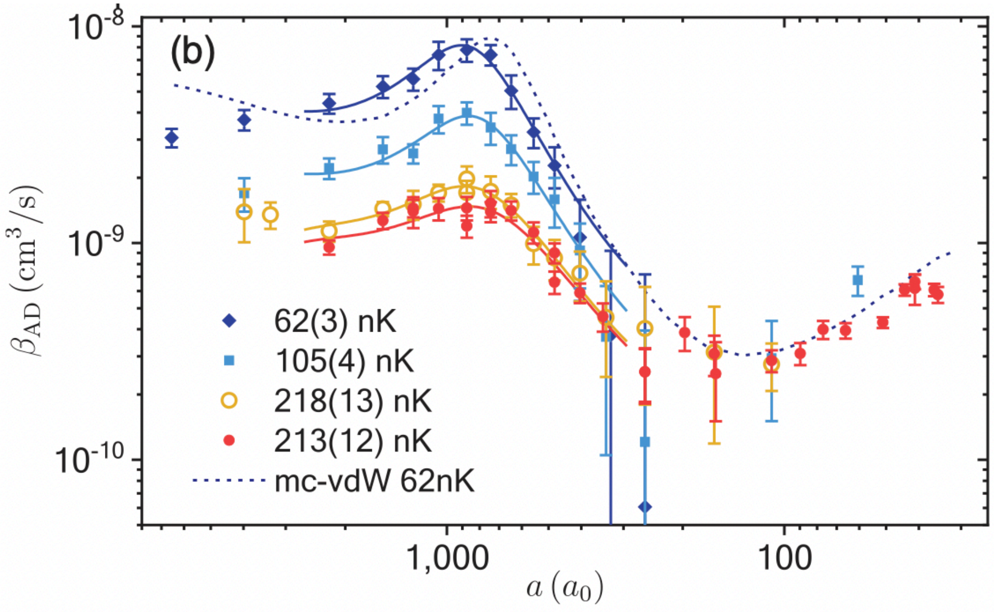
Atom-molecule Relaxation (a>0)



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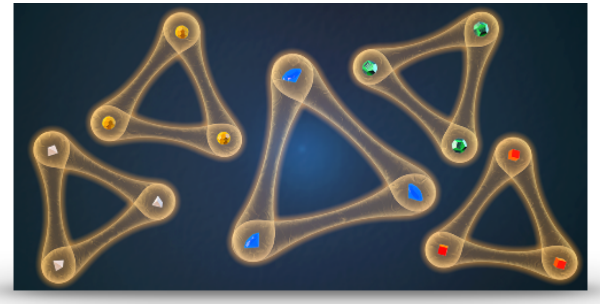

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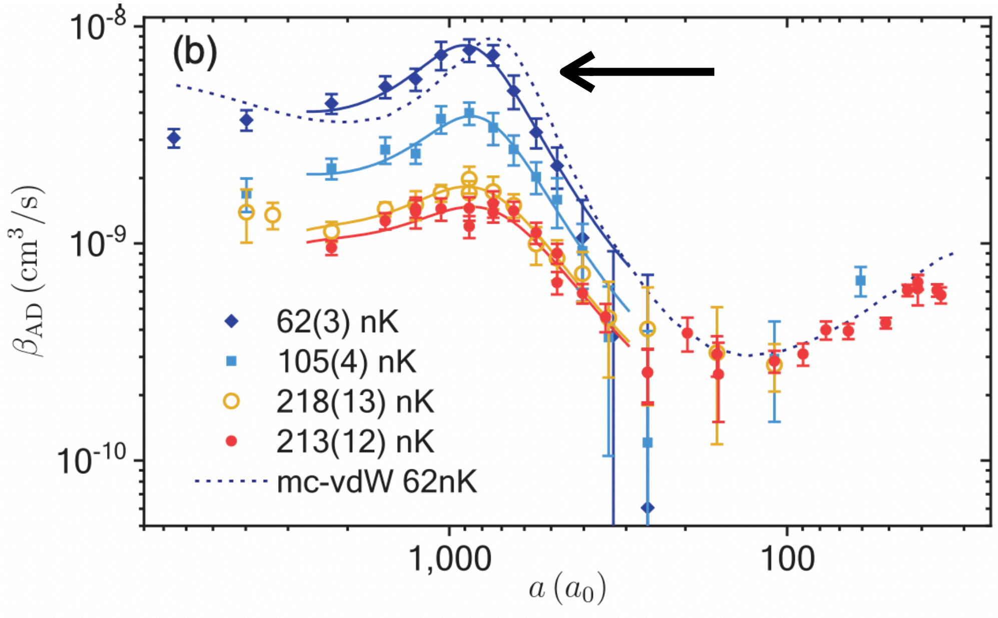
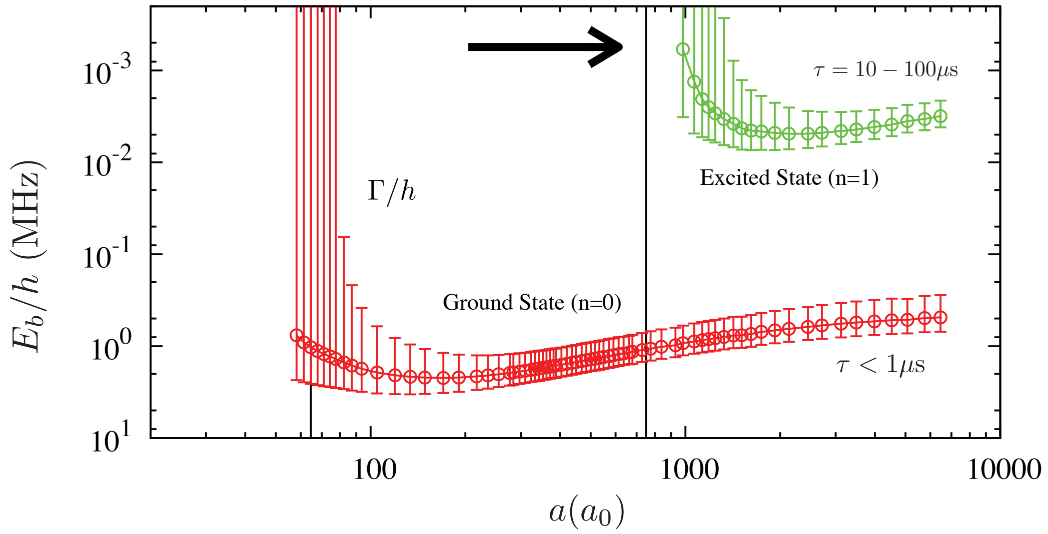
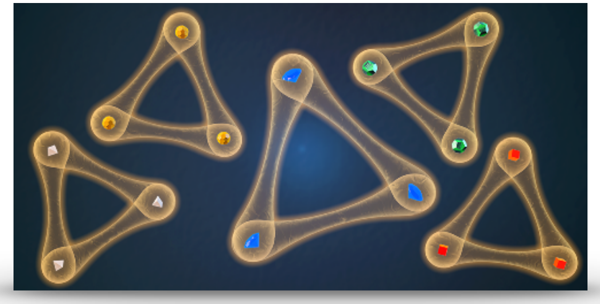


Trimer Binding Energy (Ed-Et)



Efimov Physics for 39K atoms at JILA

39K3 Efimov states are “anomalous”



Precision Test of the Limits to Universality in Few-Body Physics
Chapurin, Xie, Van de Graaff, Popowski, D’Incao, Julienne, Ye, and Cornell,
PRL 123, 233402 (2019)

Observation of Efimov Universality across a Nonuniversal Feshbach Resonance in 39K
Xie , Van de Graaff, Chapurin, Frye, Hutson, D’Incao, Julienne, Ye, Cornell,
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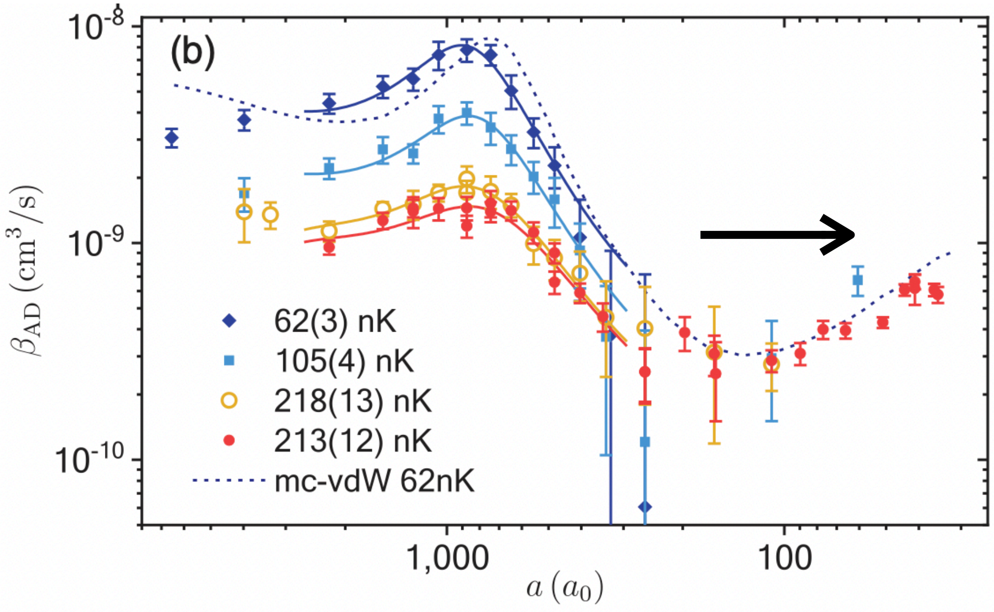
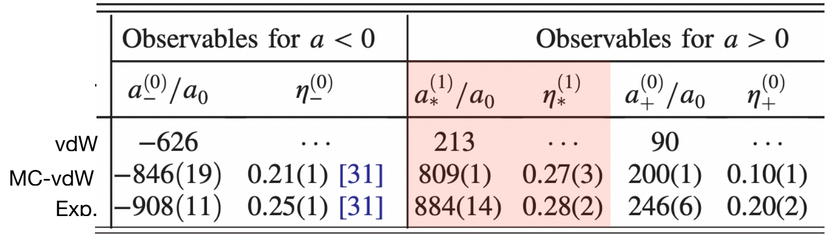
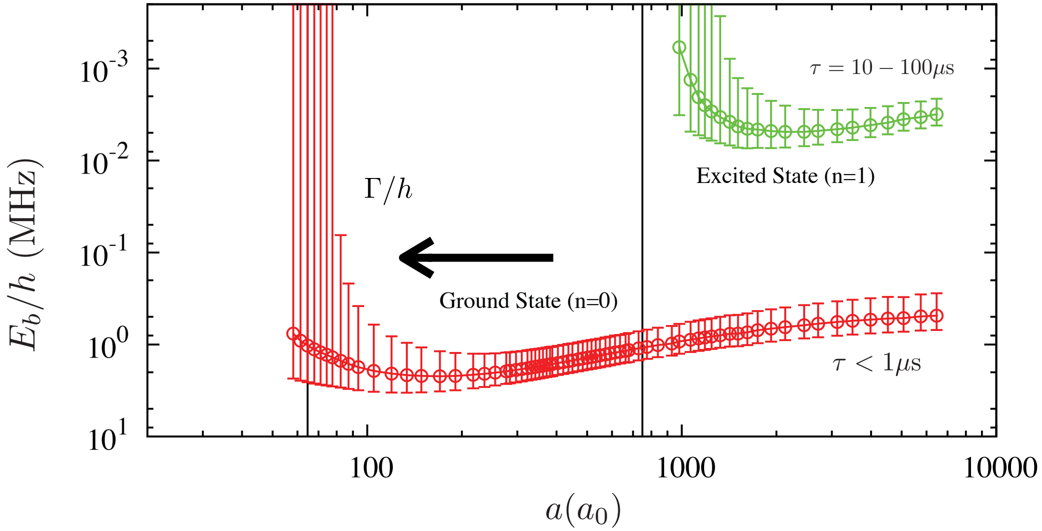
Atom-molecule Relaxation (a>0)





	Observables for $a<0$		Observables for $a>0$			
	$a_-^{(0)}/a_0$	$\eta_-^{(0)}$	$a_*^{(1)}/a_0$	$\eta_*^{(1)}$	$a_+^{(0)}/a_0$	$\eta_+^{(0)}$
vdW	−626	...	213	...	90	...
MC-vdW	−846(19)	0.21(1) [31]	809(1)	0.27(3)	200(1)	0.10(1)
Exp.	−908(11)	0.25(1) [31]	884(14)	0.28(2)	246(6)	0.20(2)

Trimer Binding Energy (Ed-Et)



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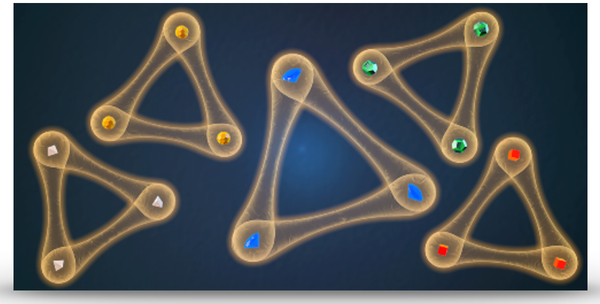

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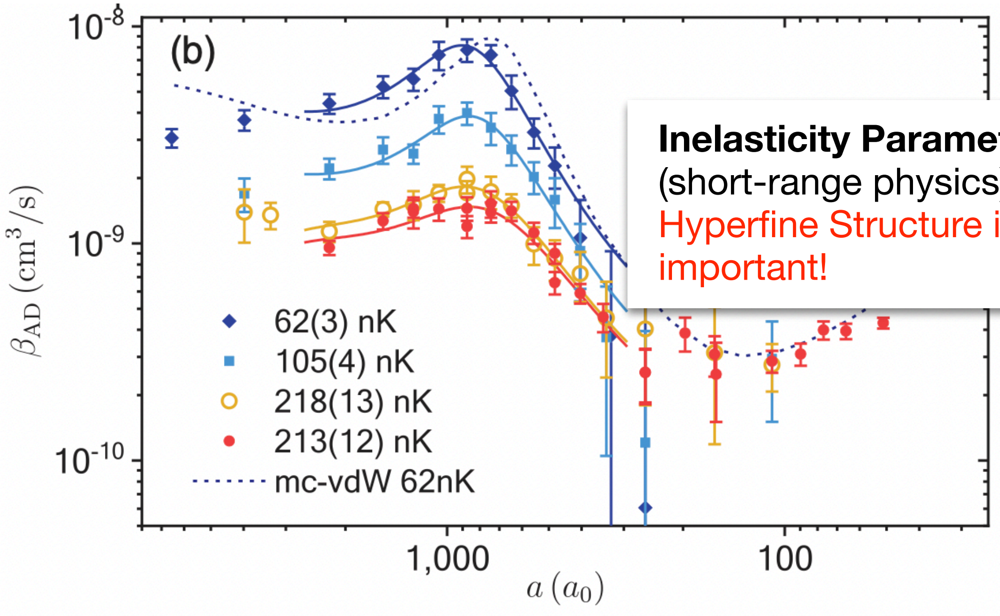
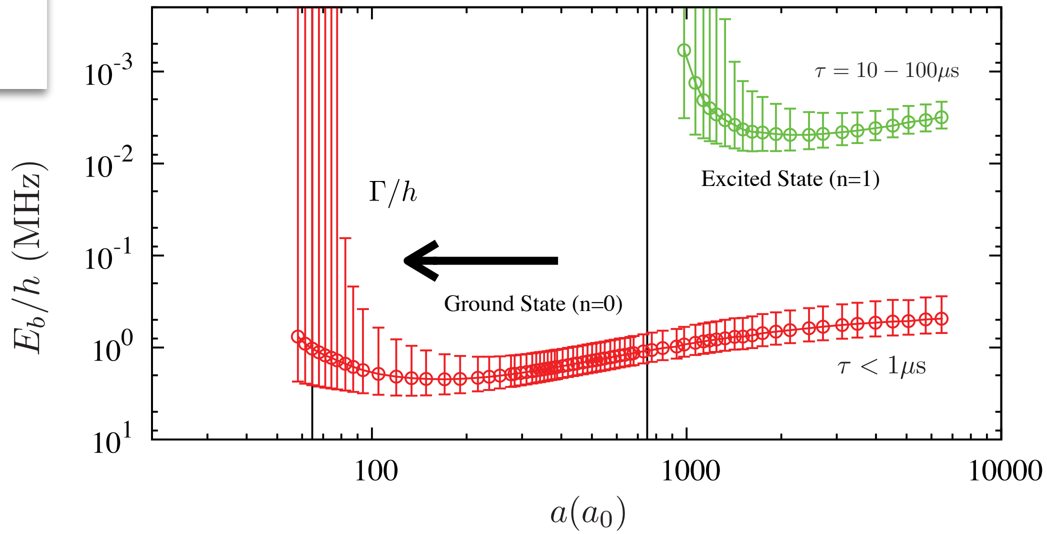
Future Experiments and Applications:
Important to know not only the location of features but also lifetimes and decay rates
…the search for better conditions has began!

Atom-molecule Relaxation (a>0)



Inelasticity Parameter
(short-range physics)
Hyperfine Structure is important!

Trimer Binding Energy (Ed-Et)



87Rb/85Rb Three-body Recombination

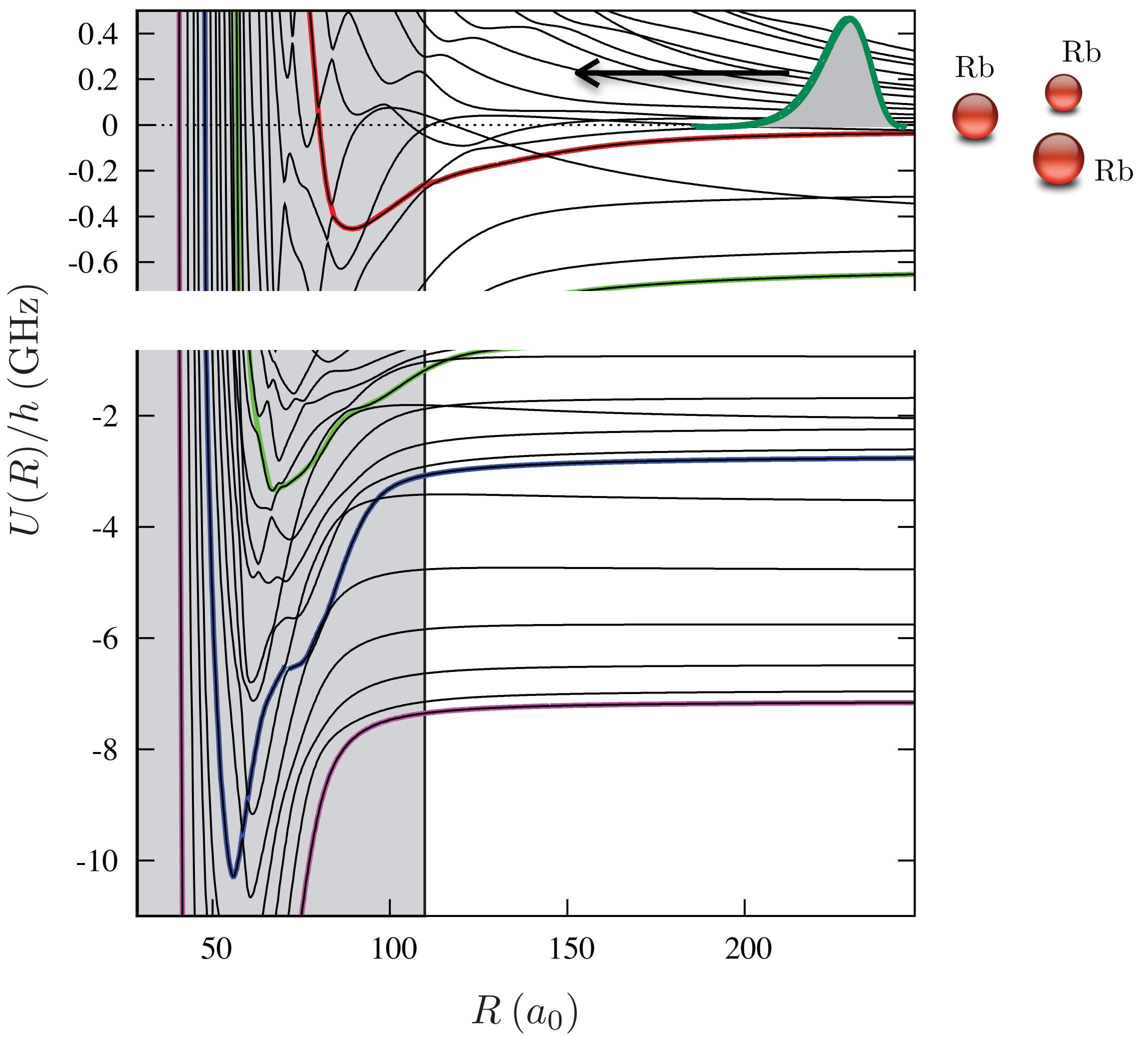
(initiated on KITP-2016)

Ultracold Chemical Reactions

Accessing Final Products

State-to-state chemistry for three-body recombination in an ultracold rubidium gas
Wolf, Deiß, Krükow, Tiemann, Ruzic, Wang, D'Incao, Julienne, and Denschlag
Science 358 921 (2017)

(Hyperspherical potentials for 87Rb3 atoms)



As usual, the experiment prepares a ultracold sample of ultracold Rubidium atoms in a specific hyperfine state

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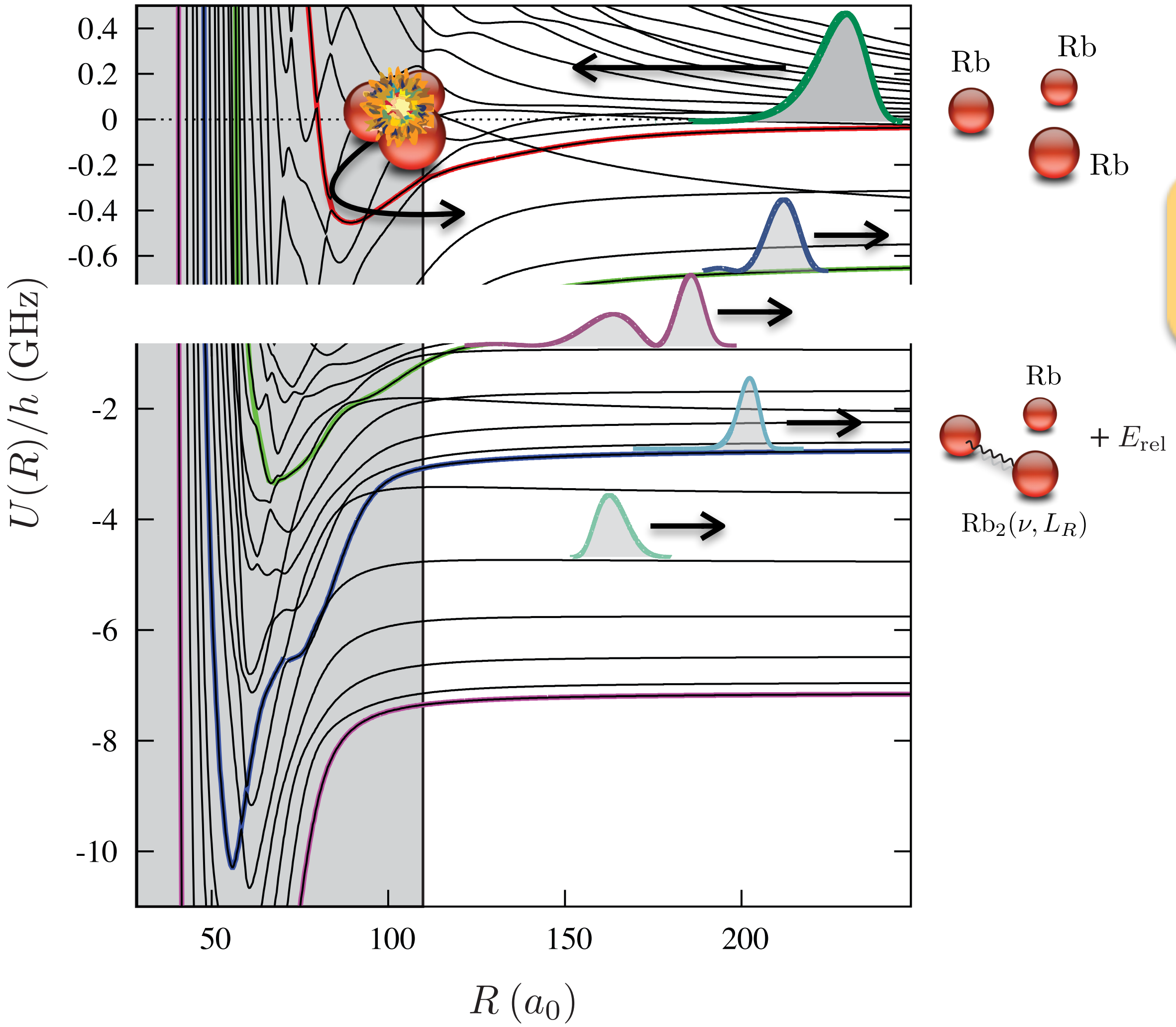

Atoms react to form diatomic molecules. At this point, usual experiments only observe atomic losses

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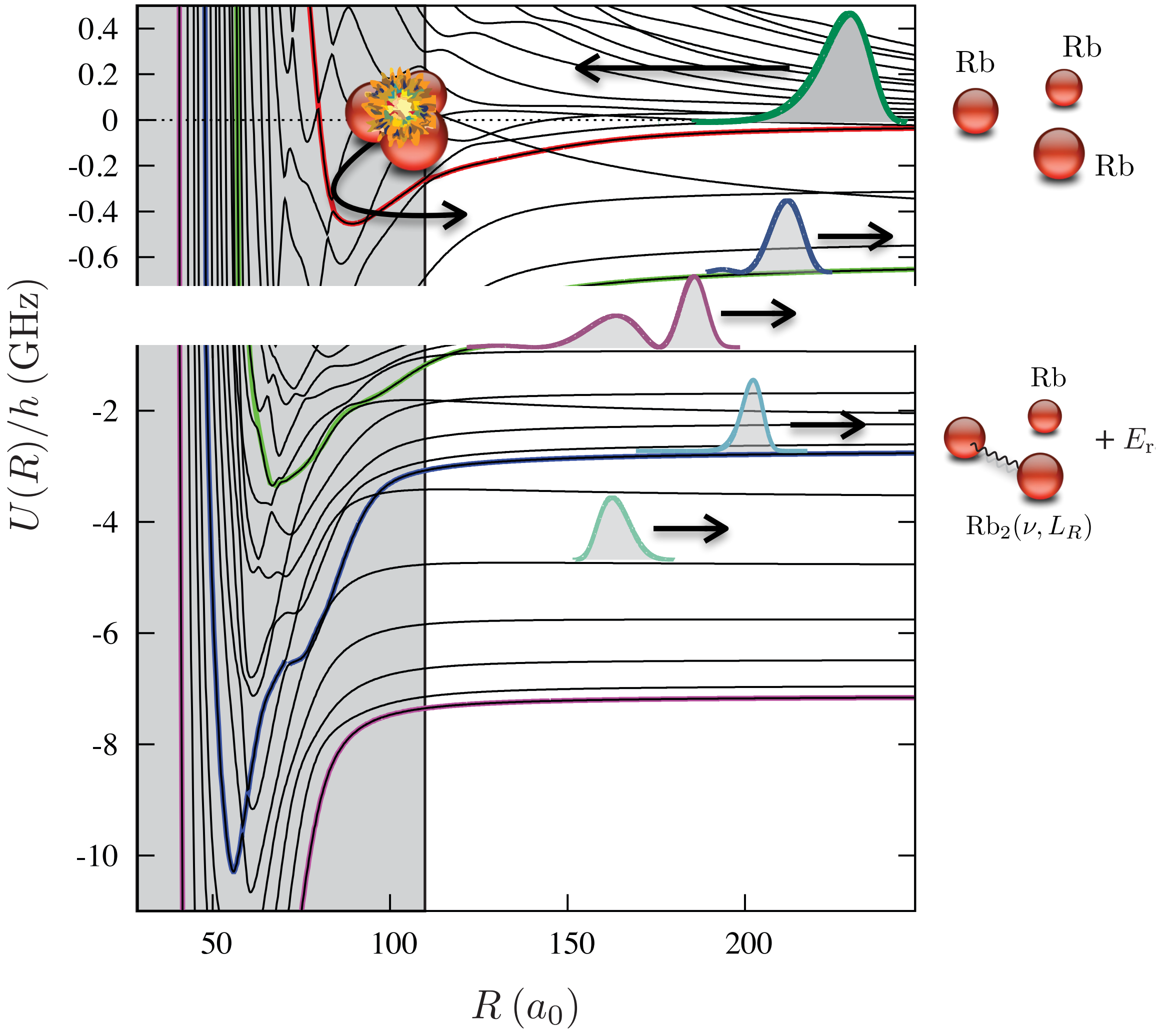

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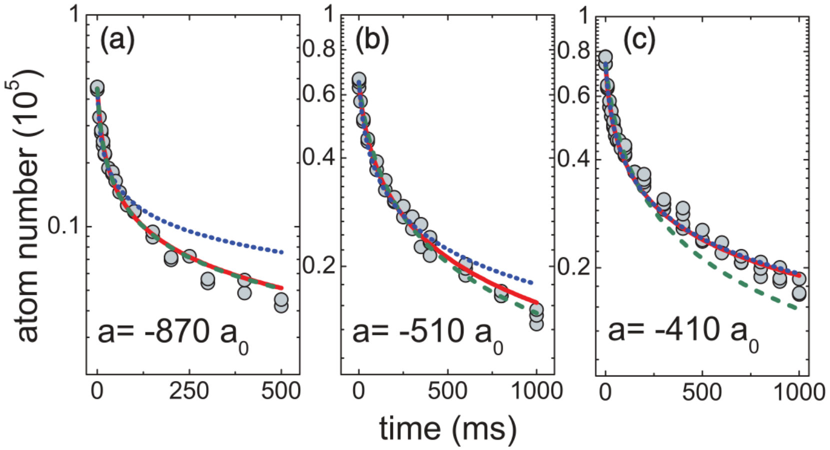
Atom Losses

Ferlaino, et.al PRL 2009



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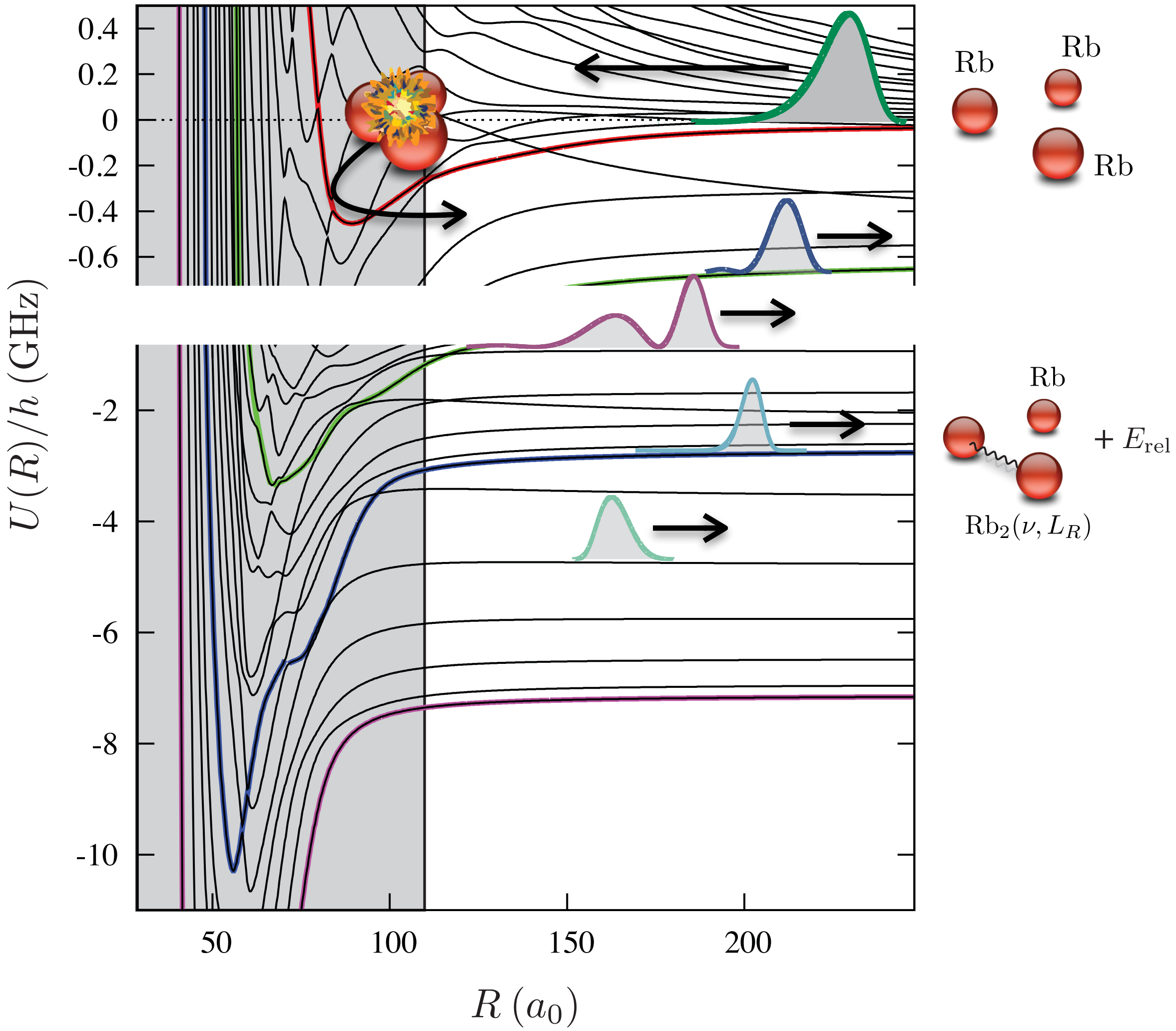
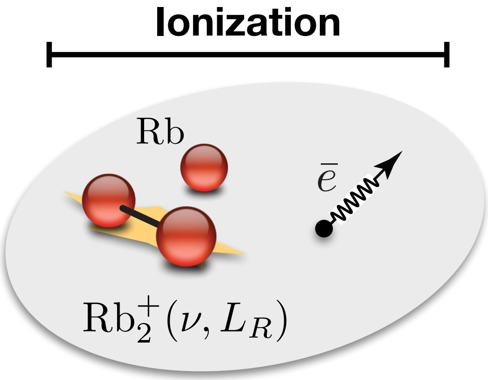


However, reactions occur in a presence of a laser field which selectively **ionize molecules**



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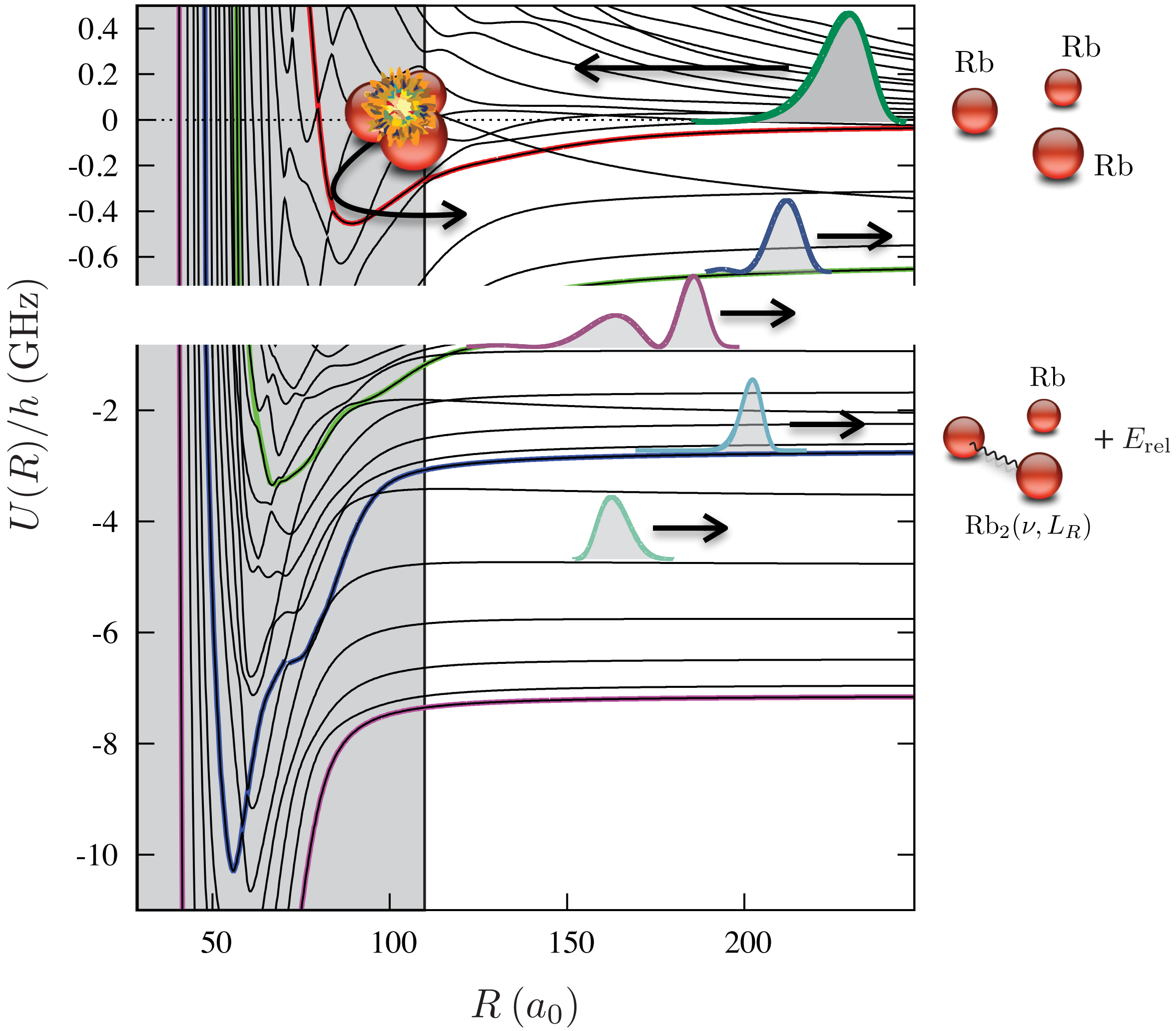
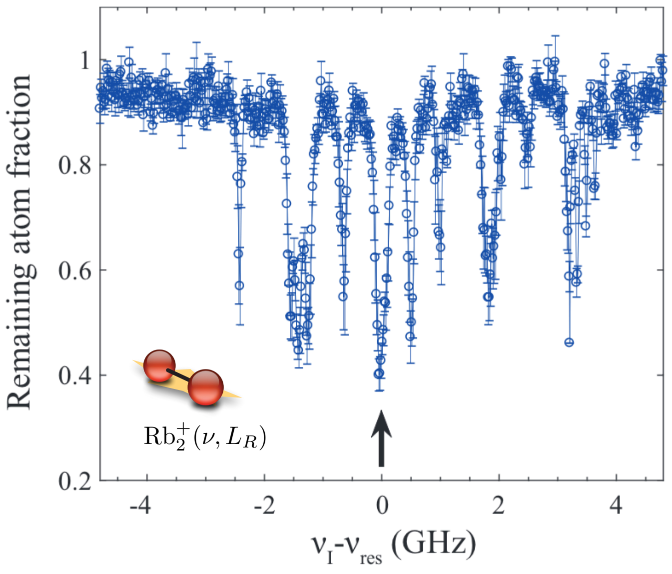


However, reactions occur in a presence of a laser field which selectively **ionize molecules**

(molecular ion signal)



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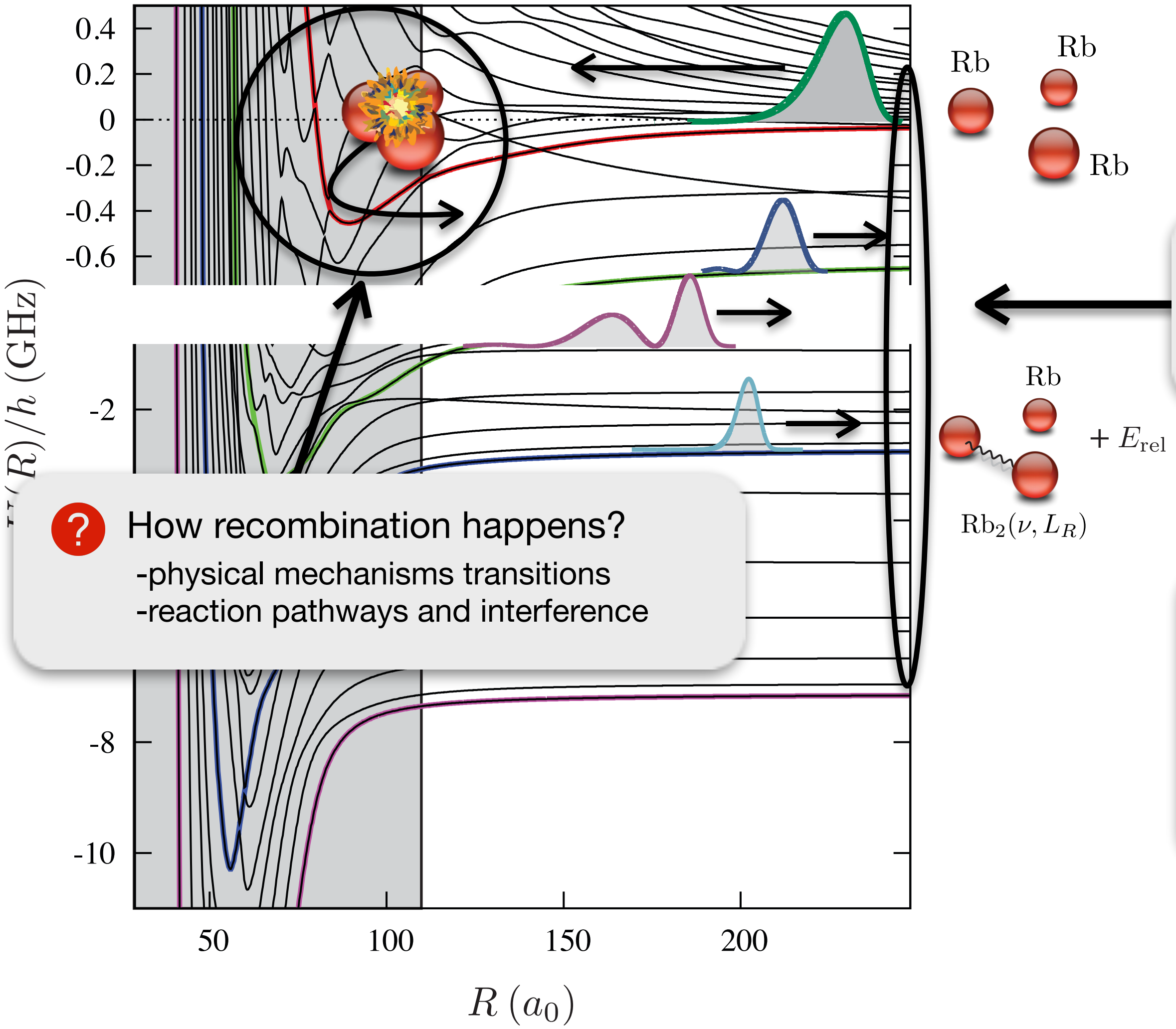


? How recombination happens?
- physical mechanisms transitions
- reaction pathways and interference

? Product state distribution?
- vibrational and rotational structure
- spin dependence

? Universality and propensity rules?

vs

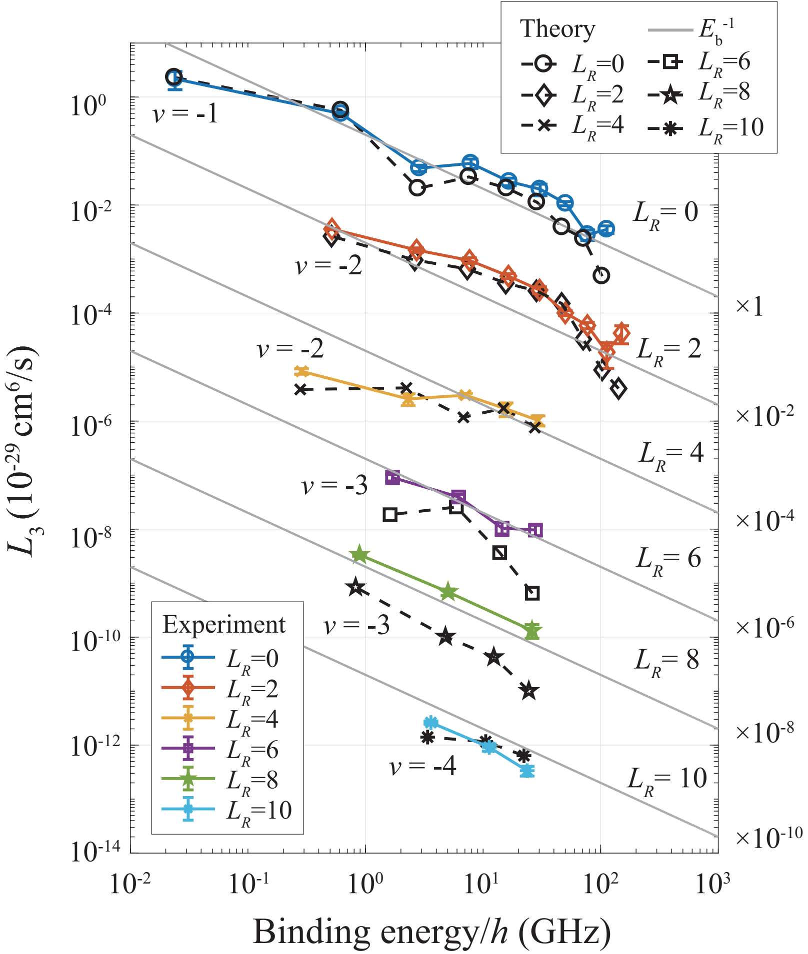
Final State Distribution of Three-body Recombination

Energy-scaling Propensity Rule

Energy-scaling of the product state distribution for three-body recombination of ultracold atoms
Haze, D’Incao, Dorer, Li, Deiß, Tiemann, Julienne, and Denschlag
in preparation (2022)

Propensity rule: 1/Eb state distribution of molecular states…
(previously unknown)

87Rb Recombination



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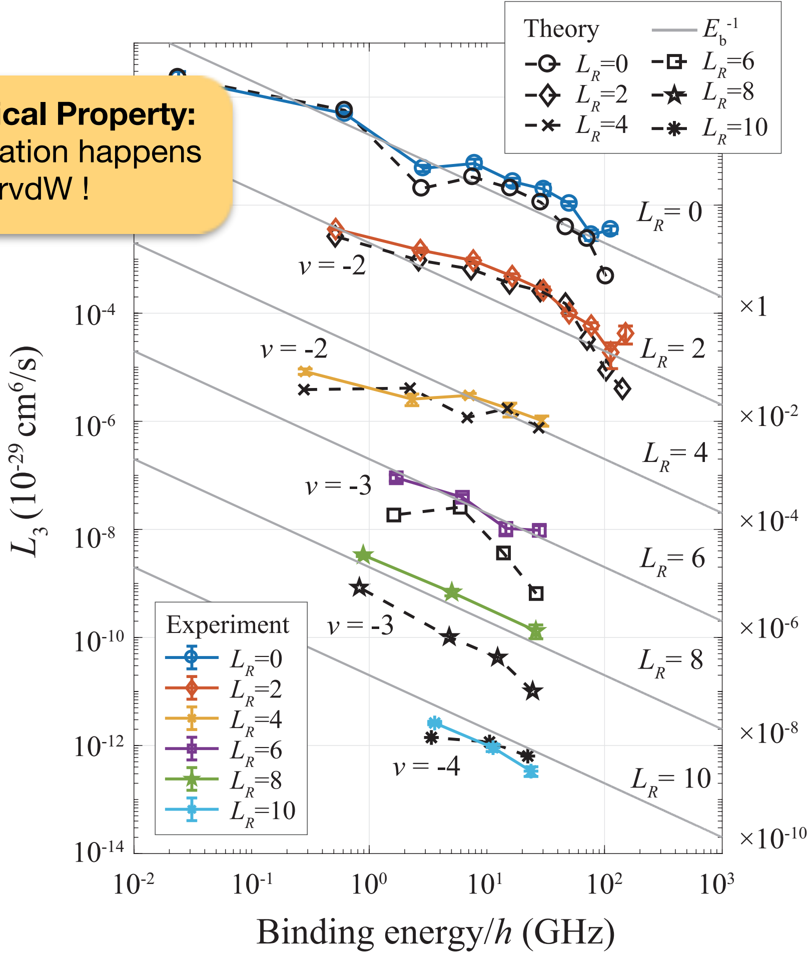
D'Incao & Julienne, in prep.
(propensity rules and reaction pathways)

$$L_3^{(f)} \propto \underbrace{\frac{1}{E_b^{(f)}}}_{\text{Long-range physics}} \underbrace{\sum_{jk} \sin^2[\Delta\phi_{jk}^{(f)}/2]}_{\text{Short-range physics (interference)}}$$

87Rb Recombination



Key Physical Property:
Recombination happens when R~2rvdW !

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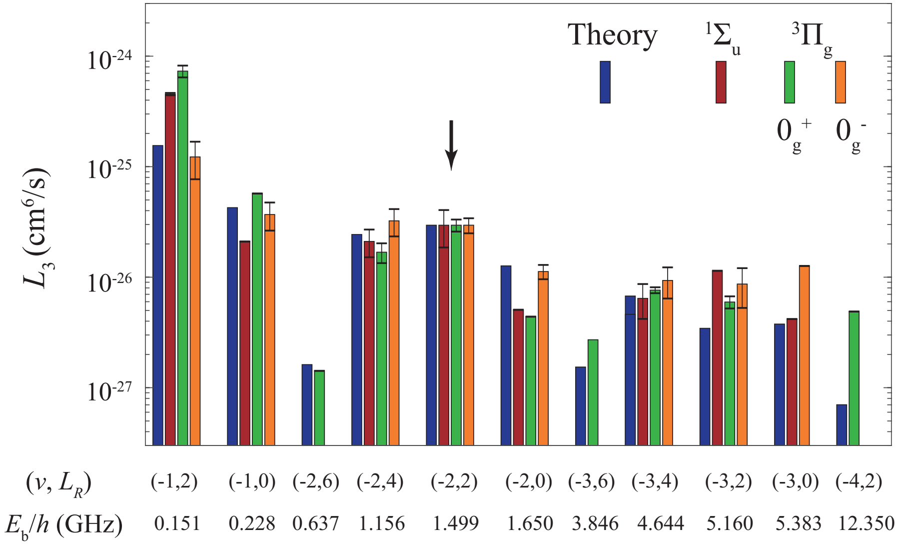
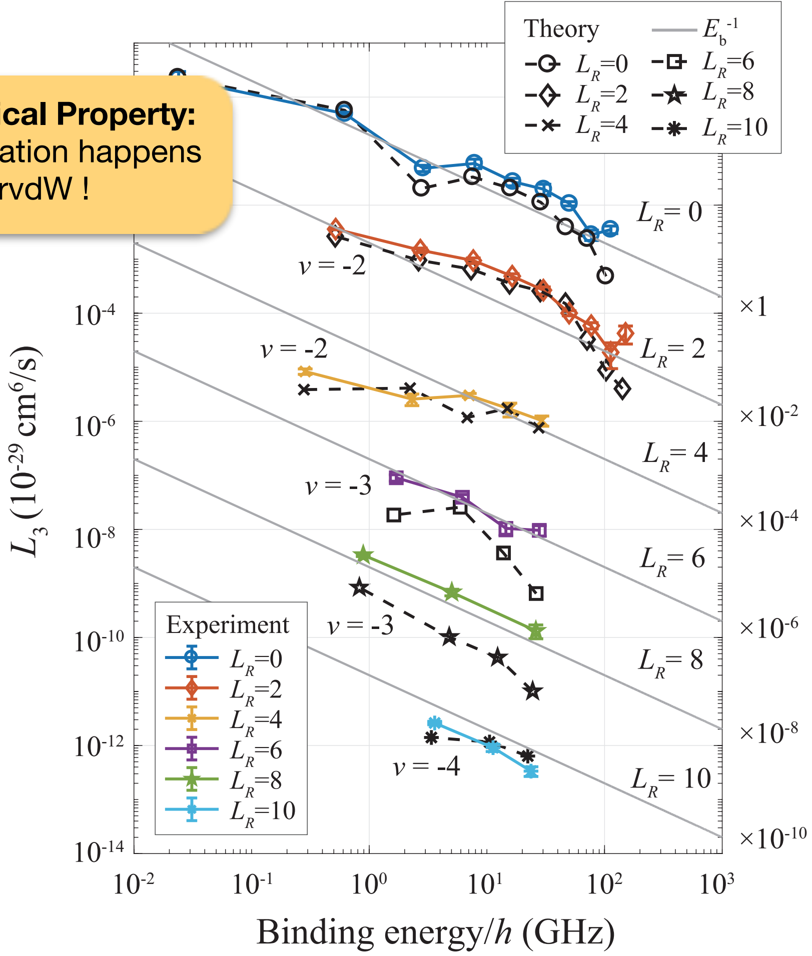
85Rb Recombination



Haze, et al.,
PRL **128** 133401
(2022)

87Rb Recombination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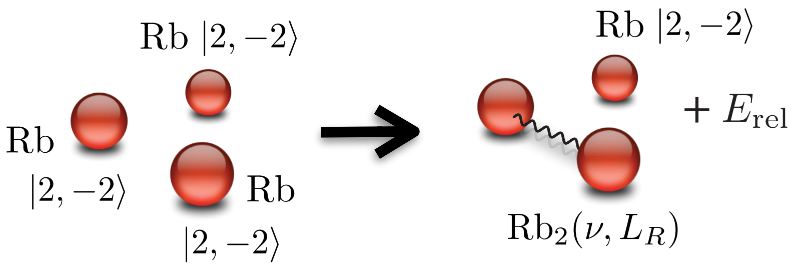

$$
\begin{aligned}
|F_{2b}(f_1 f_2)\rangle &= |422\rangle \\
&= |2,-2\rangle|2,-2\rangle
\end{aligned}
$$

Only molecules whose spins are same than those of the atoms

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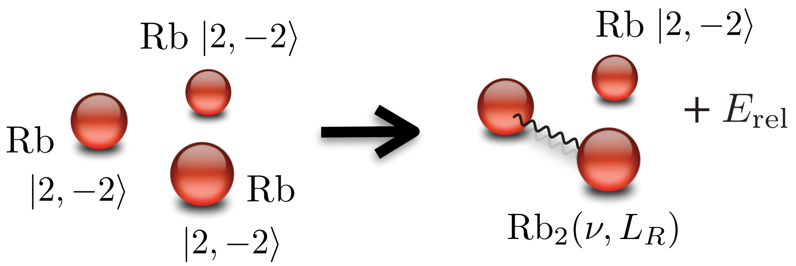

$$|F_{2b}(f_1 f_2)\rangle = |422\rangle$$
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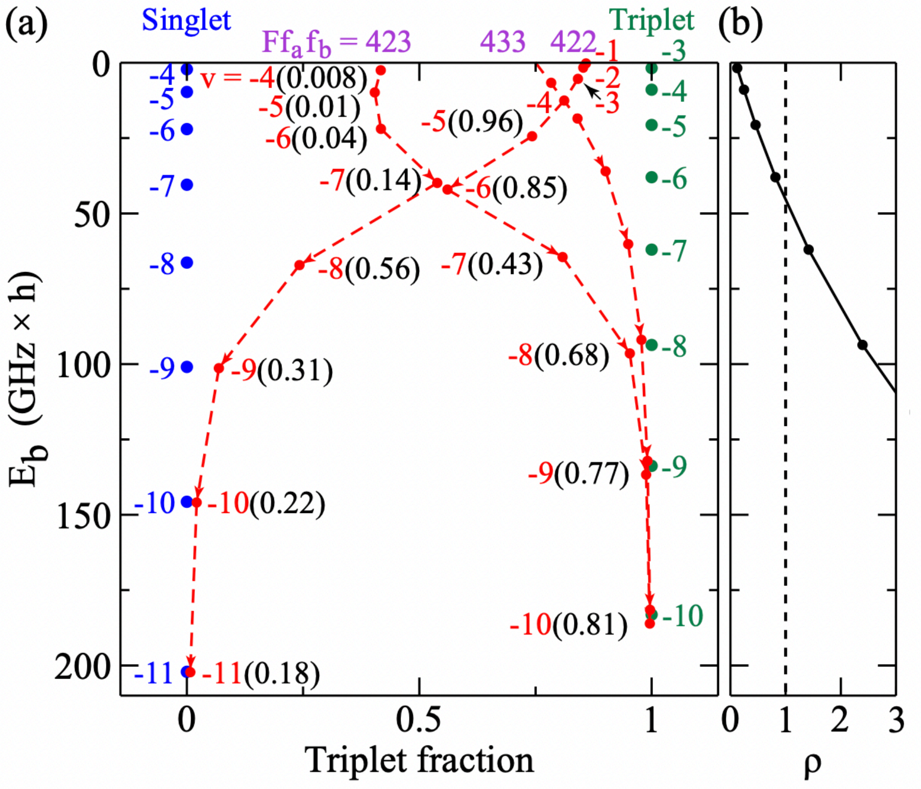
85Rb Molecular Spectrum



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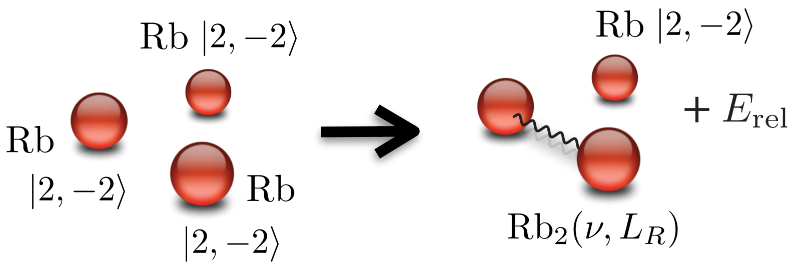

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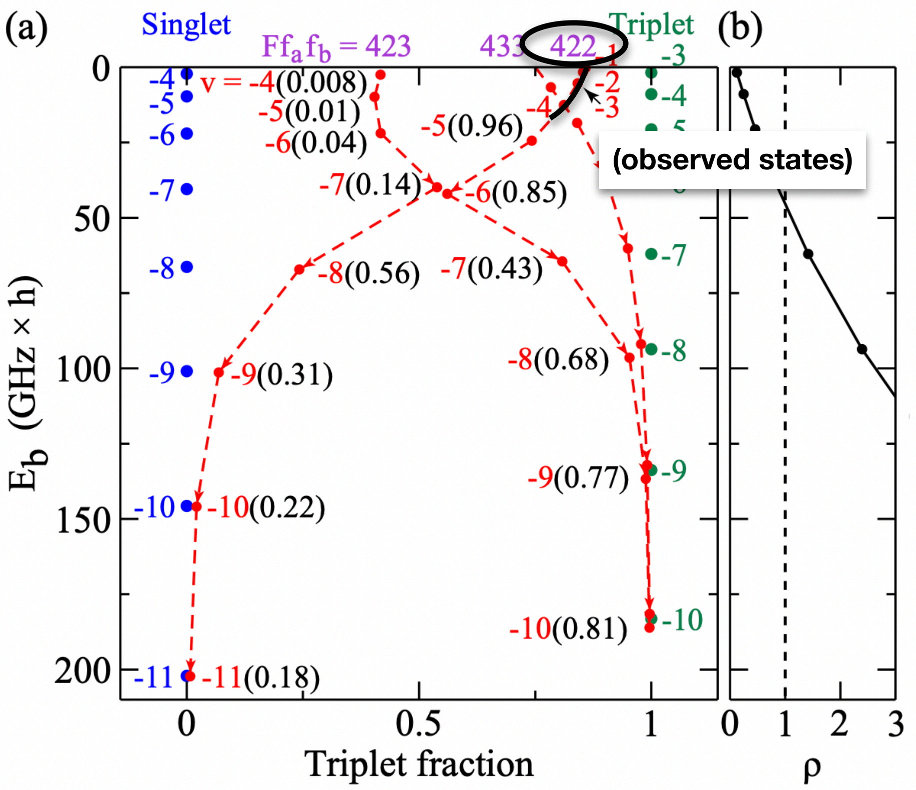

(observed states)

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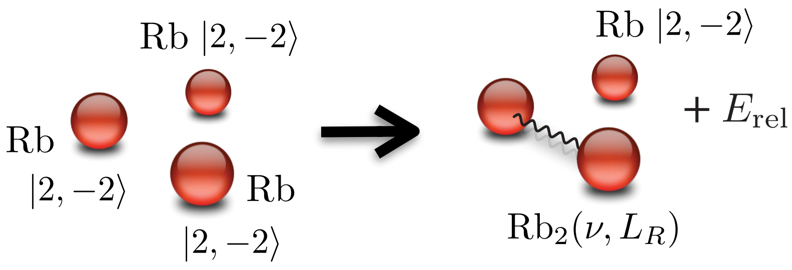

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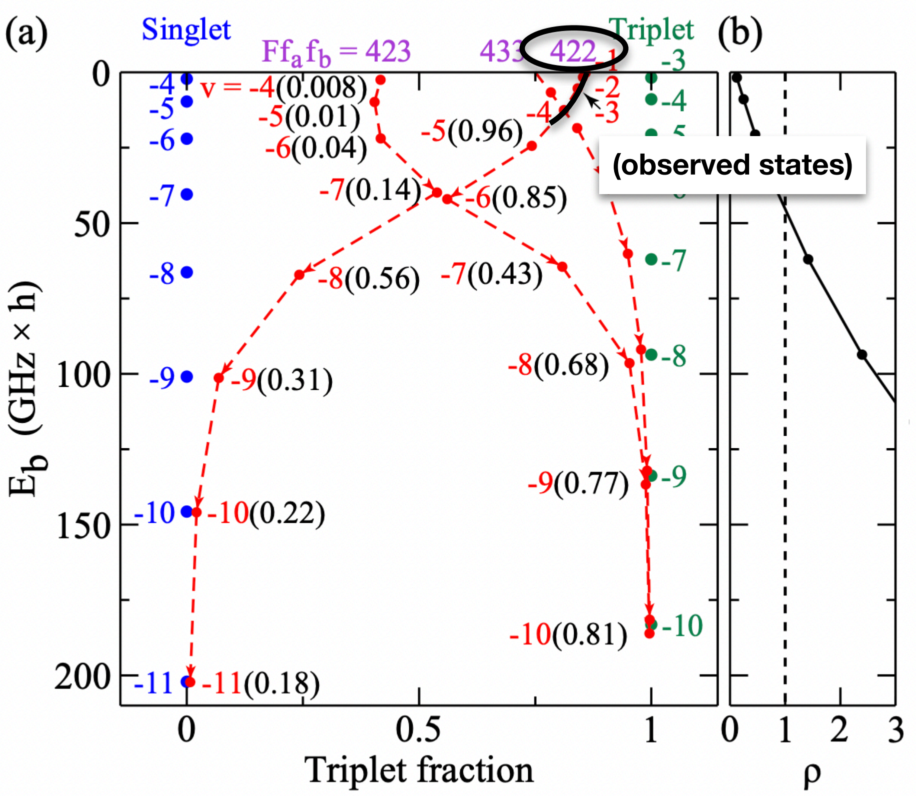

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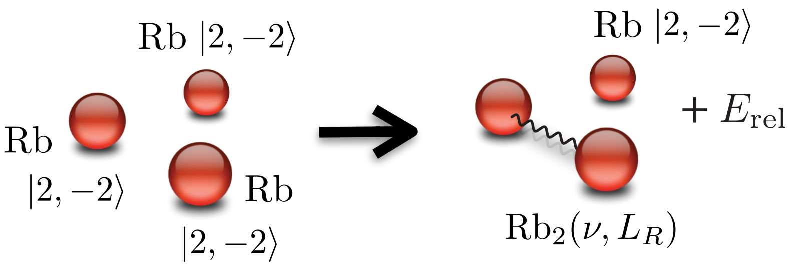

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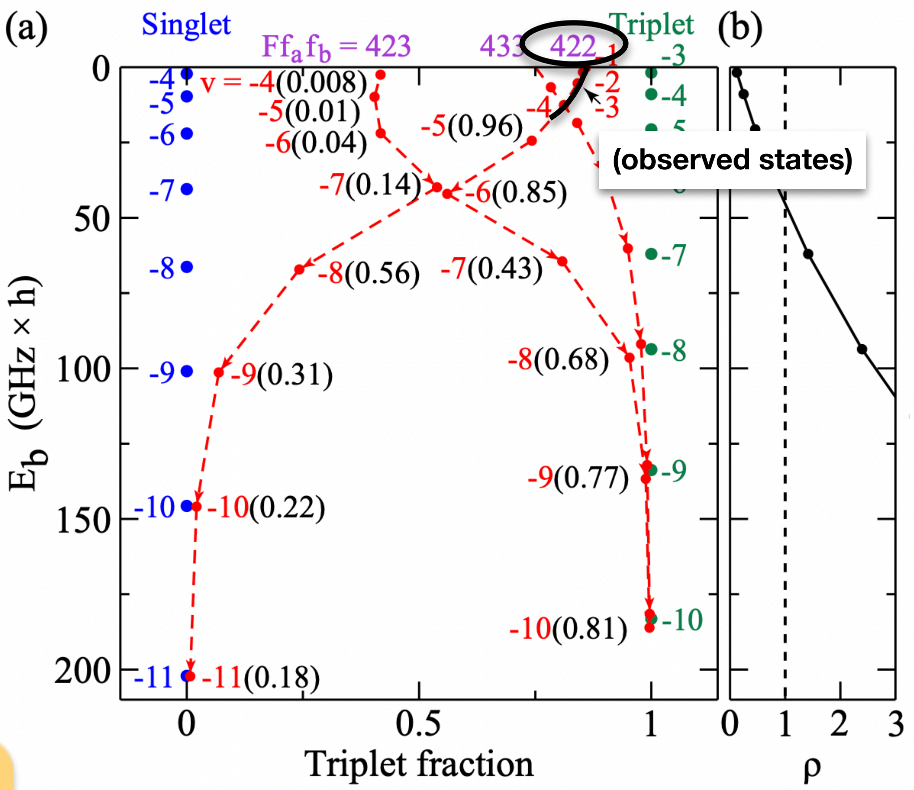
Only molecules whose spins are same than those of the atoms

Key Physical Property: Recombination happens when R~2rvdW !

Single channel models are good for 85Rb and 87Rb whenever spin-conservation rule holds!

85Rb Molecular Spectrum



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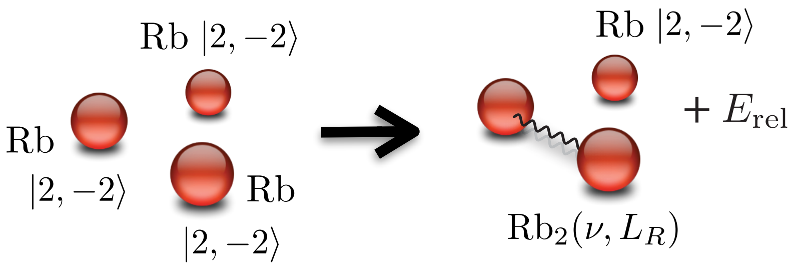
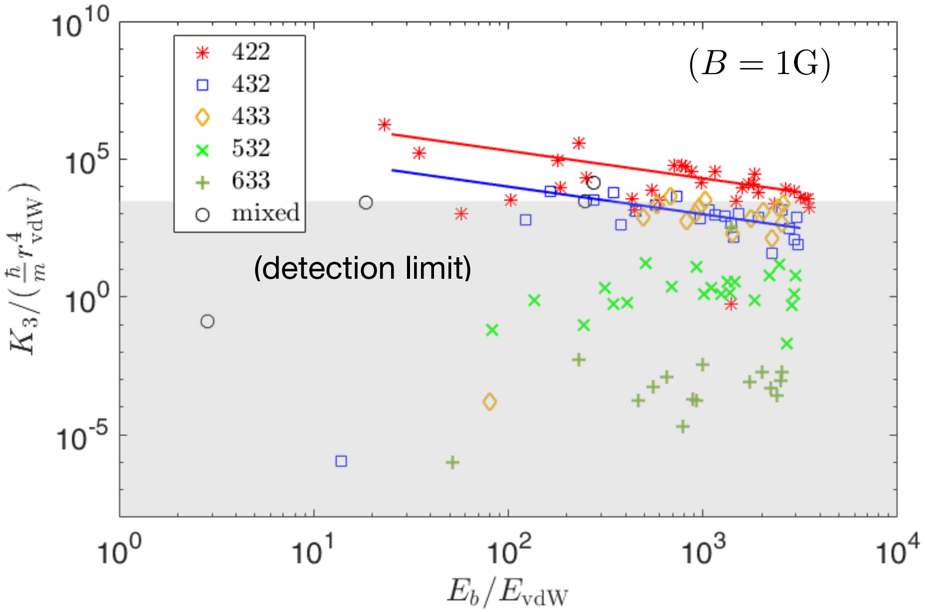
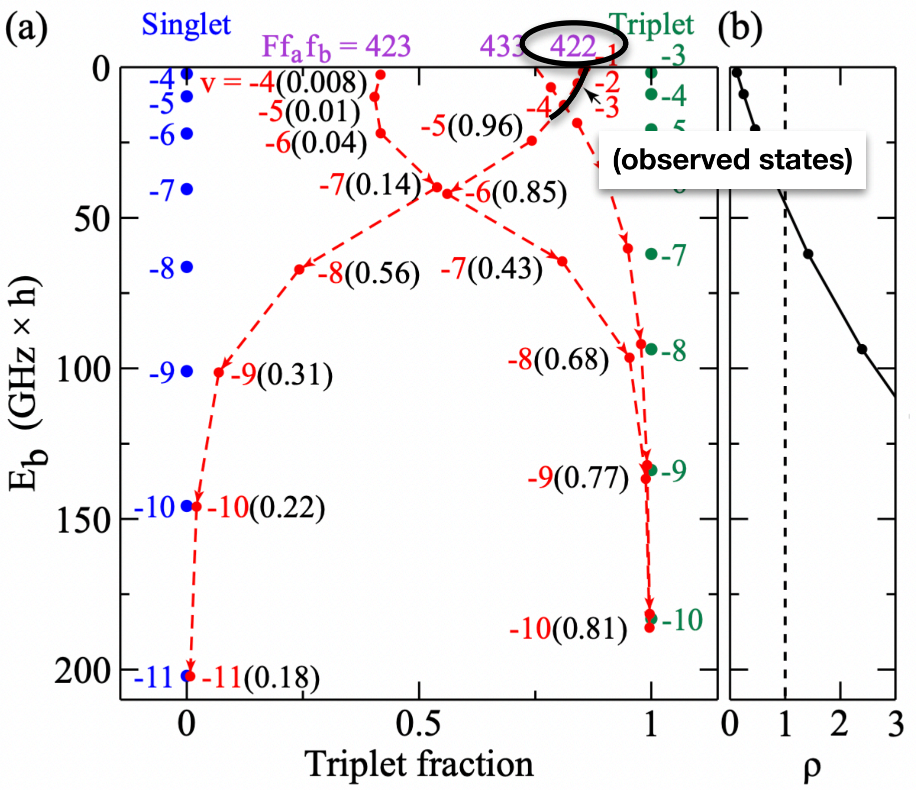


85Rb Recombination (Theo)



(detection limit)

85Rb Molecular Spectrum



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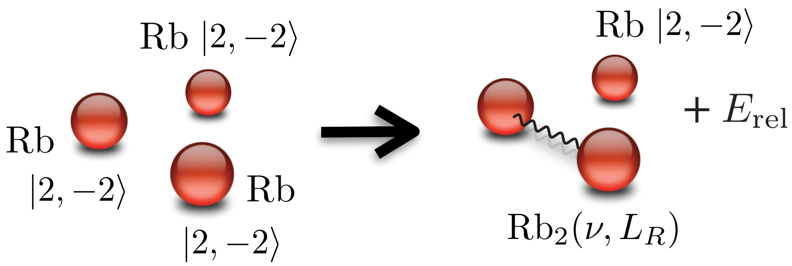

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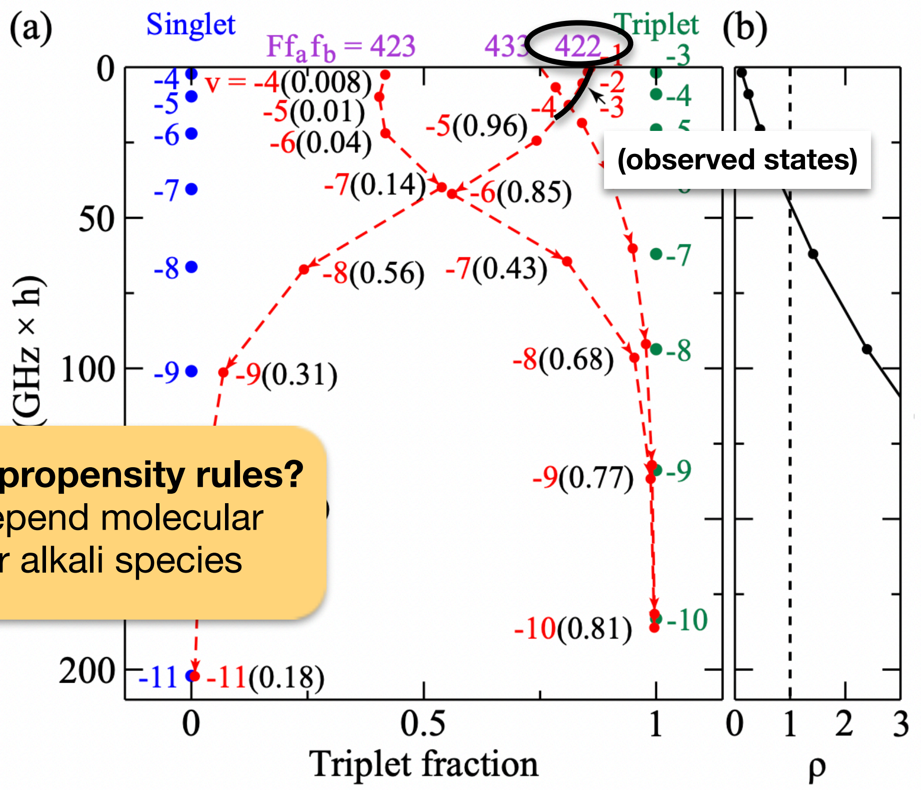

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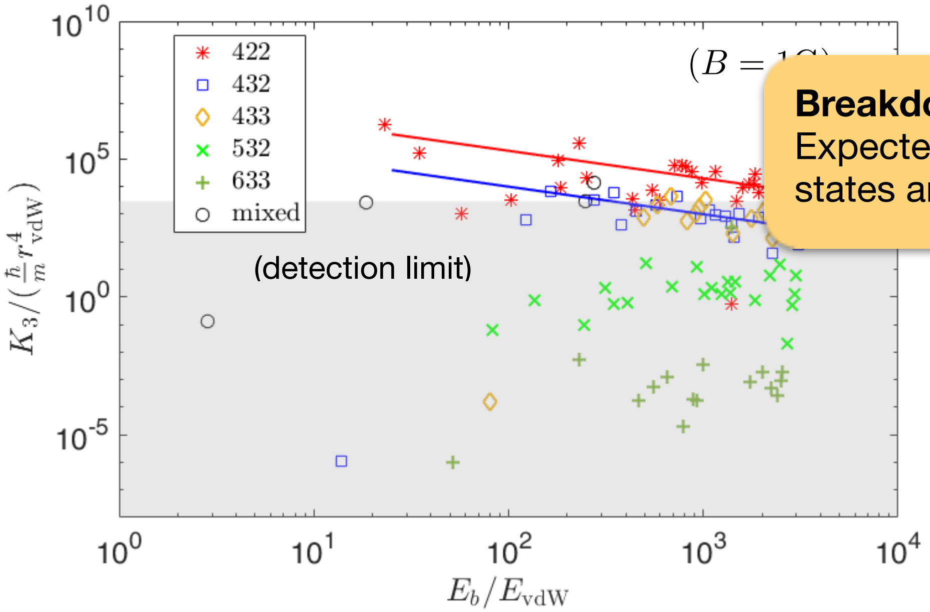

Breakdown of propensity rules?
Expected for depend molecular states and other alkali species

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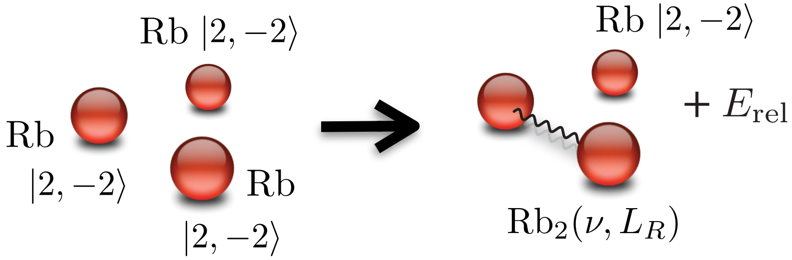

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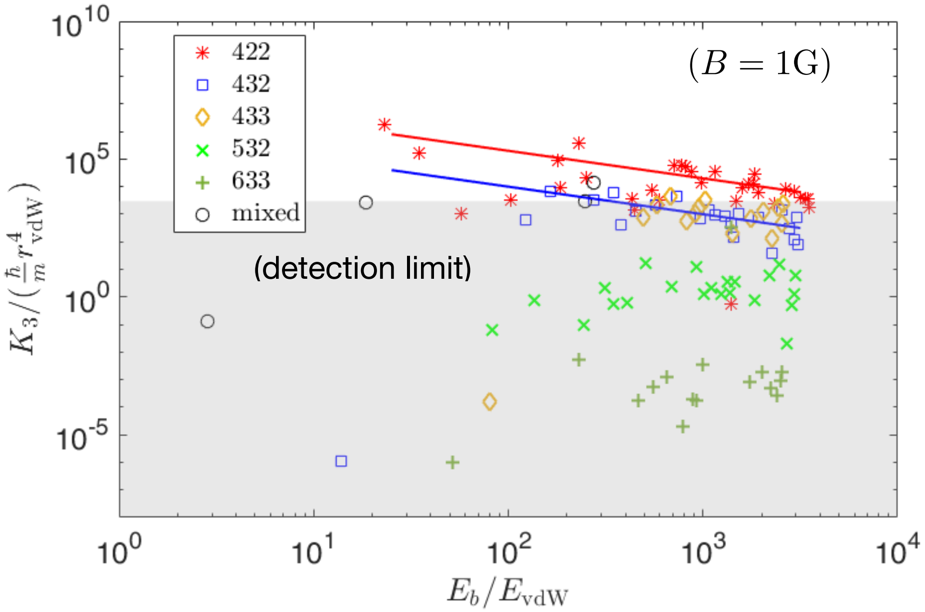

Efimov states in 85Rb

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Klauss, Xie, Lopez-Abadia, D'Incao, Hadzibabic, Jin, Cornell
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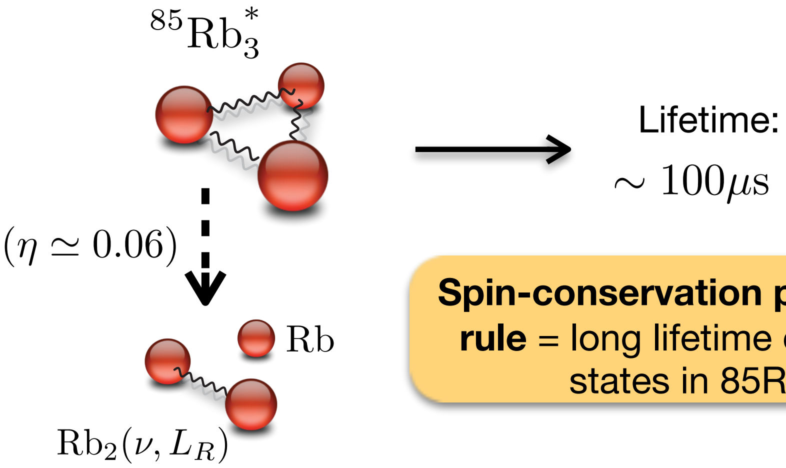

Spin-conservation propensity rule = long lifetime of Efimov states in 85Rb?

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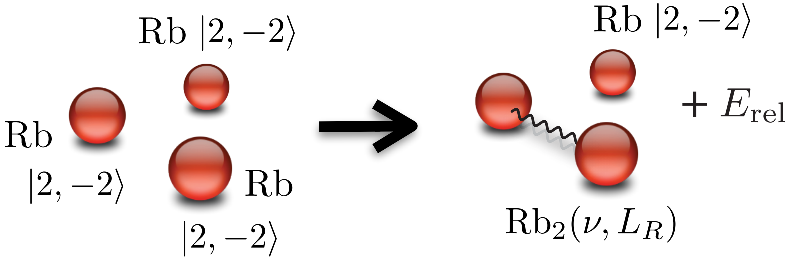

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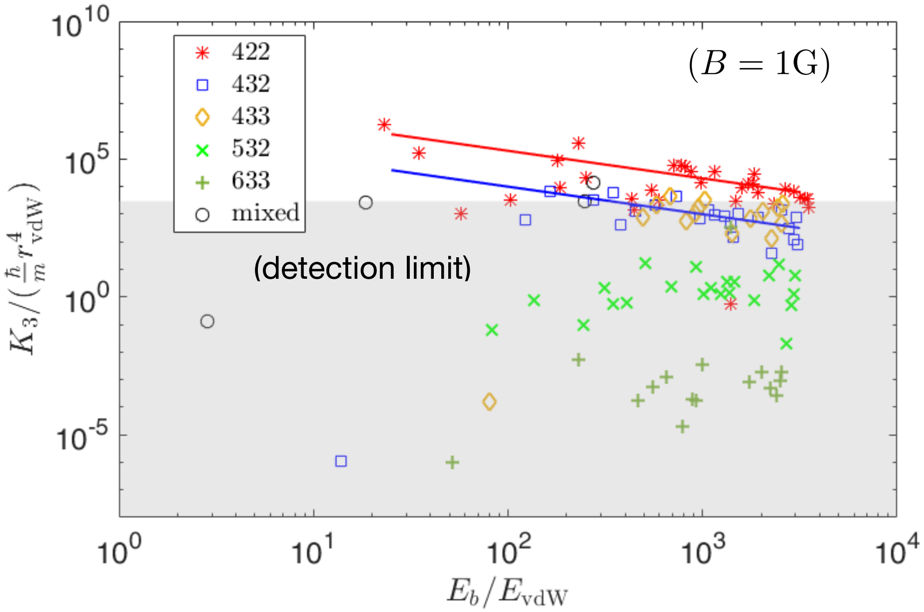

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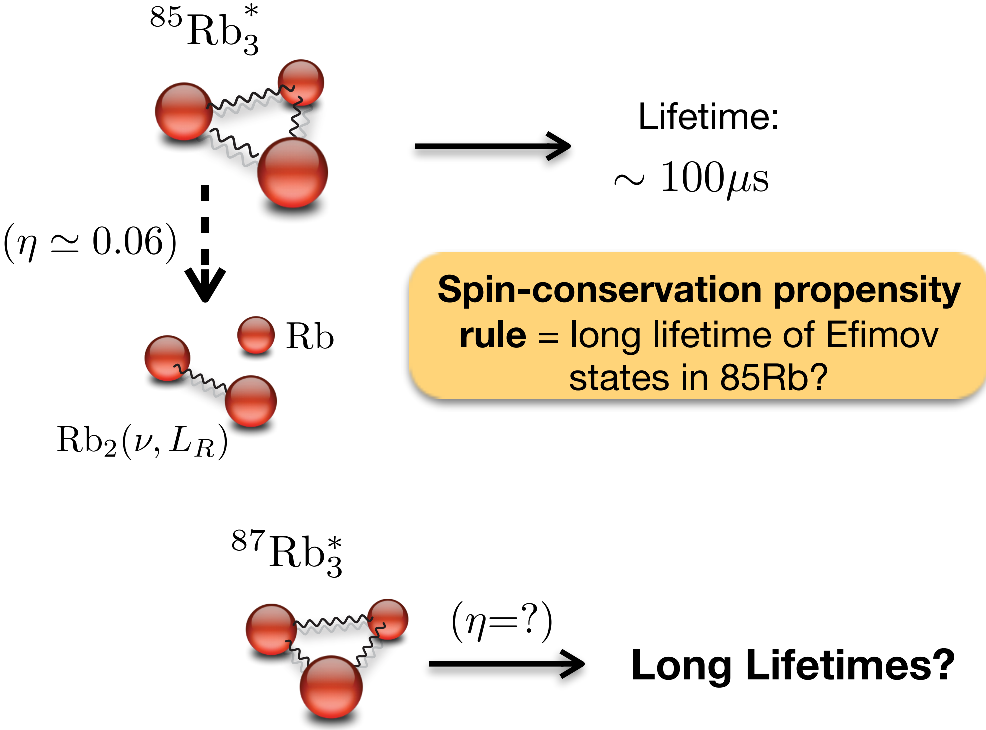

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Long Lifetimes?

Final State Distribution of Three-body Recombination

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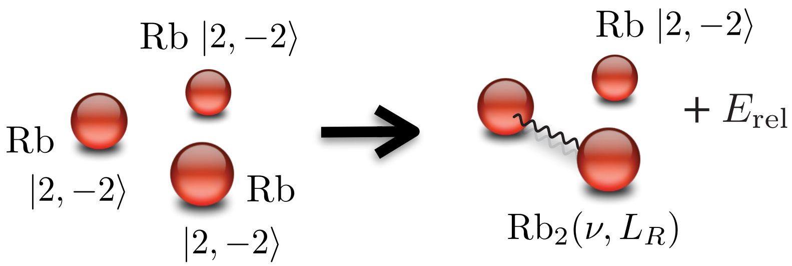

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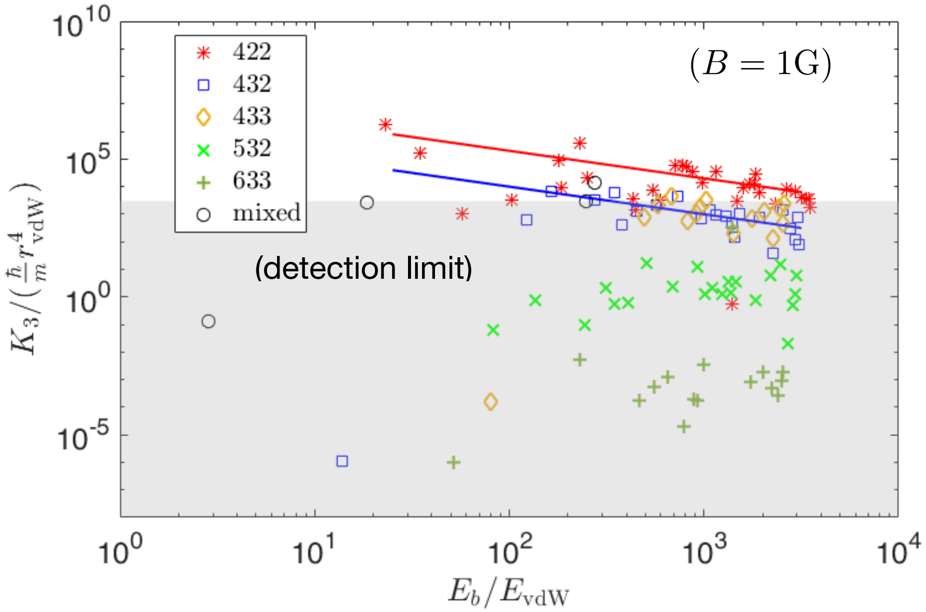
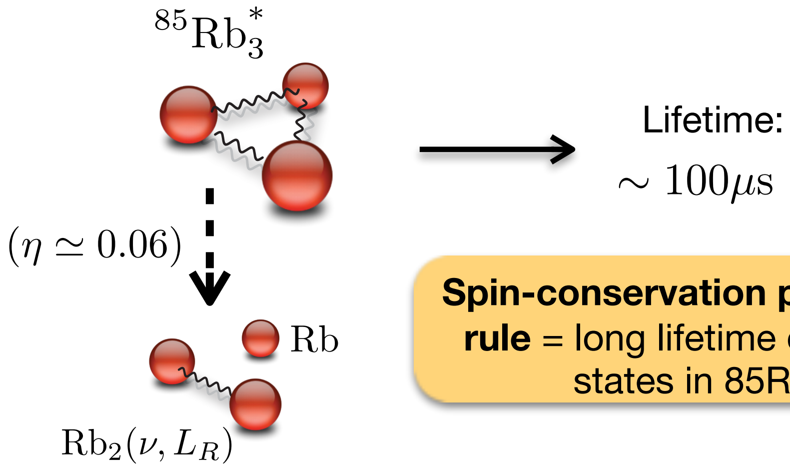


Efimov states in 85Rb

Observation of Efimov Molecules Created from a Resonantly Interacting Bose Gas
Klauss, Xie, Lopez-Abadia, D’Incao, Hadzibabic, Jin, Cornell
PRL 119, 143401 (2017)



Spin-conservation propensity rule = long lifetime of Efimov states in 85Rb?

One (or more) step(s) closer to:

- coherent control of chemical processes
- suppression of reactions (stability of condensates)
- chemically reactive quantum phases
- **...details matter!**

Few-body Physics for 7Li Atoms

(…where short- and long-range meet!?)

Efimov Physics For 7Li Atoms

van der Waals Universality

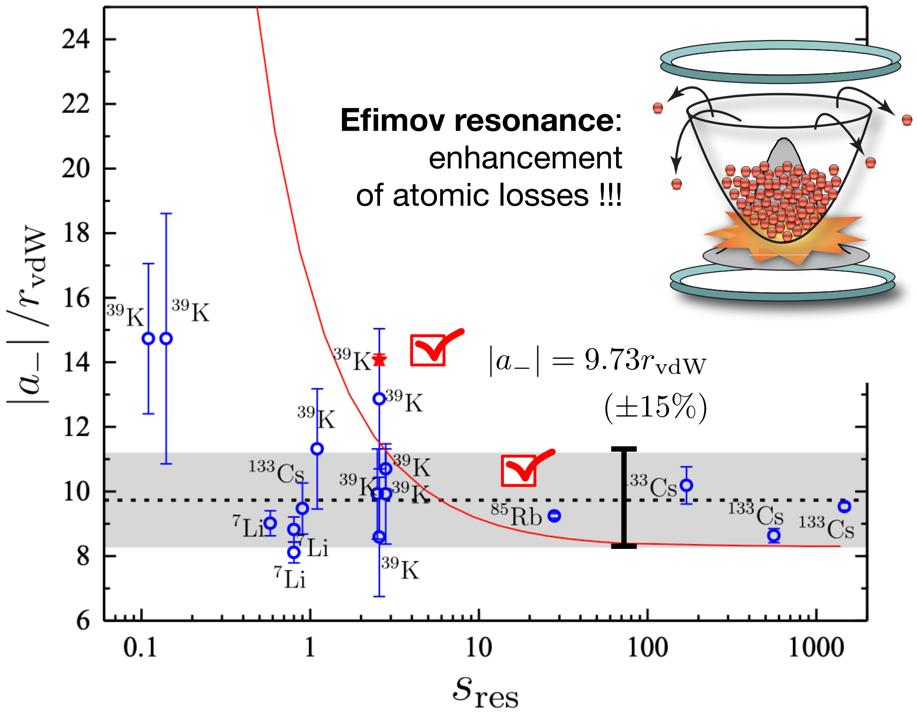
Refers to the Efimov physics obtained using (single channel) vdW interactions, -C6/r^6, leading to a three-body parameter depending only on rvdW.

Ultracold Gases Experiments

$\boxed{s_{\mathrm{res}}}$ **Resonance Strength**

$s_{\mathrm{res}} \gg 1$: strong (broad)

$s_{\mathrm{res}} \ll 1$: weak (narrow)



Efimov resonance:
enhancement
of atomic losses !!!

$|a_-| = 9.73 r_{\mathrm{vdW}}$
$(\pm 15\%)$

Efimov Physics For 7Li Atoms

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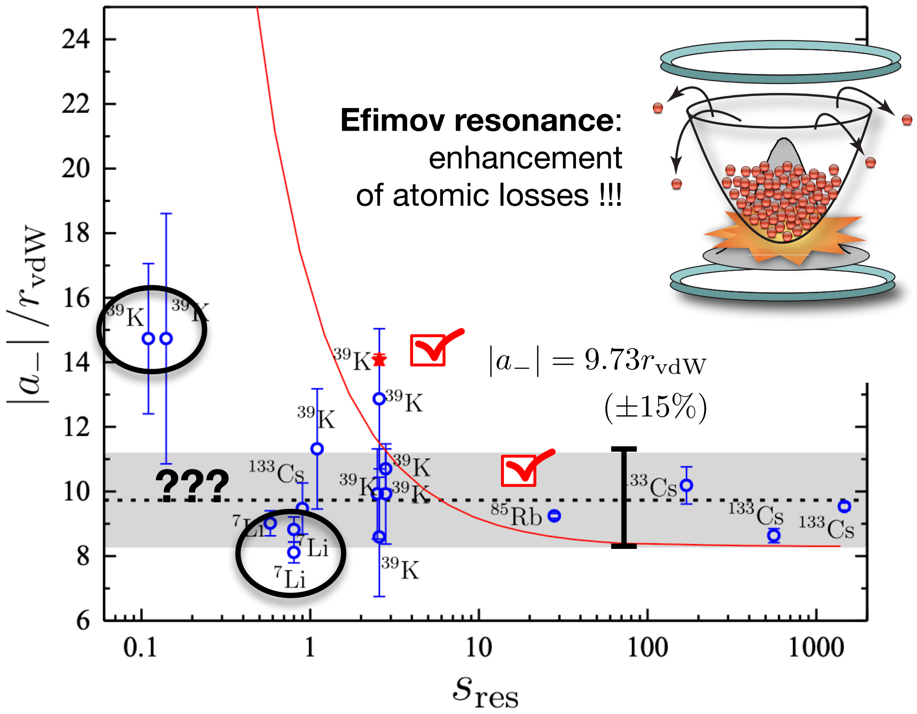
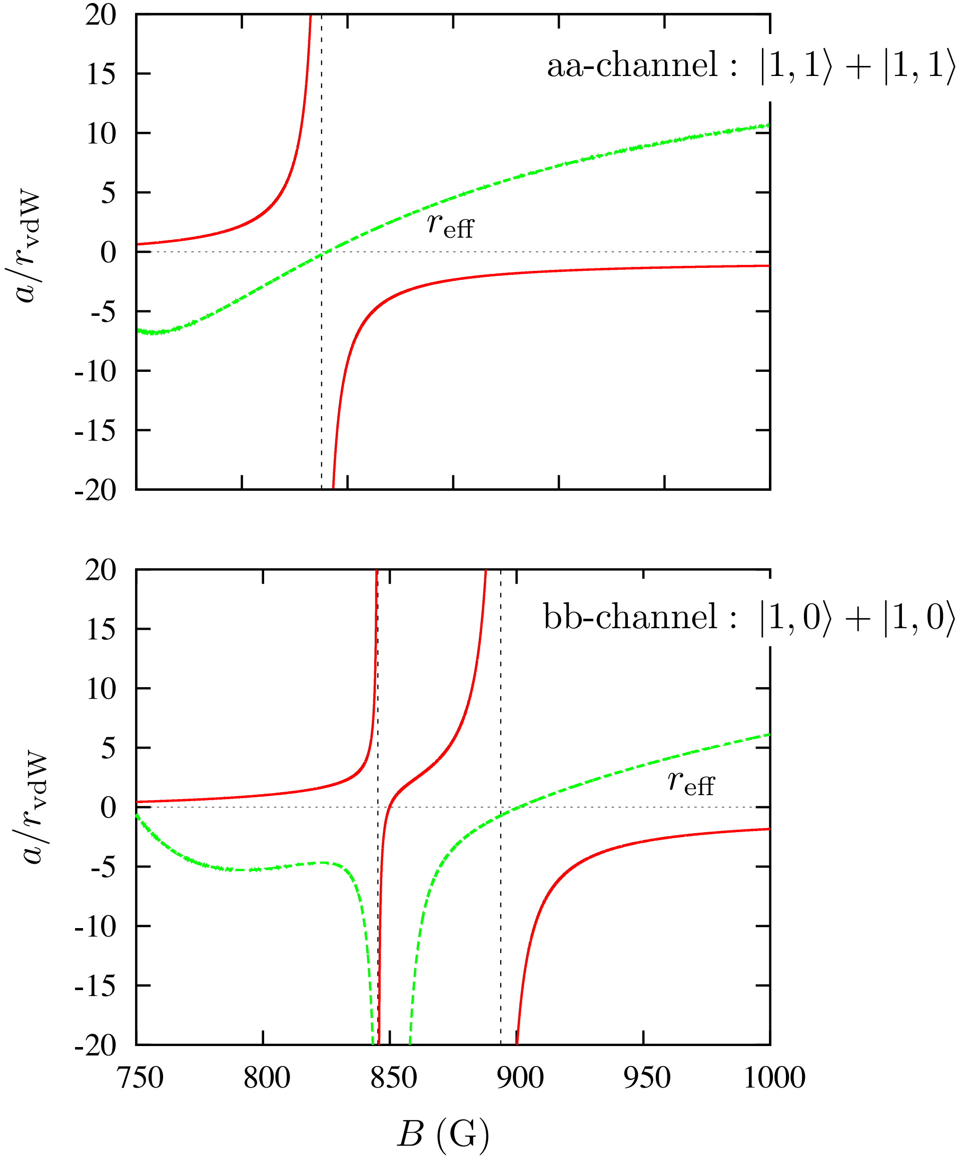


Narrow Resonances Alters Efimov Physics

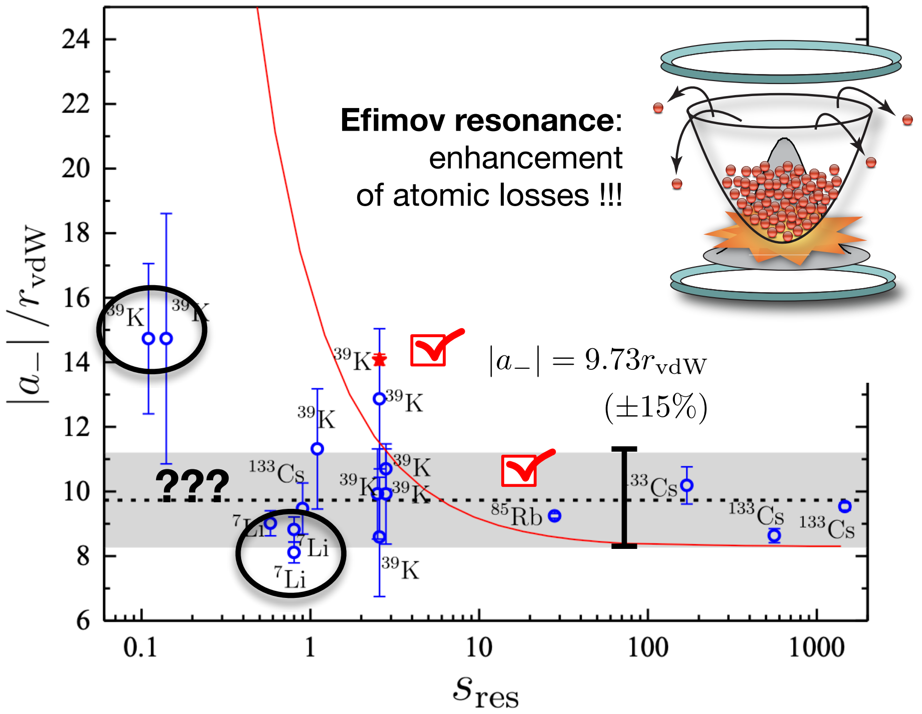
Petrov, PRL 93, 143201 (2004)
Wang, D'Incao, Esry, PRA 83, 042710 (2011)
Schmidt, Rath, Zwerger, EPJB 85, 386 (2012)

Efimov Physics For 7Li Atoms

Feshbach Resonances for 7Li



Ultracold Gases Experiments



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Pollack, Dries, and Hulet, Science, 326, 1683 (2009)
Gross, Shotan, Kokkelmans, and Khaykovich, PRL 103, 163202 (2009)
Gross, Shotan, Kokkelmans, and Khaykovich, PRL 105, 103203 (2010)
Dyke, Pollack, and Hulet, PRA 88, 023625 (2013)

Efimov Physics For 7Li Atoms

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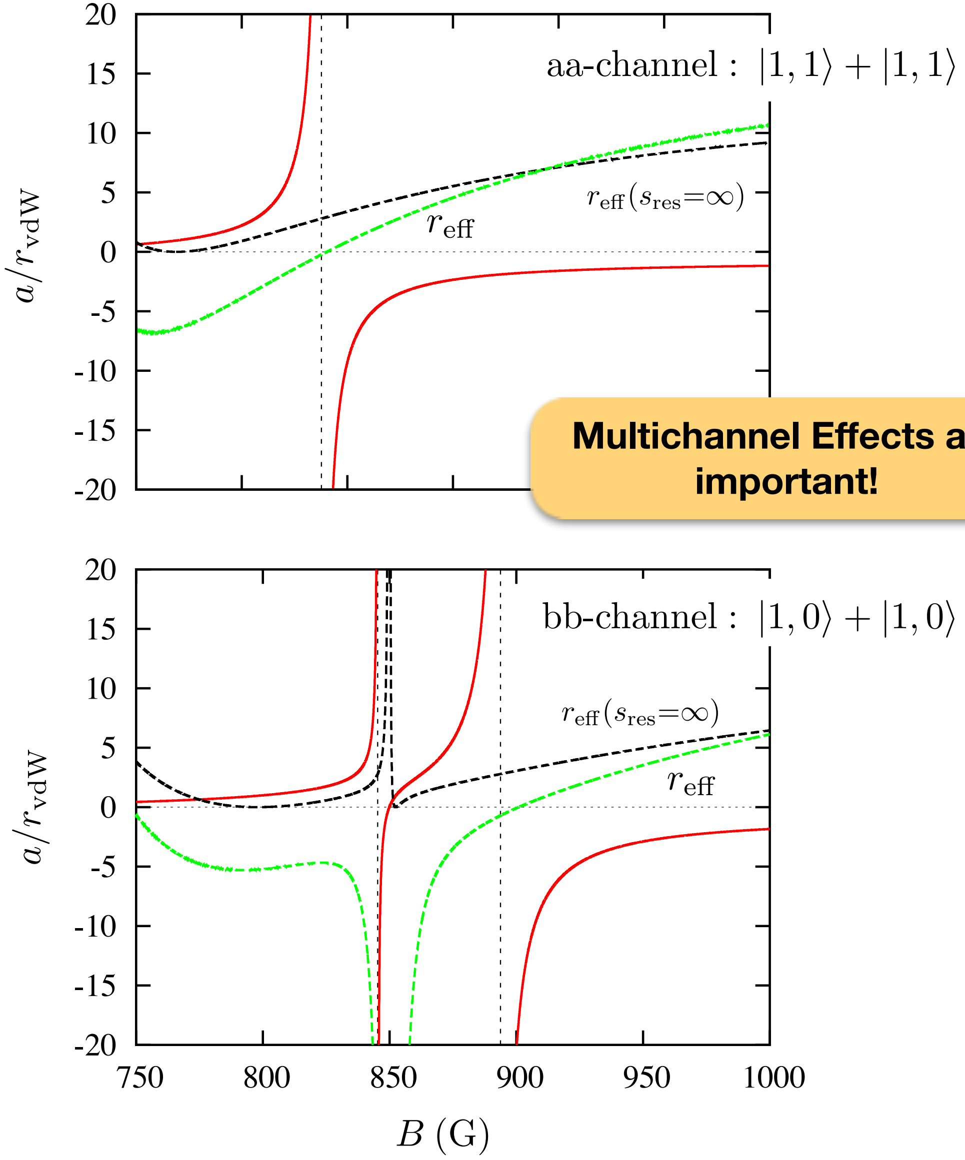
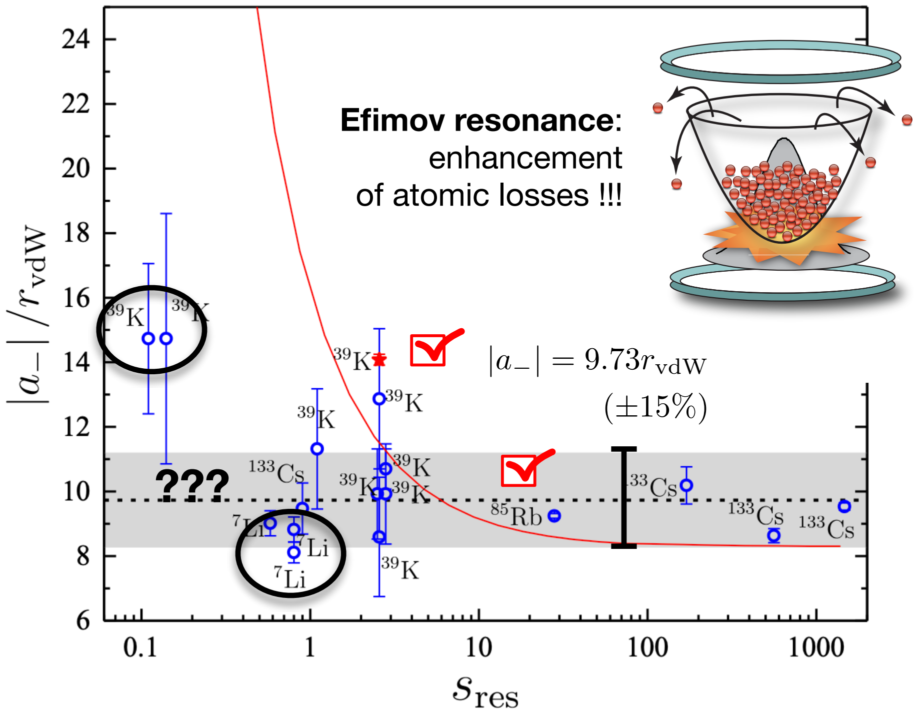


Multichannel Effects are important!

Ultracold Gases Experiments



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Three-body Recombination for 7Li

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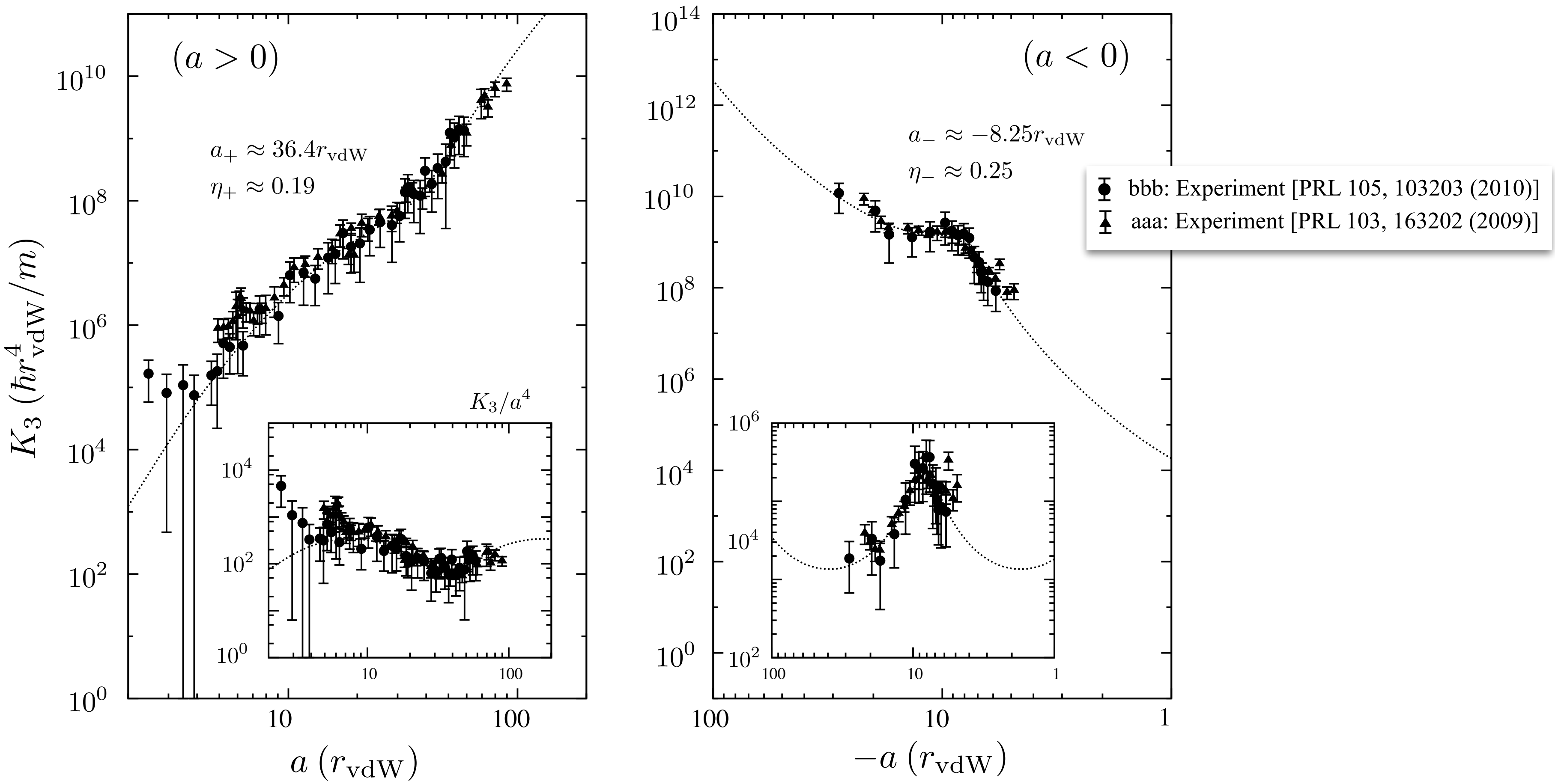

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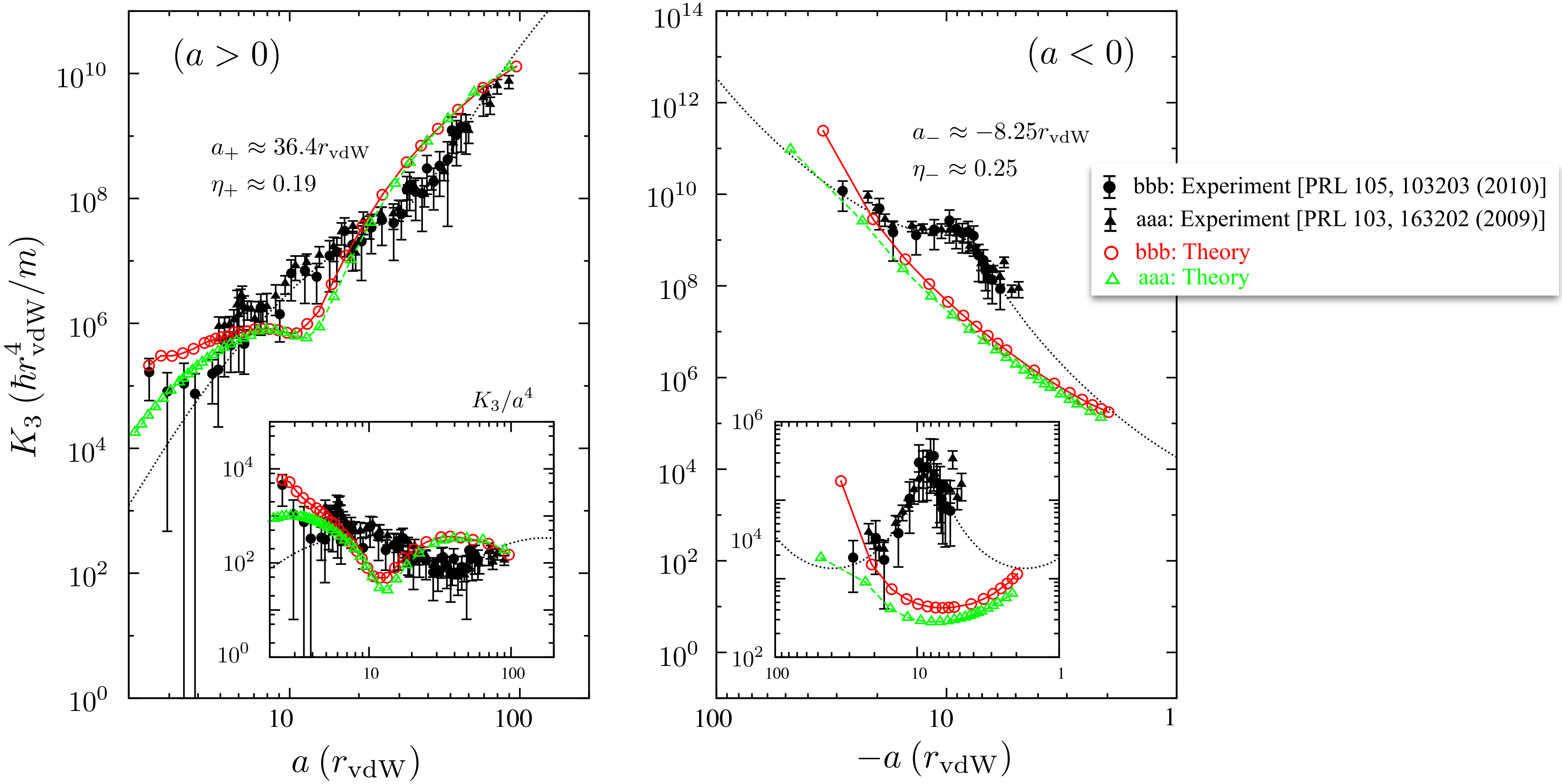

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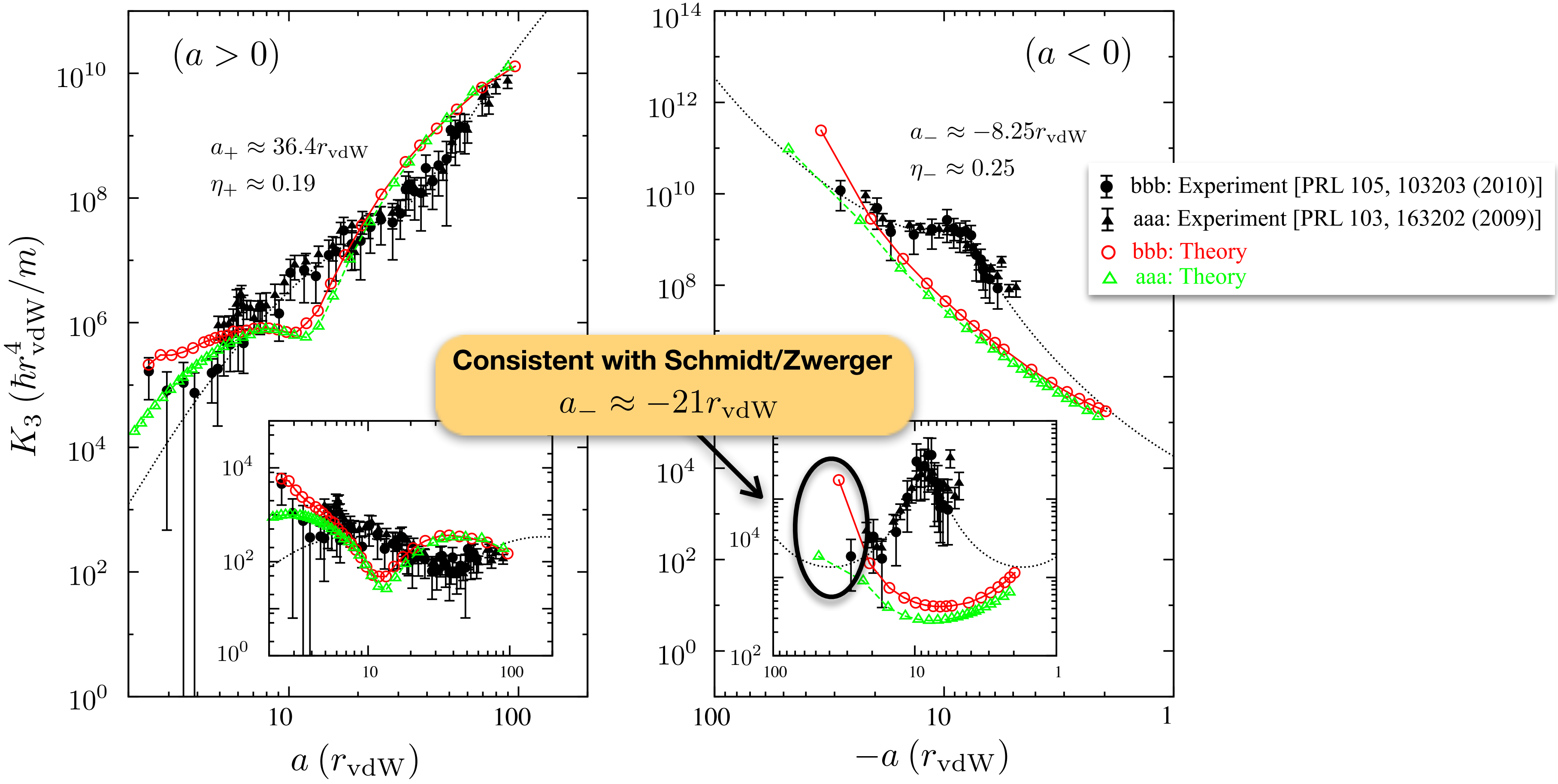

Consistent with Schmidt/Zwerger

$a_- \approx -21 r_{\rm vdW}$

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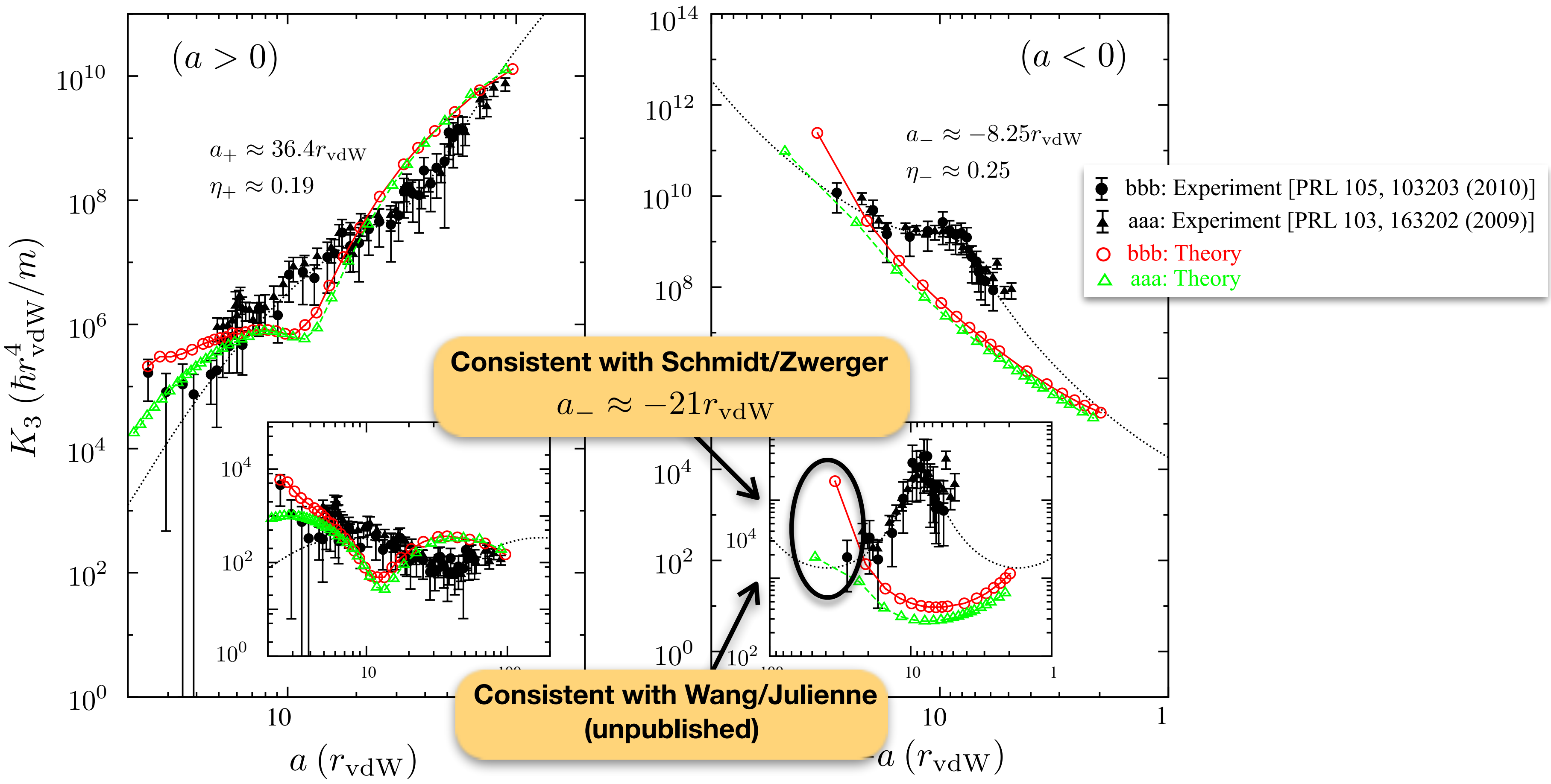

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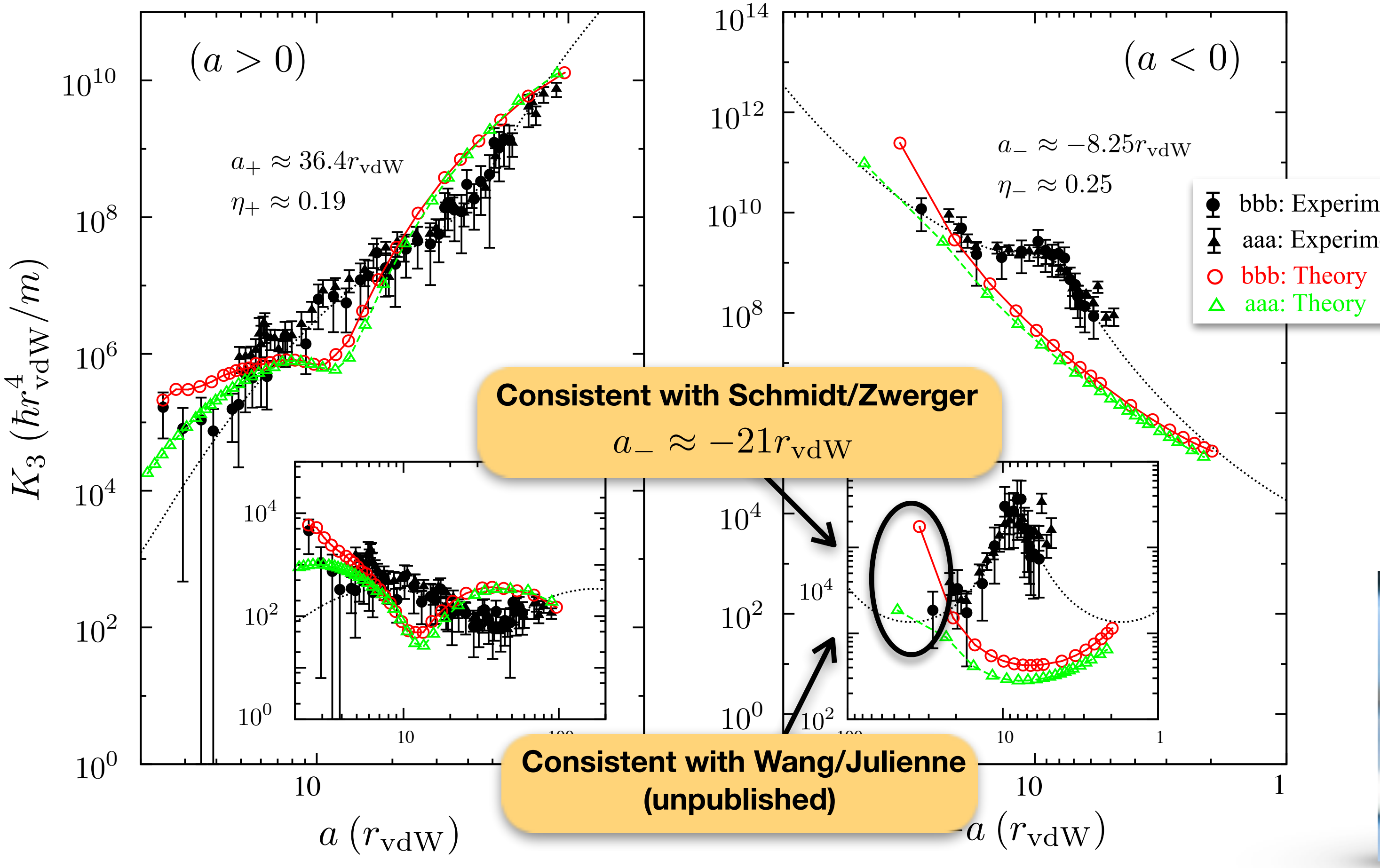

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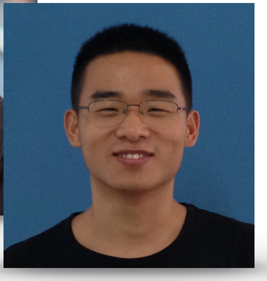
Similar results also for Servaas's group…


Servaas Kokkelmans


Jinglun Li (Ulm)

Efimov Physics For 7Li Atoms

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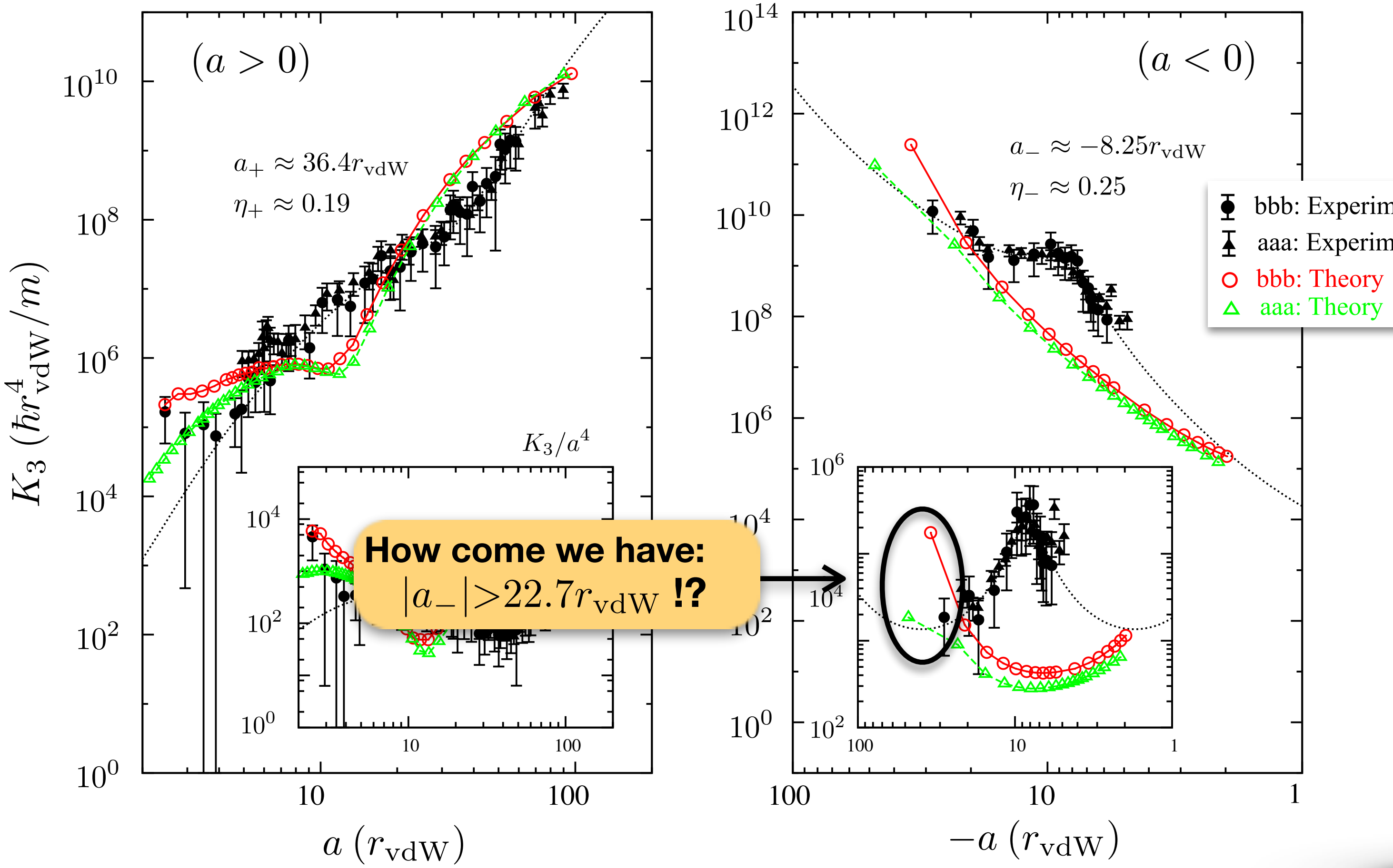
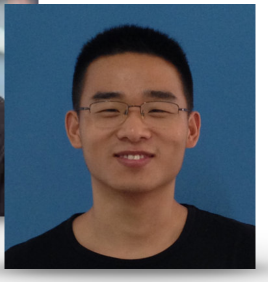


How come we have: $|a_-| > 22.7 r_{\mathrm{vdW}}$ **!?**

Similar results also for Servaas's group…

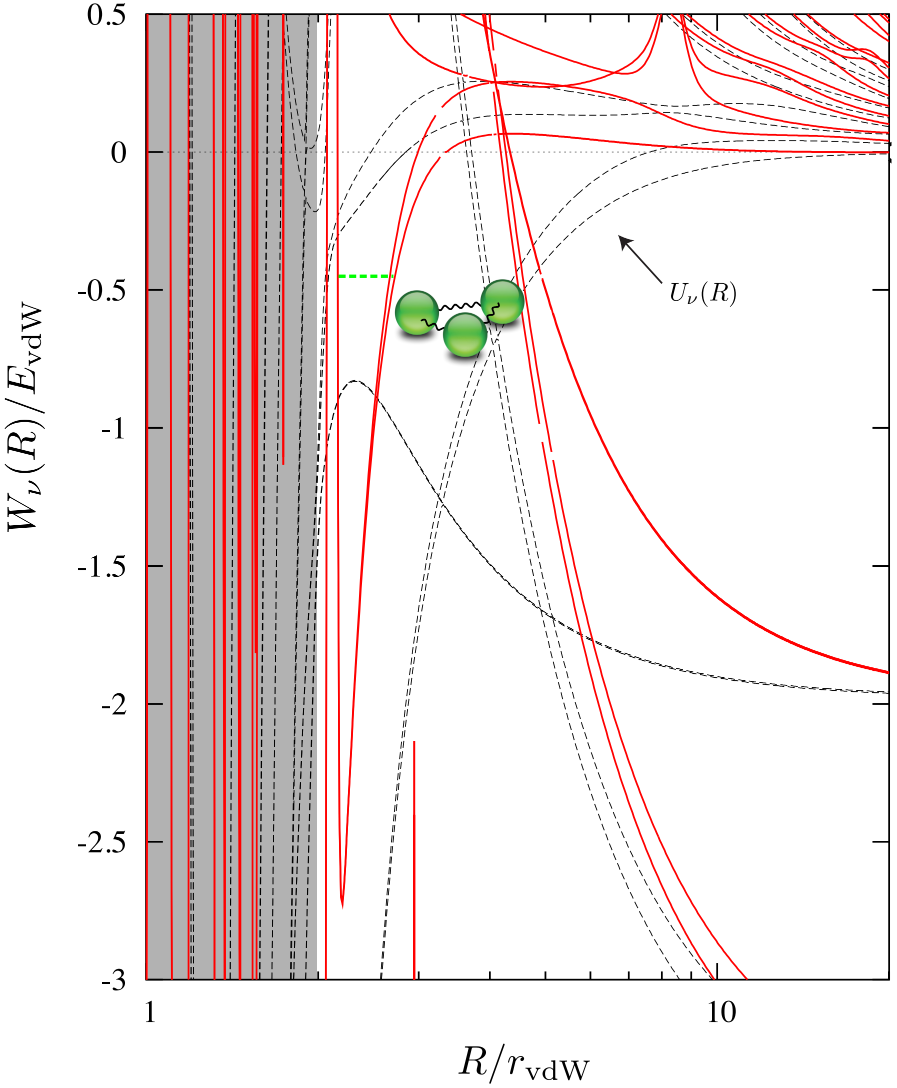
Servaas Kokkelmans



Jinglun Li (Ulm)

Efimov Physics For 7Li Atoms

Hyperspherical Potentials for 7Li



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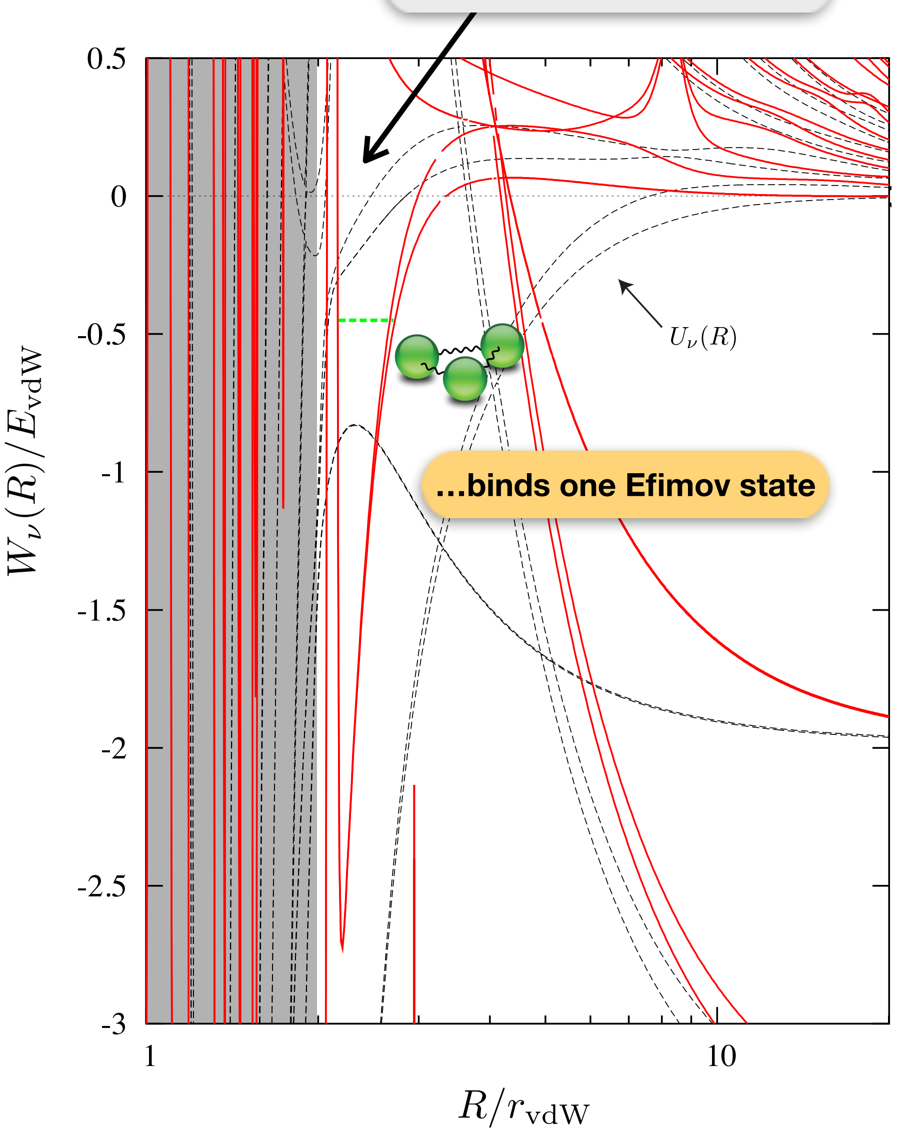
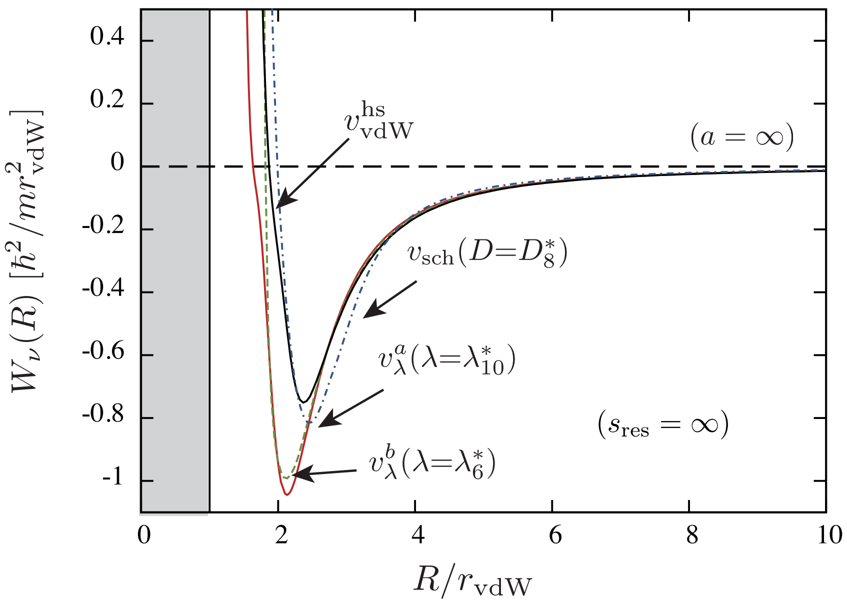

Typical Universal vdW barrier

...binds one Efimov state

Broad Resonances:

Wang, D’Incao, Esry, Greene, PRL 108, 263001 (2012)



Efimov Physics For 7Li Atoms

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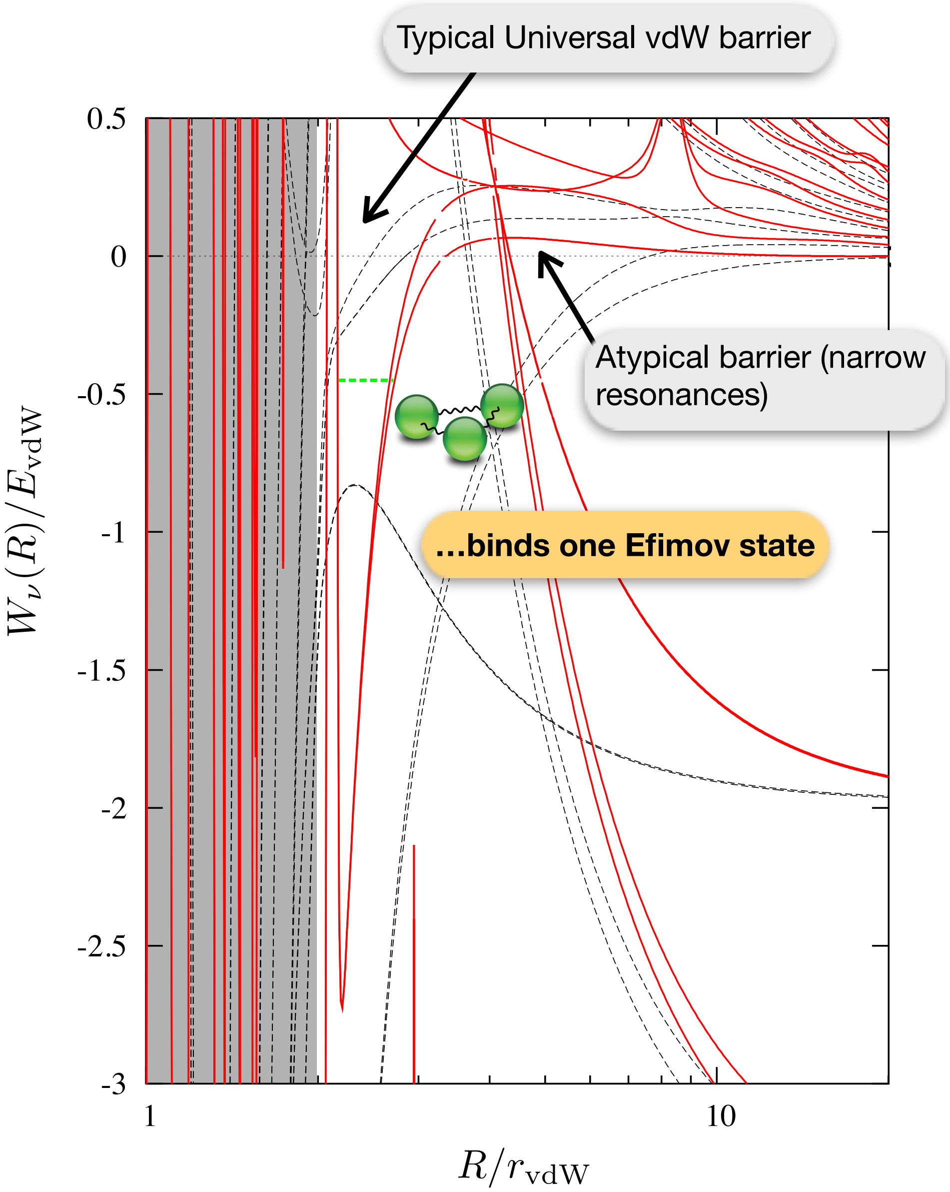

Theory for Narrow Resonances:

Petrov, PRL 93, 143201 (2004)
Wang, D'Incao, Esry, PRA 83, 042710 (2011)

Efimov Physics For 7Li Atoms

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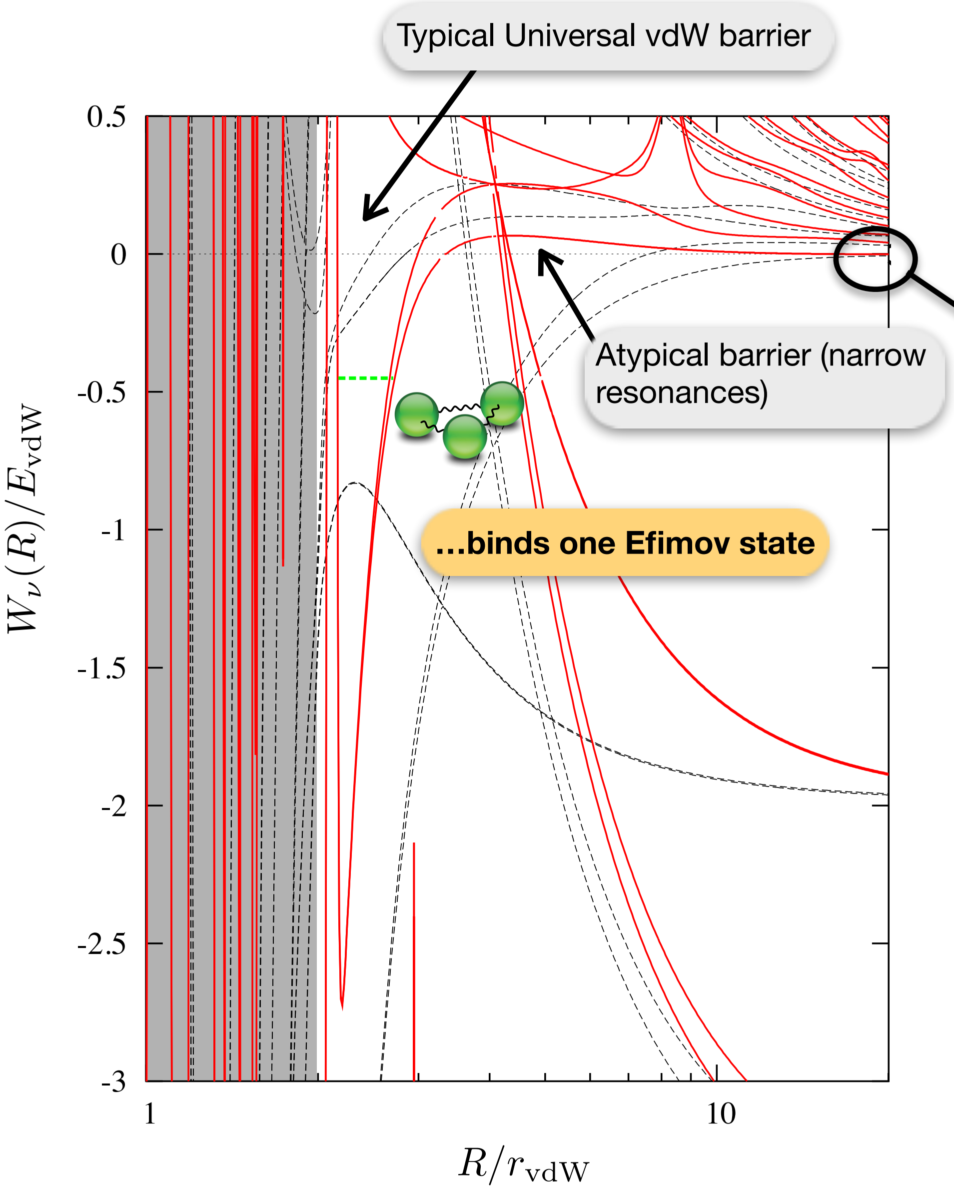

Typical Universal vdW barrier

Atypical barrier (narrow resonances)

...binds one Efimov state

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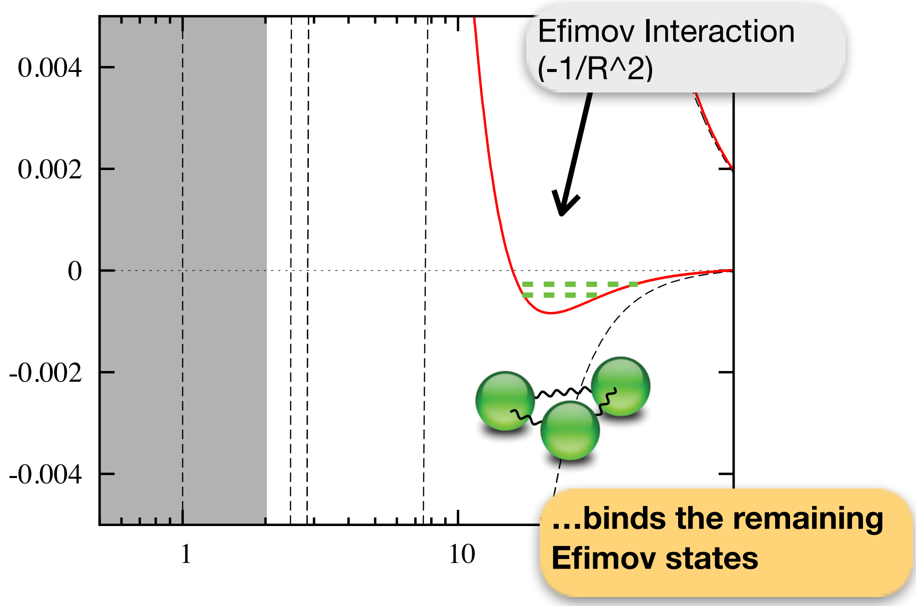

Efimov Interaction (-1/R^2)

...binds the remaining Efimov states

Efimov Physics For 7Li Atoms

What is different about 7Li?

…small Hyperfine Splitting

Species	$E_{\mathrm{hf}}/E_{\mathrm{vdW}}$
^{7}Li	1.25
^{23}Na	22.8
^{39}K	21.7
^{85}Rb	501.5
^{87}Rb	1122.5
^{133}Cs	3456.2

…spin physics is important!

Efimov Physics For 7Li Atoms

What is different about 7Li?

… small van der Waals length [from Chin, *et al.*, RMP 82, 1225 (2010)]

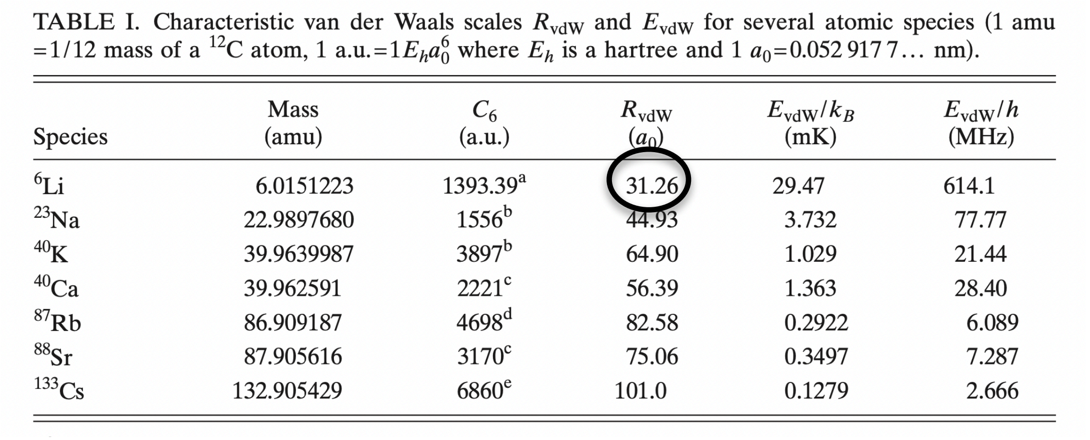

TABLE I. Characteristic van der Waals scales R_{vdW} and E_{vdW} for several atomic species (1 amu $=1/12$ mass of a ^{12}C atom, 1 a.u.$=1E_h a_0^6$ where E_h is a hartree and 1 $a_0=0.052\,917\,7\ldots$ nm).

Species	Mass (amu)	C_6 (a.u.)	R_{vdW} (a_0)	E_{vdW}/k_B (mK)	E_{vdW}/h (MHz)
^{6}Li	6.0151223	1393.39[a]	31.26	29.47	614.1
^{23}Na	22.9897680	1556[b]	44.93	3.732	77.77
^{40}K	39.9639987	3897[b]	64.90	1.029	21.44
^{40}Ca	39.962591	2221[c]	56.39	1.363	28.40
^{87}Rb	86.909187	4698[d]	82.58	0.2922	6.089
^{88}Sr	87.905616	3170[c]	75.06	0.3497	7.287
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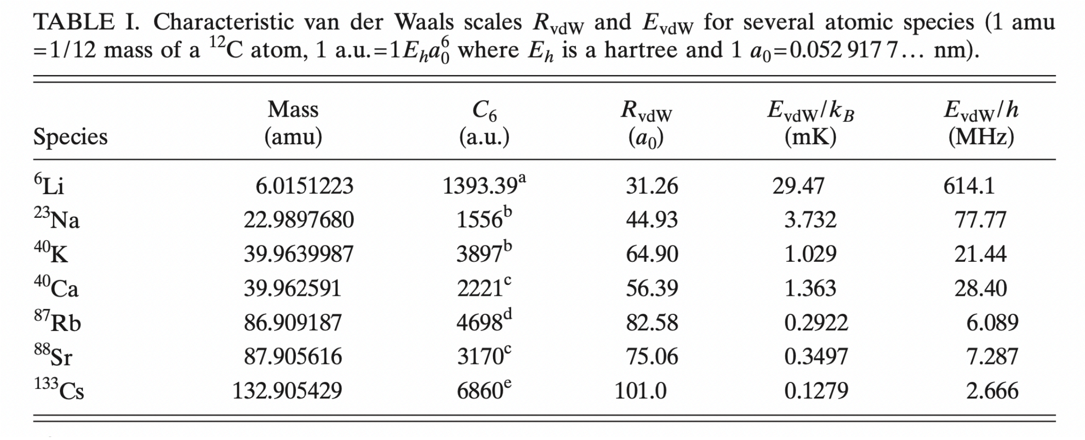

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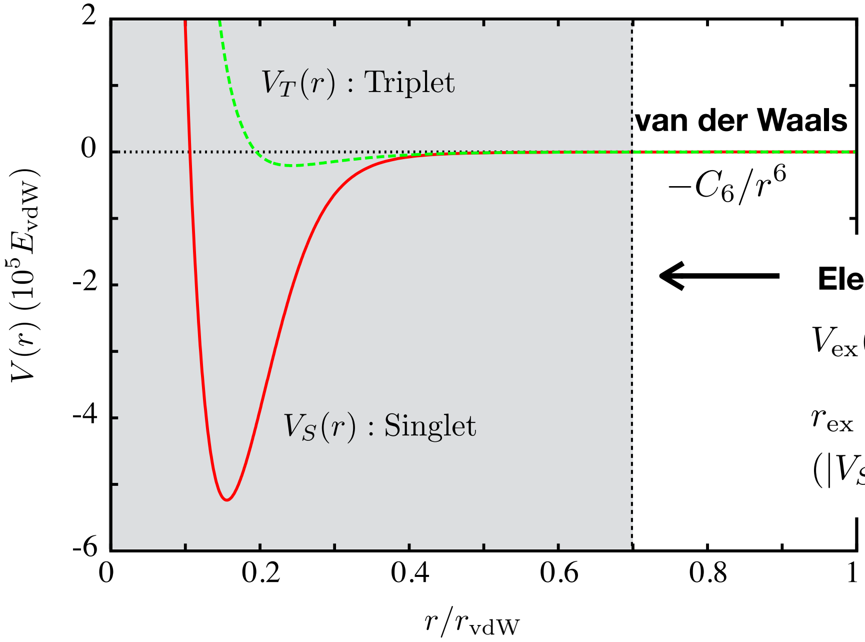

Comparable values for r_vdW and r_ex. Thus, strong electronic interactions

Electronic Exchange

$$V_{\text{ex}}(r) \approx A_{\text{ex}} r^{\lambda} \exp[-r/\beta]$$

$$r_{\text{ex}} \approx 20a_0$$

$$(|V_S(r) - V_T(r)| = E_{\text{vdW}})$$

Efimov Physics For 7Li Atoms

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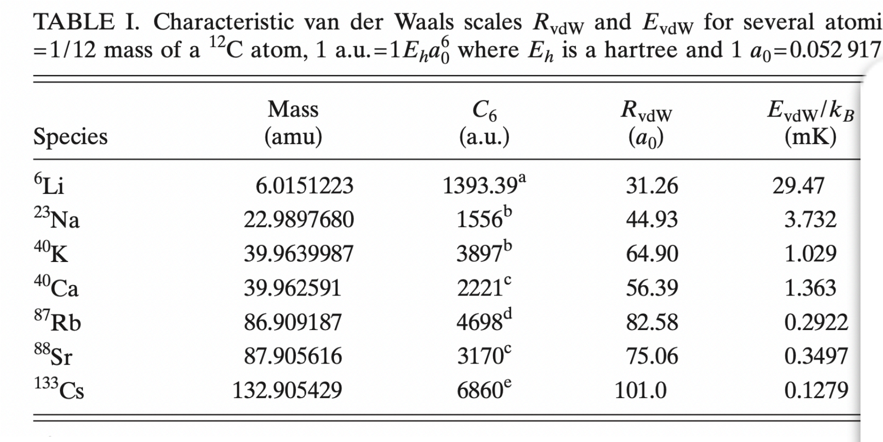

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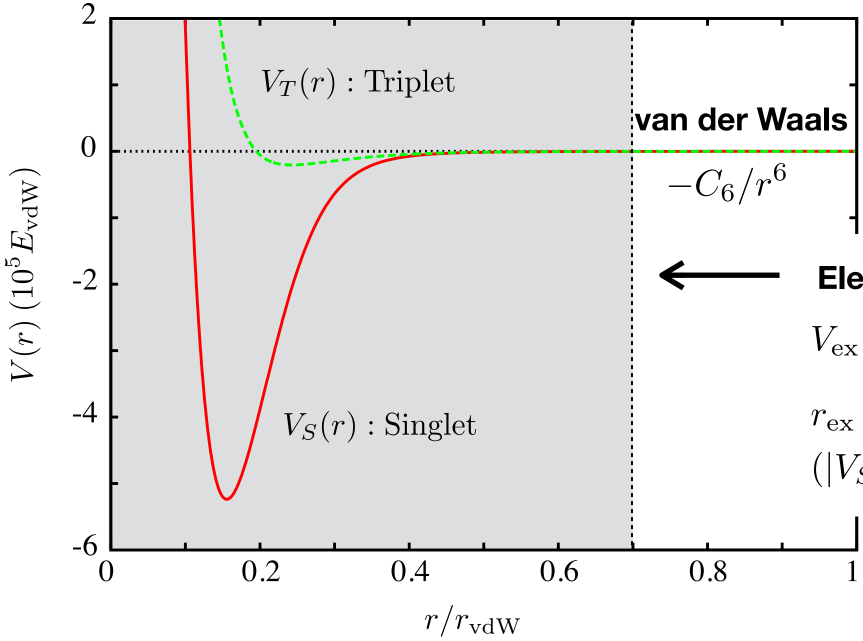


←

Electronic

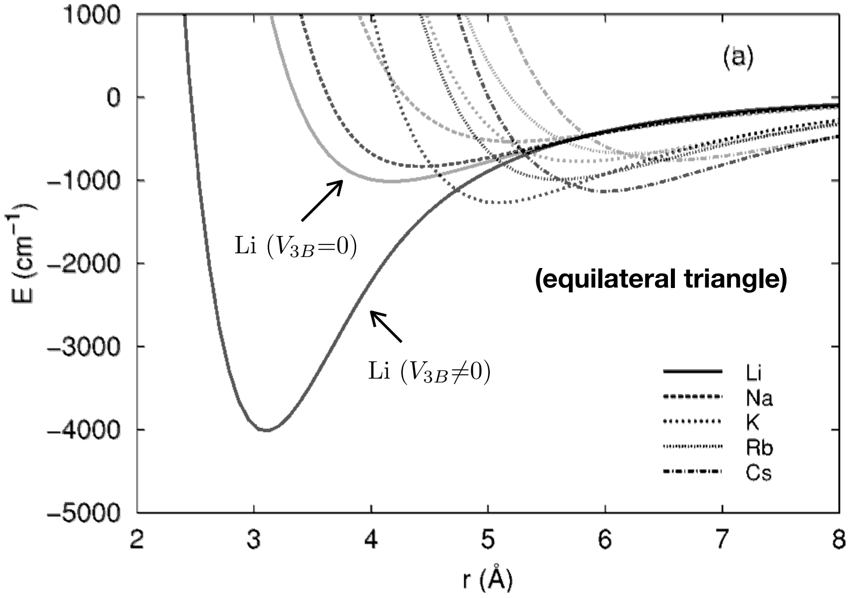
$V_{\rm ex}(r) \approx A_{\rm e}$

$r_{\rm ex} \approx 20a_0$

$(|V_S(r) - V_T(r)| = E_{\rm vdW})$

… strong Three-body interactions

[from Soldan, *et al.*, PRA 67, 054702 (2003)]



(equilateral triangle)

Efimov Physics For 7Li Atoms

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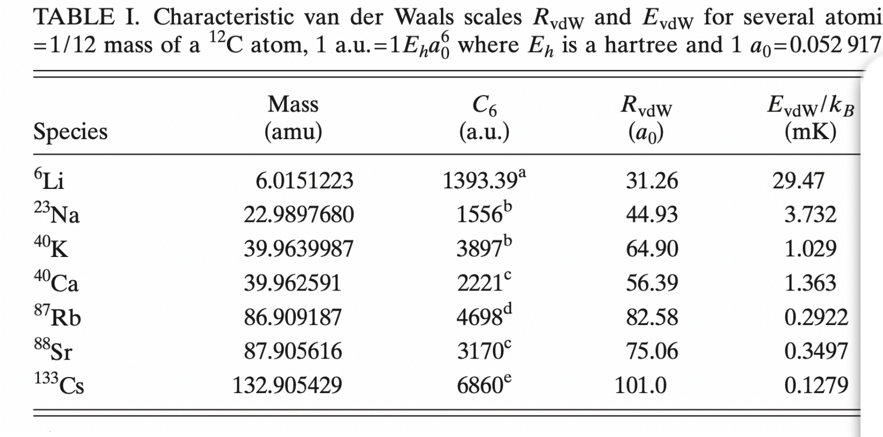
… small van der Waals length

[from Chin, *et al.*, RMP 82, 1225 (2010)]



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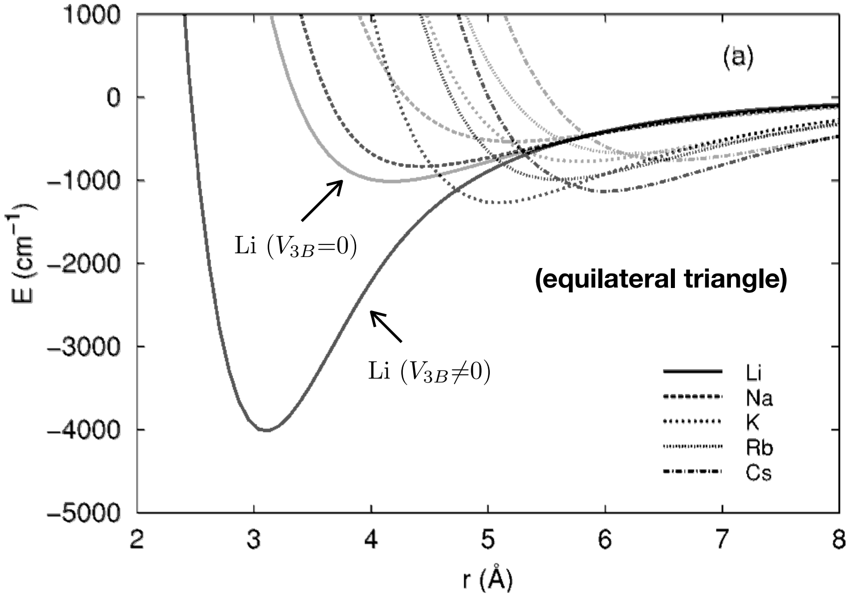

(equilateral triangle)

…calculations near r_vdW are coming

(KITP-2022)

Tomza's group…

Michal Tomza

Jacek Gebala

Efimov Physics For 7Li Atoms

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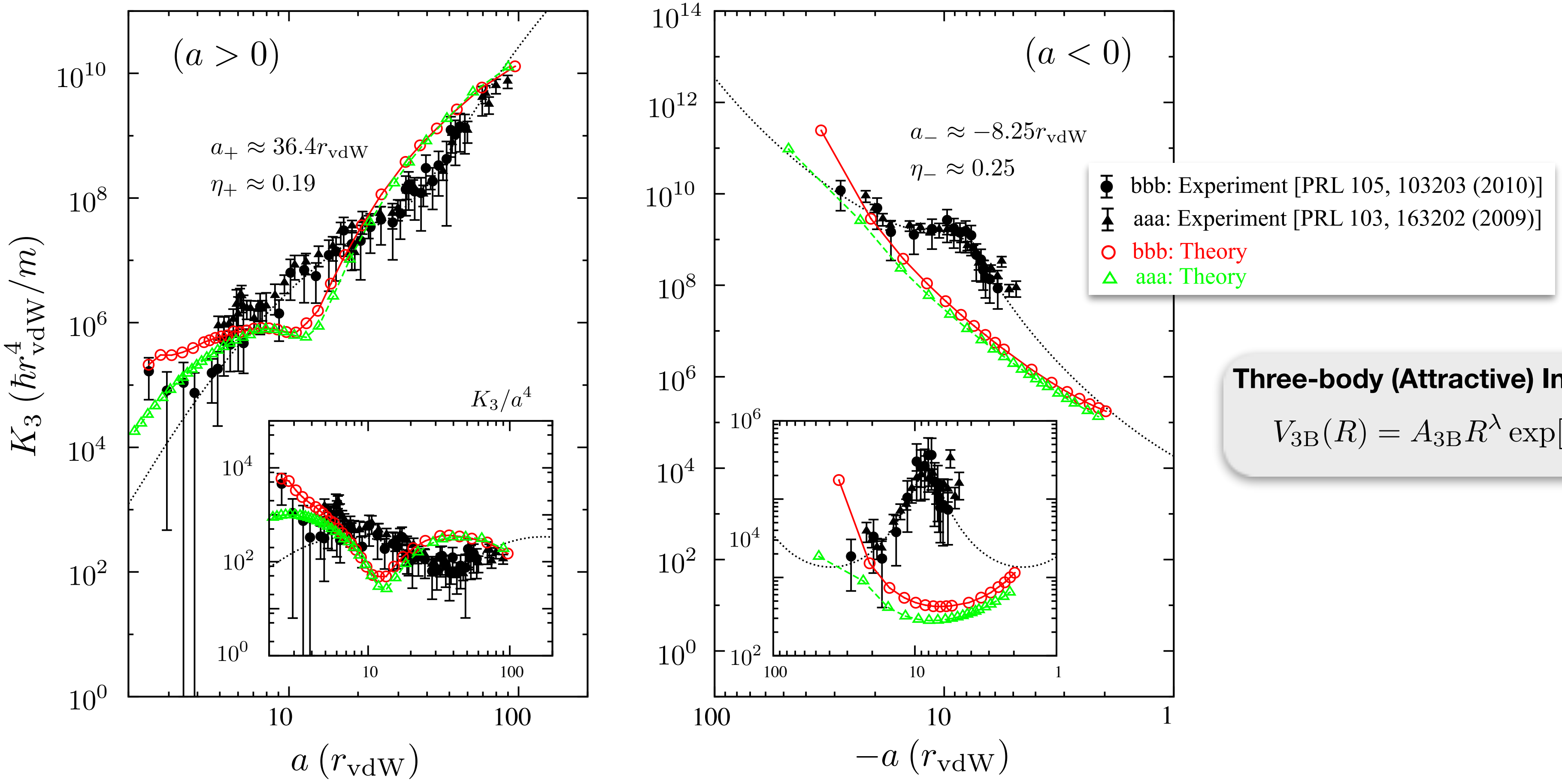

Three-body (Attractive) Interaction

$$V_{3\mathrm{B}}(R) = A_{3\mathrm{B}} R^{\lambda} \exp[-R/\beta]$$

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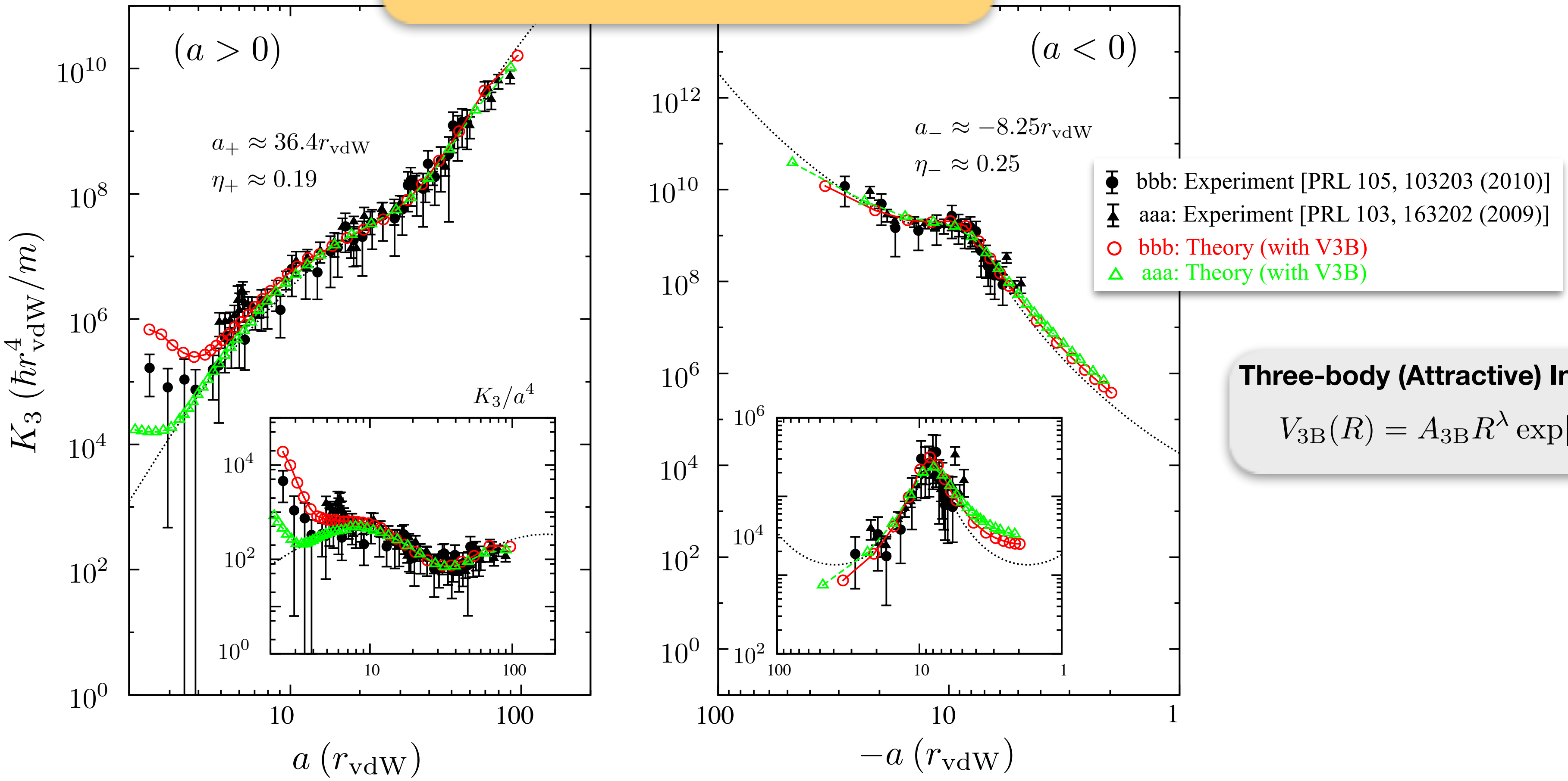

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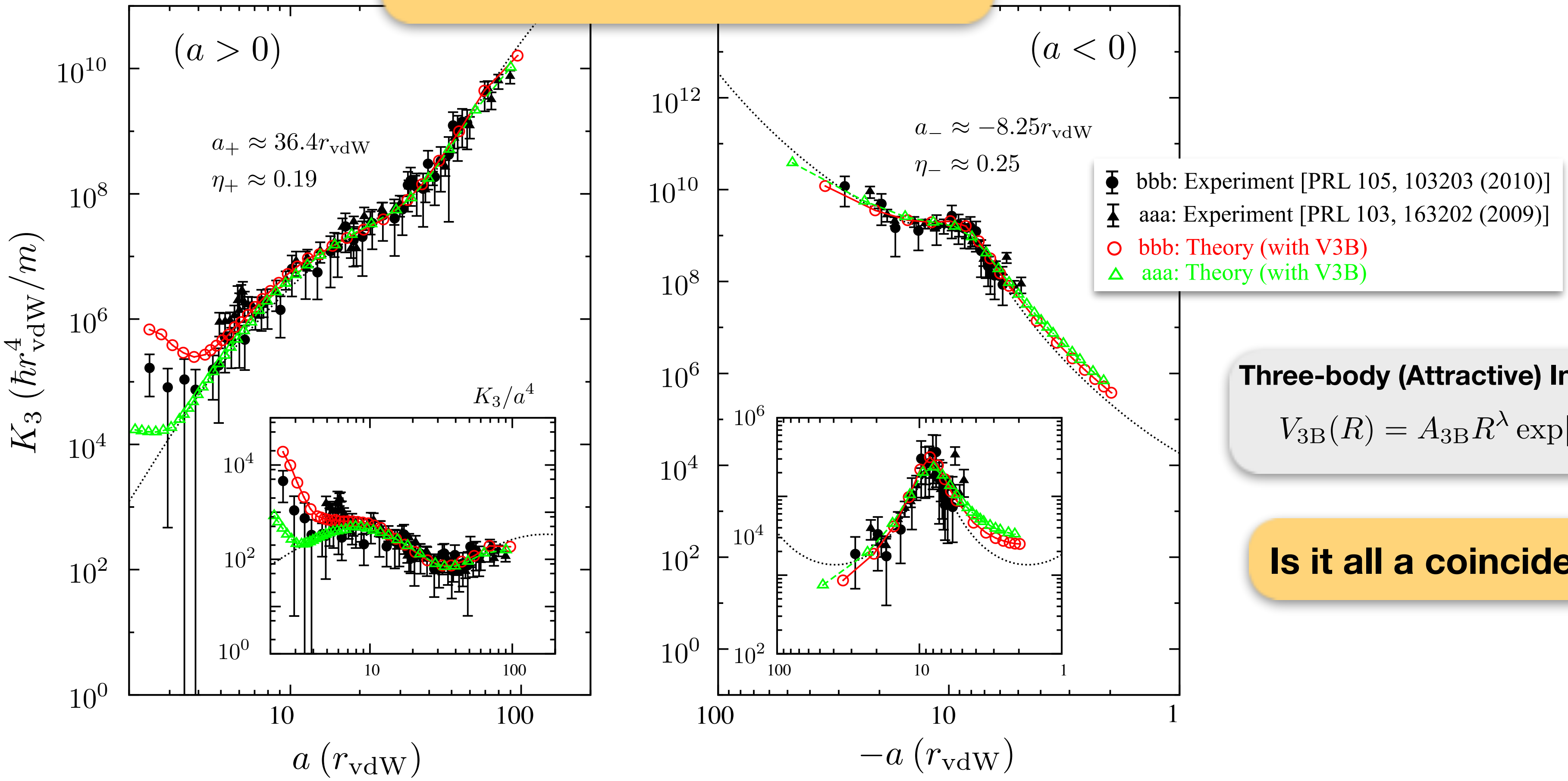

Three-body (Attractive) Interaction

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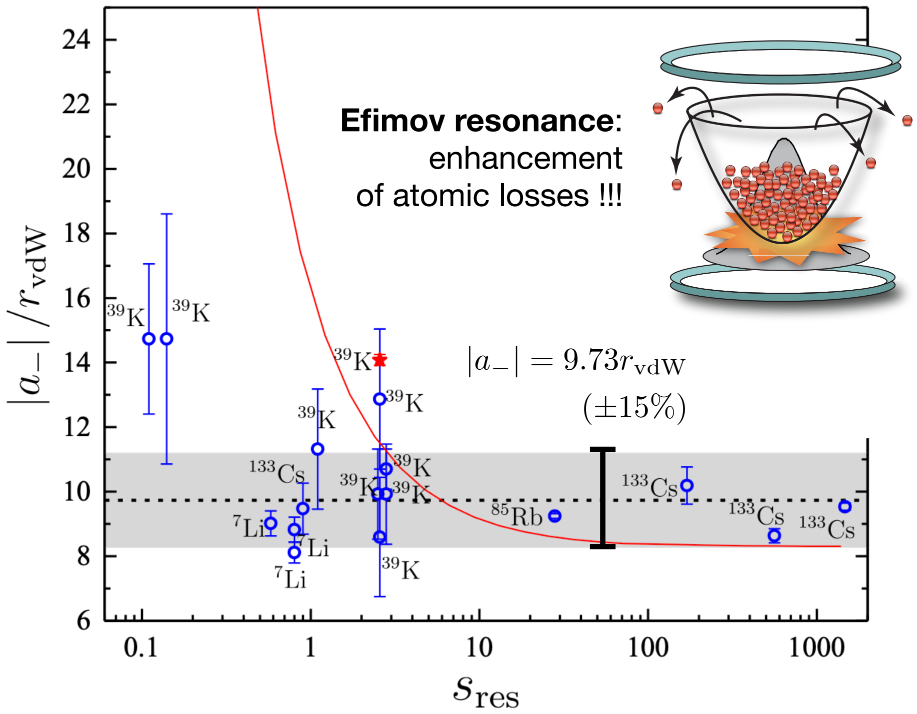
Is it all a coincidence!?

Summary (Opportunities and Challenges)

- **Still much to understand** on Universality and the various multichannel and short-range aspects of it

- **Realistic models** are necessary investigate the physics controlling universality on few-body systems but also to understand decay rates and lifetimes

- **Few-body physics** can help to answer fundamental question in an unambiguous, clean, and precise way



Efimov resonance: enhancement of atomic losses !!!

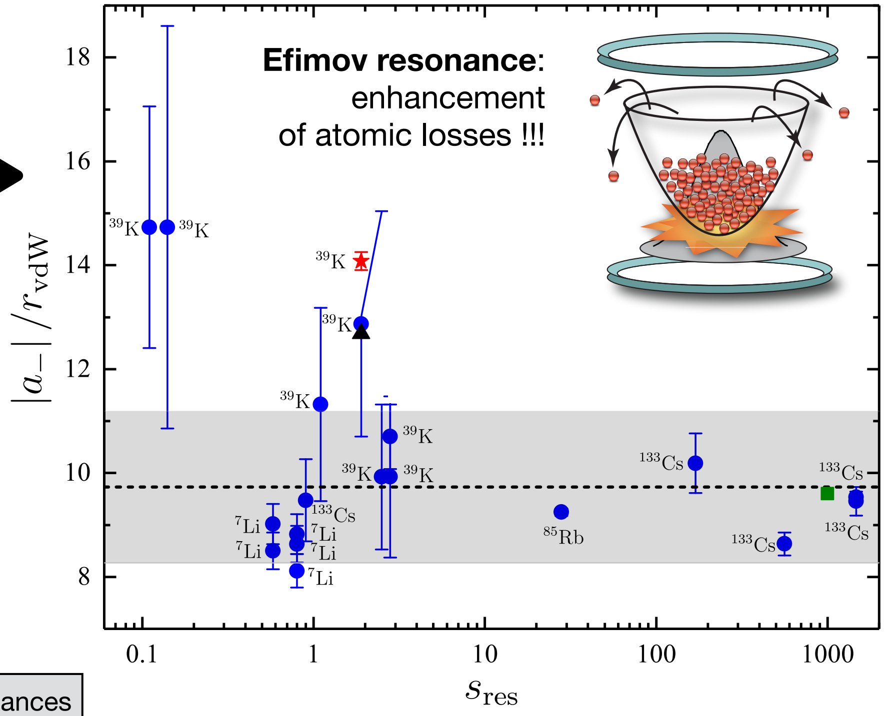
- **Connections to experiments** has been and will continue to be critical for the development of quantum control of reactive processes

Backup Slides

A new universal picture

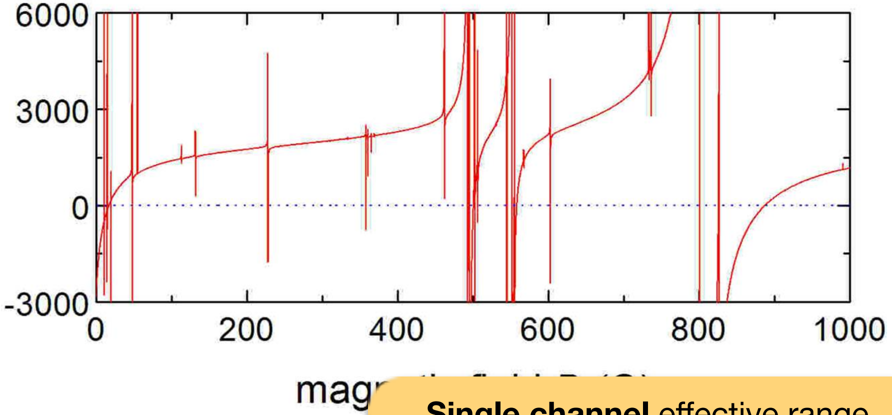
van der Waals Universality

Refers to the Efimov physics obtained using (single channel) vdW interactions, -C6/r^6, which leads to a three-body parameter depending solely on rvdW.



Feshbach resonances come in various flavors!

Fano-Feshbach resonances for 133Cs



$$\boxed{s_{\rm res}}$$

Resonance Strength

$s_{\rm res} \gg 1$: strong (broad)

$s_{\rm res} \ll 1$: weak (narrow)

Single channel effective range

multichannel properties

Physically…

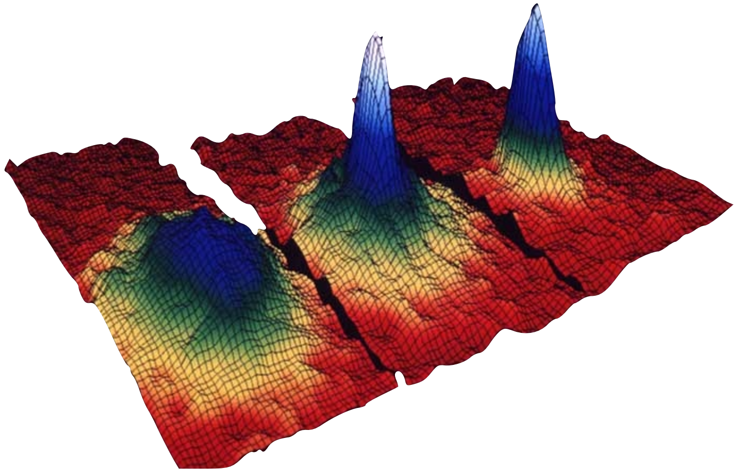
$$r^*_{\rm eff}(B) = \overbrace{r_{\rm eff}(a(B))} - \frac{4\pi}{\Gamma(1/4)^2}\overbrace{\frac{r_{\rm vdW}}{s_{\rm res}}\left(1-\frac{a_{\rm bg}}{a(B)}\right)}$$

$s_{\rm res} \gg 1 \rightarrow r^*_{\rm eff}(B) \equiv r_{\rm eff}(a(B))$

$s_{\rm res} \ll 1 \rightarrow r^*_{\rm eff}(B) \not\equiv r_{\rm eff}(a(B))$

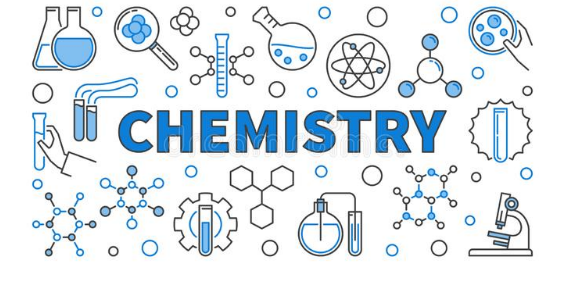
… a new laboratory for chemistry

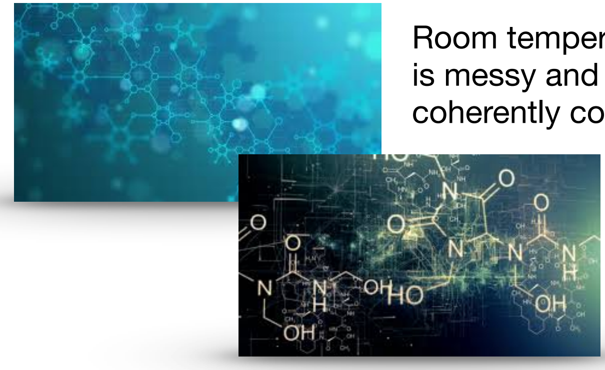
Ultracold Atomic/Molecular Gases



Ultracold temperatures, low density, quantum state selectivity, …

Ultracold Chemical Reactions

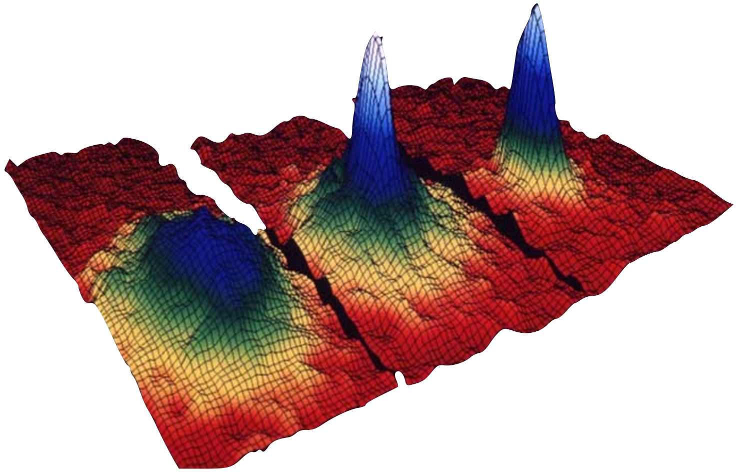




Room temperature chemistry is messy and difficult to coherently control!

… a new laboratory for chemistry

Ultracold Atomic/Molecular Gases



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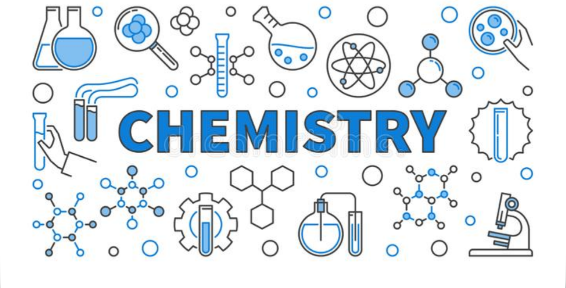
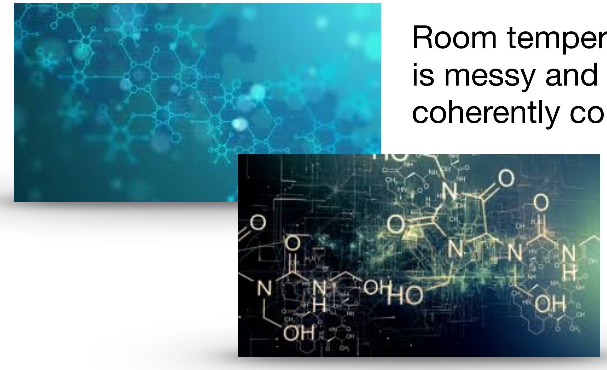
Ultracold Chemical Reactions

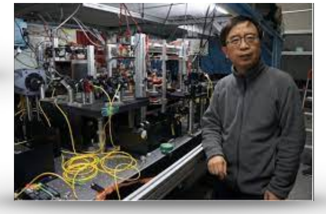




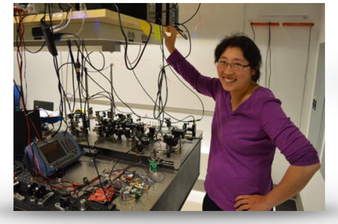
Room temperature chemistry is messy and difficult to coherently control!

Experiments in State-to-State Chemistry

Prof. Johannes H. Denschlag
(Ulm University, Germany)



Prof. Pan Jianwei
(University of Science and Technology of China, USTC)



Prof. Kang-Kuen Ni
(Harvard University, USA)

Challenging experiments…

- high phase-space densities
- fast detection schemes
- mapping many atomic and molecular transitions
- etc…