KITP Discussion May 18, 2022

Molecular interactions and reactions for diatomics and triatomics

Paul S. Julienne

Joint Quantum Institute, NIST and The University of Maryland

NIST

Joint Quantum Institute

Molecules

1. 2-body
   - Very accurate, coupled channels, bound + scattering
   - Long-range potential (van der Waals length, energy)
   - Weakly bound, near threshold (e.g., Feshbach molecules)
   - Near ground state (deeply bound, "normal")

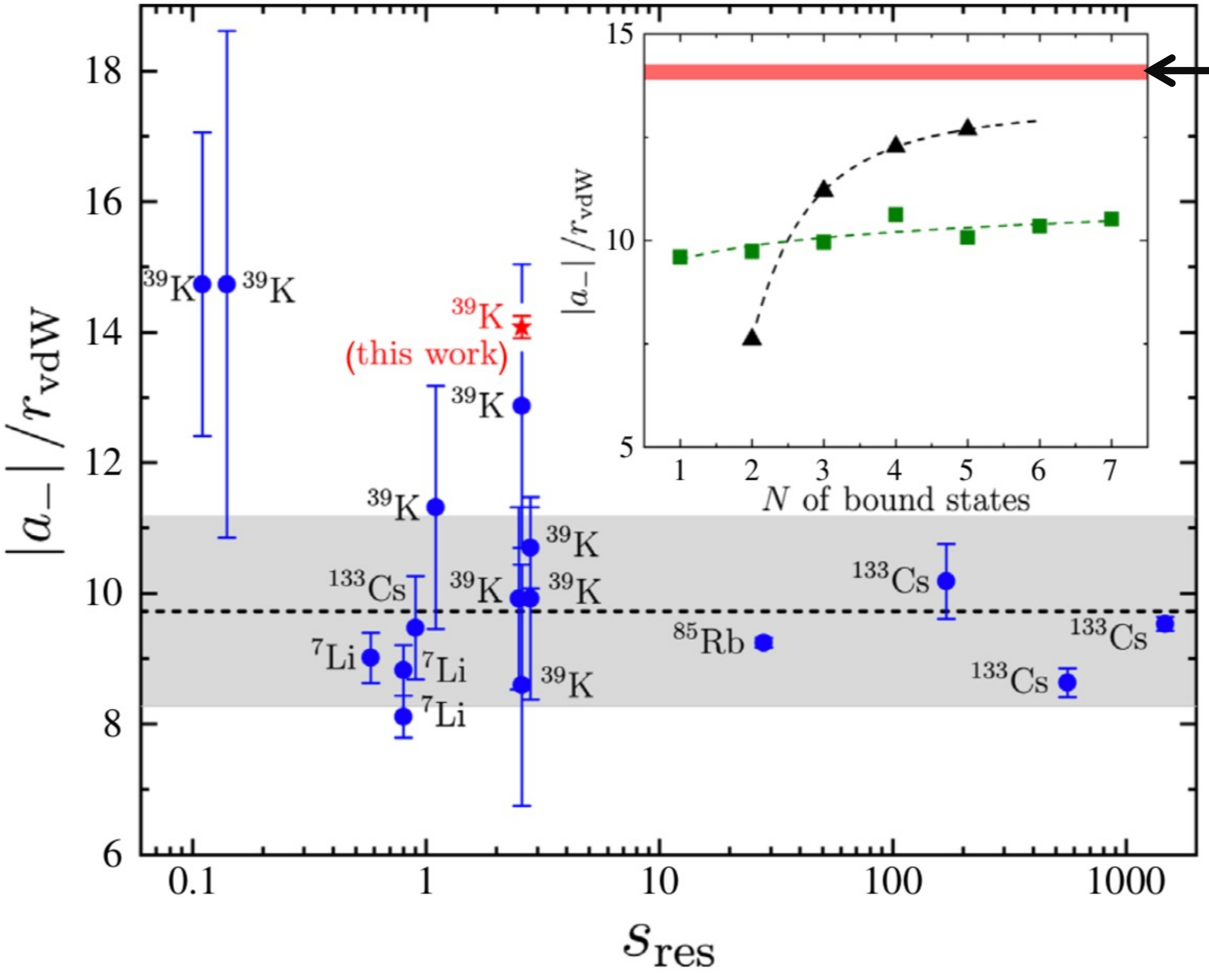
2. 3-body
   - Weakly bound, near threshold (Efimov, universality?)
   - 3-body recombination
     - Loss rate, magnitude, "shape" vs B or T
     - Product distributions-–role of spin
   - Atom-dimer collisions (Efimov, chemistry)
   - Accurate 3-body calculations: pairwise long-range 2-body + numerical

3. "4-body"
   - Chemical reactions of diatomics
   - Universal rates
   - Resonance spectrum (chaotic or non-chaotic)?
   - Product distributions

Precision Test of the Limits to Universality in Few-Body Physics

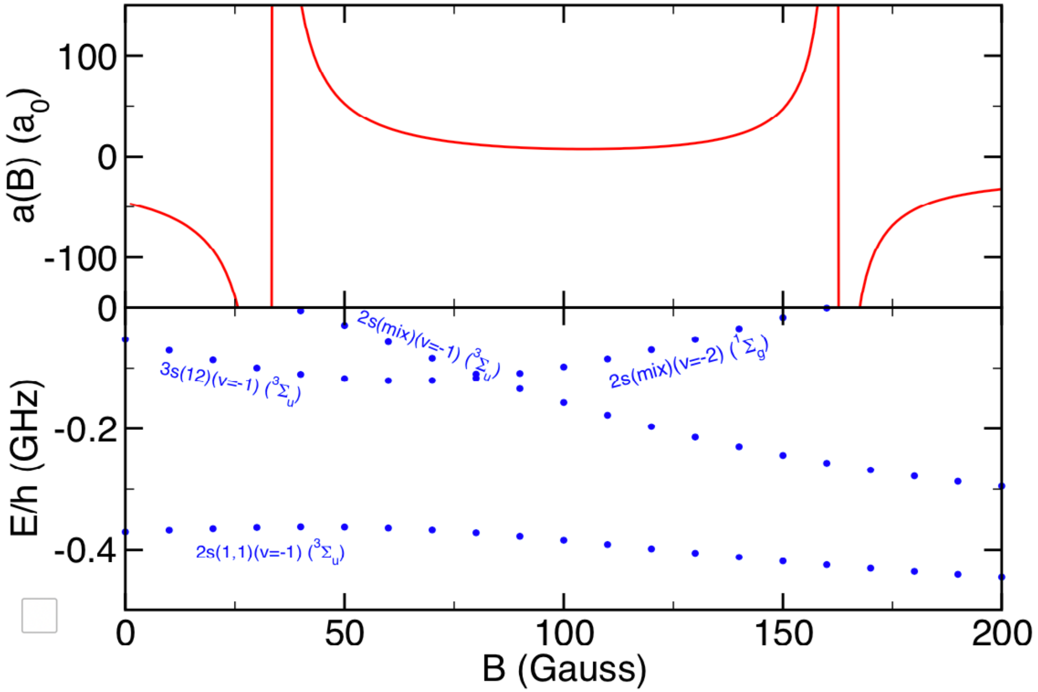
Phys. Rev. Lett. 123, 233402 (2019)

Roman Chapurin,[1] Xin Xie,[1] Michael J. Van de Graaff,[1] Jared S. Popowski,[1] José P. D'Incao,[1]
Paul S. Julienne,[2] Jun Ye,[1] and Eric A. Cornell[1]

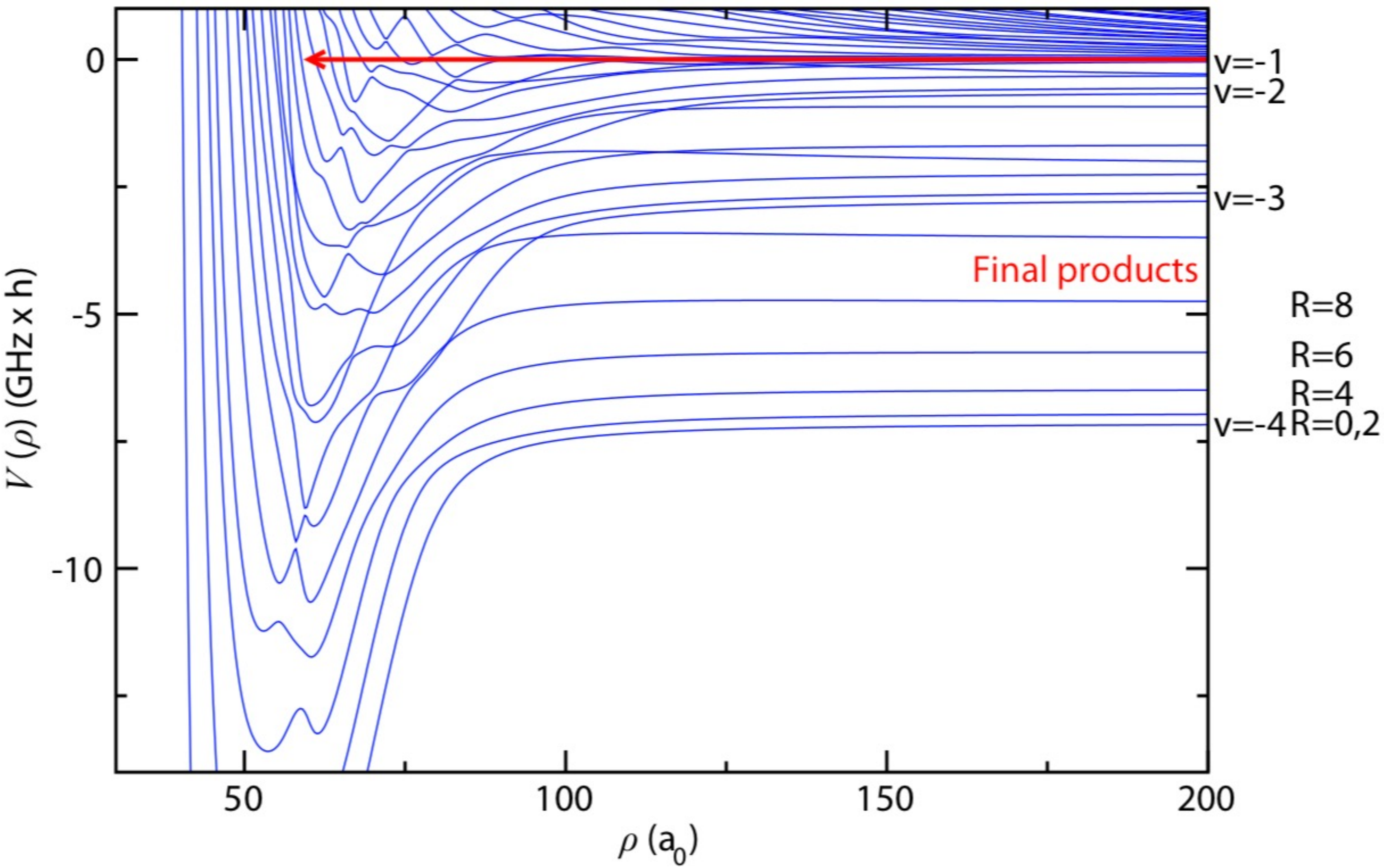


Secker, Li, Mestrom, Kokkelmans,
Phys. Rev. A **103**, 022825 (2021)
Numerical, multichannel AGS

$^{39}K_2$ cc channel



Adiabatic hyperspherical potential energy curves, $^{87}Rb_3$
4 s-wave bound states

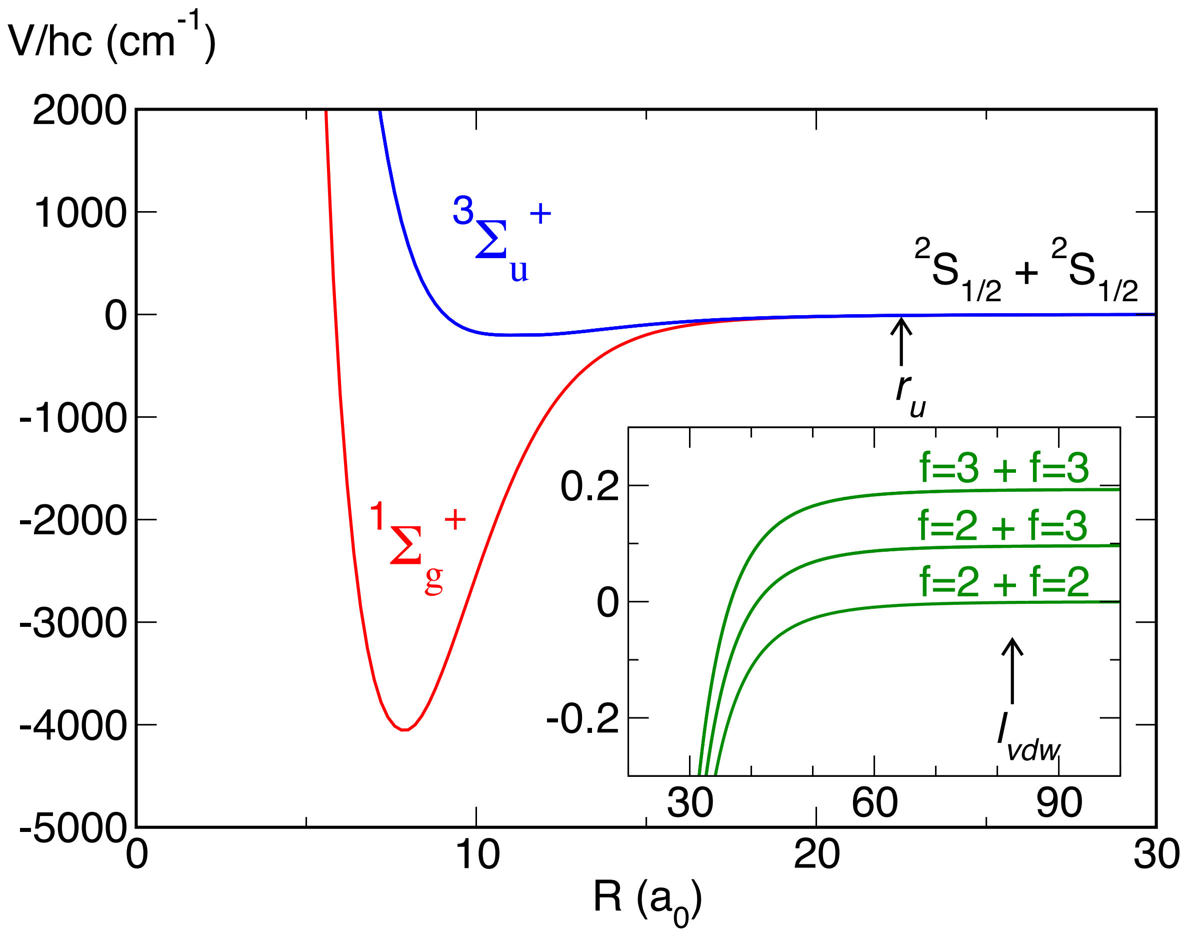


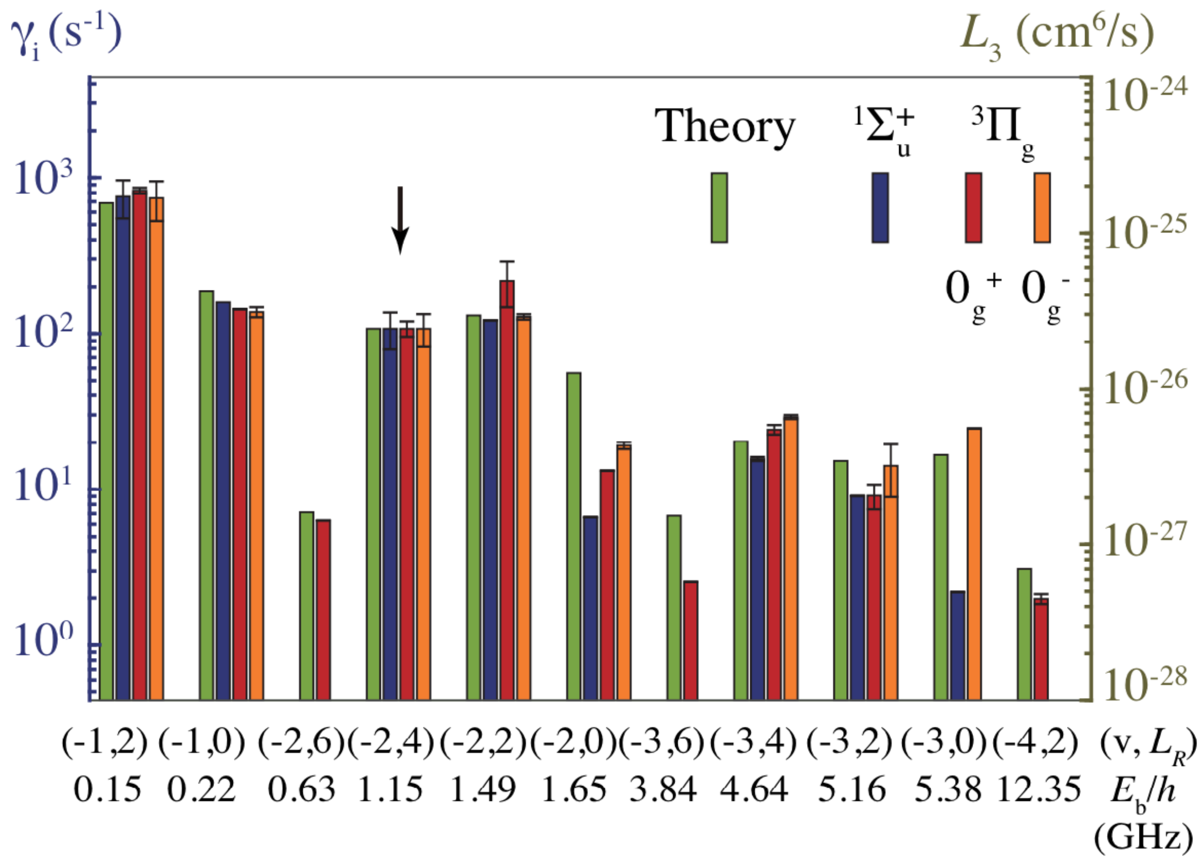
Wolf et al, Science 358, 921 (2017), Supplementary Material

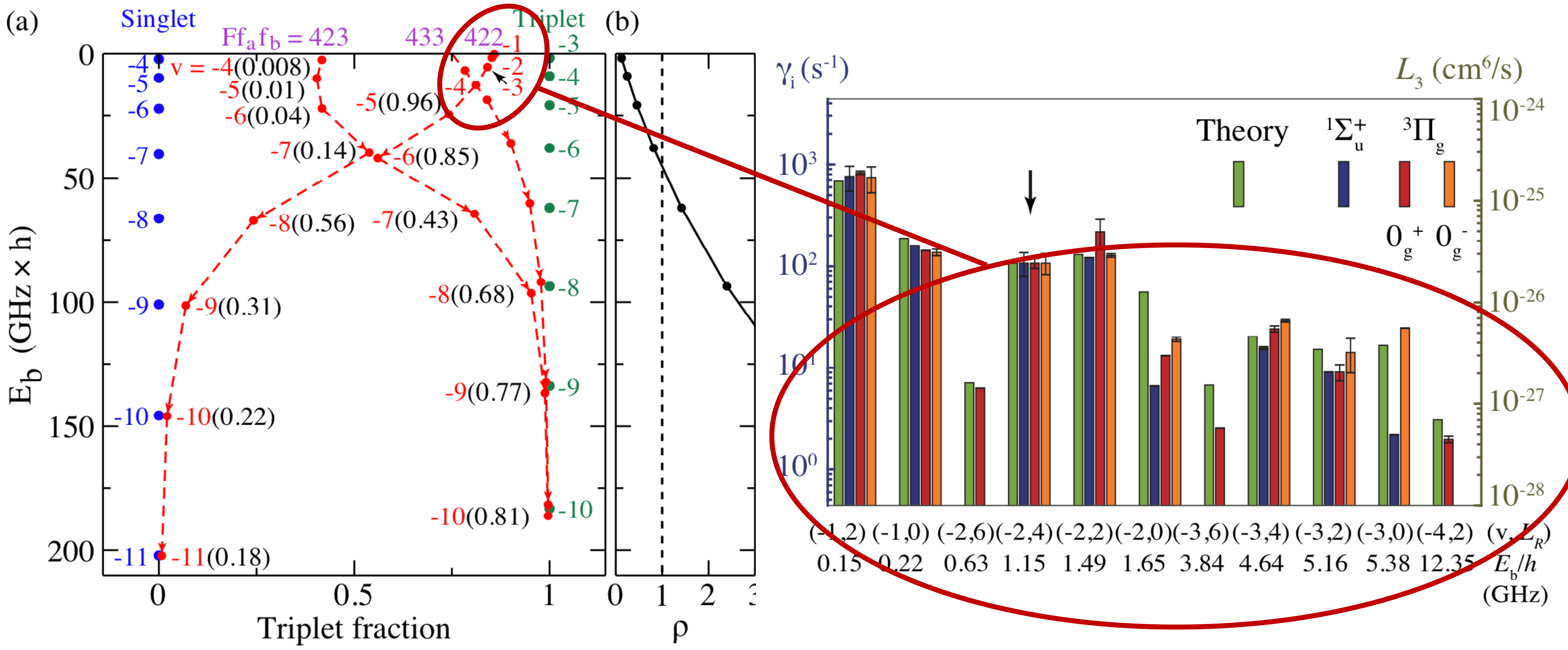
Spin-Conservation Propensity Rule for Three-Body Recombination of Ultracold Rb Atoms

Phys. Rev. Lett. 128, 133401 (2022)

Shinsuke Haze,[1,*] José P. D'Incao,[1,2] Dominik Dorer,[1] Markus Deiß,[1] Eberhard Tiemann,[3]
Paul S. Julienne,[1,4] and Johannes Hecker Denschlag[1,†]

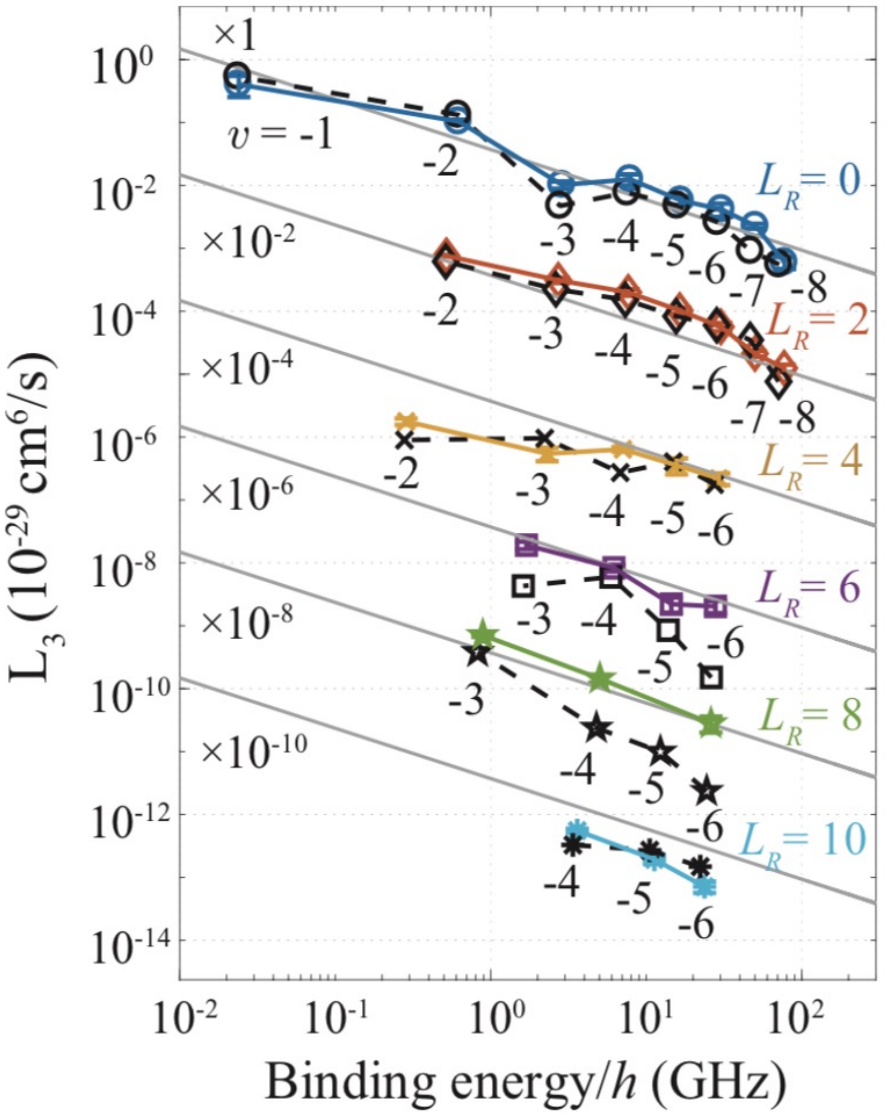


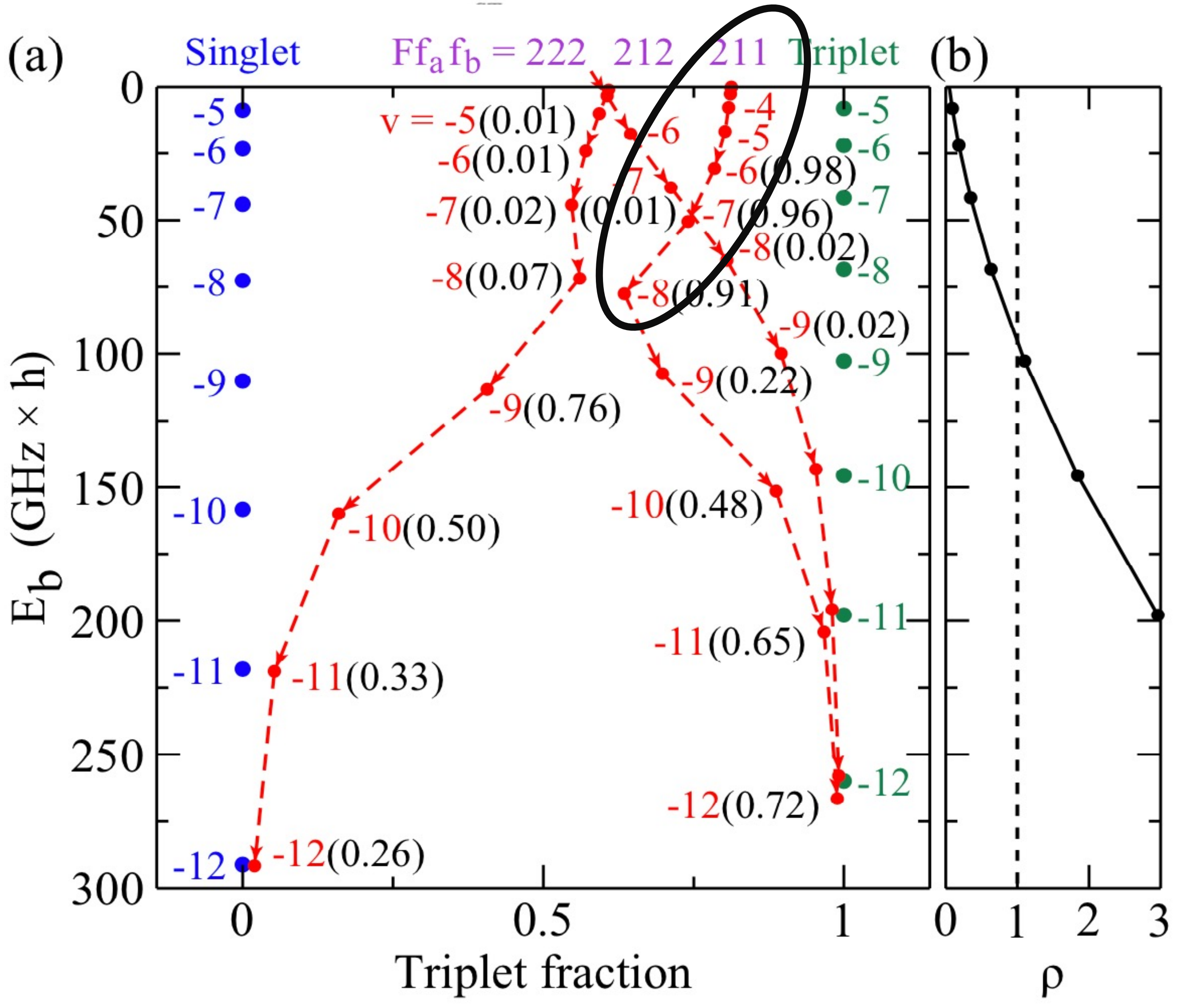



(a)
Singlet
Ff_a f_b = 423
433
422
Triplet
Triplet fraction
E_b (GHz × h)
v = -4(0.008)
-5(0.01)
-6(0.04)
-7(0.14)
-8(0.56)
-9(0.31)
-10(0.22)
-11(0.18)
-5(0.96)
-6(0.85)
-7(0.43)
-8(0.68)
-9(0.77)
-10(0.81)
(b)
ρ
γ_i (s^-1)
L_3 (cm^6/s)
Theory
^1Σ_u^+
^3Π_g
0_g^+ 0_g^-
(-1,2) (-1,0) (-2,6) (-2,4) (-2,2) (-2,0) (-3,6) (-3,4) (-3,2) (-3,0) (-4,2) (v, L_R)
0.15 0.22 0.63 1.15 1.49 1.65 3.84 4.64 5.16 5.38 12.35 E_b/h (GHz)

Energy-scaling of the product state distribution for three-body recombination of ultracold atoms

Shinsuke Haze,[1] José P. D'Incao,[1,2] Dominik Dorer,[1] Jinglun Li,[1] Markus Deiß,[1] Eberhard Tiemann,[3] Paul S. Julienne,[4] and Johannes Hecker Denschlag[1]





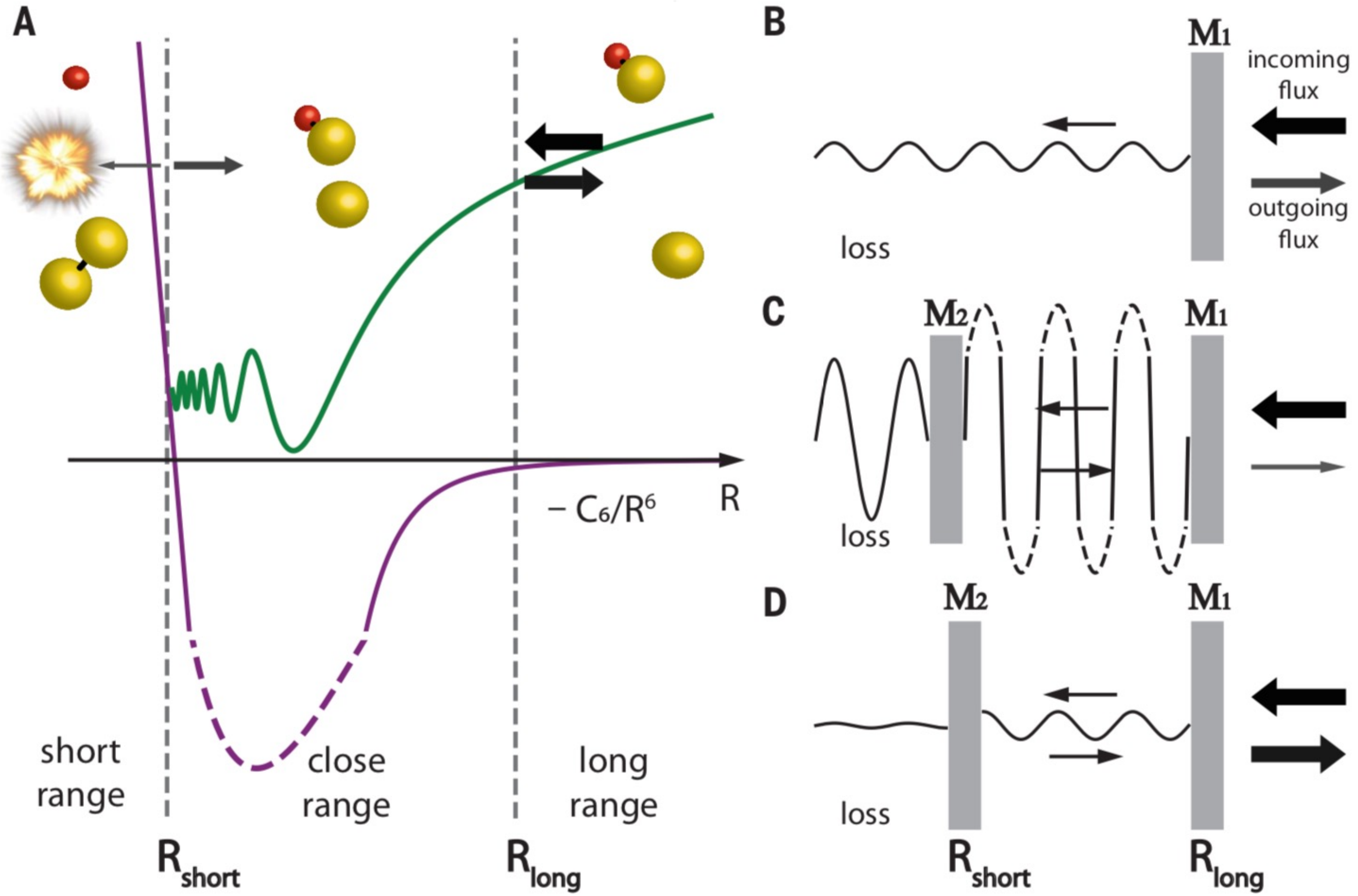
ULTRACOLD CHEMISTRY

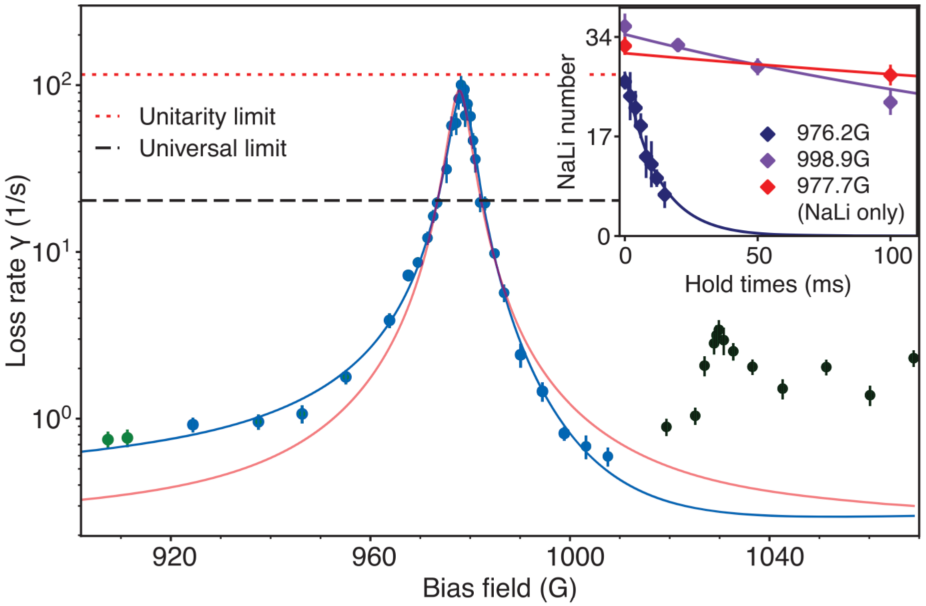
Control of reactive collisions by quantum interference

Na + NaLi

Science 375, 1006 (2022)

Hyungmok Son[1,2]*, Juliana J. Park[1], Yu-Kun Lu[1], Alan O. Jamison[3], Tijs Karman[4], Wolfgang Ketterle[1]

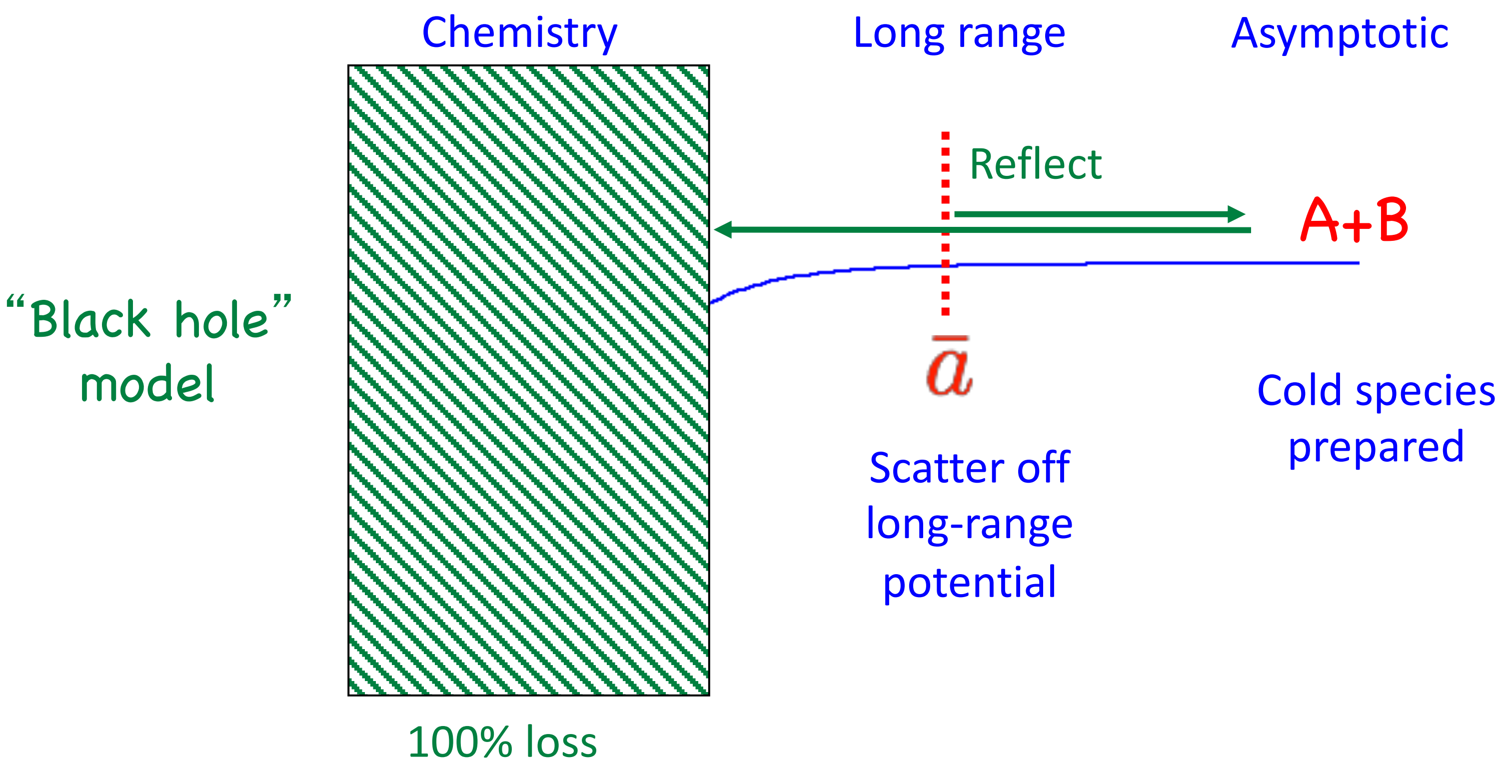




$$\tilde{a} = \bar{a}\left(s + y\frac{1+(1-s)^2}{i + y(1-s)}\right) \equiv \alpha - i\beta$$

"Universal" van der Waals capture model

Quantum version of classical Langevin (1905) and Gorin (1938) models



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

Identical fermions (p-wave): $$K^{\text{loss}}_{\ell=1}(T) = 1513\,\bar{a}^3\,\frac{k_B T}{h}$$

Gao , PRA 78, 012702(2008); PRL 105, 263203(2010); Idziaszek, PSJ (2010); Frye, PSJ, Hutson, New J. Phys. 17, 045019 (2015)

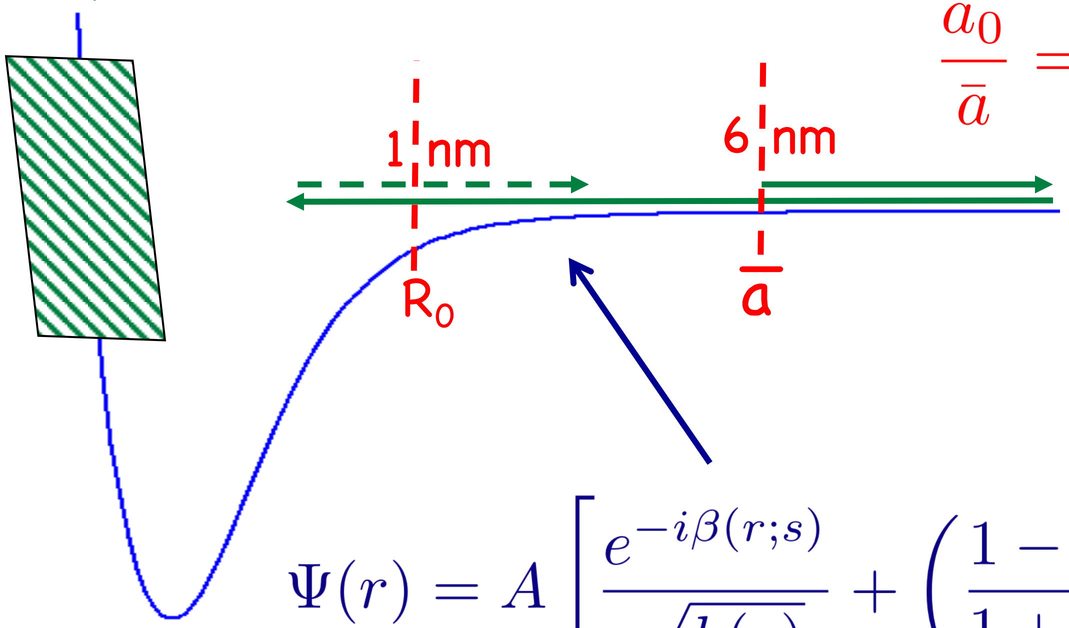
"grey hole" reaction rate theory

Partial Absorption
$0 \le y \le 1$

Parameterised by
$s = a/\bar{a}$ and y

vdW: analytic

$$\frac{\tilde{a}_0}{\bar{a}} = s + y\frac{1+(1-s)^2}{i+y(1-s)}$$



$$\Psi(r) = A\left[\frac{e^{-i\beta(r;s)}}{\sqrt{k(r)}} + \left(\frac{1-y}{1+y}\right)\frac{e^{+i\beta(r;s)}}{\sqrt{k(r)}}\right]$$

Universal(vdW) "black hole": $\tilde{a}_0 = \bar{a}(1-i)$ when $y \to 1$

$$\tilde{a}_1 = \bar{a}_1(k\bar{a})^2(-1-i)$$

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

Gao , PRA 78, 012702(2008); PRL 105, 263203(2010); Idziaszek, PSJ (2010); Frye, PSJ, Hutson, New J. Phys. 17, 045019 (2015)

Article

Precision test of statistical dynamics with state-to-state ultracold chemistry

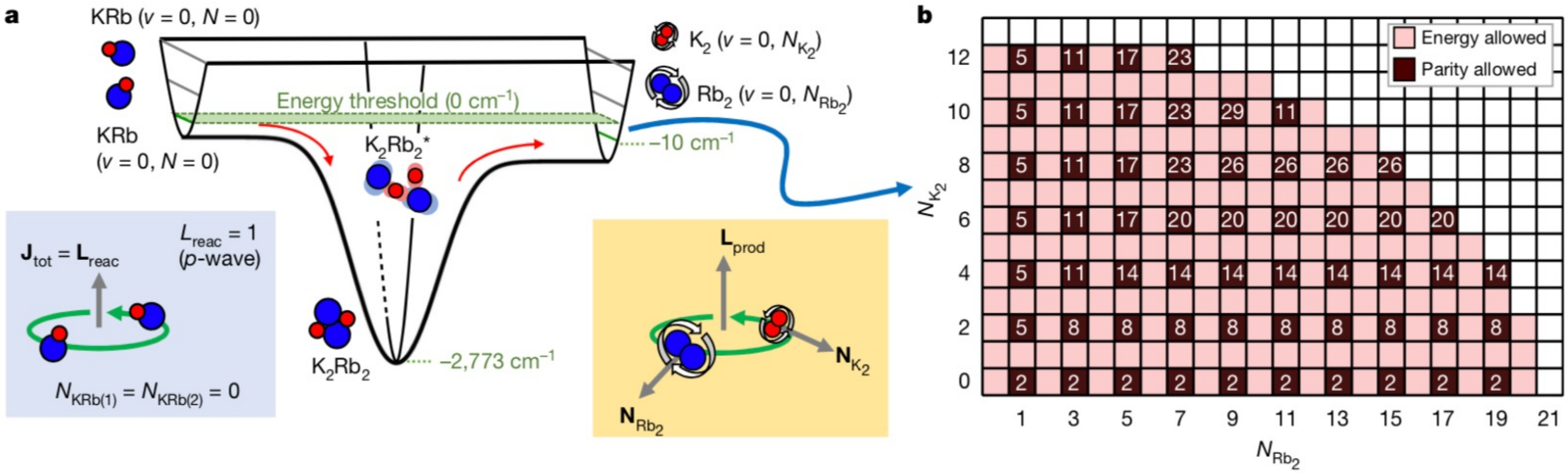
Nature 593, 380 (2021)

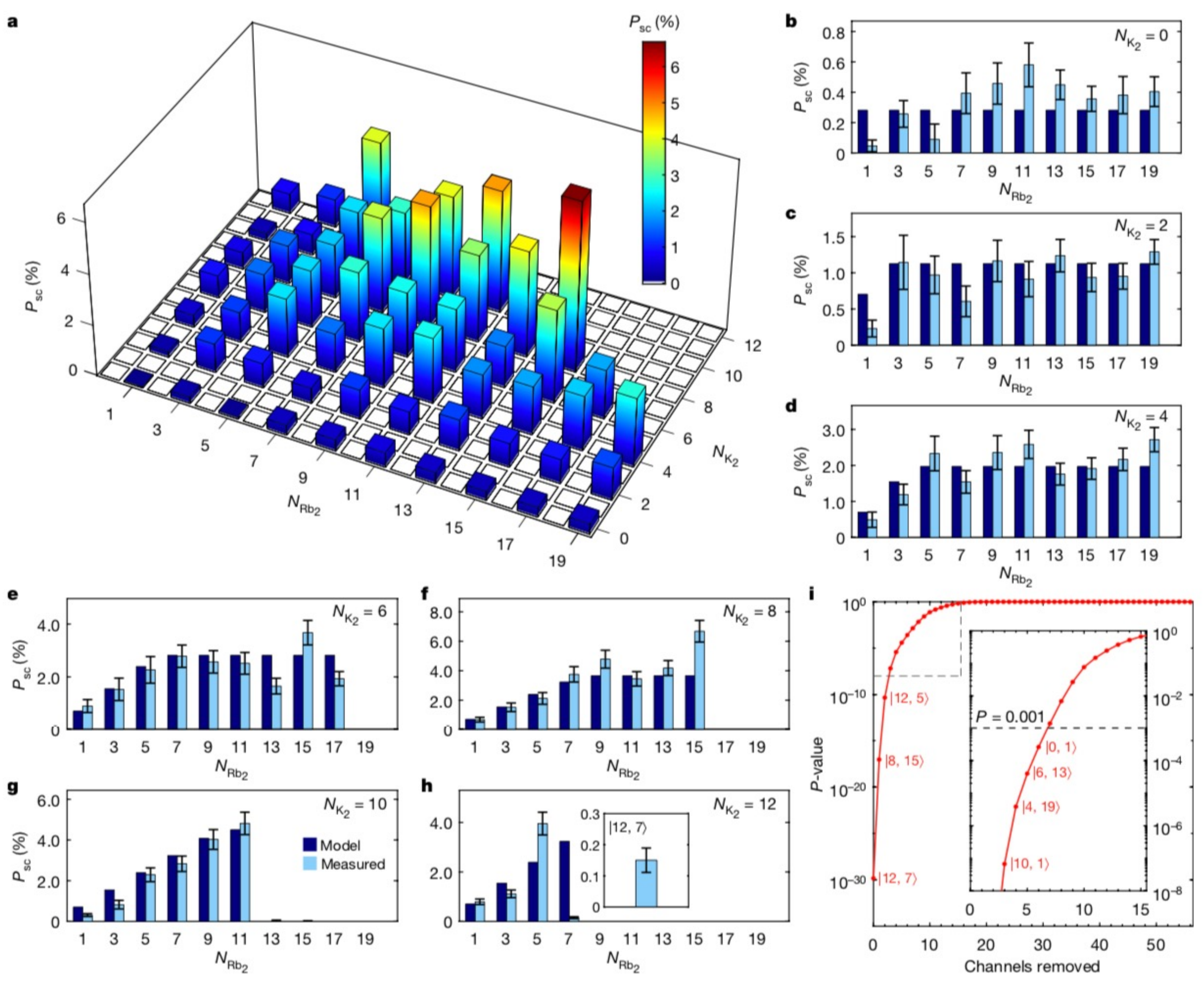
https://doi.org/10.1038/s41586-021-03459-6

Received: 12 January 2021

Accepted: 16 March 2021

Yu Liu[1,2,3,6,7]✉, Ming-Guang Hu[1,2,3,7], Matthew A. Nichols[1,2,3], Dongzheng Yang[4], Daiqian Xie[4], Hua Guo[5] & Kang-Kuen Ni[1,2,3]✉




a
P_{sc} (%)
N_{Rb_2}
N_{K_2}
b
$N_{K_2} = 0$
c
$N_{K_2} = 2$
d
$N_{K_2} = 4$
e
$N_{K_2} = 6$
f
$N_{K_2} = 8$
g
$N_{K_2} = 10$
Model
Measured
h
$N_{K_2} = 12$
|12, 7⟩
i
P-value
Channels removed
$P = 0.001$
|12, 5⟩
|8, 15⟩
|12, 7⟩
|0, 1⟩
|6, 13⟩
|4, 19⟩
|10, 1⟩