

KITP Conference on Correlated States in Degenerate Atomic Gases, April 25, 2007

Some Perspectives on Ultracold
Atomic and Molecular Interactions
and their Control

Paul S. Julienne

Atomic Physics Division, NIST
Joint Quantum Institute, NIST/U. Md

Thanks to

Roman Ciurylo (Torun), Pascal Naidon (NIST), Bo Gao (U. Toledo),

Eite Tiesinga (NIST), Svetlana Kotochigova (Temple/NIST)

Thorsten Köhler (Oxford)

Carlos Sa de Mello (JQI/Georgia Tech), Menderes Iskin (Georgia Tech)

And experimentalist colleagues

M. Kitagawa, K. Enomoto, K. Kasa, Y. Takahashi (Kyoto University)

T. Zelevinsky, M. M. Boyd, A. D. Ludlow, T. Ido, A. Pe'er,

J. Zirbel, S. Ospelkaus, D. Jin, J. Ye (JILA/NIST)

Looking for good students/postdocs
Joint Quantum Institute
NIST / University of Maryland

<http://www.jqi.umd.edu/>
<http://physics.nist.gov/>

Cold atoms and molecules

Widely used in forefront experiments

Bose gases and BEC

Fermi gases, BEC-BCS crossover

Lattices and reduced dimensional structures

Control scattering properties

by static or dynamic electromagnetic fields

depends on specific physical systems available

Complex calculations required

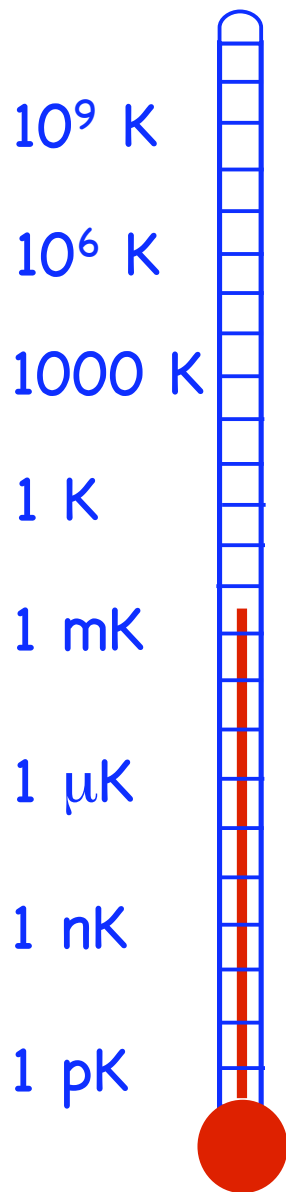
coupled channels scattering

ab initio structure and properties

But remain amenable to simple models

Universal--parameterized by $a(B)$ and mass

Based on long range potentials



Interior of sun

Surface of sun
Room temperature

Outer space (3K)
Cold He

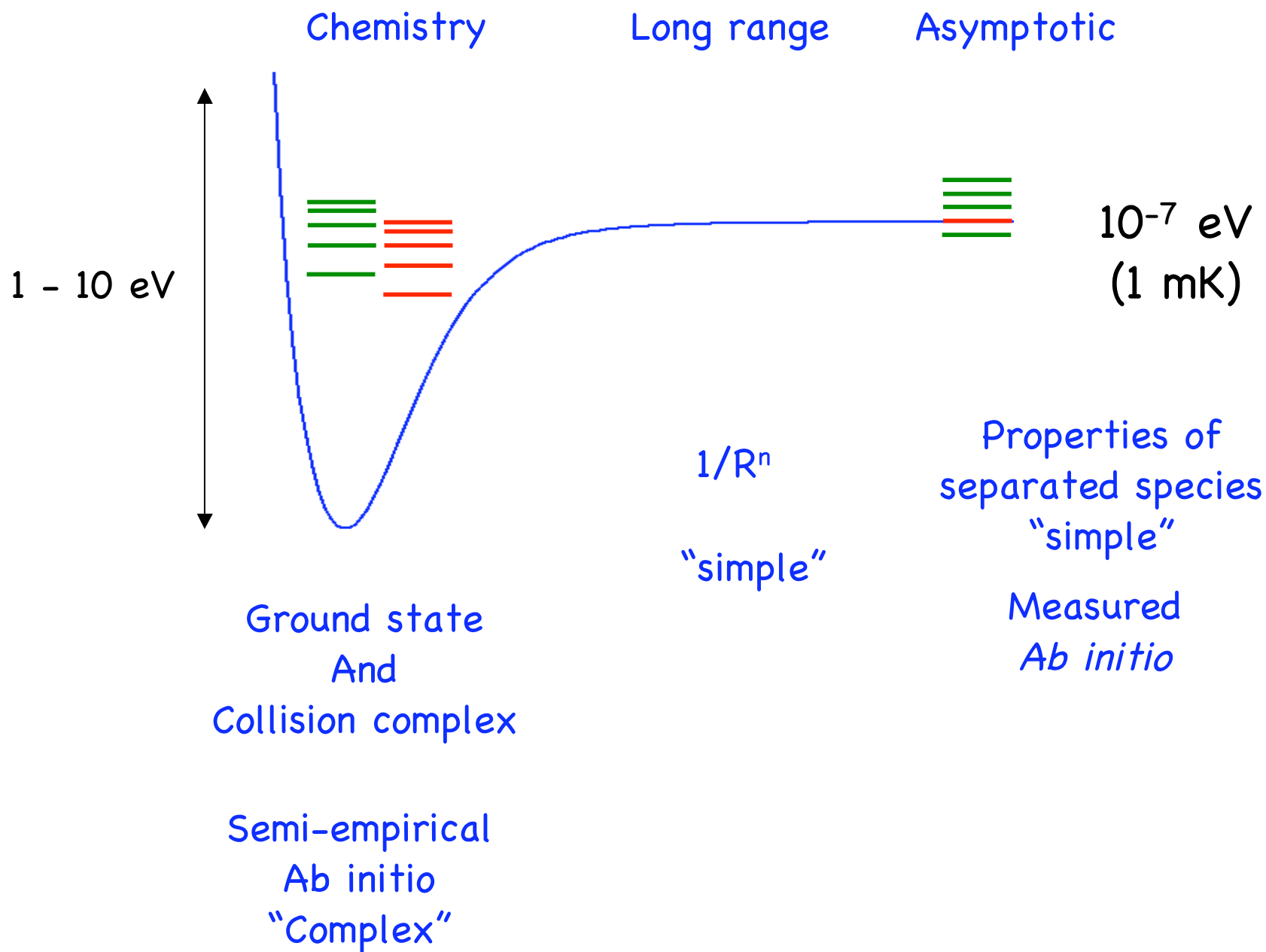
Laser cooled atoms

Atomic clock atoms

Fermionic quantum gases

Bose-Einstein condensates

Molecules
↓
Buffer gas cooling
Decelerated beams
Photoassociated atoms
Feshbach molecules
Molecular BEC



s-wave Threshold Collisions Summary

Complex scattering length $a - ib$
(from exact $E \rightarrow 0$ S-matrix element)

$$\text{Elastic collision } \sigma = 4\pi(a^2 + b^2)$$

$$\text{Inelastic collision } K = \sigma v = (2h/\mu)b$$

$$K_{\text{loss}} = \frac{2h}{\mu}b = 10^{-10} \text{ cm}^3/\text{s} \frac{b(a_0)}{\mu(\text{amu})}$$

Typical values: "Allowed" $b \sim 10\text{-}100 a_0$

"Forbidden" $b \ll 1 a_0$

Upper bound $4b = k^{-1} = \lambda/2\pi$

How fast are inelastic cold collisions (Maxwell-Boltzmann)?

$$\frac{dn}{dt} = -2Kn^2 = -\frac{1}{\tau}n \quad \text{where} \quad \frac{1}{\tau} = 2Kn$$

$$K = \frac{1}{Q_T} \frac{k_B T}{h} \sum_{\ell} (2\ell + 1) \langle |S(E)|^2 \rangle$$

$$\text{where} \quad \frac{1}{Q_T} = \Lambda_T^3 = \left(\frac{h}{2\pi\mu k_B T} \right)^{\frac{3}{2}}$$

Q_T = translational partition function

Λ_T = thermal de Broglie wavelength

Probability $|S|^2 < 1$
Dynamical factor

$$\frac{1}{\tau} = 2Kn = 2 \underbrace{(n\Lambda_T^3)}_{\text{Phase Space density}} \underbrace{\frac{k_B T}{h}}_{\text{Upper bound}} \underbrace{f}_{\text{Dynamics}}$$

$$\frac{k_B T}{h} = 21 \text{ kHz at } 1 \mu\text{K}$$

“Size” of $-C_6/R^6$ van der Waals potential $V(R)$

$$R_{\text{vdw}} = \frac{1}{2} \left(\frac{2\mu C_6}{\hbar^2} \right)^{\frac{1}{4}} \quad \text{or} \quad \bar{a} = \frac{\Gamma(3/4)}{\Gamma(5/4)} R_{\text{vdw}} = 0.956 R_{\text{vdw}}$$

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

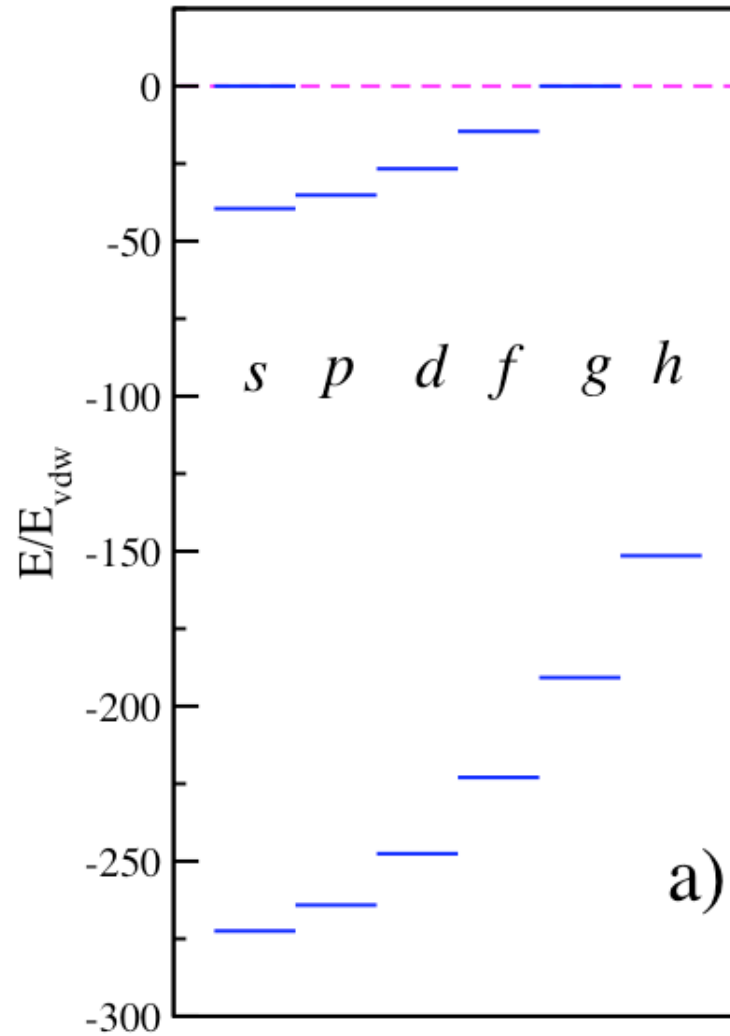
G. F. Gribakin and V. V. Flambaum
Phys. Rev. A 48, 546 (1993)

	$R_{\text{vdw}}(a_0)$	$E_{\text{vdw}}(\text{mK})$
${}^6\text{Li}$	31	29
${}^{40}\text{K}$	65	1.0
${}^{85}\text{Rb}$	83	0.35
${}^{133}\text{Cs}$	101	0.13

See Jones, Lett, Tiesinga, Julienne, Rev. Mod. Phys. 78, 483 (2006)

Bound states from van der Waals theory

$$a = \pm\infty$$



Adapted from Gao, Phys. Rev. A 62, 050702 (2000); Figure from E. Tiesinga

Effective range and bound states of vdW $V(R)$

Effective range expansion of $\eta(E)$

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

$$r_0 = 2.918 \dots \bar{a} \left(1 - 2\frac{\bar{a}}{a} + 2\left(\frac{\bar{a}}{a}\right)^2 \right)$$

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

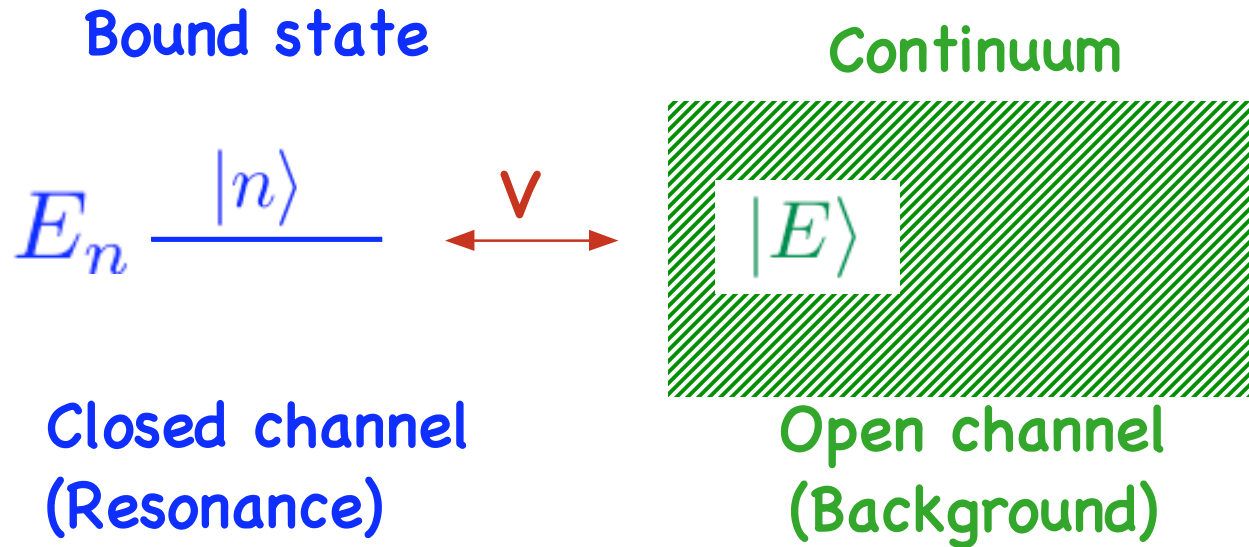
$$E_{-1} = \frac{\hbar^2}{2\mu(a - \bar{a})^2}$$

G. F. Gribakin and V. V. Flambaum
Phys. Rev. A 48, 546 (1993)
Gao, J. Phys. B 37, 4273 (2004)

See P. Naidon, E. Tiesinga, W. F. Mitchell, and P. S. Julienne, "Effective-range description of a Bose gas under strong one- or two-dimensional confinement," N. J. Phys. 9, 19 (2007).

Resonant Scattering Picture

(U. Fano, Phys. Rev. 124, 1866 (1961))



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

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

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

shift δE_n

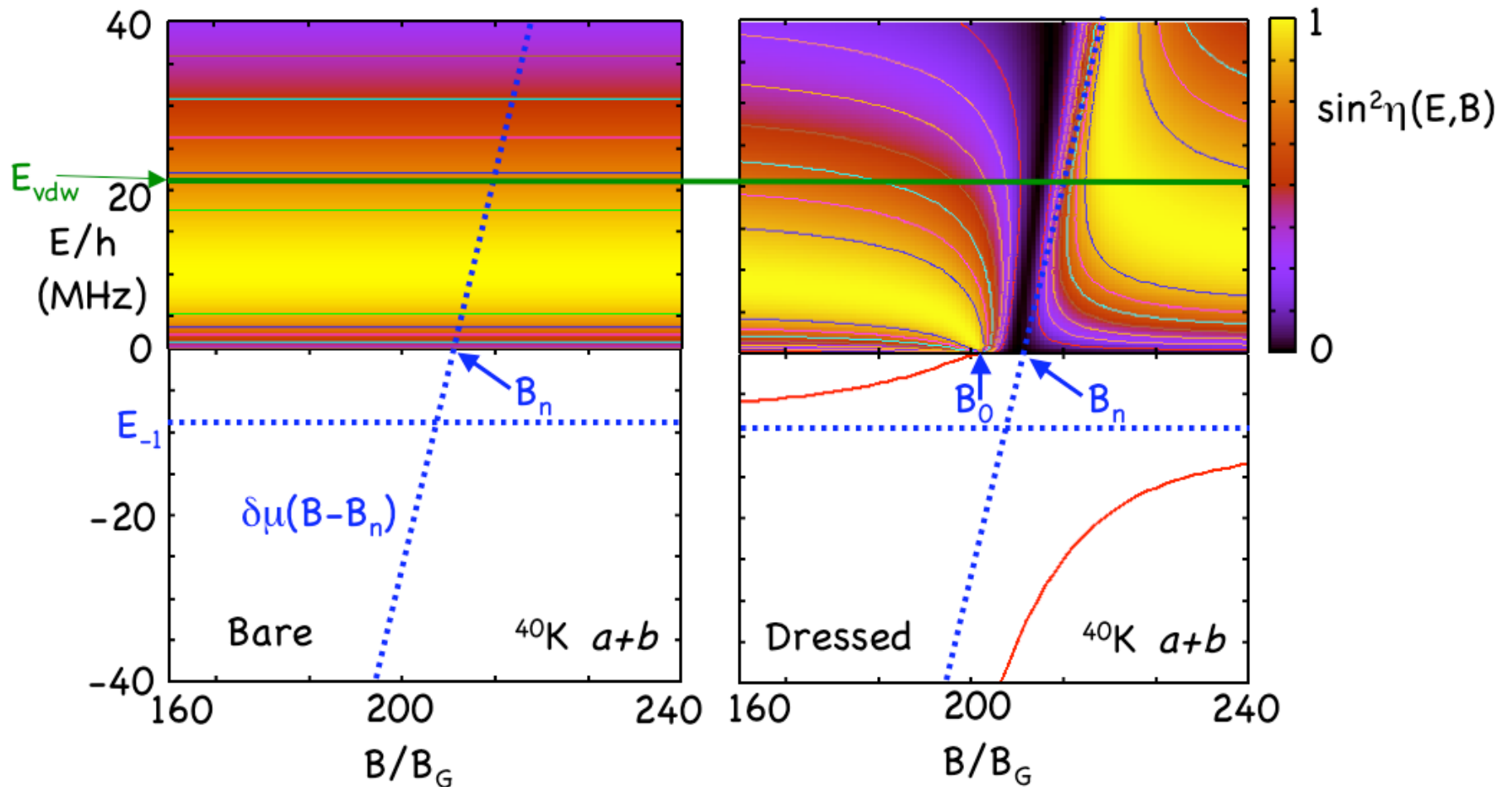
Analytic van der Waals theory reproduces ALL scattering versus E and B in the ultracold domain as compared to full coupled channels calculations.

Julienne and Gao, in *Atomic Physics 20* (AIP), p. 216, or physics/0609013

$$\eta_{\text{res}} = -\tan^{-1} \frac{\frac{1}{2}\Gamma(E)}{E - \delta\mu(B - B_n) - \delta E_n(E)}$$

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

$$\delta E_n(E) = -\frac{1}{2}\bar{\Gamma}\tan\lambda(E)$$



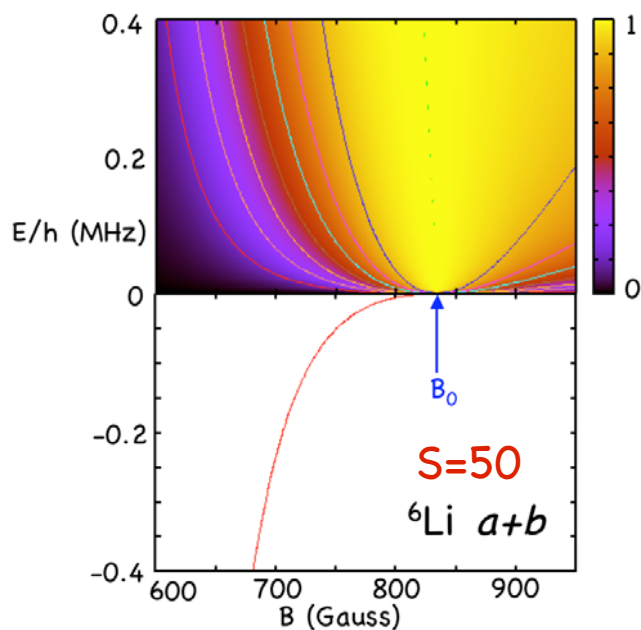
Open or closed channel dominated?

$$S = \frac{a_{bg}}{\bar{a}} \frac{\delta\mu \Delta}{E_{vdW}}$$

Köhler, Goral, Julienne,
Rev. Mod. Phys. 78, 1311 (2006)

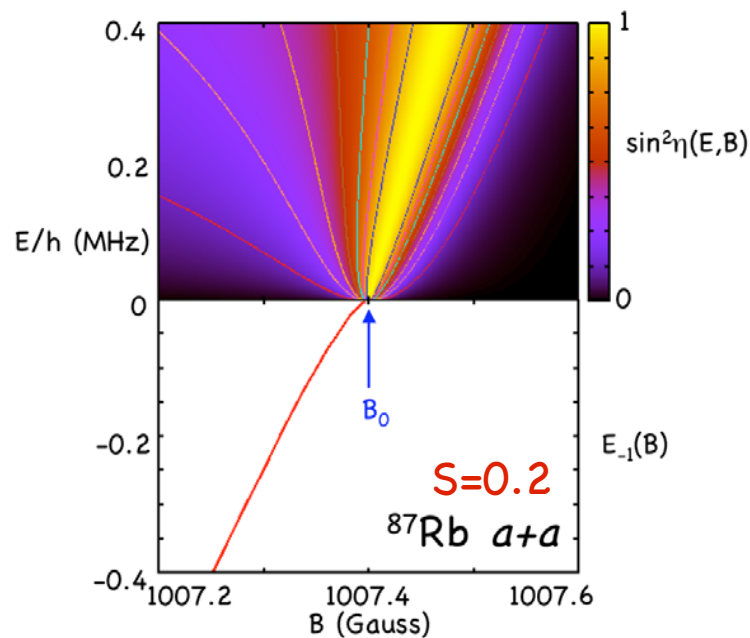
Open: $S \gg 1$
Universal, $Z \ll 1$
over $\approx \Delta$

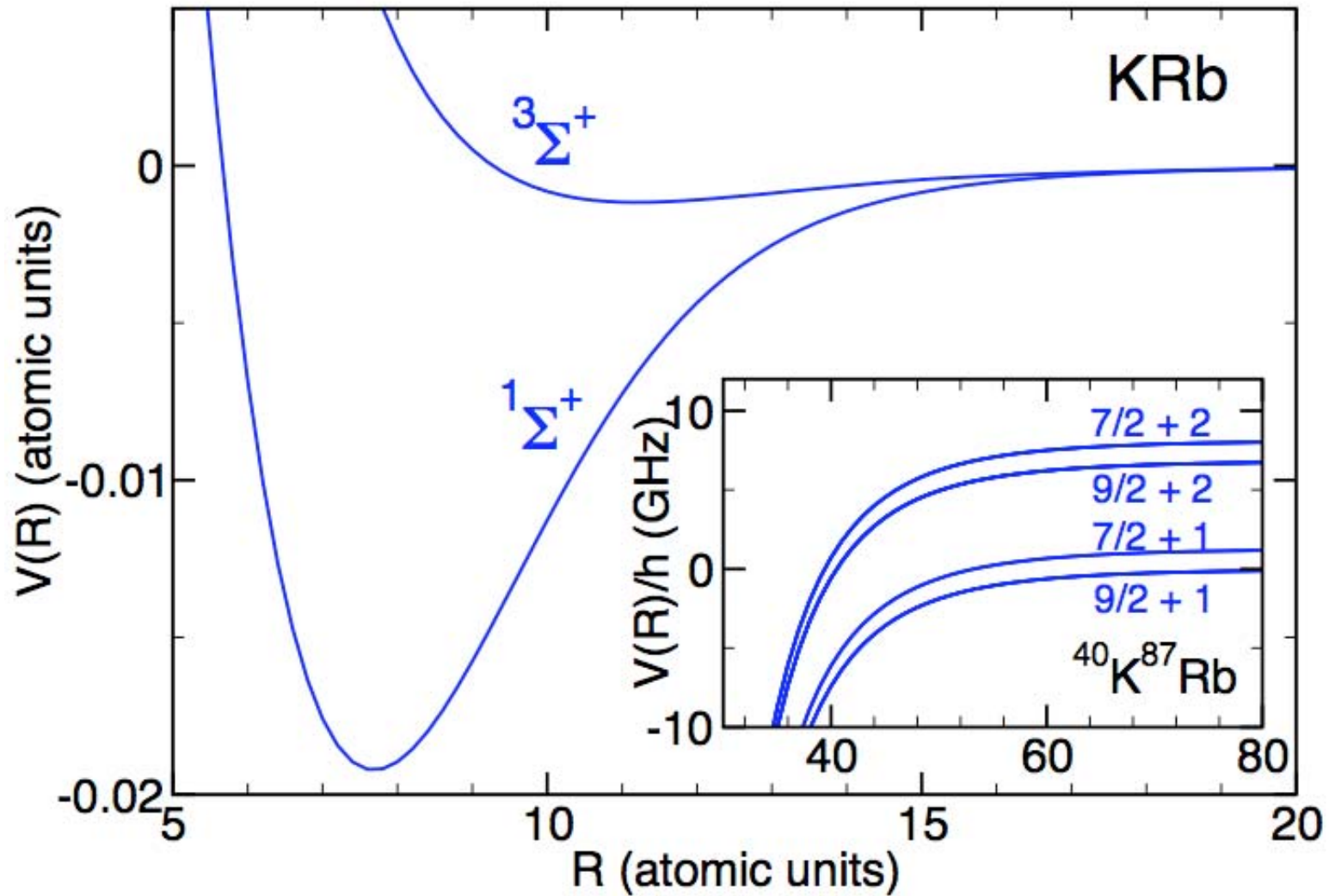
$\Gamma(E) \gg E$ when $E < E_{vdw}$



Closed: $S \ll 1$
Not universal, $Z \approx 1$
over most of Δ

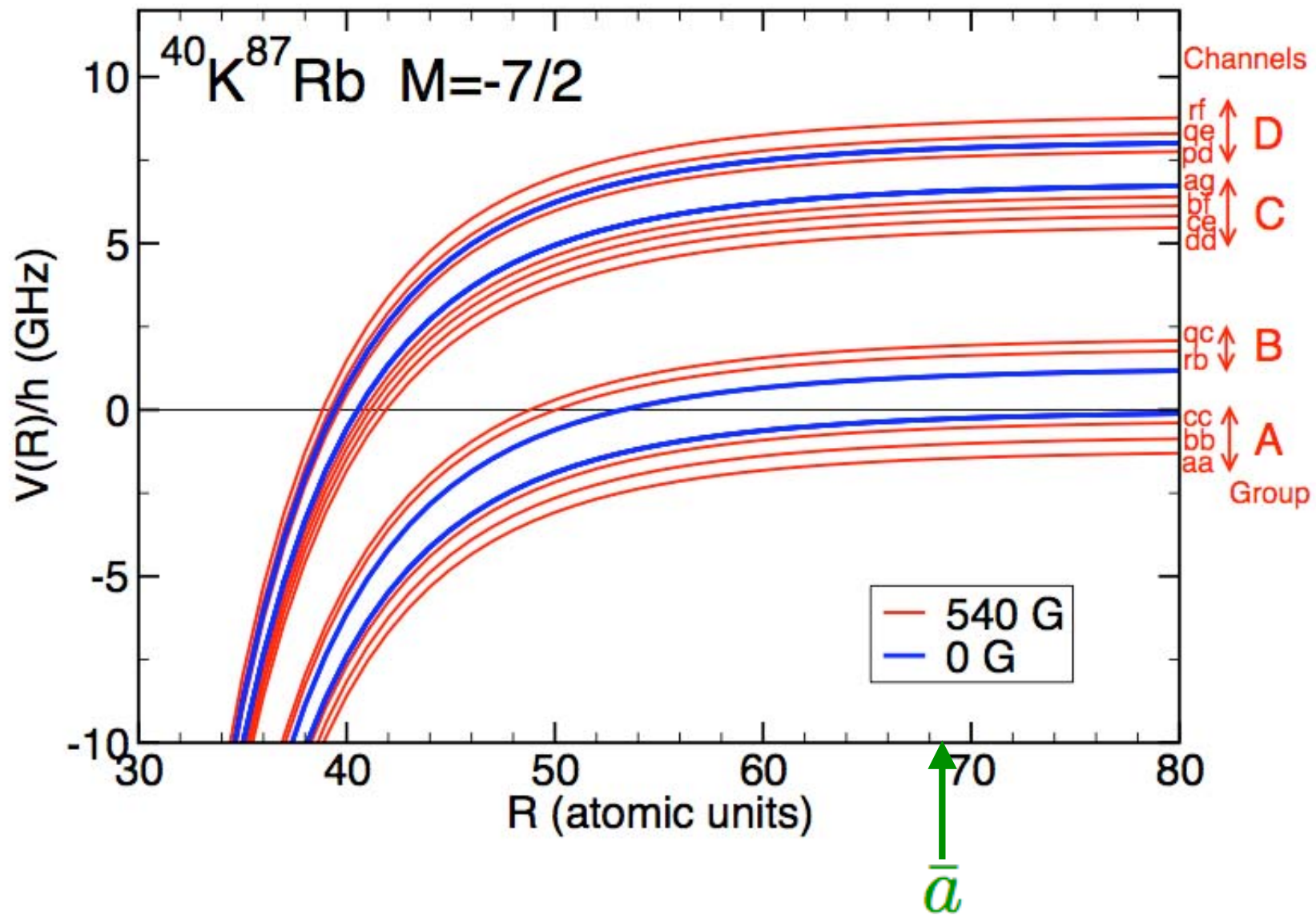
$\Gamma(E) \ll E$ when $E < E_{vdw}$



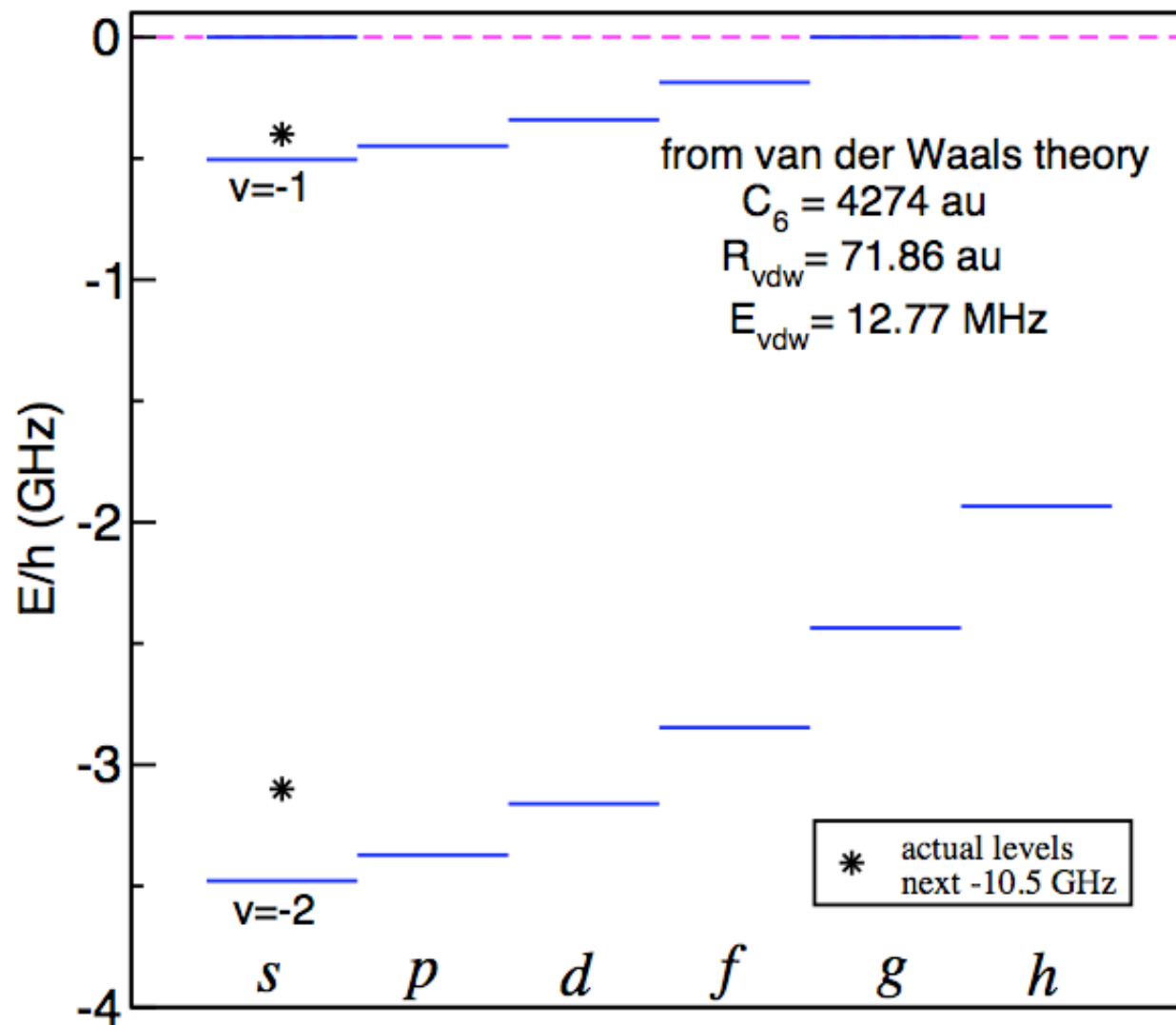


Ab initio: Kotochigova , Julienne, Tiesinga, Phys. Rev. A 68,022501 (2003).

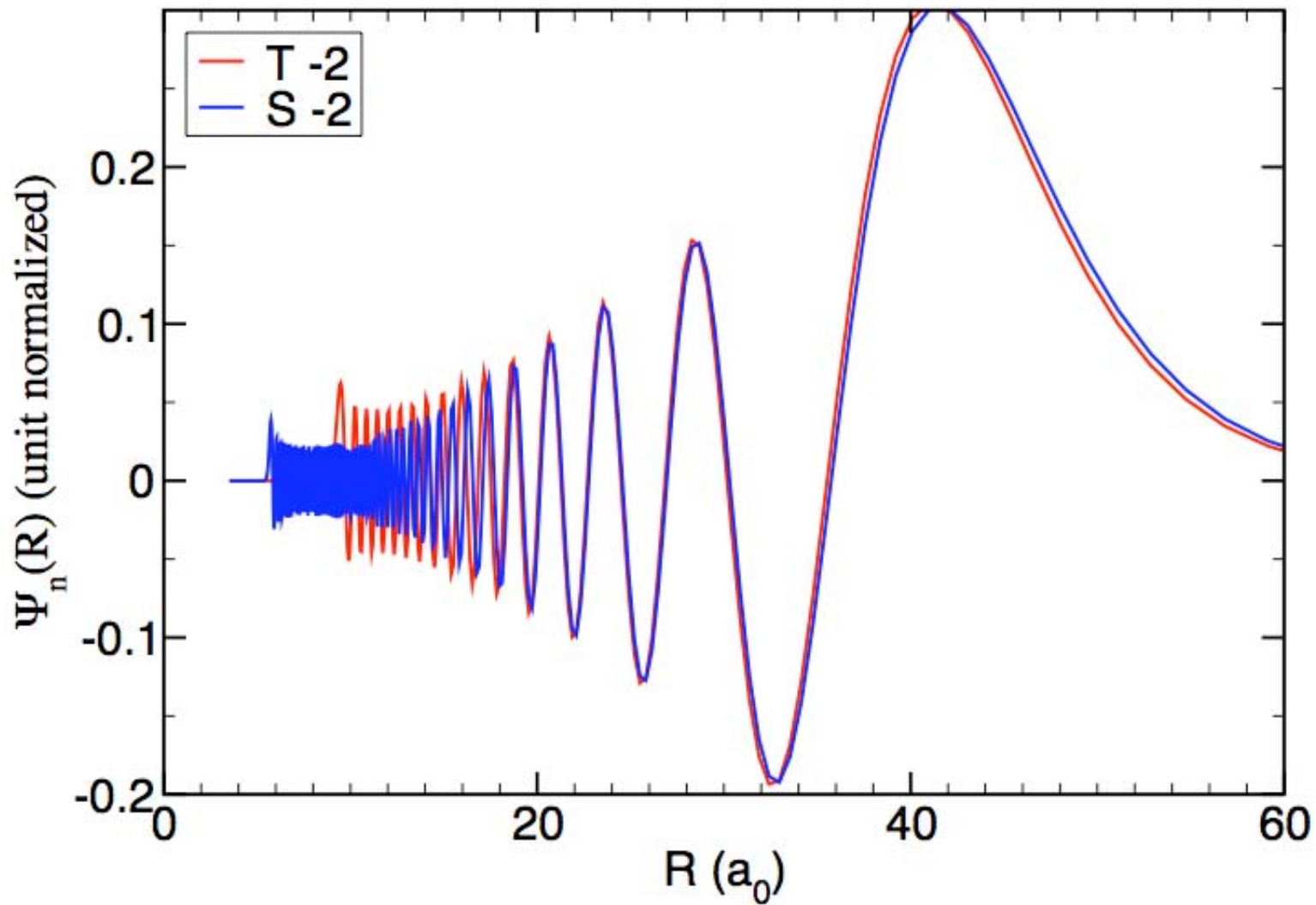
See also Aymar & Dulieu, JCP, 122, 204302(2005)



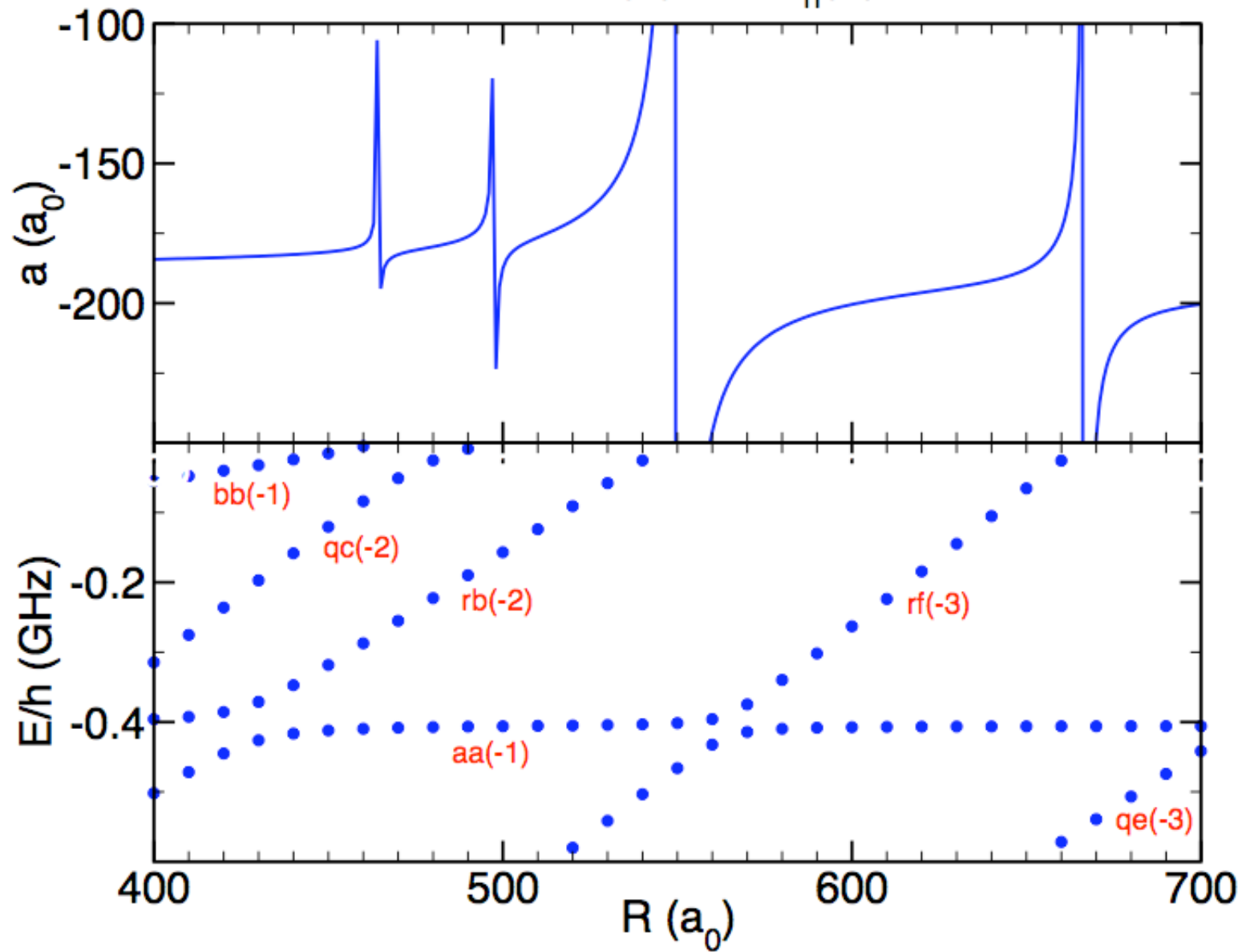
$^{40}\text{K}^{87}\text{Rb}$ energy level "bins"



$^{40}\text{K}^{87}\text{Rb}$ $n=-2$ levels
single channel $\Psi_n(R)$

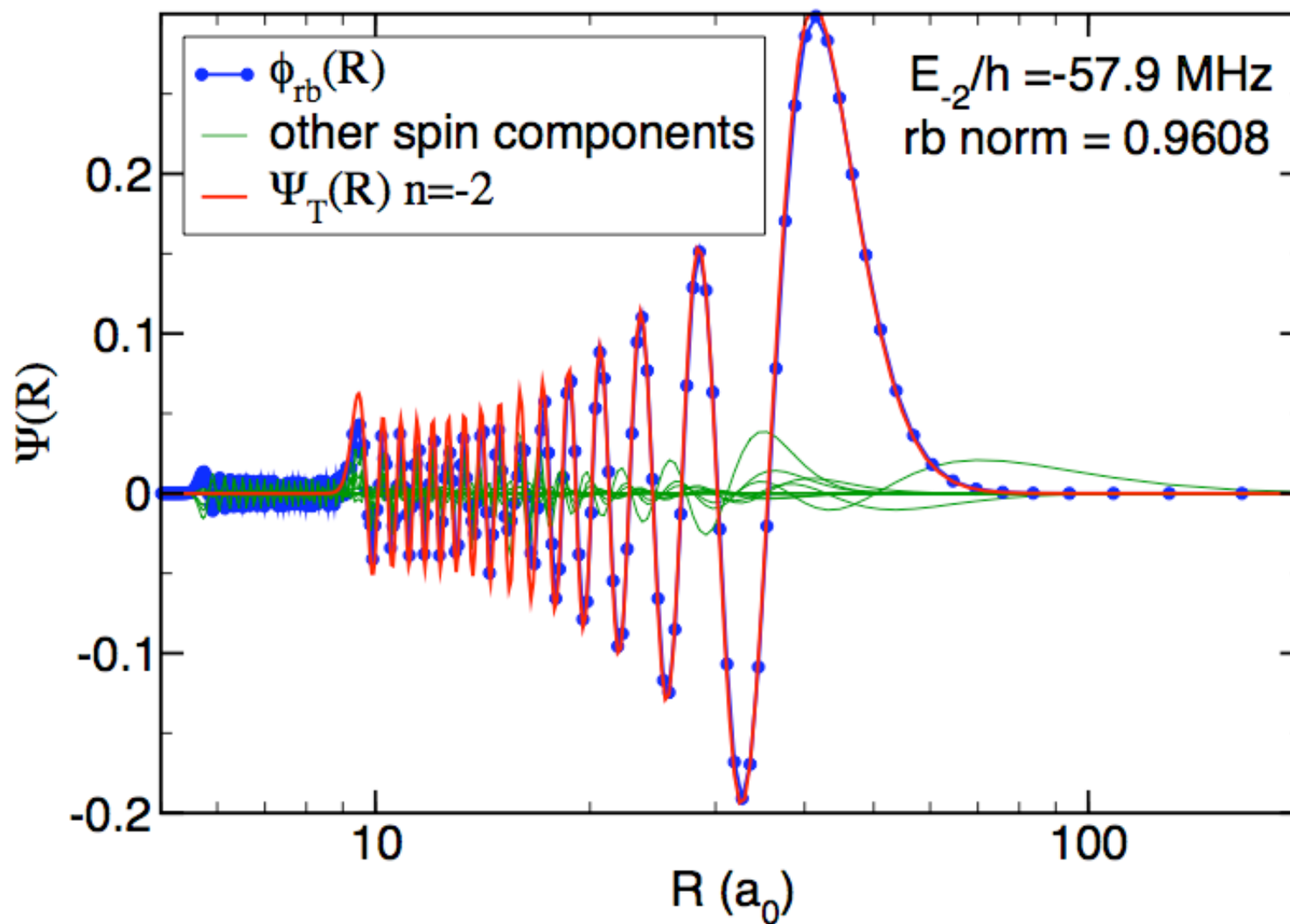


$^{40}\text{K}^{87}\text{Rb}$ $a(B)$ and $E_n(B)$ vs. B

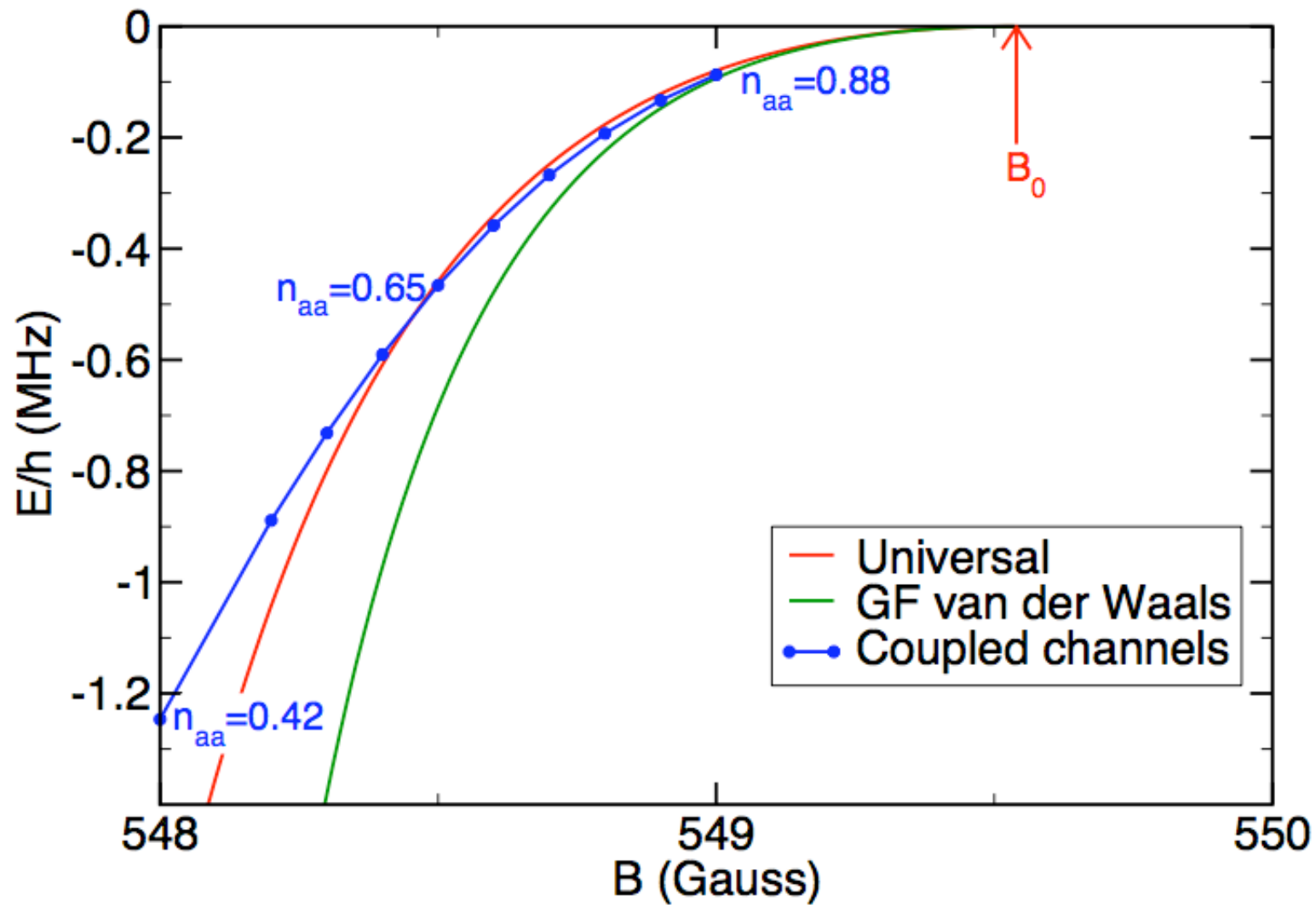


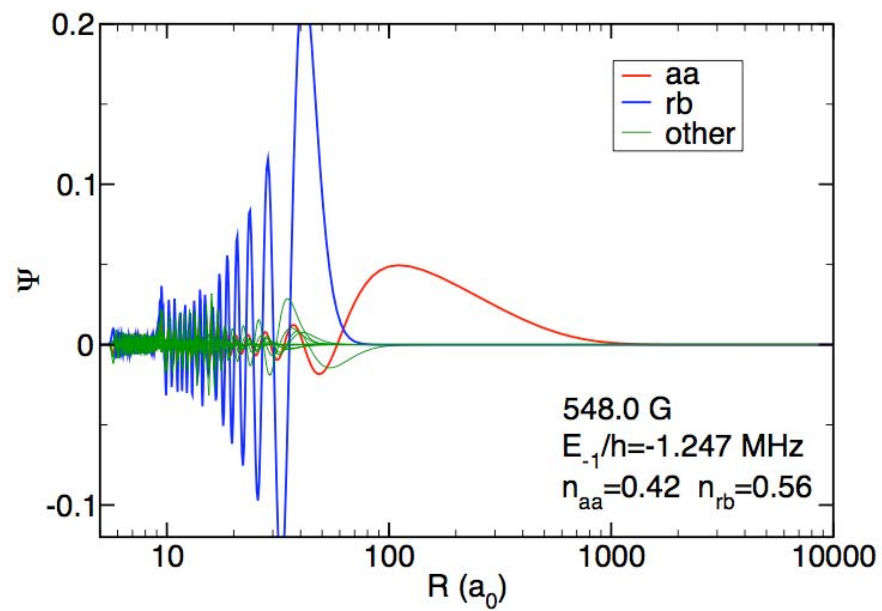
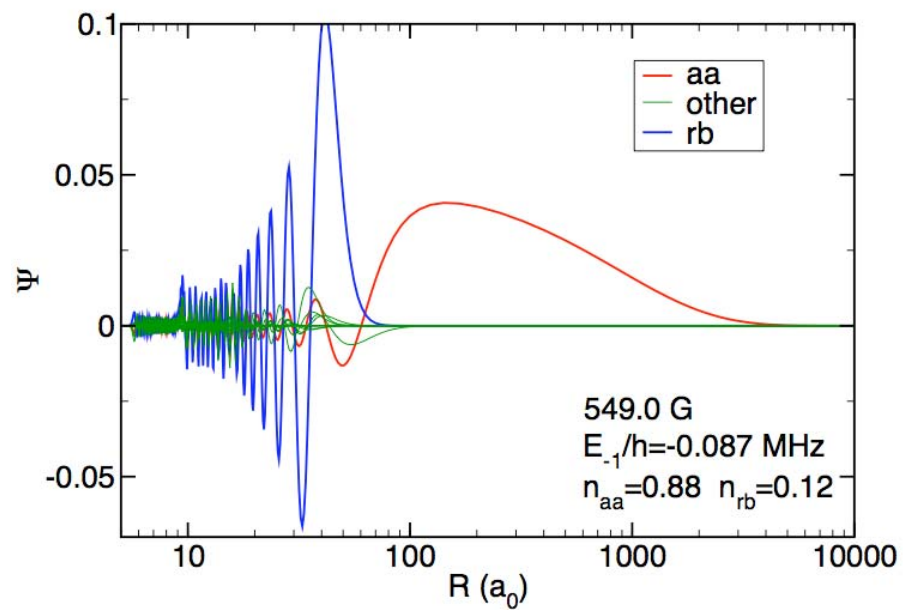
$^{40}\text{K}^{87}\text{Rb}$ rb(-2) level 530 G

Coupled channels calculation with 12 spin channels



$^{40}\text{K}^{87}\text{Rb}$ {aa(s0), rb(-2s0)} M=-7/2 bound state





PERIODIC TABLE
Atomic Properties of the Elements

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

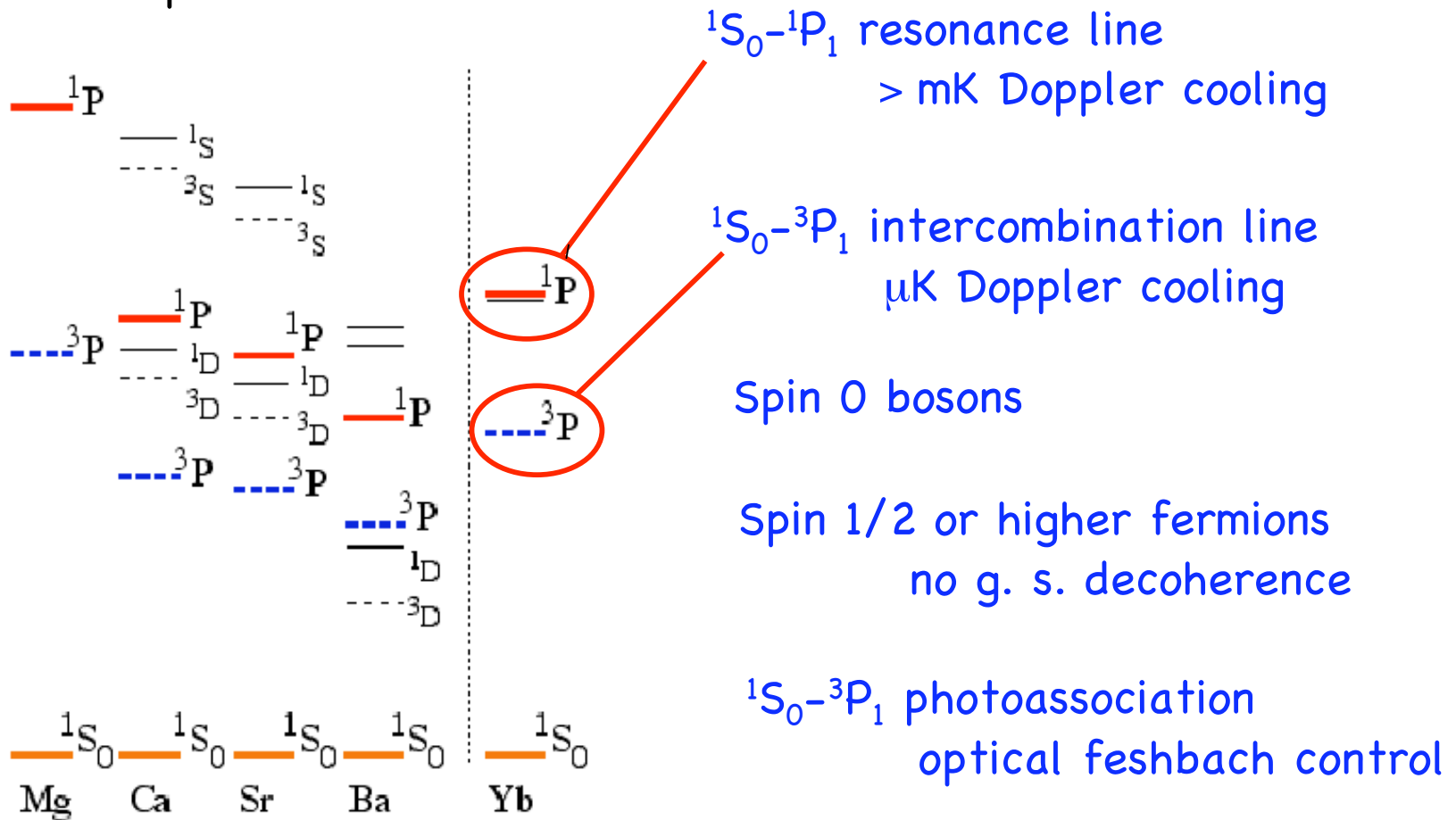
Group II

Ytterbium

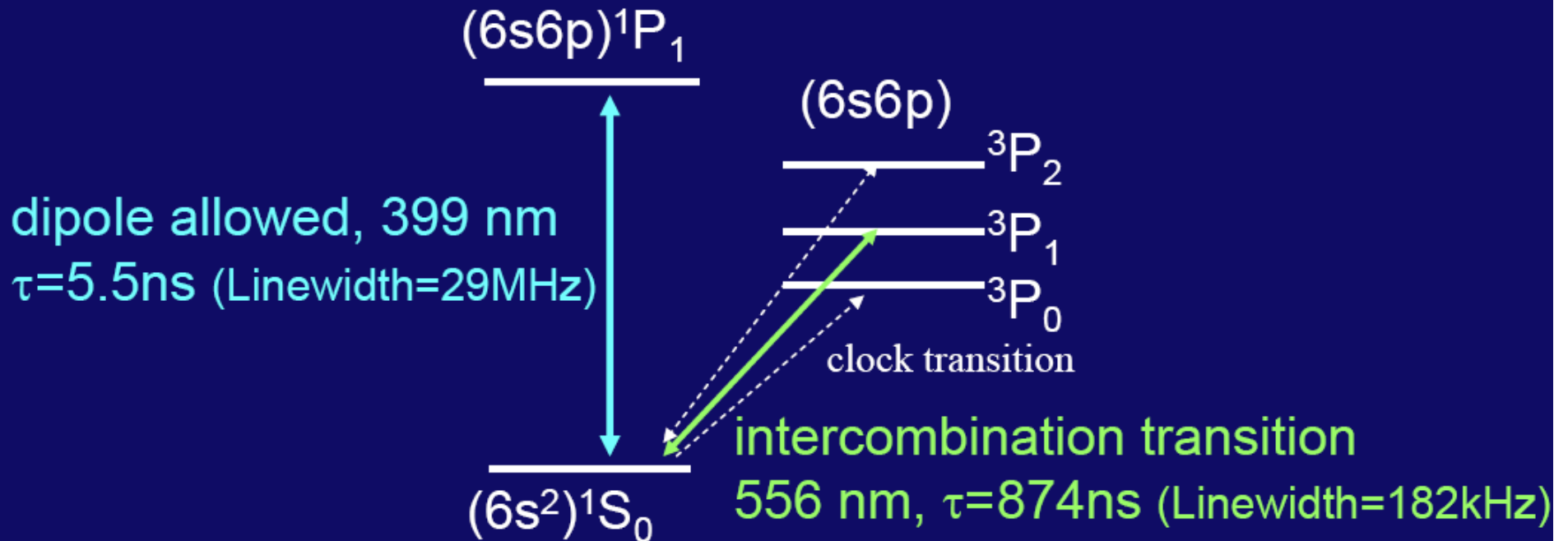
1 IA 1 H Hydrogen 1.00794 1s	2 IIA 2 He Helium 4.002602 1s ²																	18 VIIIA 2 He Helium 4.002602 1s ²					
3 Li Lithium 6.941 1s ² 2s ¹	Be Beryllium 9.012182 1s ² 2s ²																	B Boron 10.811 1s ² 2s ² 2p ¹	C Carbon 12.0107 1s ² 2s ² 2p ²	N Nitrogen 14.0067 1s ² 2s ² 2p ³	O Oxygen 15.9994 1s ² 2s ² 2p ⁴	F Fluorine 18.9984032 1s ² 2s ² 2p ⁵	Ne Neon 20.1797 1s ² 2s ² 2p ⁶
11 Na Sodium 22.989770 [Ne]3s ¹	12 Mg Magnesium 24.3050 [Ne]3s ²																	13 Al Aluminum 26.981538 [Ne]3s ² 3p ¹	14 Si Silicon 28.0855 [Ne]3s ² 3p ²	15 P Phosphorus 30.973761 [Ne]3s ² 3p ³	16 S Sulfur 32.065 [Ne]3s ² 3p ⁴	17 Cl Chlorine 35.453 [Ne]3s ² 3p ⁵	18 Ar Argon 39.948 [Ne]3s ² 3p ⁶
19 K Potassium 39.0983 [Ar]4s ¹	20 Ca Calcium 40.078 [Ar]4s ²	21 Sc Scandium 44.955910 [Ar]3d ¹ 4s ²	22 Ti Titanium 47.867 [Ar]3d ² 4s ²	23 V Vanadium 50.9415 [Ar]3d ³ 4s ²	24 Cr Chromium 51.9961 [Ar]3d ⁵ 4s ¹	25 Mn Manganese 54.938049 [Ar]3d ⁵ 4s ²	26 Fe Iron 55.845 [Ar]3d ⁶ 4s ²	27 Co Cobalt 58.933200 [Ar]3d ⁷ 4s ²	28 Ni Nickel 58.6934 [Ar]3d ⁸ 4s ²	29 Cu Copper 63.546 [Ar]3d ¹⁰ 4s ¹	30 Zn Zinc 65.408 [Ar]3d ¹⁰ 4s ²	31 Ga Gallium 69.723 [Ar]3d ¹⁰ 4s ² 4p ¹	32 Ge Germanium 72.64 [Ar]3d ¹⁰ 4s ² 4p ²	33 As Arsenic 74.92160 [Ar]3d ¹⁰ 4s ² 4p ³	34 Se Selenium 78.96 [Ar]3d ¹⁰ 4s ² 4p ⁴	35 Br Bromine 79.904 [Ar]3d ¹⁰ 4s ² 4p ⁵	36 Kr Krypton 83.796 [Ar]3d ¹⁰ 4s ² 4p ⁶						
37 Rb Rubidium 85.4678 [Kr]5s ¹	38 Sr Strontium 87.62 [Kr]5s ²	39 Y Yttrium 88.90505 [Kr]4d ¹ 5s ²	40 Zr Zirconium 91.224 [Kr]4d ² 5s ²	41 Nb Niobium 92.90638 [Kr]4d ⁴ 5s ¹	42 Mo Molybdenum 95.94 [Kr]4d ⁵ 5s ¹	43 Tc Technetium (98) [Kr]4d ⁵ 5s ²	44 Ru Ruthenium 101.07 [Kr]4d ⁷ 5s ¹	45 Rh Rhodium 102.90550 [Kr]4d ⁸ 5s ¹	46 Pd Palladium 106.42 [Kr]4d ¹⁰	47 Ag Silver 107.8682 [Kr]4d ¹⁰ 5s ¹	48 Cd Cadmium 112.411 [Kr]4d ¹⁰ 5s ²	49 In Indium 114.818 [Kr]4d ¹⁰ 5s ² 5p ¹	50 Sn Tin 118.710 [Kr]4d ¹⁰ 5s ² 5p ²	51 Sb Antimony 121.750 [Kr]4d ¹⁰ 5s ² 5p ³	52 Te Tellurium 127.60 [Kr]4d ¹⁰ 5s ² 5p ⁴	53 I Iodine 126.90447 [Kr]4d ¹⁰ 5s ² 5p ⁵	54 Xe Xenon 131.293 [Kr]4d ¹⁰ 5s ² 5p ⁶						
55 Cs Cesium 132.90545 [Xe]6s ¹	56 Ba Barium 137.327 [Xe]6s ²	72 Hf Hafnium 178.49 [Xe]4f ¹⁴ 5d ² 6s ²	73 Ta Tantalum 180.9479 [Xe]4f ¹⁴ 5d ³ 6s ²	74 W Tungsten 183.84 [Xe]4f ¹⁴ 5d ⁴ 6s ²	75 Re Rhenium 186.207 [Xe]4f ¹⁴ 5d ⁵ 6s ²	76 Os Osmium 190.23 [Xe]4f ¹⁴ 5d ⁶ 6s ²	77 Ir Iridium 192.217 [Xe]4f ¹⁴ 5d ⁷ 6s ²	78 Pt Platinum 195.078 [Xe]4f ¹⁴ 5d ⁹ 6s ¹	79 Au Gold 196.96657 [Xe]4f ¹⁴ 5d ¹⁰ 6s ¹	80 Hg Mercury 200.59 [Xe]4f ¹⁴ 5d ¹⁰ 6s ²	81 Tl Thallium 204.3833 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ¹	82 Pb Lead 207.2 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ²	83 Bi Bismuth 208.98038 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ³	84 Po Polonium (209) [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁴	85 At Astatine (210) [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁵	86 Rn Radon (222) [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁶							
87 Fr Francium (223) [Rn]7s ¹	88 Ra Radium (226) [Rn]7s ²	104 Rf Rutherfordium (261) [Rn]5f ¹⁴ 6d ² 7s ²	105 Db Dubnium (262) [Rn]5f ¹⁴ 6d ³ 7s ²	106 Sg Seaborgium (266) [Rn]5f ¹⁴ 6d ⁴ 7s ²	107 Bh Bohrium (264) [Rn]5f ¹⁴ 6d ⁵ 7s ²	108 Hs Hassium (277) [Rn]5f ¹⁴ 6d ⁶ 7s ²	109 Mt Meitnerium (268) [Rn]5f ¹⁴ 6d ⁷ 7s ²	110 Uun Ununium (281) [Rn]5f ¹⁴ 6d ⁸ 7s ²	111 Uuu Unununium (272) [Rn]5f ¹⁴ 6d ⁹ 7s ²	112 Uub Ununbium (285) [Rn]5f ¹⁴ 6d ¹⁰ 7s ²	114 Uuq Ununquadium (289) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ²	116 Uuh Ununhexium (293) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁴	118 Uuo Ununoctium (294) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁶										
		Lanthanides										Actinides											
		57 La Lanthanum 138.9055 [Xe]5d ¹ 6s ²	58 Ce Cerium 140.90765 [Xe]4f ¹ 5d ¹ 6s ²	59 Pr Praseodymium 140.90765 [Xe]4f ³ 6s ²	60 Nd Neodymium 144.24 [Xe]4f ⁴ 6s ²	61 Pm Promethium (145) [Xe]4f ⁵ 6s ²	62 Sm Samarium 150.36 [Xe]4f ⁶ 6s ²	63 Eu Europium 151.964 [Xe]4f ⁷ 6s ²	64 Gd Gadolinium 157.25 [Xe]4f ⁷ 5d ¹ 6s ²	65 Tb Terbium 158.92534 [Xe]4f ⁹ 6s ²	66 Dy Dysprosium 162.500 [Xe]4f ¹⁰ 6s ²	67 Ho Holmium 164.93032 [Xe]4f ¹¹ 6s ²	68 Er Erbium 167.259 [Xe]4f ¹² 6s ²	69 Tm Thulium 168.9342 [Xe]4f ¹³ 6s ²	70 Yb Ytterbium 173.04 [Xe]4f ¹⁴ 6s ²	71 Lu Lutetium 174.967 [Xe]4f ¹⁴ 5d ¹ 6s ²							
		89 Ac Actinium (227) [Rn]5f ⁷ 6d ¹ 7s ²	90 Th Thorium 232.0381 [Rn]6d ² 7s ²	91 Pa Protactinium 231.03688 [Rn]5f ² 6d ¹ 7s ²	92 U Uranium 238.02891 [Rn]5f ³ 6d ¹ 7s ²	93 Np Neptunium (237) [Rn]5f ⁴ 6d ¹ 7s ²	94 Pu Plutonium (244) [Rn]5f ⁶ 7s ²	95 Am Americium (247) [Rn]5f ⁷ 7s ²	96 Cm Curium (247) [Rn]5f ⁷ 6d ¹ 7s ²	97 Bk Berkelium (247) [Rn]5f ⁹ 7s ²	98 Cf Californium (251) [Rn]5f ¹⁰ 7s ²	99 Es Einsteinium (252) [Rn]5f ¹¹ 7s ²	100 Fm Fermium (257) [Rn]5f ¹² 7s ²	101 Md Mendelevium (258) [Rn]5f ¹³ 7s ²	102 No Nobelium (259) [Rn]5f ¹⁴ 7s ²	103 Lr Lawrencium (262) [Rn]5f ¹⁴ 7s ² 7p ¹							

Atomic Number: 58
Ground-state Level: $4f^1$
Symbol: **Ce**
Name: Cerium
Atomic Weight: 140.116
Ground-state Configuration: $[Xe]4f^1 5s^2$
Ionization Energy (eV): 5.5387

Group II Atoms



Level Diagram of Yb



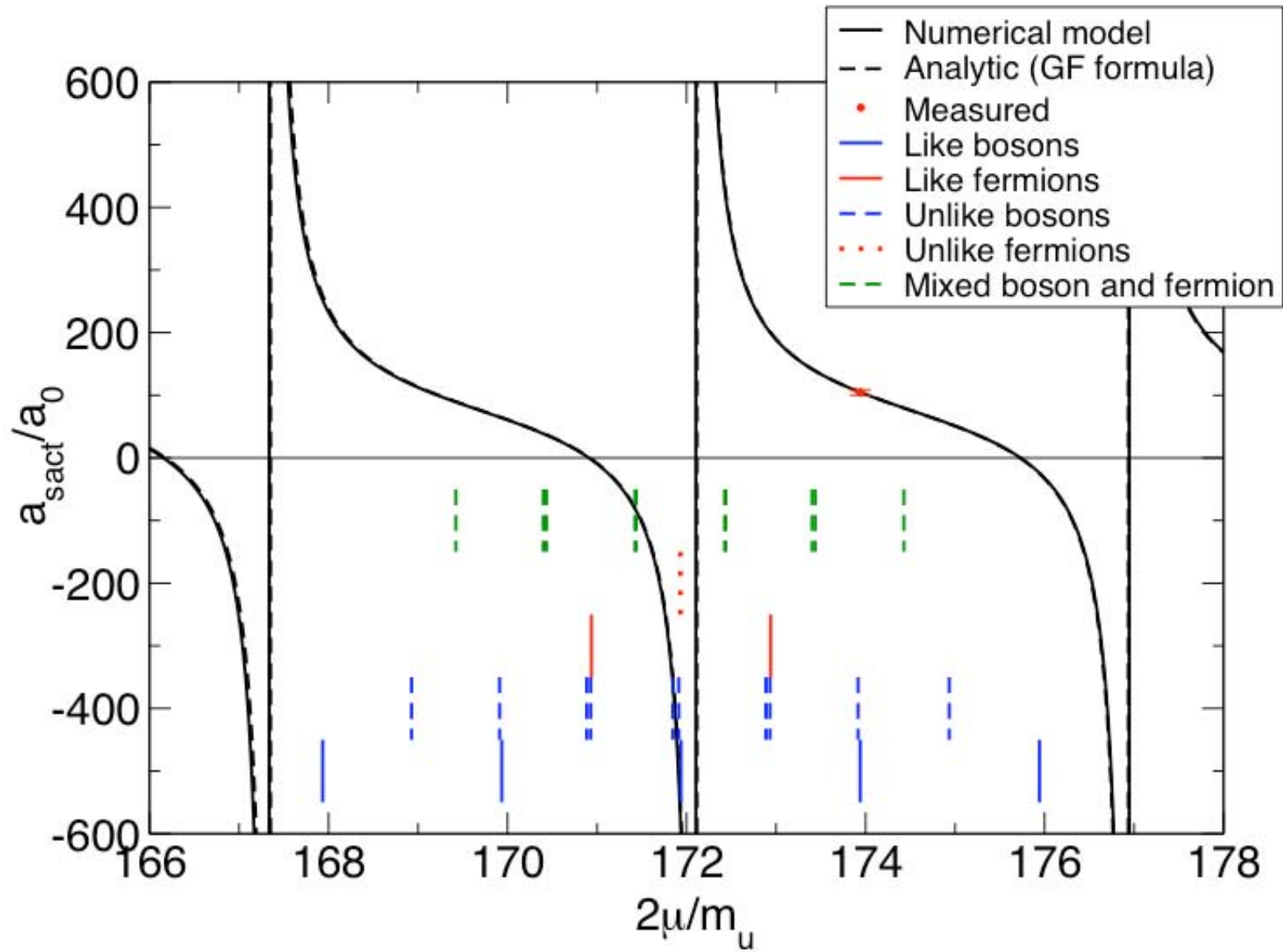
From Enomoto et al

Mass number	168	170	171	172	173	174	176
Nuclear spin <i>i</i>	0	0	1/2	0	5/2	0	0
Abundance(%)	0.13	3.05	14.3	21.9	16.2	31.8	12.7

Scattering lengths for Yb ground state model (in a_0 units)

	168	170	171	172	173	174	176
168	252(6)	117(1)	89(1)	65(1)	39(1)	2(2)	-360(30)
170	117	64(1)	37(1)	-2(2)	-81(4)	-520(50)	209(4)
171	89	37	-3(2)	-84(5)	-580(60)	430(20)	142(2)
172	65	-2	-84	-600(60)	420(20)	201(3)	106(1)
173	39	-81	-580	420	199(3)	139(2)	80(1)
174	2	-520	430	201	139	105(1)	55(1)
176	-360	209	142	106	80	55	-24(2)

Variation of scattering length with mass



Model: LJ 6-12 + C_8 van der Waals
 1 potential + reduced mass

$C_6=1932(4)$ au $C_8=1.9(5)\times 10^5$ Exactly 72 bound states in $^{174}\text{Yb}_2$

Isotope	vib, rot	Eb [MHz]	Error [MHz]	Eb [MHz]	Dev [MHz]
N	176 v=1,J=0	-70.404	0.011	-70.405	-0.001
	v=1,J=2	-37.142	0.013	-37.118	0.024
C_6	174 v=1,J=0	-10.612	0.038	-10.642	-0.030
	v=2,J=0	-325.607	0.018	-325.607	0.000
C_8	v=2,J=2	-268.575	0.021	-268.576	-0.001
	173 v=1,J=0	-1.539	0.074	-1.613	-0.074
	172 v=1,J=0	-123.269	0.026	-123.349	-0.080
	v=1,J=2	-81.786	0.019	-81.879	-0.093
	171 v=1,J=0	-64.418	0.040	-64.548	-0.130
	v=1,J=2	-31.302	0.050	-31.392	-0.090
	170 v=1,J=0	-27.661	0.023	-27.755	-0.094
	v=1,J=2	-3.651	0.026	-3.683	-0.032

Gribakin and Flambaum

Phys. Rev. A 48, 546 (1993)

$$a = \bar{a} \left(1 - \tan \left(\Phi - \frac{\pi}{8} \right) \right)$$

$$\bar{a} = \frac{1}{2^{3/2}} \frac{\Gamma(3/4)}{\Gamma(5/4)} \left(\frac{2\mu C_6}{\hbar^2} \right)^{1/4}$$

$$\Phi = \int_{r_{in}}^{\infty} \left(\frac{2\mu}{\hbar^2} (-V(R)) \right)^{1/2} dR$$

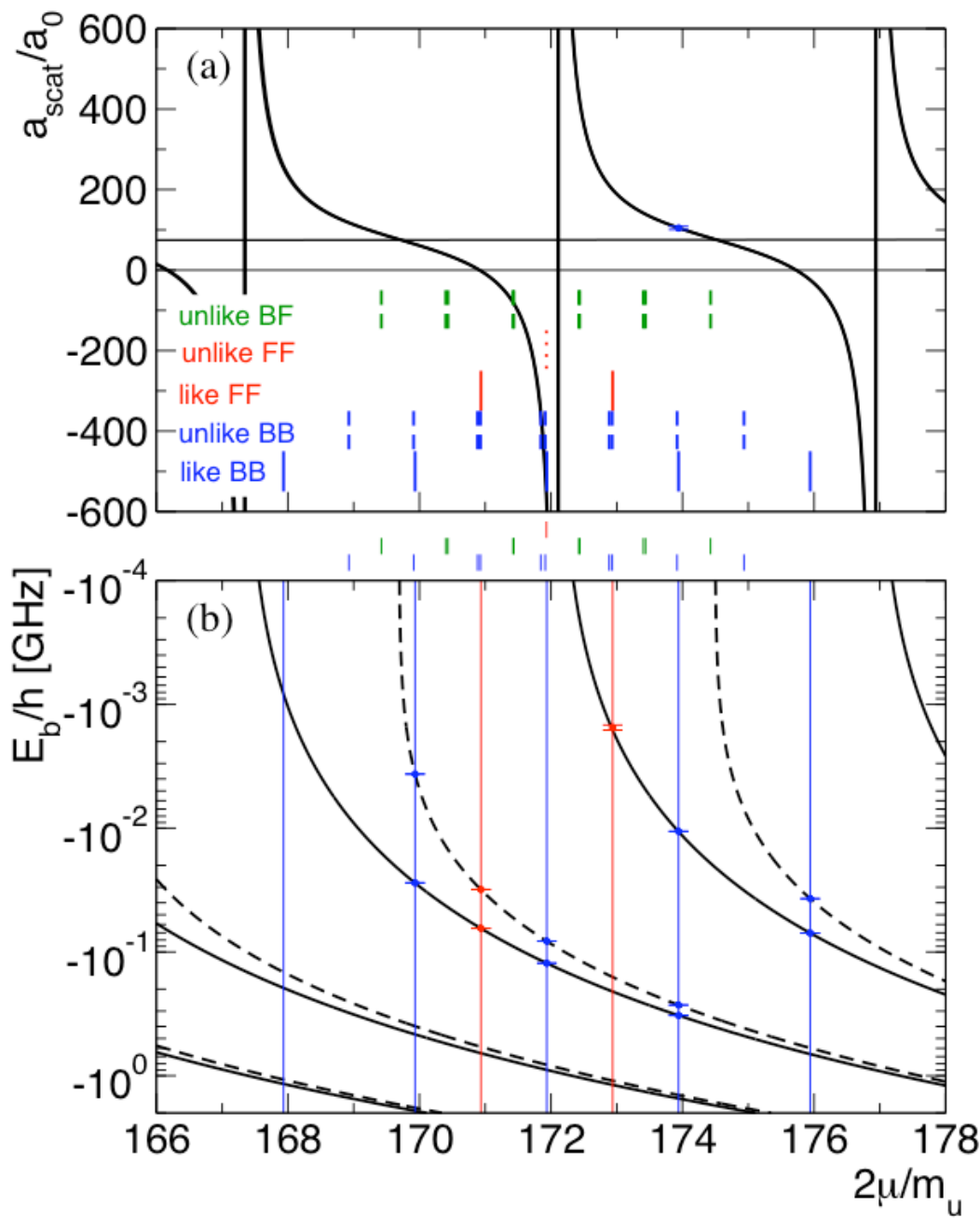
$$\text{Number of bound states in } V(R) = \text{Int} \left[\frac{\Phi}{\pi} - \frac{5}{8} \right] + 1$$

Pure van der Waals theory

(GF and B. Gao)

$$V(R) = \infty \text{ for } 0 < R \leq R_{in}$$

$$V(R) = -\frac{C_6}{R^6} \text{ for } R_{in} < R \leq \infty$$



Scattering
length

Bound
states

Species	Spin	% Abundance
---------	------	-------------

^{84}Sr	0	0.56
------------------	---	------

^{86}Sr	0	9.86
------------------	---	------

^{87}Sr	9/2	7.00
------------------	-----	------

^{88}Sr	0	82.58
------------------	---	-------

^{196}Hg	0	0.15
-------------------	---	------

^{198}Hg	0	9.98
-------------------	---	------

^{199}Hg	1/2	16.87
-------------------	-----	-------

^{200}Hg	0	23.10
-------------------	---	-------

^{201}Hg	3/2	13.19
-------------------	-----	-------

^{202}Hg	0	29.86
-------------------	---	-------

^{204}Hg	0	6.87
-------------------	---	------

^{130}Ba	0	0.11
-------------------	---	------

^{132}Ba	0	0.10
-------------------	---	------

^{134}Ba	0	2.42
-------------------	---	------

^{135}Ba	3/2	6.59
-------------------	-----	------

^{136}Ba	0	7.85
-------------------	---	------

^{137}Ba	3/2	11.23
-------------------	-----	-------

^{138}Ba	0	71.71
-------------------	---	-------