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Some Perspectives on Ultracold Atomic and Molecular Interactions and their Control

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

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

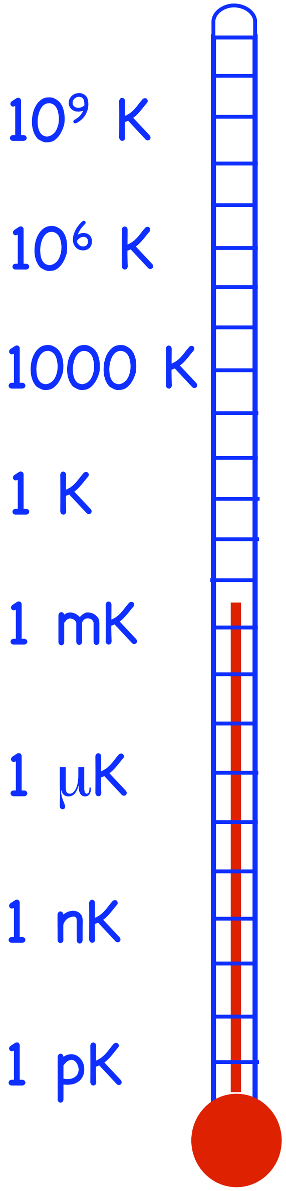
Cold atoms and molecules

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

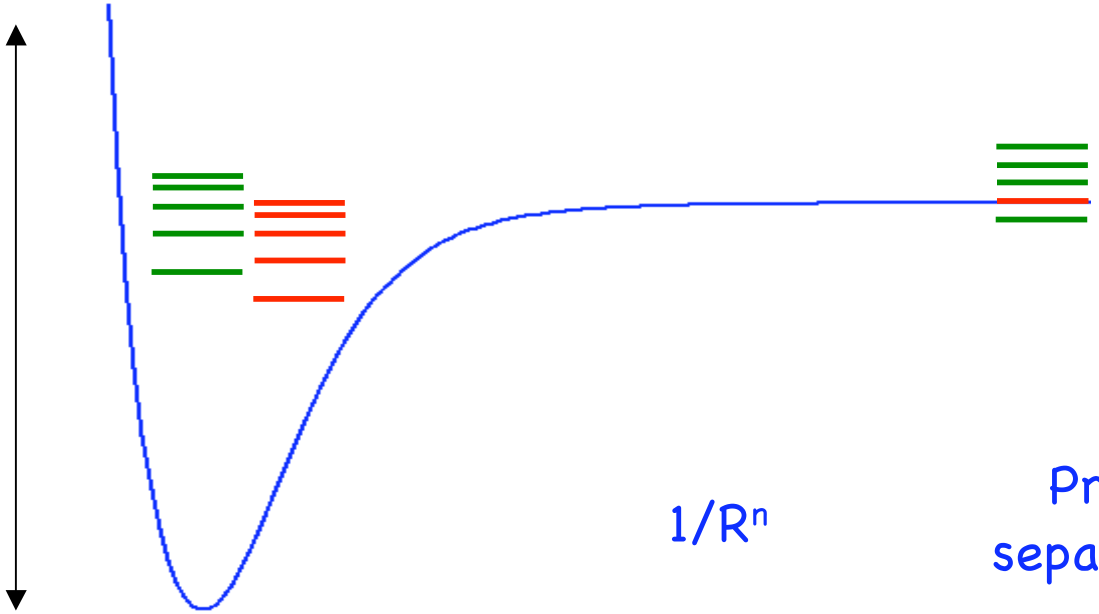
Feshbach molecules

Molecular BEC

Chemistry

Long range

Asymptotic



1 - 10 eV

10^{-7} eV
(1 mK)

Ground state
And
Collision complex

Semi-empirical
Ab initio
"Complex"

$1/R^n$

"simple"

Properties of
separated species
"simple"

Measured
Ab initio

s-wave Threshold Collisions Summary

Complex scattering length $a - ib$

(from exact E->0 S-matrix element)

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

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

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

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)?

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

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

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

Q_T = translational partition function

Λ_T = thermal de Broglie wavelength

Probability $|S|^2 < 1$

Dynamical factor

$$\frac{1}{\tau} = 2Kn = 2\,(n\Lambda_T^3)\,\frac{k_B T}{h}\,f$$

Phase Space density

Upper bound

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)

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

or

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

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

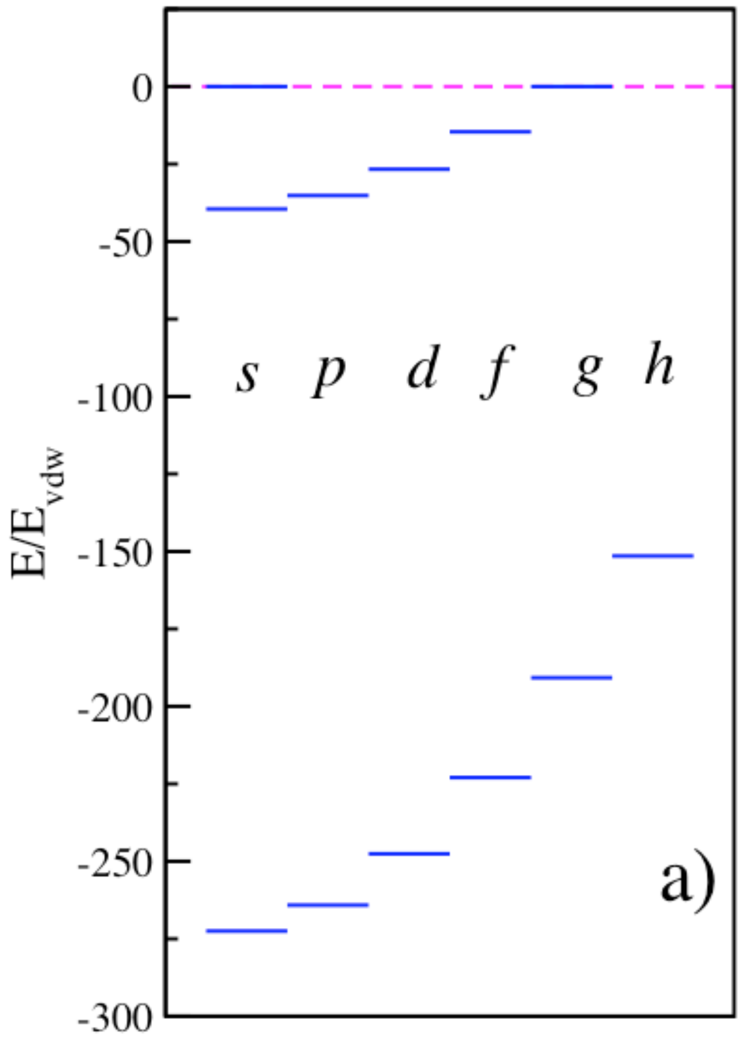
$$E_{\mathrm{vdw}} = \frac{\hbar^2}{2\mu R_{\mathrm{vdw}}^2}$$

	$R_{vdw}(a_0)$	E_{vdw}(mK)
^{6}Li	31	29
^{40}K	65	1.0
^{85}Rb	83	0.35
^{133}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 η(E)

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

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

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

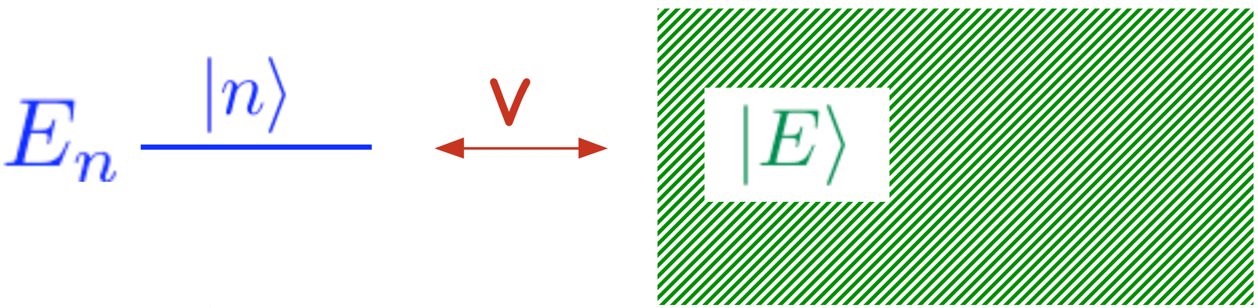
$$E_{-1} = \frac{\hbar^2}{2\mu(a-\bar{a})^2}$$

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))



Bound state

Continuum

Closed channel
(Resonance)

Open channel
(Background)

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

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

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

δE_n

shift

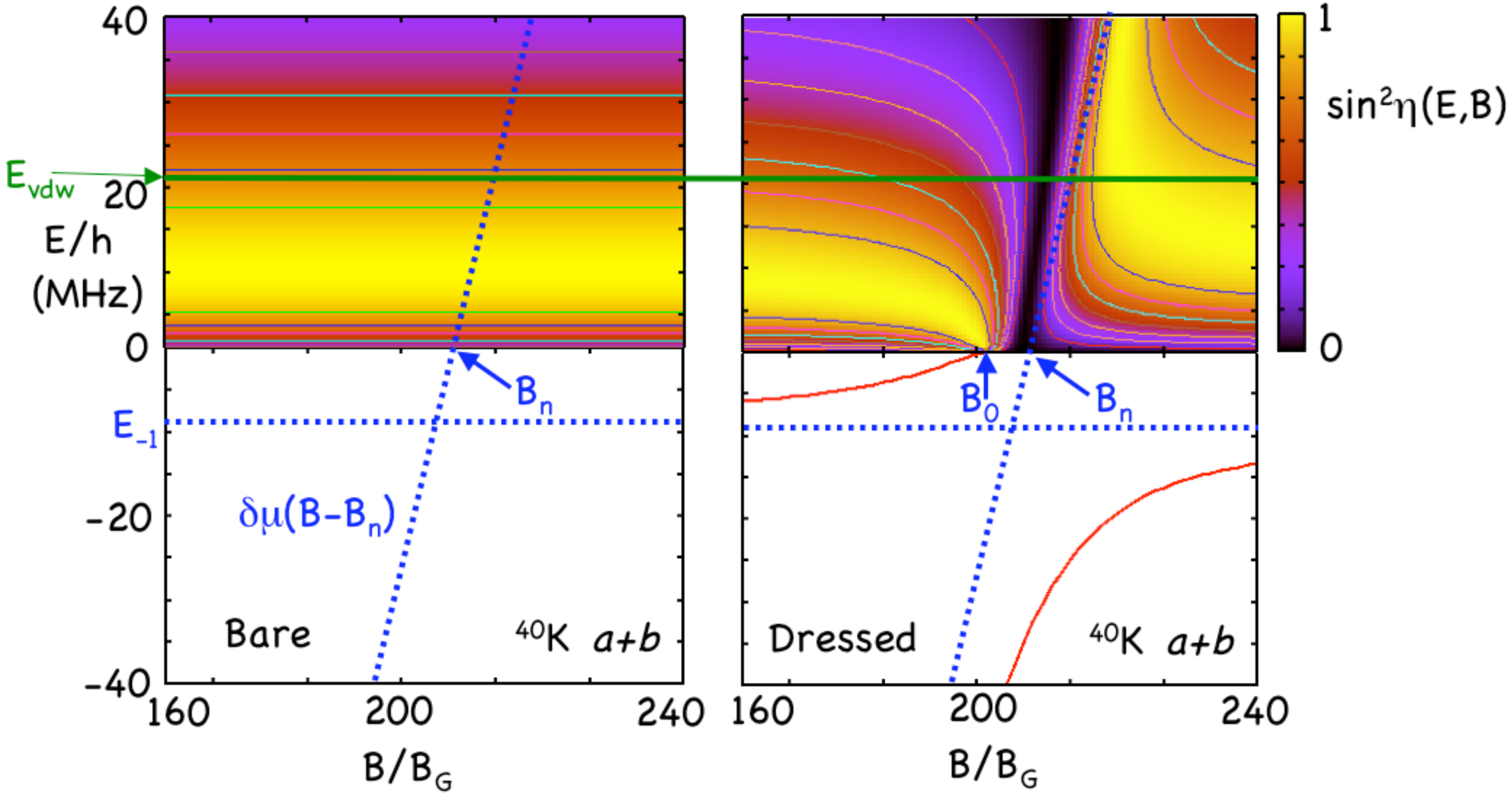
Analytic van der Waals theory reproduces ALL scattering versus E and B in the ultracold domain as compared to full coupled channels calculations.

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

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

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

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

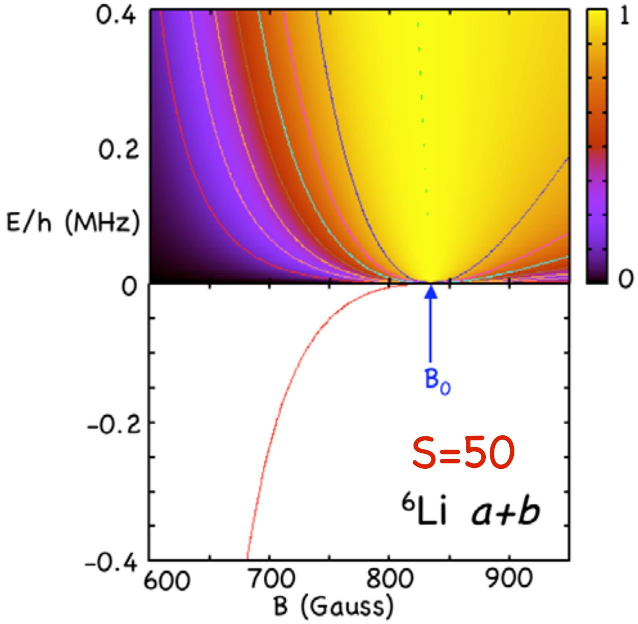


Open or closed channel dominated?

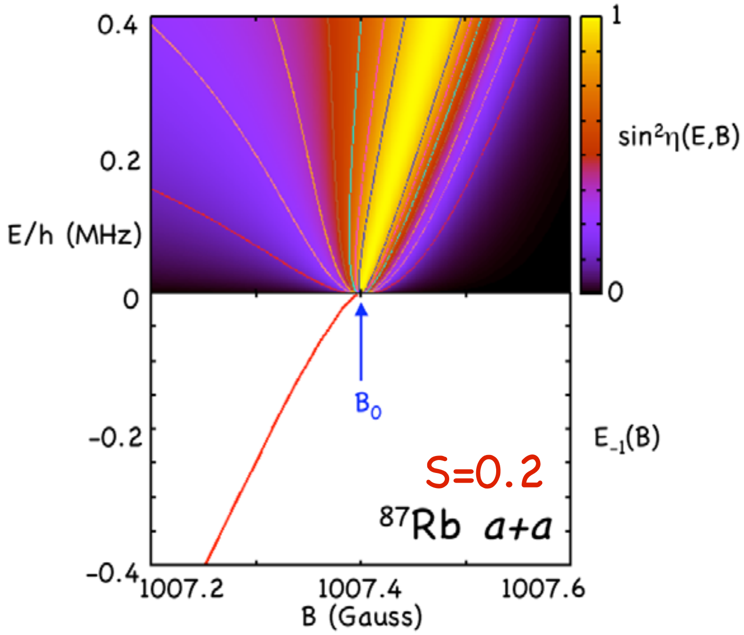
$$S = \frac{a_{\mathrm{bg}}}{\bar{a}} \frac{\delta\mu\,\Delta}{E_{\mathrm{vdW}}}$$

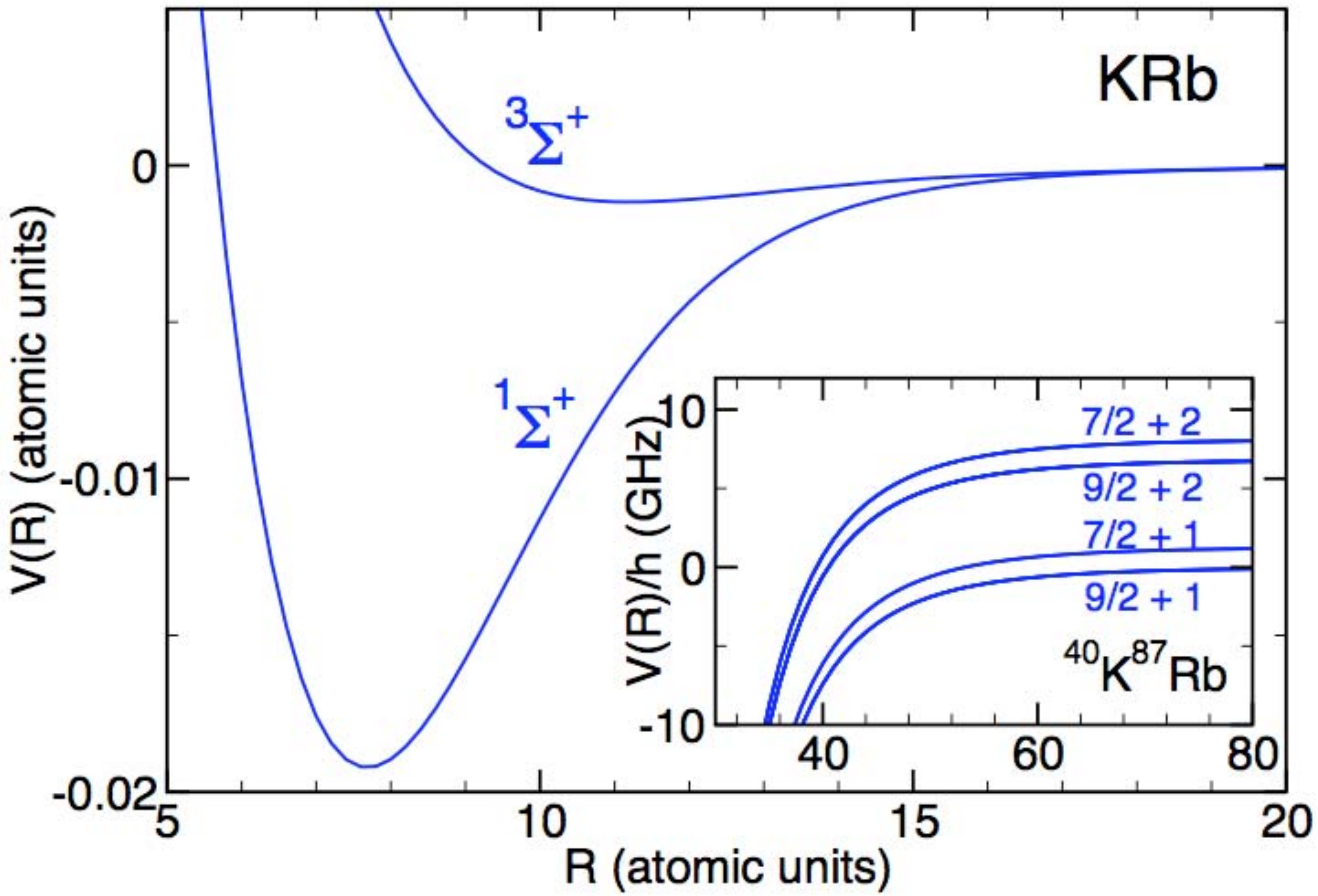
Köhler, Goral, Julienne,
Rev. Mod. Phys. 78, 1311 (2006)

Open: S >> 1
Universal, Z<<1
over ≈ Δ
Γ(E) >> E when E < E_{vdw}



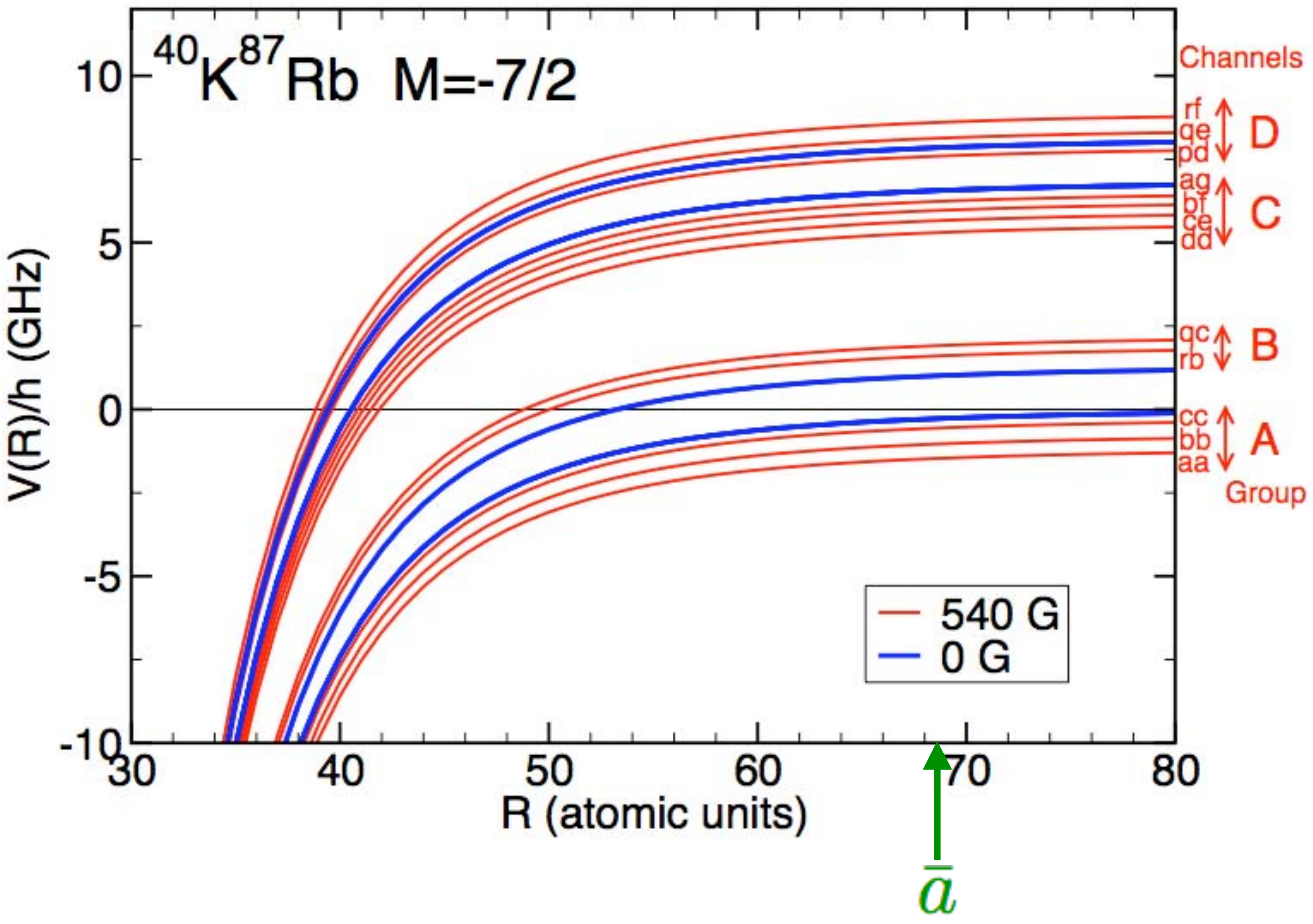
Closed: S << 1
Not universal, Z ≈ 1
over most of Δ
Γ(E) << E when E < E_{vdw}



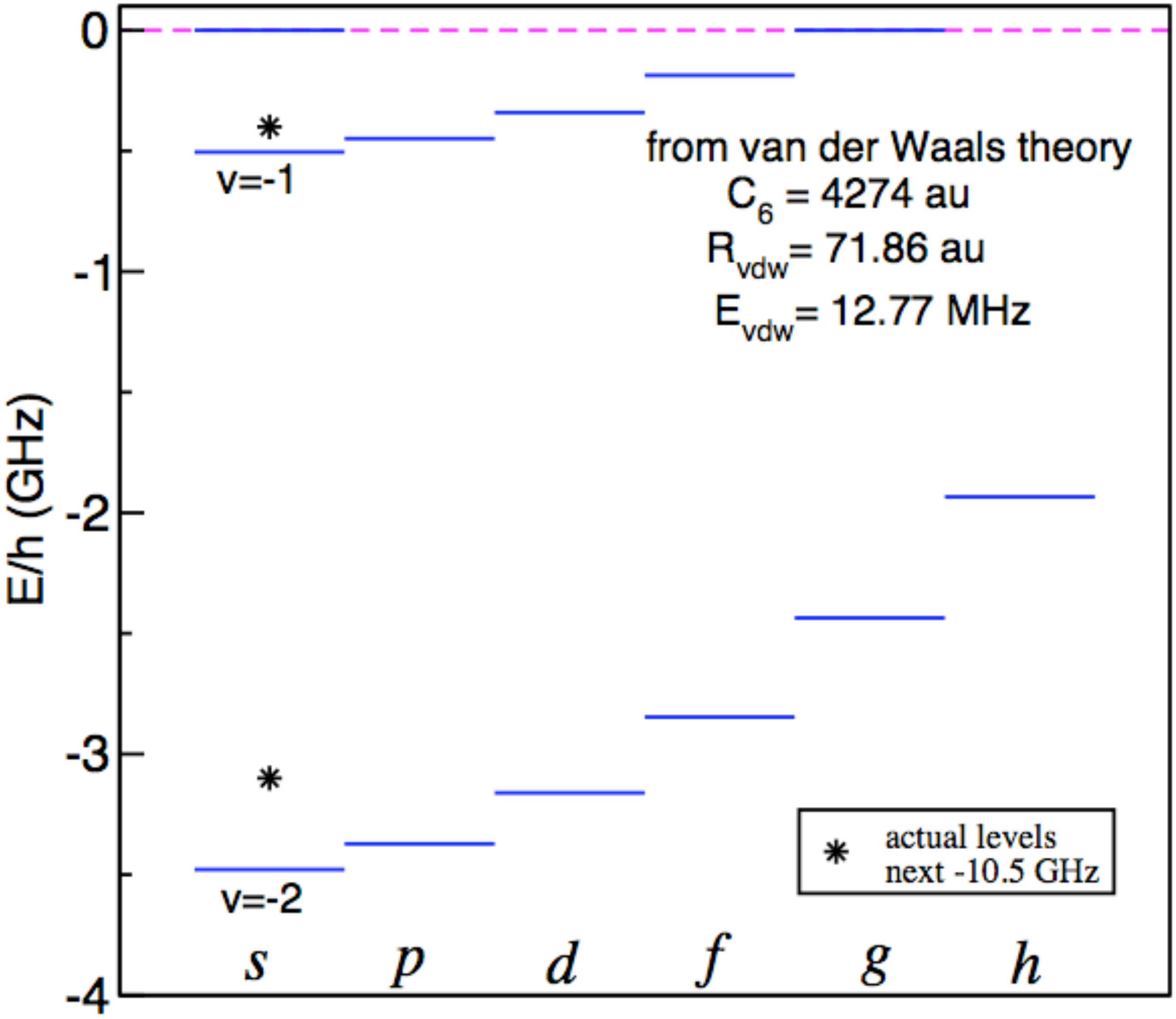


Ab initio: Kotochigova , Julienne, Tiesinga, Phys. Rev. A 68,022501 (2003).

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

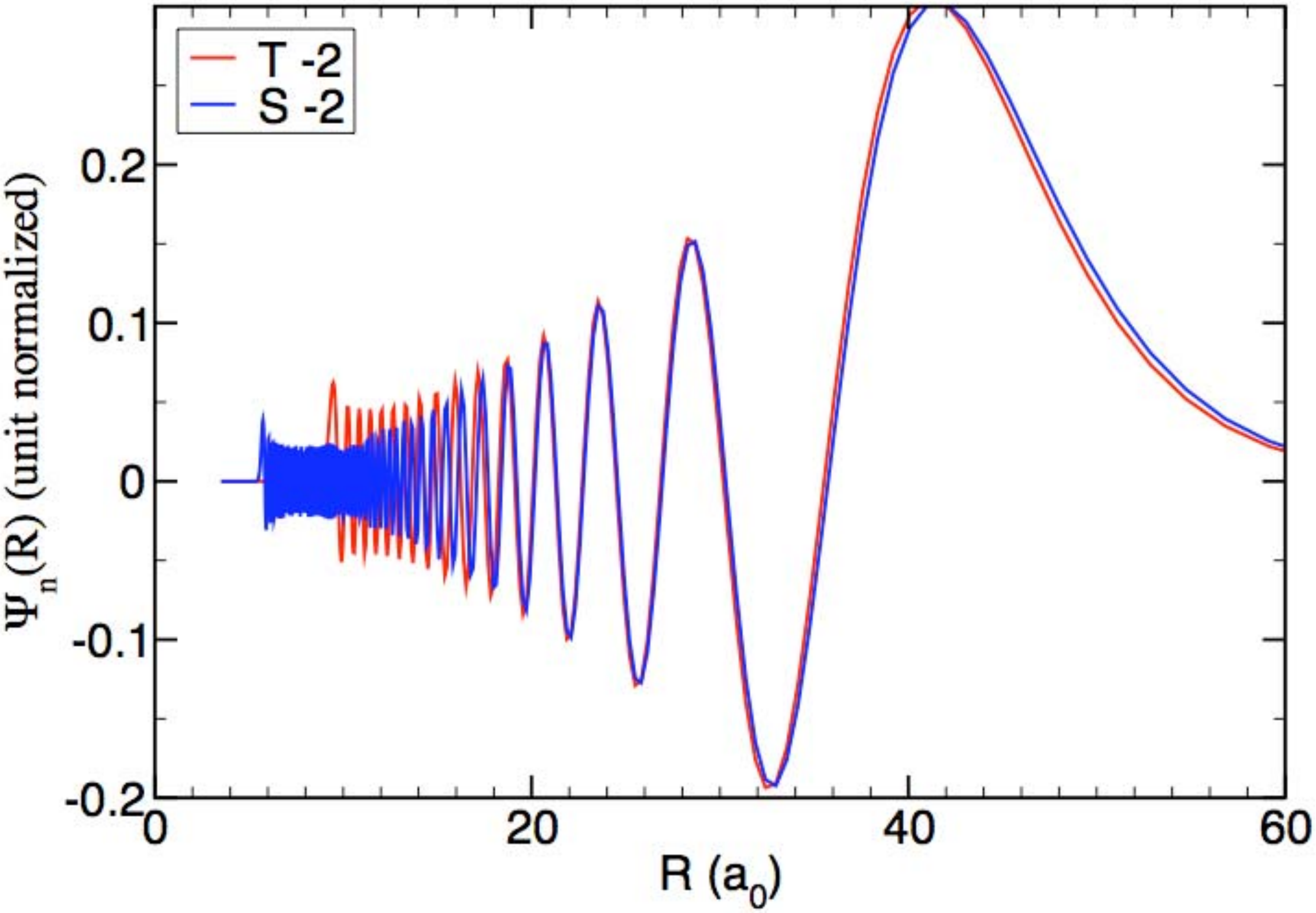

$^{40}K^{87}Rb$ M=-7/2
V(R)/h (GHz)
10
5
0
-5
-10
30
40
50
60
70
80
R (atomic units)
Channels
rf
qe
pd
D
ag
bf
ce
dd
C
qc
rb
B
cc
bb
aa
A
Group
540 G
0 G
$\bar{a}$

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



$^{40}K^{87}Rb$ n=-2 levels

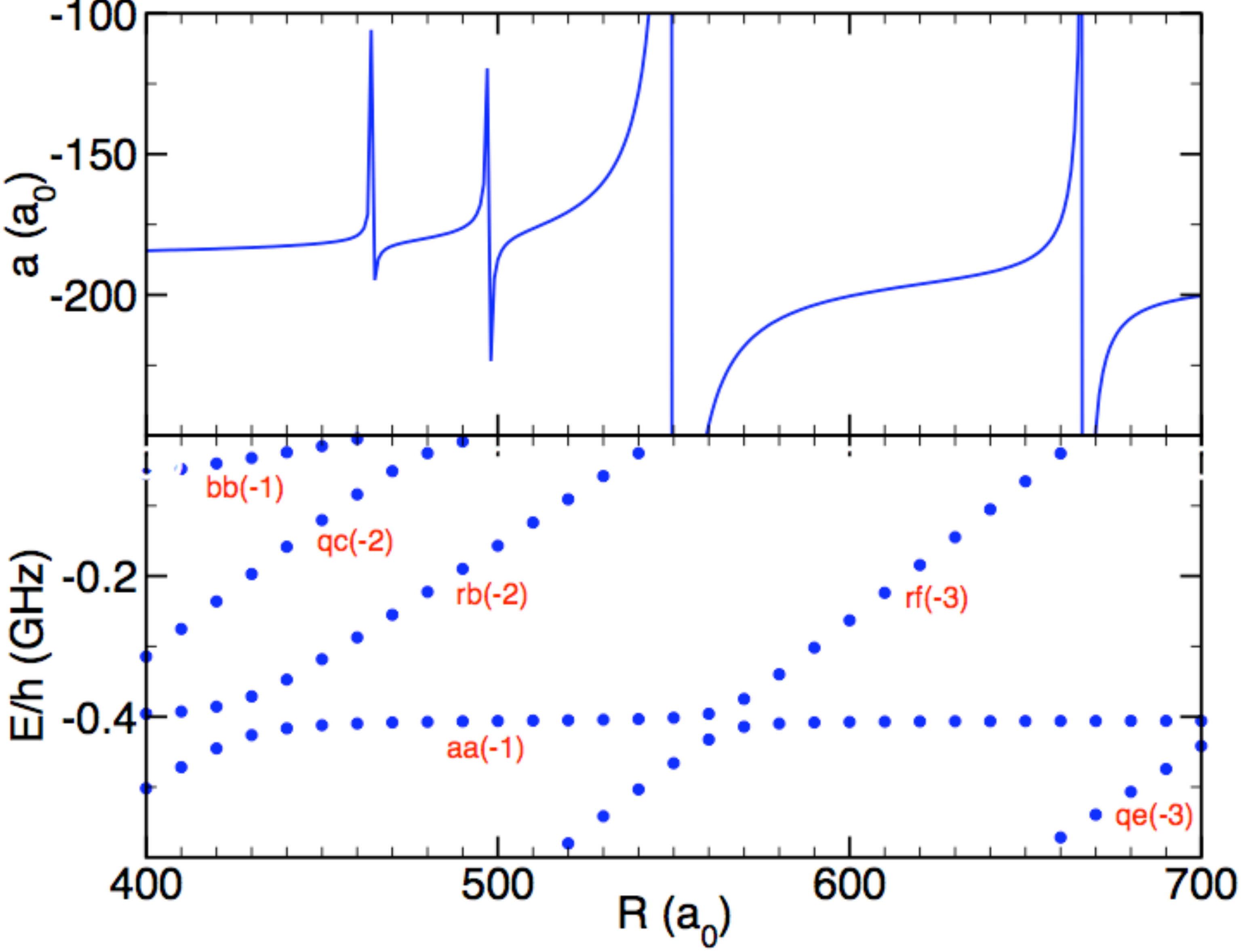
single channel $\Psi_n(R)$



$\bar{a}$

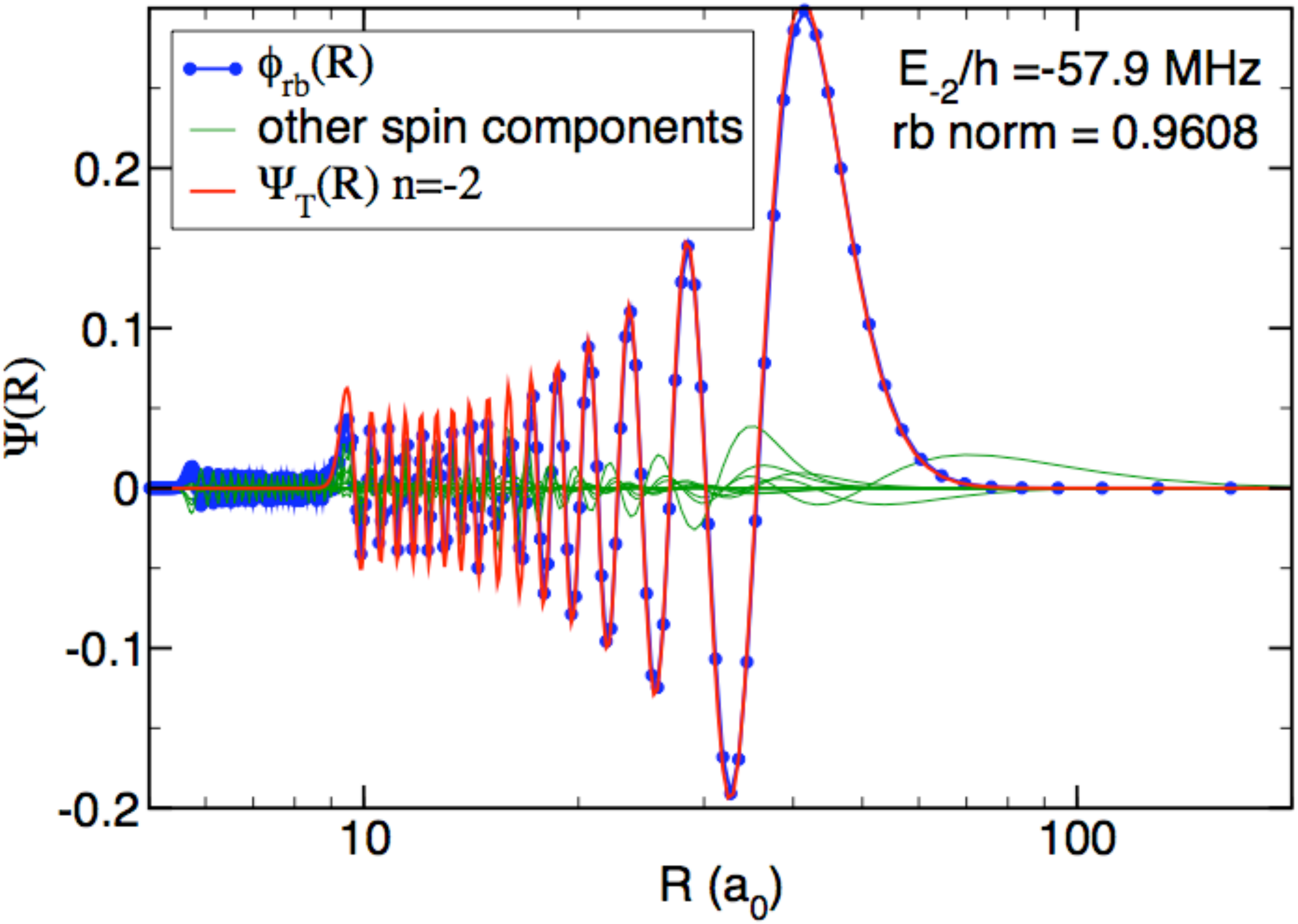
↓

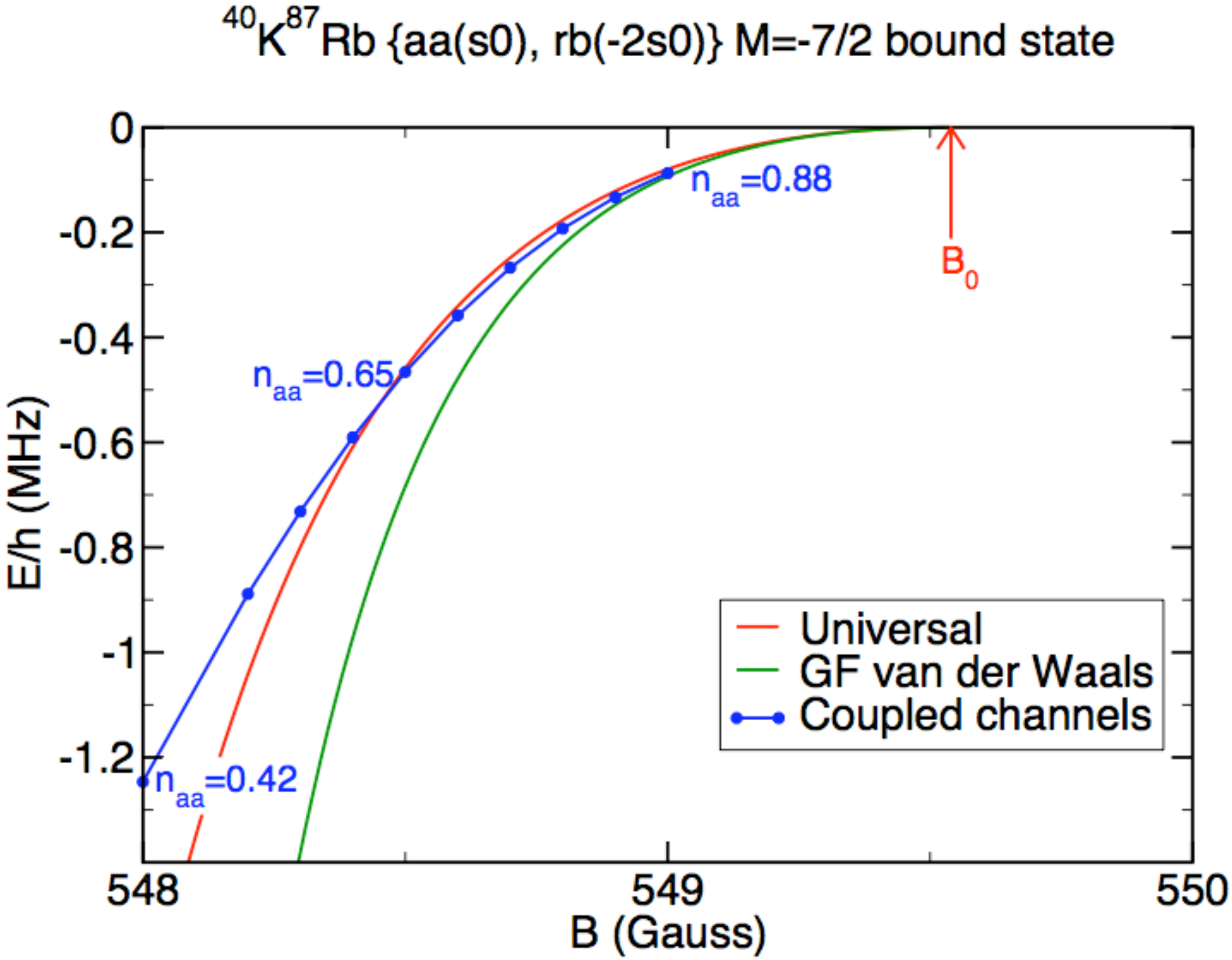
^{40}K^{87}Rb a(B) and E$_n$(B) vs. B



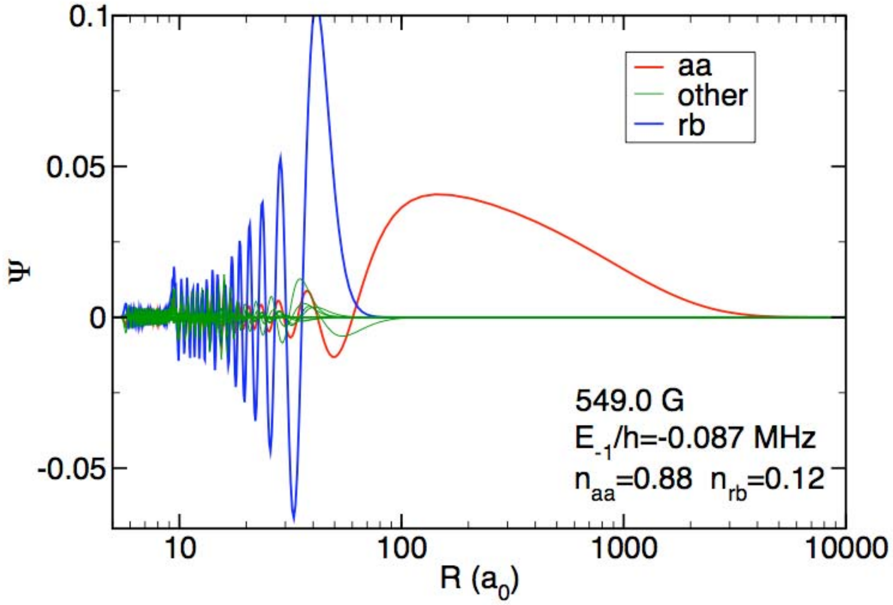
^{40}K^{87}Rb rb(-2) level 530 G

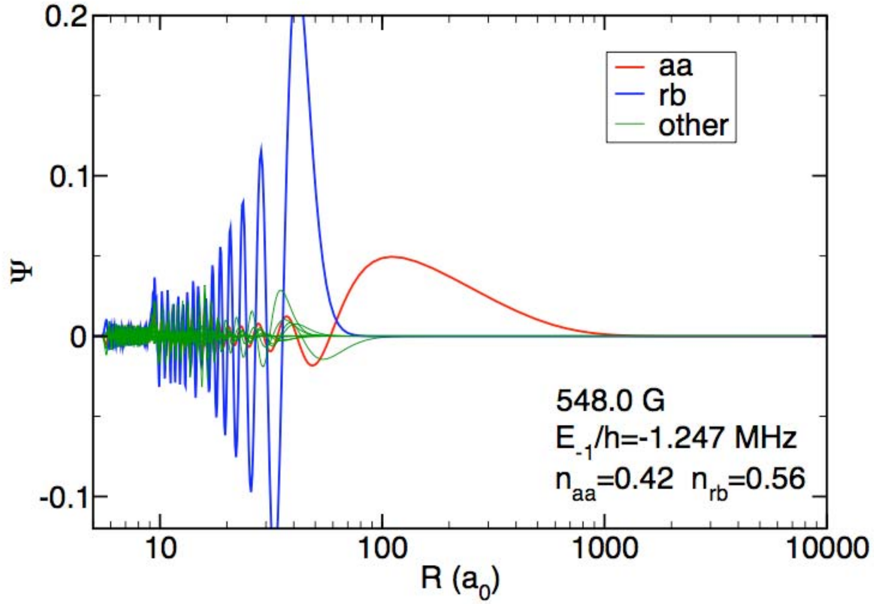
Coupled channels calculation with 12 spin channels

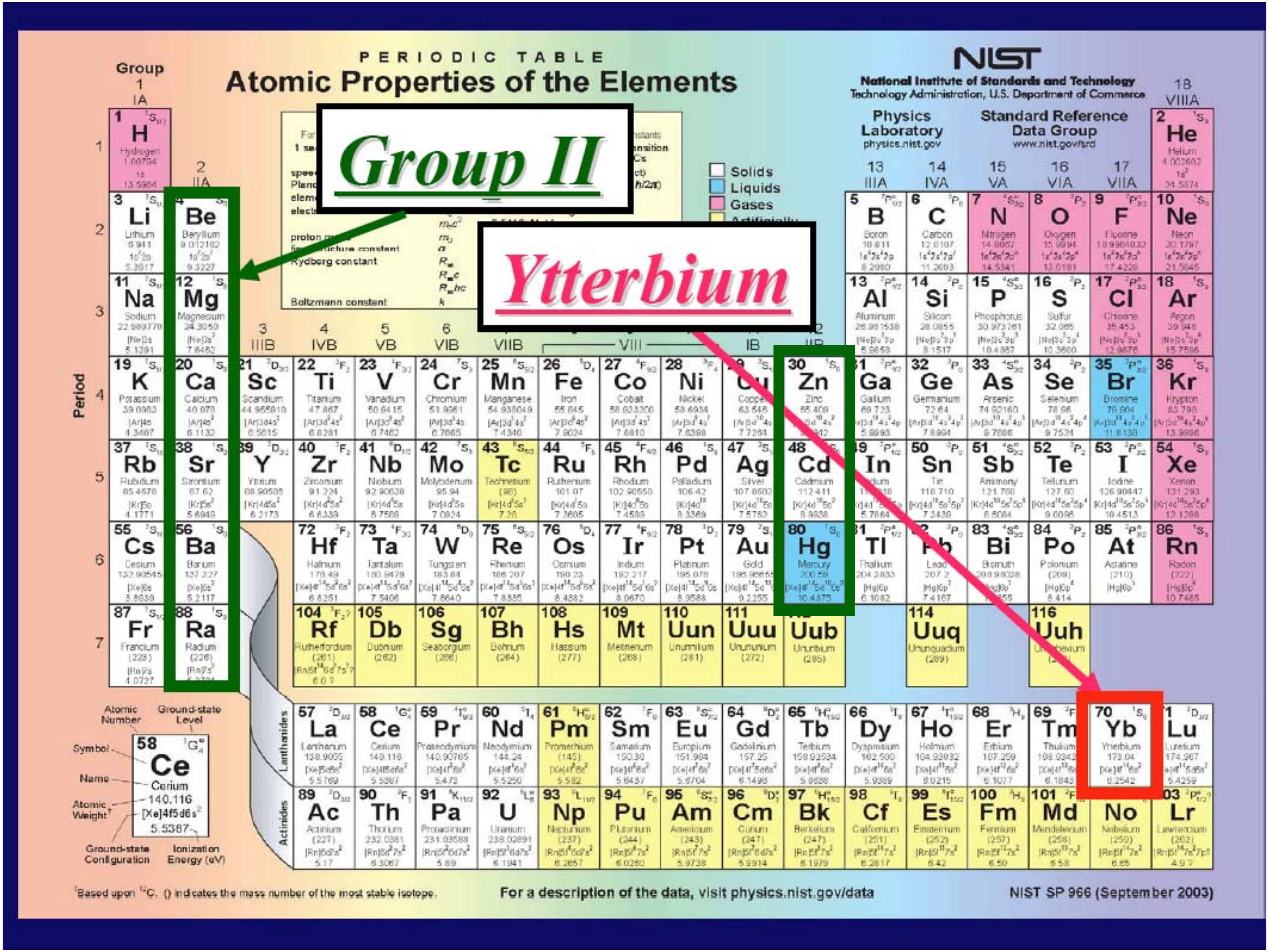




$^{40}K^{87}Rb$ {aa(s0), rb(-2s0)} M=-7/2 bound state


0.1
0.05
0
-0.05
Ψ
10
100
1000
10000
R (a_0)
aa
other
rb
549.0 G
E_{-1}/h=-0.087 MHz
n_{aa}=0.88 n_{rb}=0.12


0.2
0.1
0
-0.1
Ψ
10
100
1000
10000
R (a_0)
aa
rb
other
548.0 G
E_{-1}/h=-1.247 MHz
n_{aa}=0.42 n_{rb}=0.56



Group II

Ytterbium

PERIODIC TABLE

Atomic Properties of the Elements

NIST

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

Physics Laboratory
physics.nist.gov

Standard Reference Data Group
www.nist.gov/srd

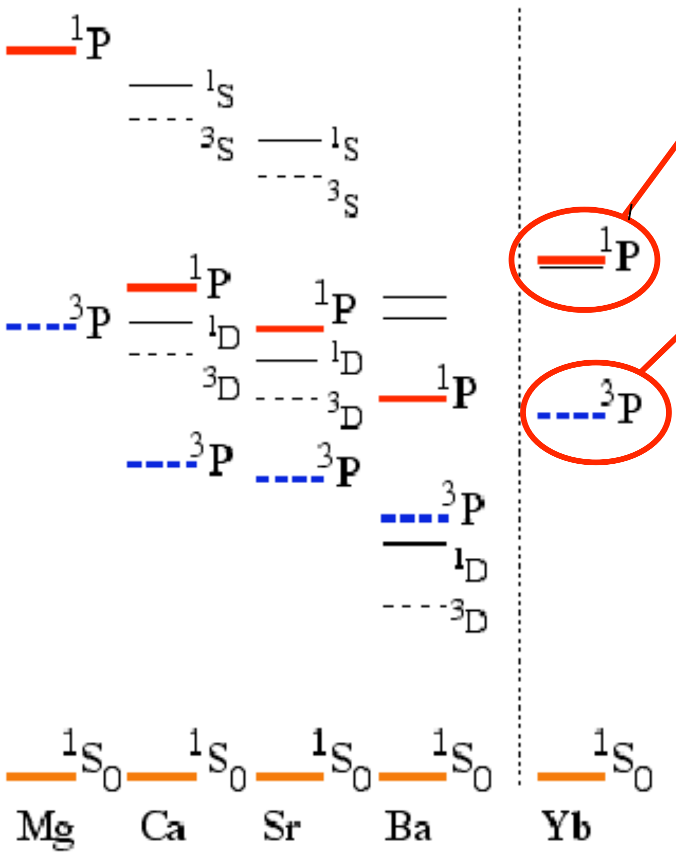
☐ Solids
🟦 Liquids
🟥 Gases

¹Based upon ¹²C. () indicates the mass number of the most stable isotope.

For a description of the data, visit physics.nist.gov/data

NIST SP 966 (September 2003)

Group II Atoms



$^1S_0$-$^1P_1$ resonance line

> mK Doppler cooling

$^1S_0$-$^3P_1$ intercombination line

μK Doppler cooling

Spin 0 bosons

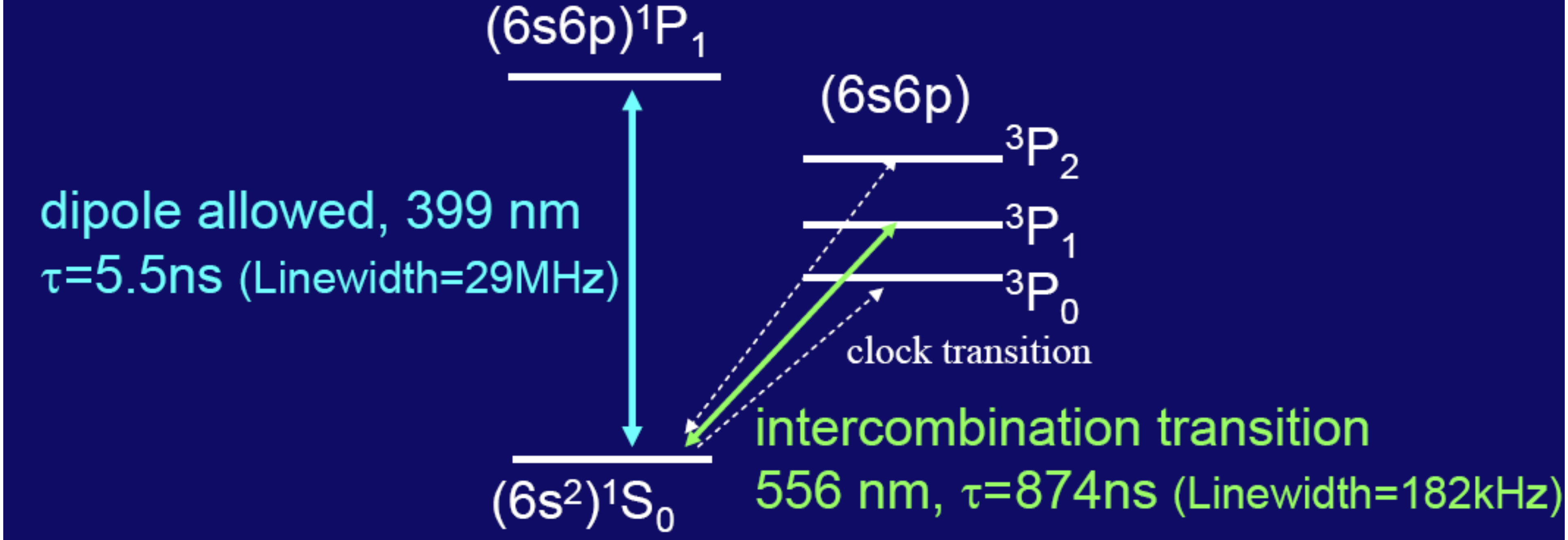
Spin 1/2 or higher fermions

no g. s. decoherence

$^1S_0$-$^3P_1$ photoassociation

optical feshbach control

Level Diagram of Yb



dipole allowed, 399 nm
τ=5.5ns (Linewidth=29MHz)

intercombination transition
556 nm, τ=874ns (Linewidth=182kHz)

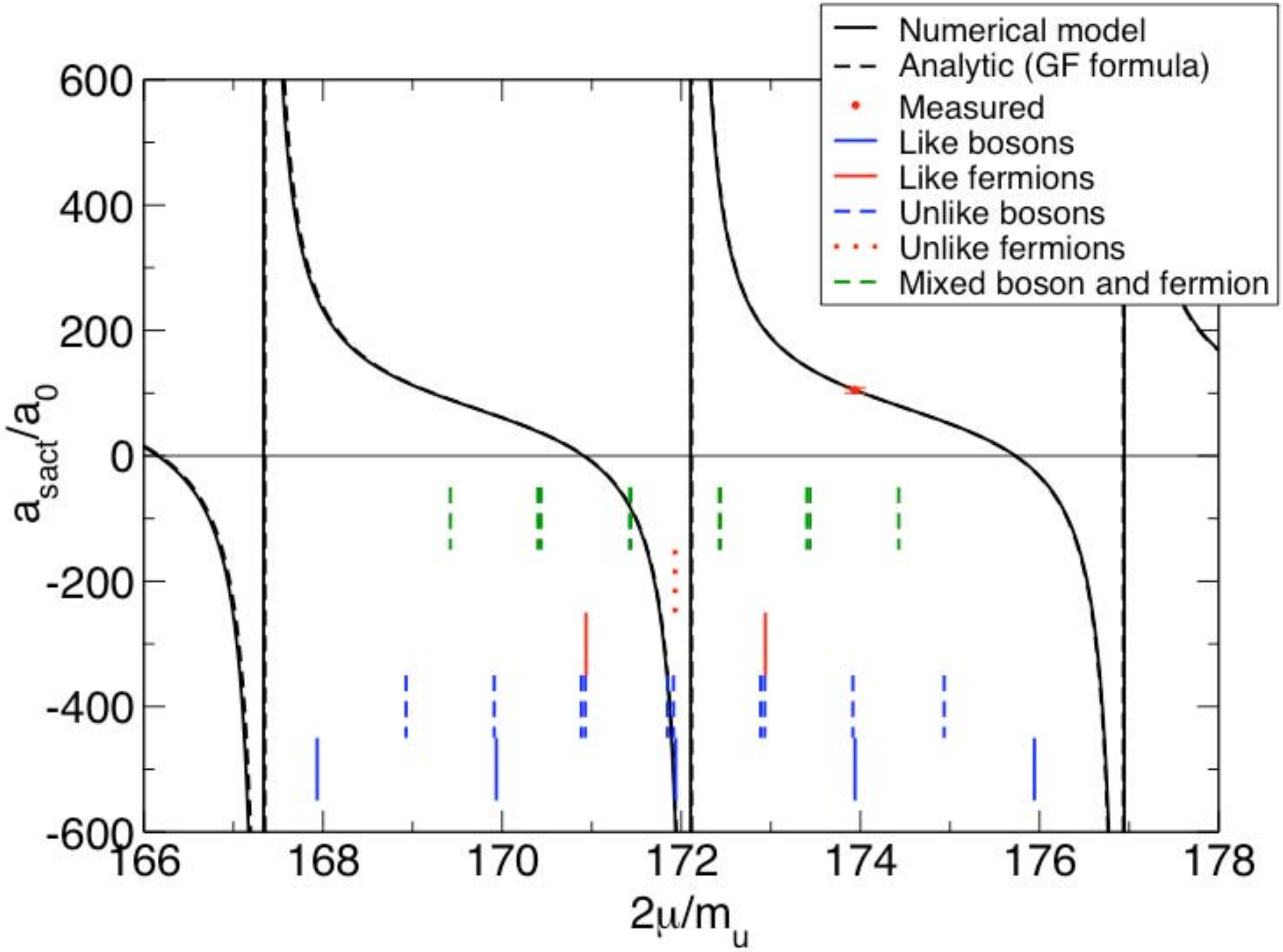
From Enomoto et al

Mass number	168	170	171	172	173	174	176
Nuclear spin *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)

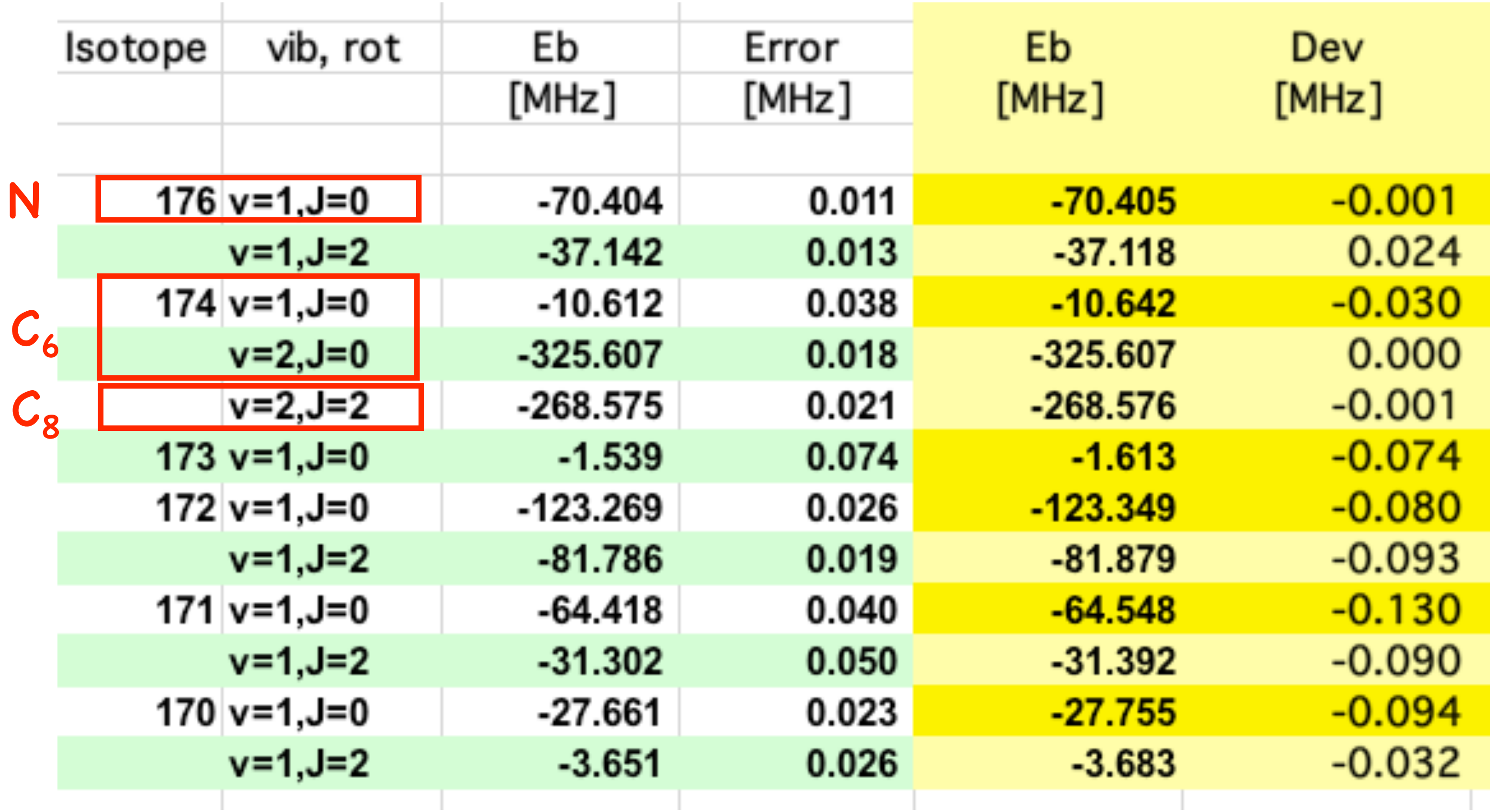
	168	170	171	172	173	174	176
168	252(6)	117(1)	89(1)	65(1)	39(1)	2(2)	-360(30)
170	117	64(1)	37(1)	-2(2)	-81(4)	-520(50)	209(4)
171	89	37	-3(2)	-84(5)	-580(60)	430(20)	142(2)
172	65	-2	-84	-600(60)	420(20)	201(3)	106(1)
173	39	-81	-580	420	199(3)	139(2)	80(1)
174	2	-520	430	201	139	105(1)	55(1)
176	-360	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)x10^5 Exactly 72 bound states in $^{174}Yb_2$



	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)

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

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

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

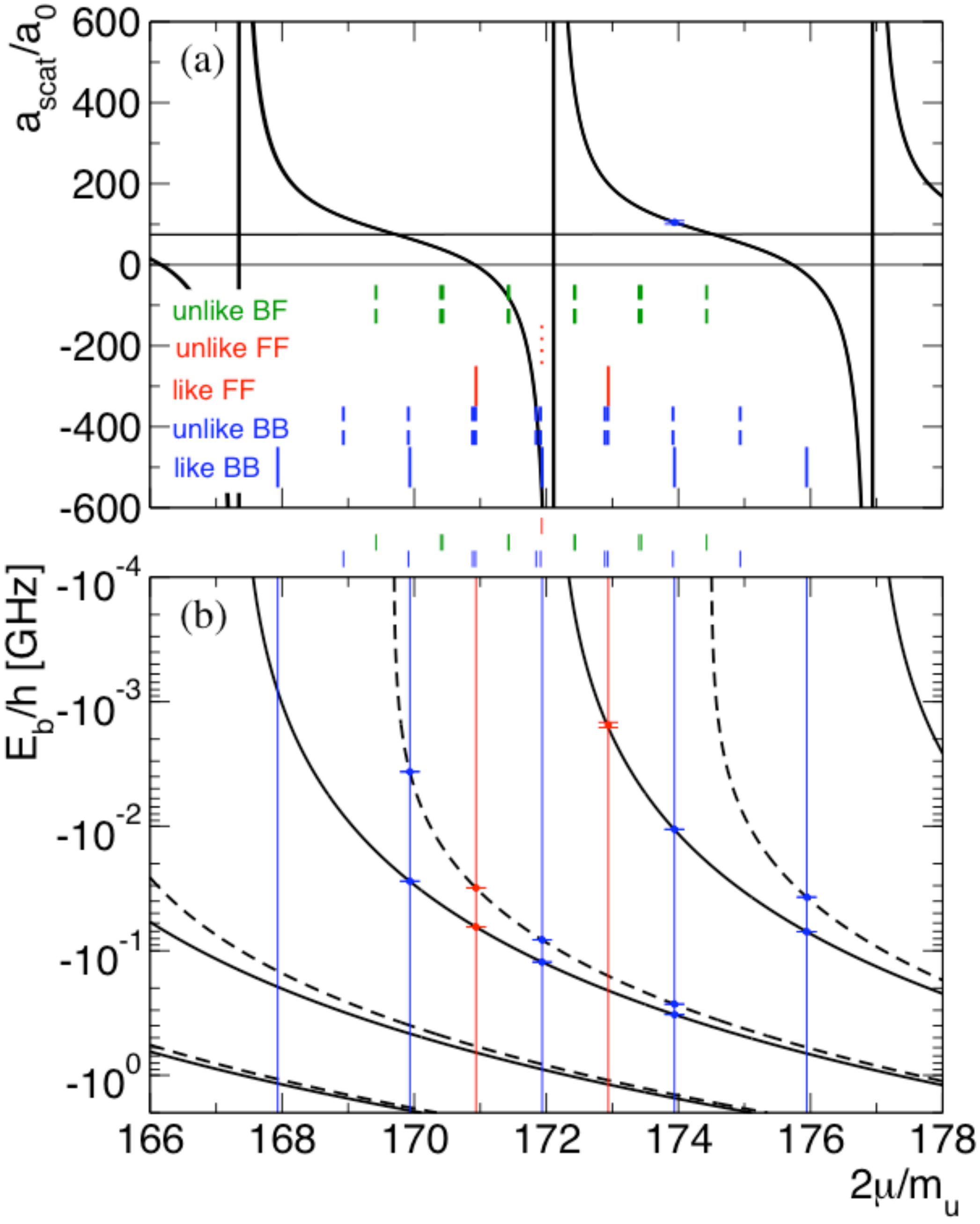
Number of bound states in V(R) = $\mathrm{Int}\left[\frac{\Phi}{\pi} - \frac{5}{8}\right] + 1$

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