

ICAP 2014 Summer School, July 31, Williamsburg

Understanding cold atomic and molecular collisions

1. Basics

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Thanks to many colleagues in theory and experiment
who have contributed to this work

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

Supported by an AFOSR MURI

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Cold Collisions

“Good” -- Essential interactions for control and measurement

“Bad” -- Source of trapped atom loss, heating, and decoherence

- Atom-atom collisions can be quantitatively understood and controlled--essential for quantum gas studies.
- Basic concepts, illustrated by examples.
- Part 1: What is a scattering length, and why is it significant? Why is the long range potential so important?
- Part 2: Magnetically tunable “Feshbach” resonances are a key to measurement and control.
- Part 3(?):What is special about molecules?
Molecules are different from atoms. What about few-body phenomena?

Some resources

PSJ, Ch. 6 of *Cold Molecules*, ed. by R. Krems et al.

also arXiv:0902.1727, threshold bound and scattering states

Chin, Grimm, PSJ, Tiesinga, Rev. Mod. Phys. 82, 1225 (2010)
review of Feshbach resonances

PSJ, Faraday Discussions 142, 361 (2009)
ultracold molecules: a case study with KRb

Kohler, Goral, PSJ, Rev. Mod. Phys. 78, 1311 (2006)
review of molecule formation through Feshbach res.

Jones, Lett, Tiesinga, PSJ, Rev. Mod. Phys. 78, 483 (2006)
review of cold atom photoassociation

PSJ and Mies, J. Opt. Soc. Am. B 6, 2257 (1989)
quantum defect theory for cold collisions

Two kinds of collision

Elastic--do not change internal state $a + b \rightarrow a + b$

- Thermalization
- Evaporation
- Mean field of BEC
- BEC-BCS crossover in Fermi gases
- Equation of state
- Phase change--quantum logic gates

Inelastic--change internal state $a + b \rightarrow a' + b' + \Delta E$

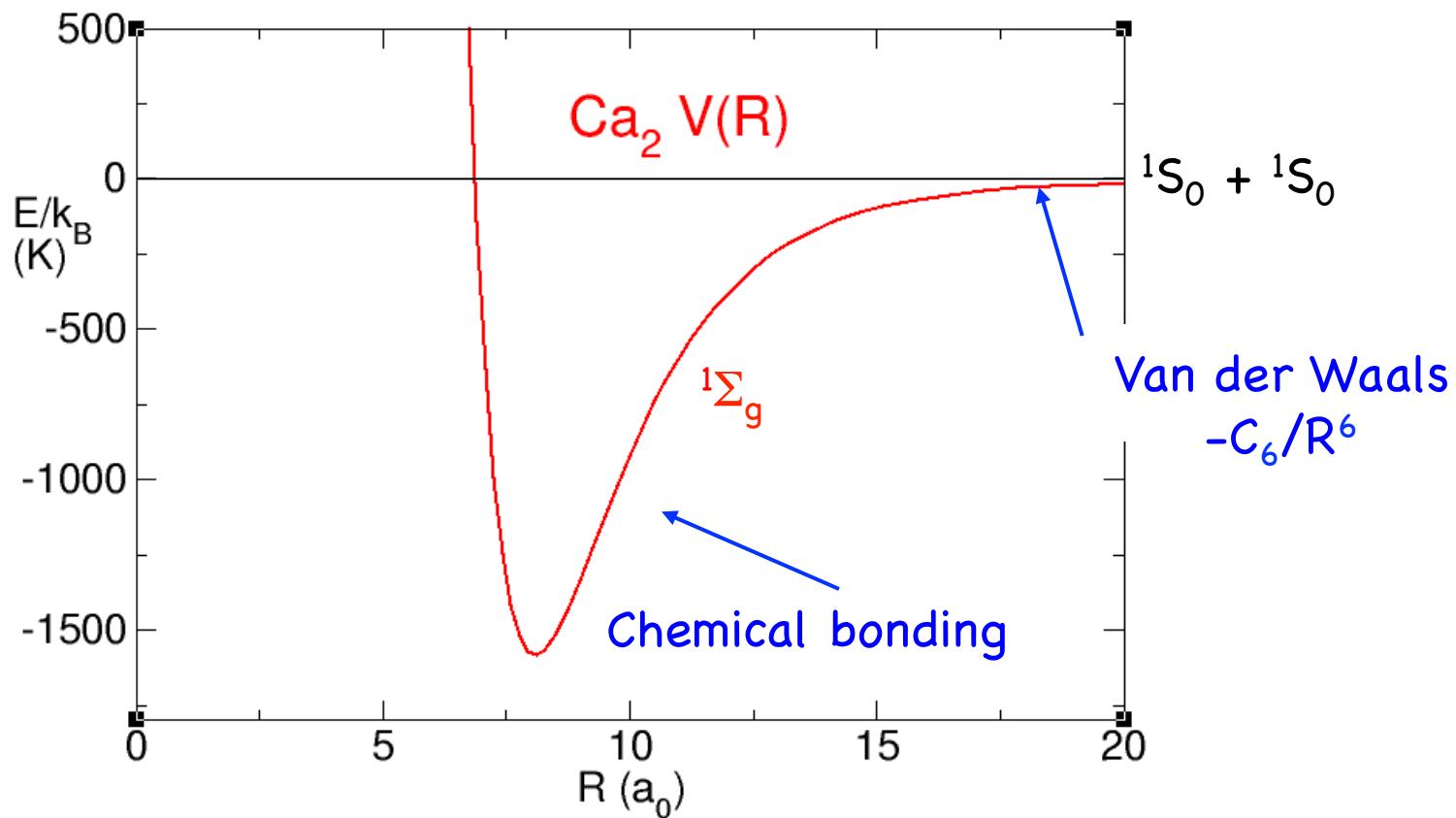
- Spin relaxation
- Loss of trapped atoms, gas lifetime
- Decoherence
- Spinor condensates ($\Delta E=0$)
- Three-body, detect resonances
- Photoassociation

Ca $4s^2$ 1S_0 atom

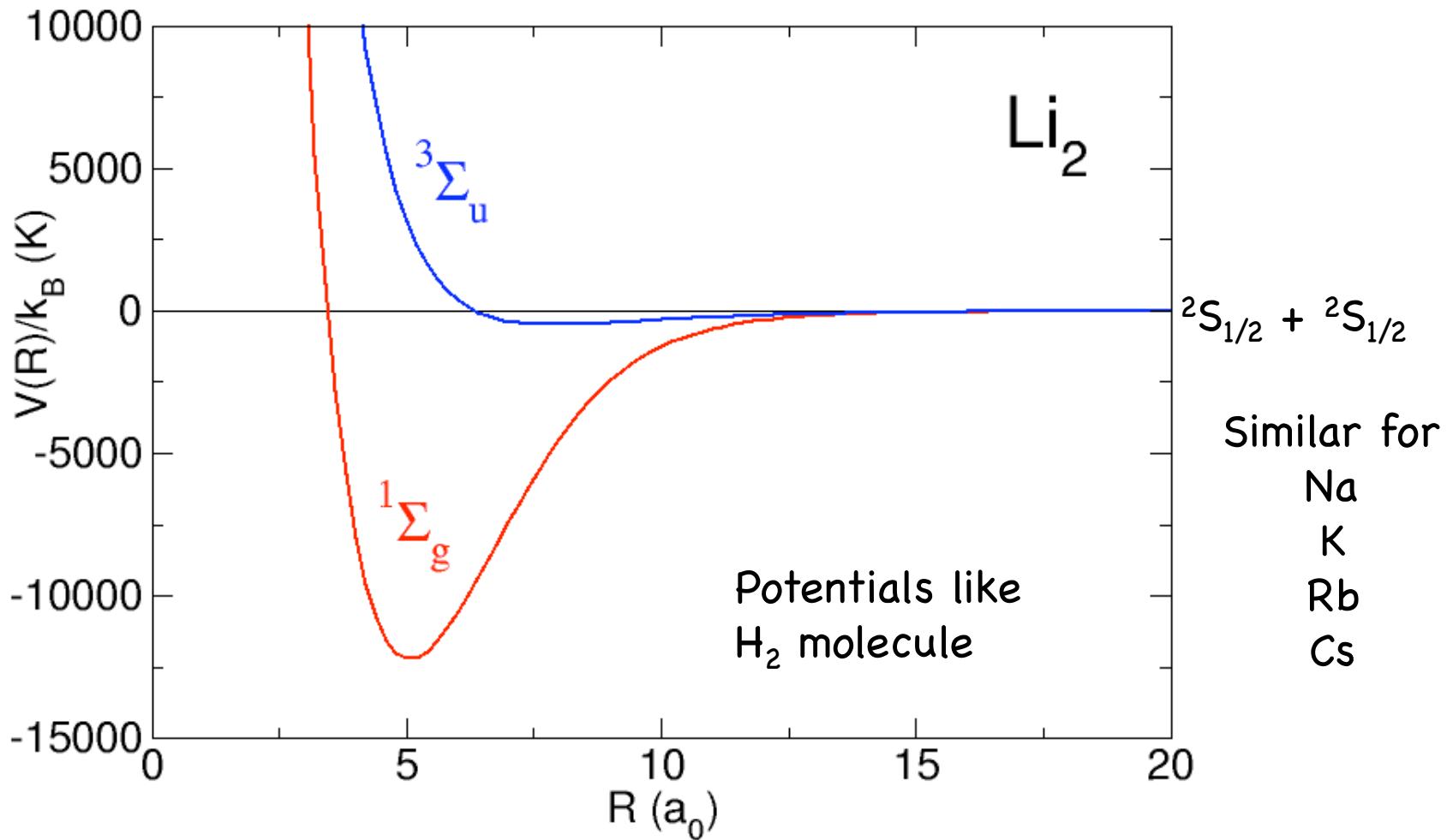
Spin degeneracy

Total angular momentum

Born-Oppenheimer approximation = potential energy curve



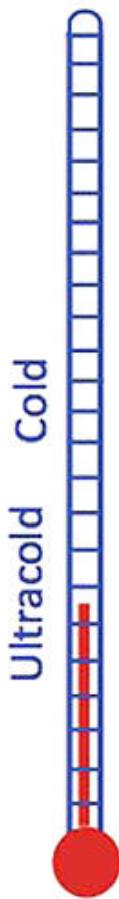
$\text{Li } 1s^2 2s \ ^2S_{1/2}$ atom



Energy
splittings

E/h

1 THz
1 GHz
1 MHz
1 kHz
1 Hz



E/k_B

10^9 K
 10^6 K
1000 K
1 K
1 mK
1 μ K
1 nK
1 pK

Interior of sun
Surface of sun
Room temperature
Liquid He
Laser cooled atoms
Optical lattice bands
Quantum gases
(Bosons or Fermions)

$$\lambda = \frac{h}{mv} \gg 1 \mu m$$

From Quéméner and Julienne, Chemical Reviews 112, 4949 (2012) *Ultracold Molecules Under Control!*

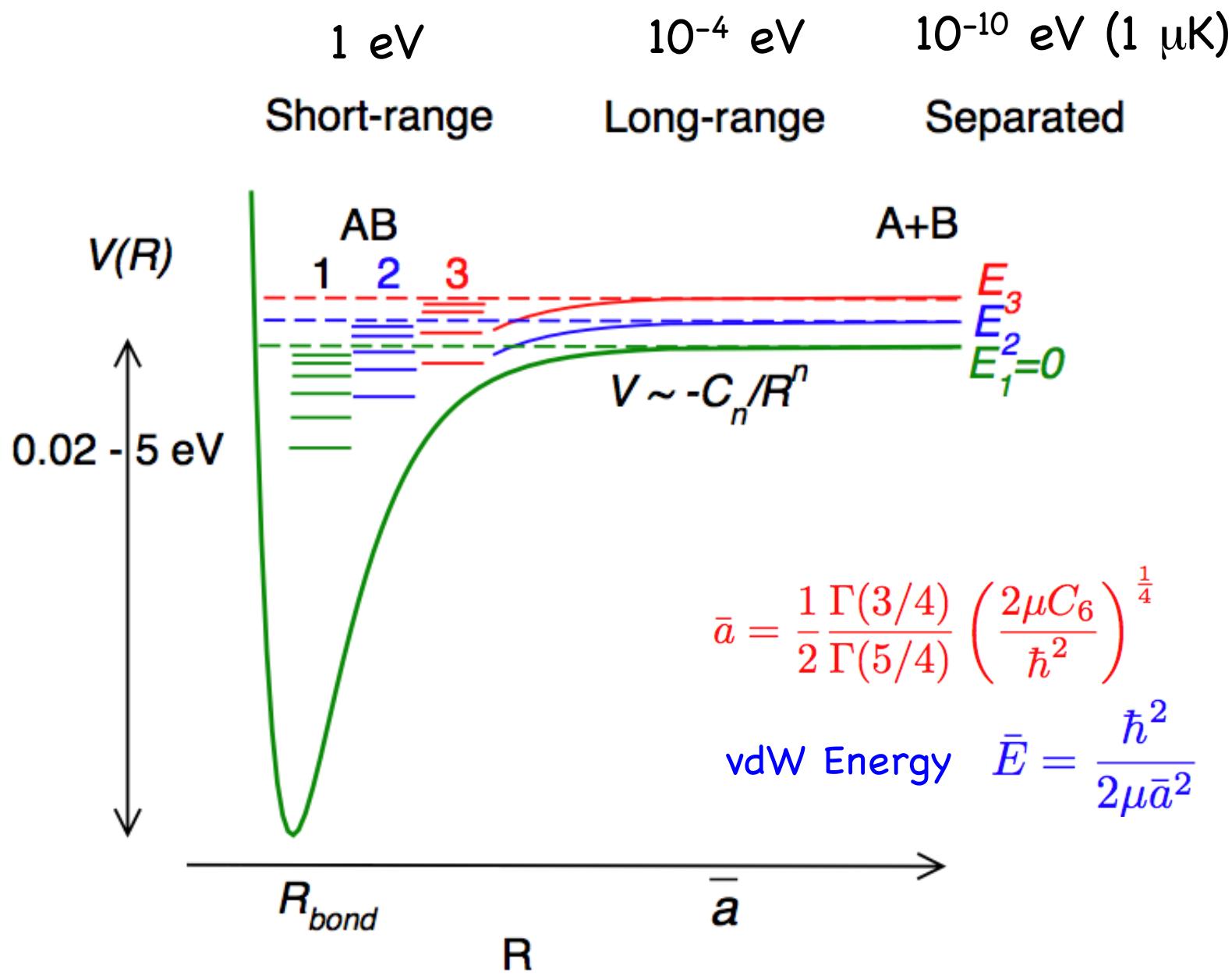


Fig. 2, PSJ Faraday Disc 142, 361 (2009)

Collision of two atoms

Separate center of mass R_{CM} and relative R motion with reduced mass μ .

Expand $\Psi(R,E)$ in relative angular momentum basis lm .

$l = 0, 1, 2 \dots$ s-, p-, d-waves, ...

Potential energy: $V(R) + \frac{\hbar\ell(\ell+1)}{2\mu R^2}$ --> phase shift $\eta_\ell(E)$

Neutral atoms (S-state): $V(R) \rightarrow -C_6/R^6$ van der Waals

Solve Schrödinger equation for bound and scattering $\Psi(R,E)$

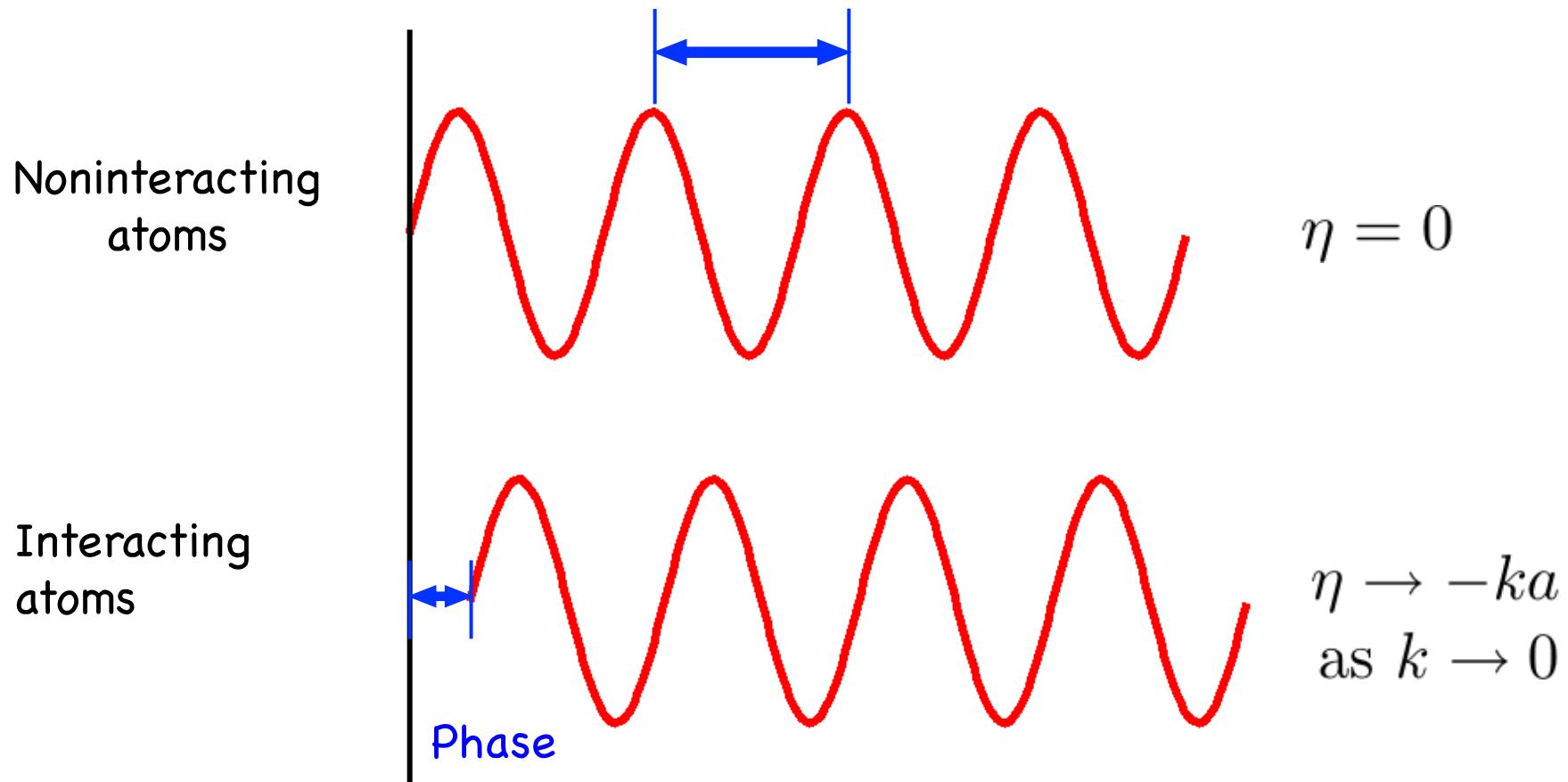
--> bound states E_n

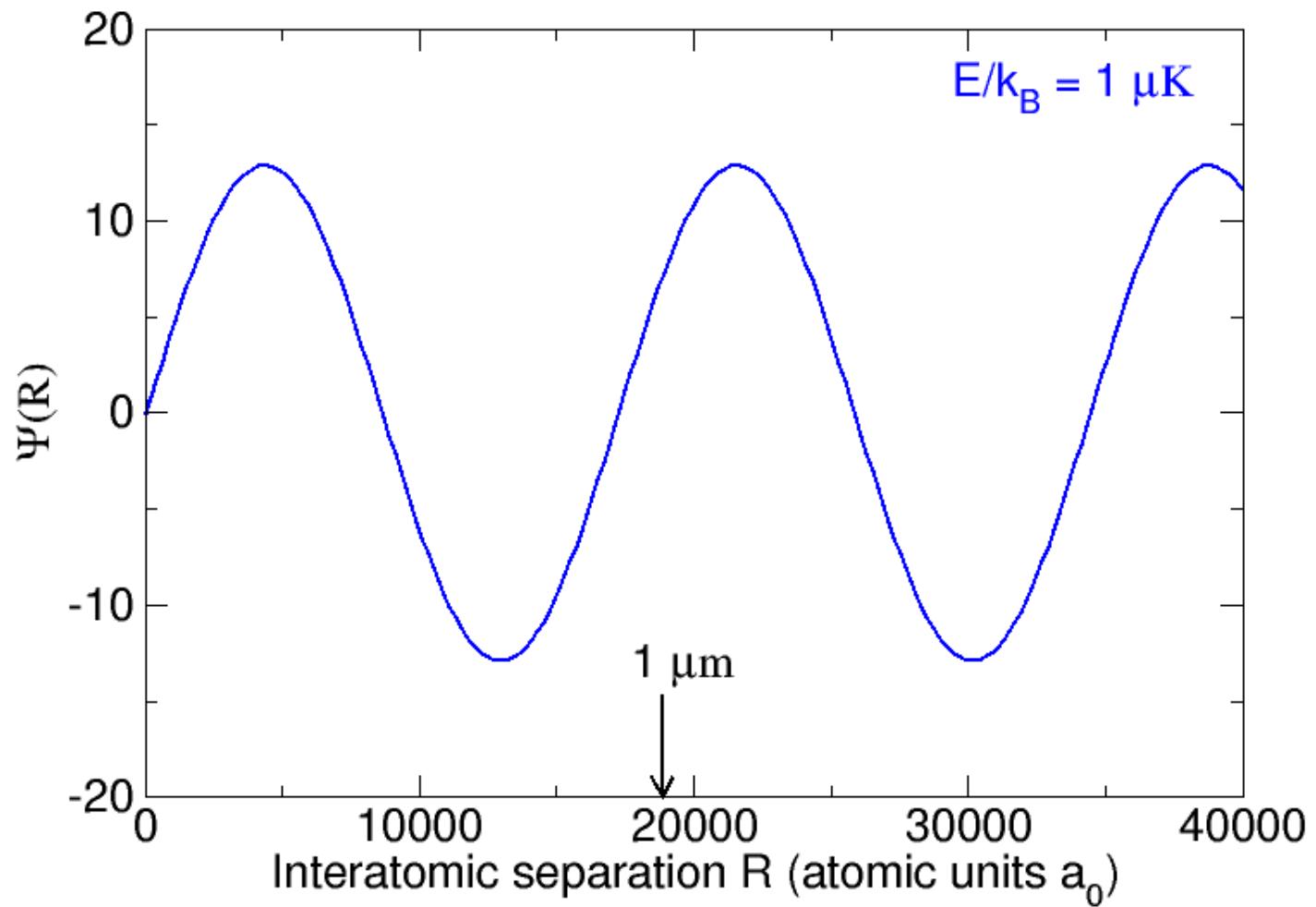
--> scattering phases, amplitudes

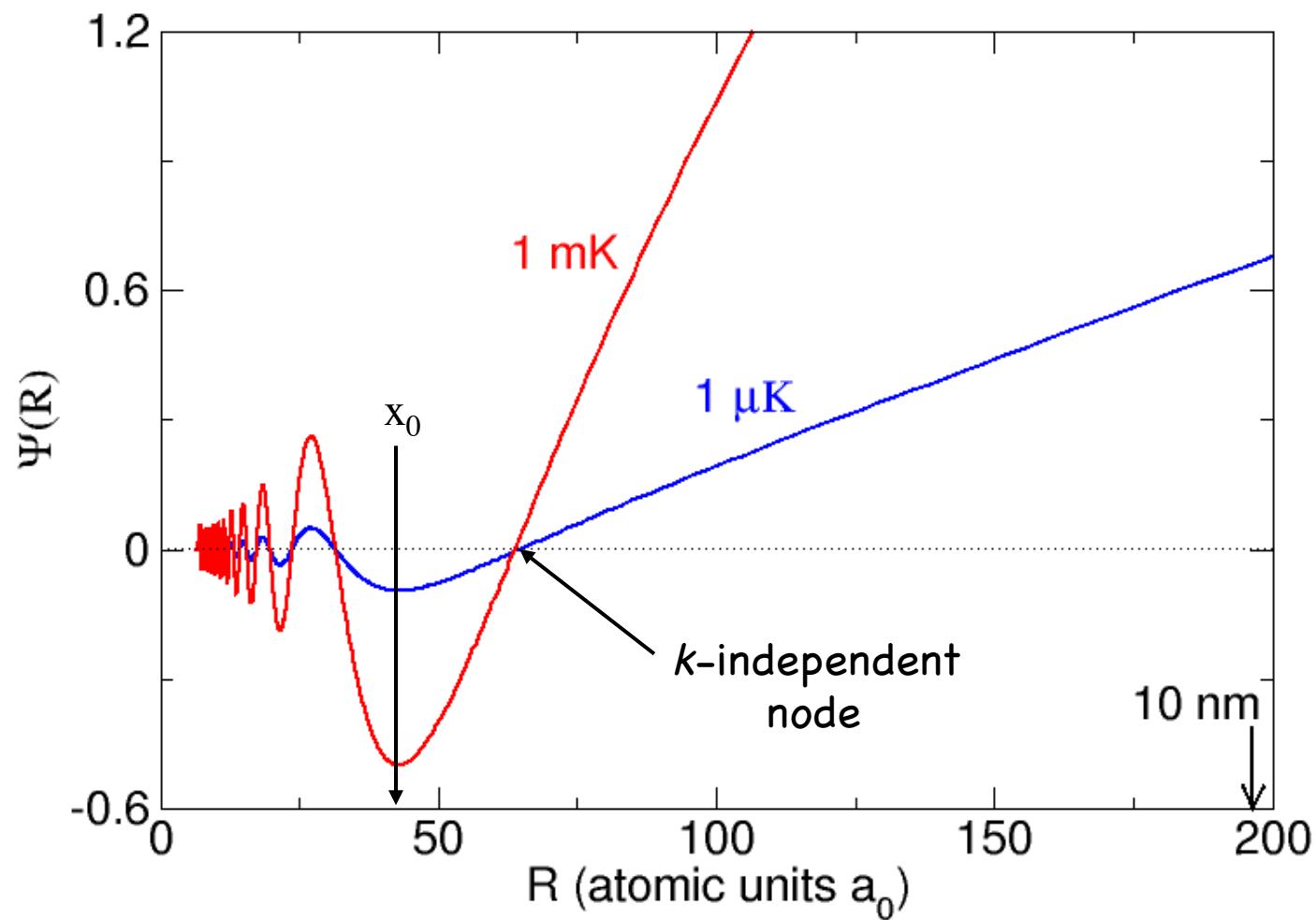
S-wave scattering phase shift

$$\Psi(R) \rightarrow \sin(kR + \eta)$$

Wavelength $\lambda = 2\pi/k$

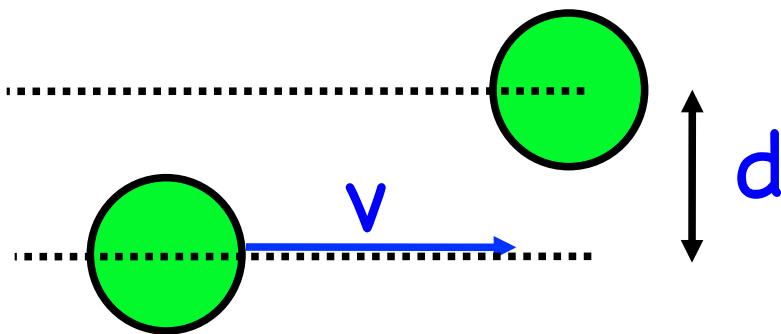






Cross section σ

Classical balls with distance of closest approach d (diameter)



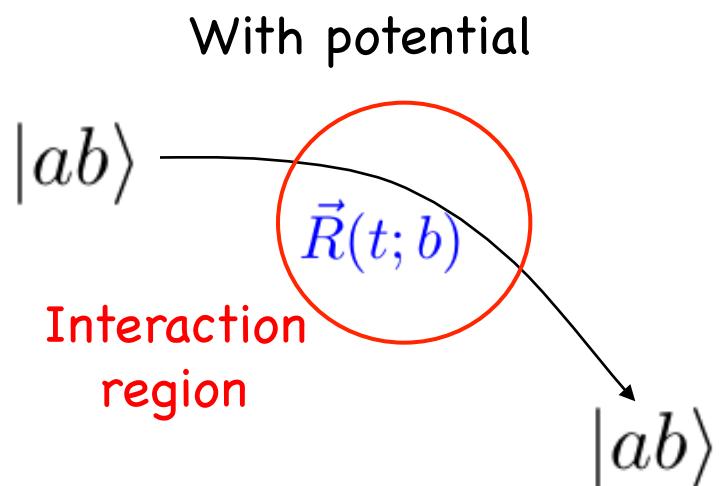
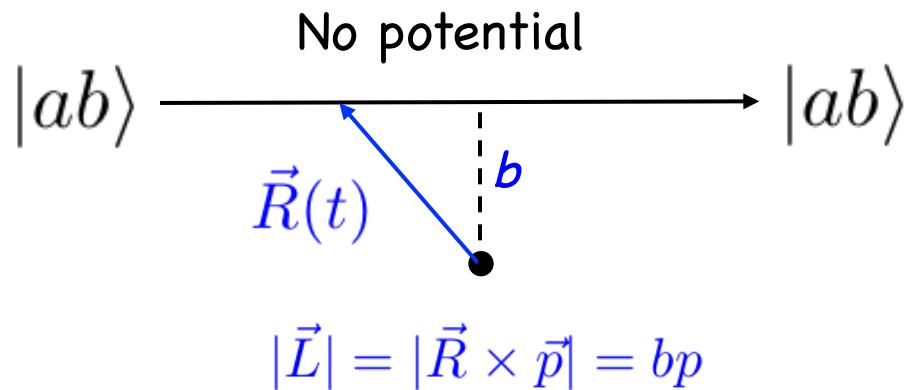
define an area with $\sigma = \pi d^2$ (10^{-12} cm^2)

and a collision rate $\Gamma = nv\sigma$ (typical: 1 s^{-1} , MOT
 10^4 s^{-1} , BEC)

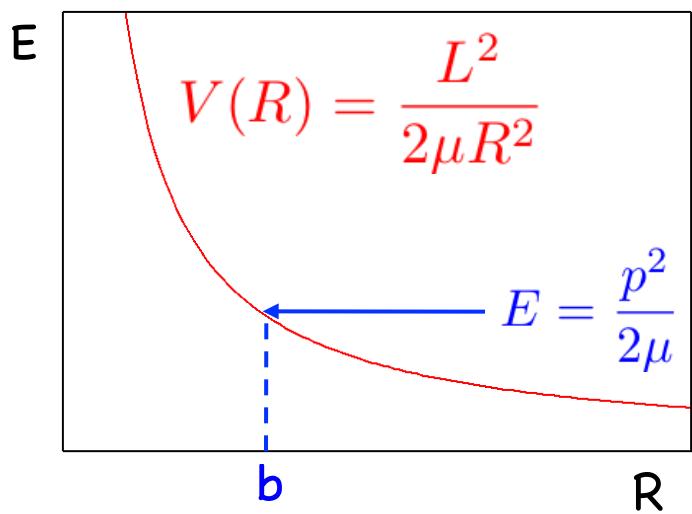
Rate constant $K = v \sigma$

Time between collisions = $1/\Gamma = 1/(Kn) \approx 1\text{s}$ (MOT), $100\mu\text{s}$ (BEC)

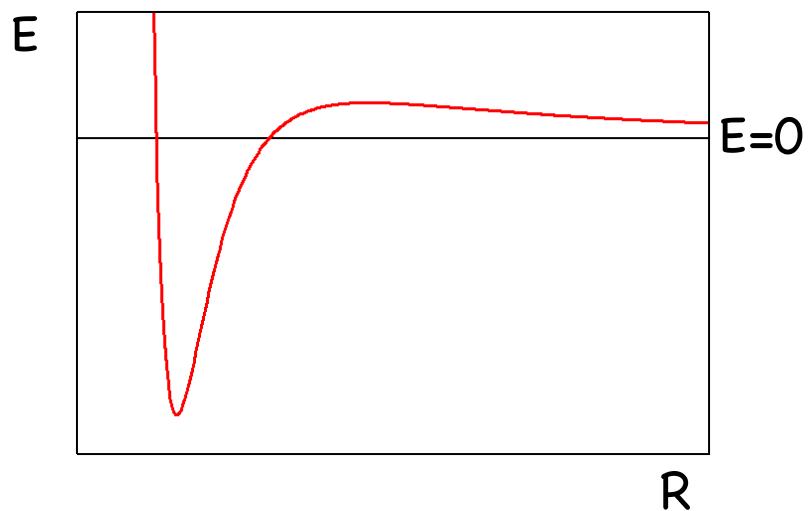
Classical picture



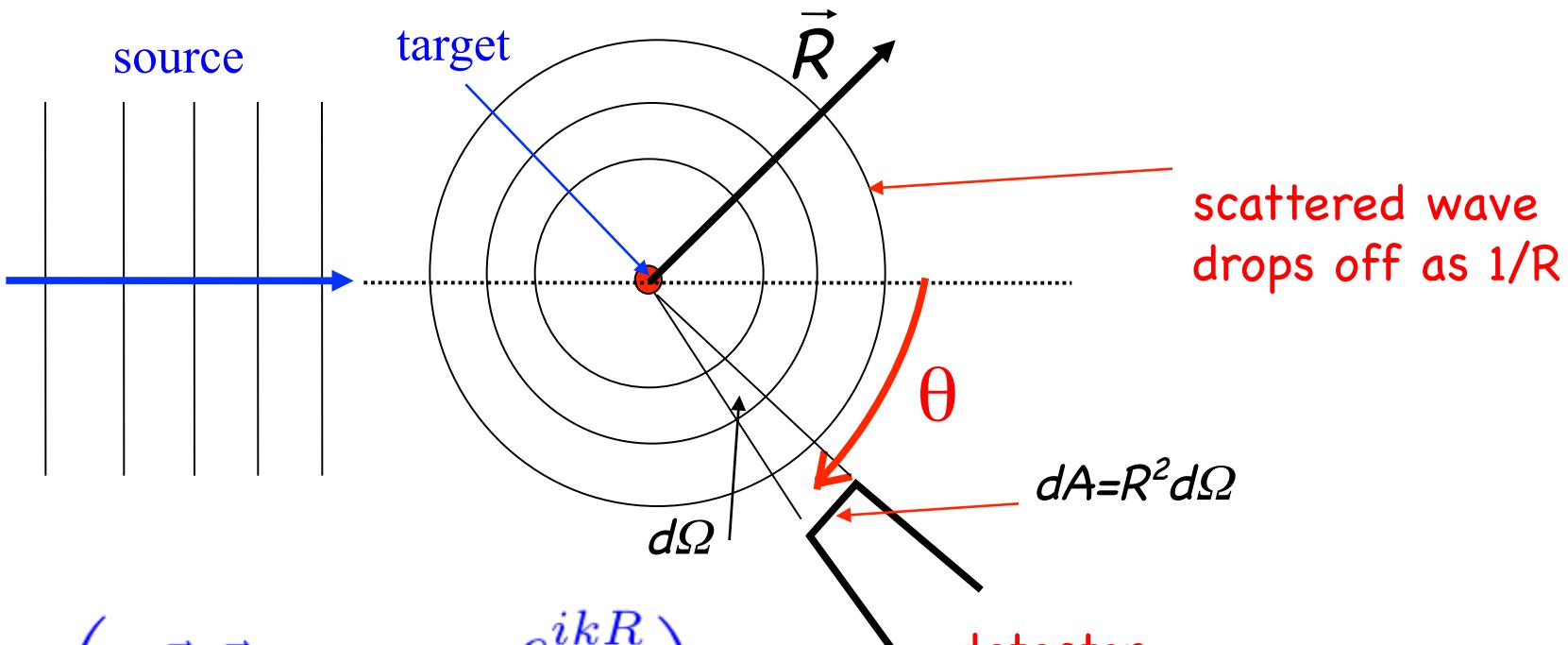
Centrifugal potential



Centrifugal barrier



Quantum scattering theory



$$\left(e^{i\vec{k} \cdot \vec{R}} + f(\Omega) \frac{e^{ikR}}{R} \right) |ab\rangle$$

atoms/s scattered flux into $d\Omega$

plane wave flux (atoms/cm²/s)

$$\begin{aligned}
 &= \frac{d\sigma}{d\Omega} = |f(\Omega)|^2 \\
 \sigma_{\text{tot}} &= \int d\Omega \frac{d\sigma}{d\Omega}
 \end{aligned}$$

Partial wave expansion

Expansion of a plane wave (Messiah, Quantum Mechanics, Vol.1, Appendix B.III):

$$e^{i\vec{k}\cdot\vec{R}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^{\ell} Y_{\ell m}^*(\hat{k}) Y_{\ell m}(\hat{R}) j_{\ell}(kR)$$

Geometric Dynamic

solution to the radial Schrödinger equation
for the centrifugal potential

At large R: $\sin(kR - \pi\ell/2)$

When $V(R)$ is present: $\sin(kR - \pi\ell/2 + \eta_{\ell}(E))$

How do we get the S-matrix, or bound states?

Coupled channels expansion:

$$\Psi_\alpha(R, E) = \sum_{\alpha'} \frac{\phi_{\alpha', \alpha}^+(R, E)}{R} |\alpha'\rangle$$

Solve matrix Schrödinger equation $\mathbf{H}\Psi(R, E) = E\Psi(R, E)$

Extract \mathbf{S} from solution at large $R \gg R_{\text{vdW}}$

Potential matrix $\mathbf{V}_{\alpha\alpha'}(R)$

$M_{\text{tot}} = M_1 + M_2 + m_\ell$ conserved

Electronic (Born-Oppenheimer) $V(R)$ does not change ℓ

Anisotropic (spin-dependent) potential changes ℓ

Collision cross section

Solve Schrödinger equation for each ℓ

Get phase shift $\eta_\ell(E)$

$$\sigma(E) = \frac{4\pi}{k^2} \sum_{\ell} (2\ell + 1) \sin^2 \eta_\ell(E)$$

Identical bosons: even ℓ

Identical fermions: odd ℓ

Nonidentical species: all ℓ

van der Waals potential:

$$\eta_\ell(E) \rightarrow -Ak \quad s\text{-wave as } k \rightarrow 0$$

$$\eta_\ell(E) \rightarrow -(A_1 k)^3 \quad p\text{-wave as } k \rightarrow 0$$

$$\eta_\ell(E) \propto k^4 \quad d\text{-wave and higher as } k \rightarrow 0$$

S-wave collision summary

If only a single s-wave channel, $S_{\alpha\alpha} = e^{2i\eta} \rightarrow e^{-2ika}$ as $k \rightarrow 0$

If inelastic channels $\alpha' \neq \alpha$ exist, unitarity ensures

$$|S_{\alpha\alpha}|^2 = 1 - \sum_{\alpha' \neq \alpha} |S_{\alpha\alpha'}|^2 = 1 - 4kb_\alpha$$

Thus, $S_{\alpha\alpha} = e^{-2ik(a-ib)}$ as $k \rightarrow 0$

Complex scattering length $a-ib$

$$\sigma_{\alpha\alpha} = 4\pi(a^2 + b^2)$$

$$K_{\text{loss}} = \sum_{\alpha' \neq \alpha} K_{\alpha\alpha'} = 2\frac{h}{\mu}b$$

Collision cross sections and rate constants

Scattering channels

Start in initial channel: $\{ab\}\ell m = \alpha$

Exit in final channel: $\{a'b'\}\ell'm' = \alpha'$

Transition amplitudes $T_{\alpha\alpha'} = \delta_{\alpha\alpha'} - S_{\alpha\alpha'}$ are expressed in terms of the elements of the unitary S-matrix

Elastic cross section $\sigma_{\alpha}^{\text{el}}(E) = \frac{\pi}{k^2} |1 - S_{\alpha\alpha}(E)|^2$

Inelastic cross section $\sigma_{\alpha}^{\text{loss}}(E) = \frac{\pi}{k^2} (1 - |S_{\alpha\alpha}(E)|^2)$

$$\sum_{\alpha' \neq \alpha} |S_{\alpha\alpha'}(E)|^2 = 1 - |S_{\alpha\alpha}(E)|^2 \quad \text{since } S \text{ is unitary.}$$

Sum over all contributing ℓm for a given $\{ab\}$ to get the TOTAL (observable) cross section.

Rate constants

Loss rate
constant

$$K_\alpha^{\text{loss}}(E) = v\sigma_\alpha^{\text{loss}}(E) = 2\frac{h}{\mu} b_\alpha(E)$$

where $b_\alpha(E) = \frac{1 - |S_{\alpha\alpha}(E)|^2}{k}$ has units of length.

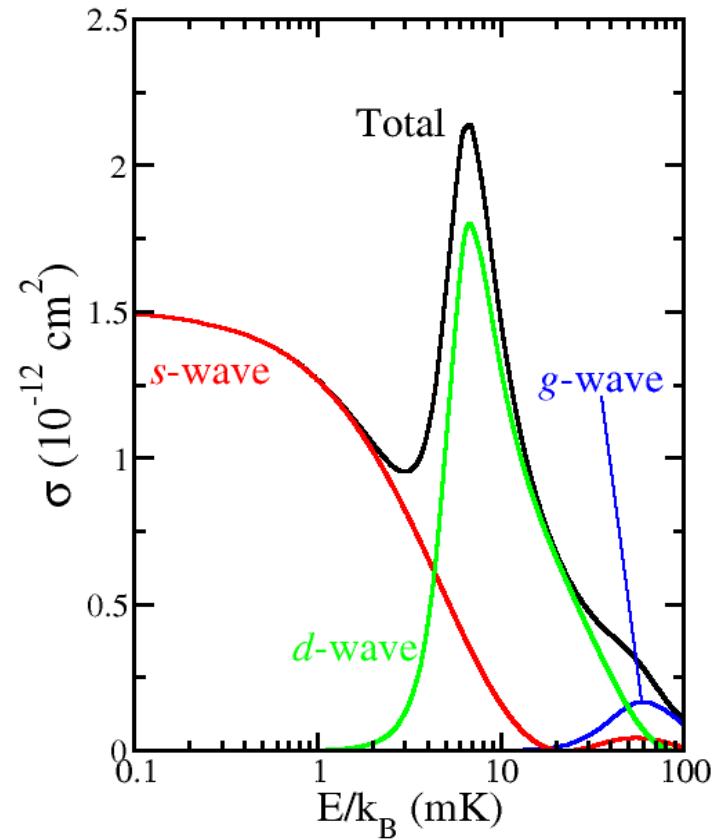
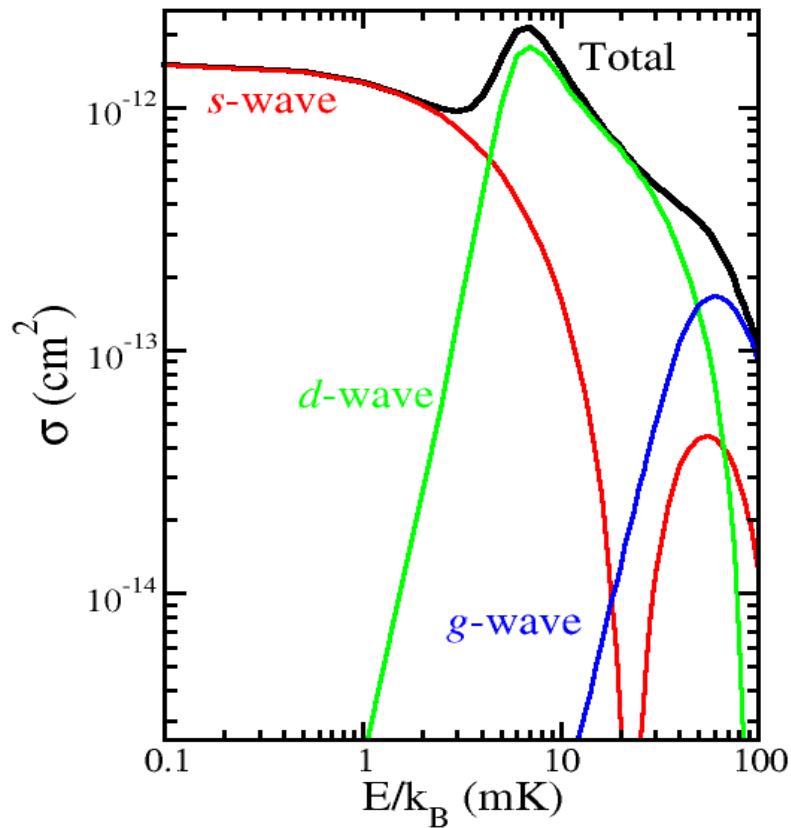
$$K_\alpha^{\text{loss}}(E) = 2\frac{h}{\mu} b_\alpha(E) = 4.2 \times 10^{-11} \text{ cm}^3/\text{s} \frac{b[a_0]}{\mu[\text{amu}]}$$

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

“Forbidden” $b \ll 1 a_0$

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

Elastic cross section σ for like Na atoms



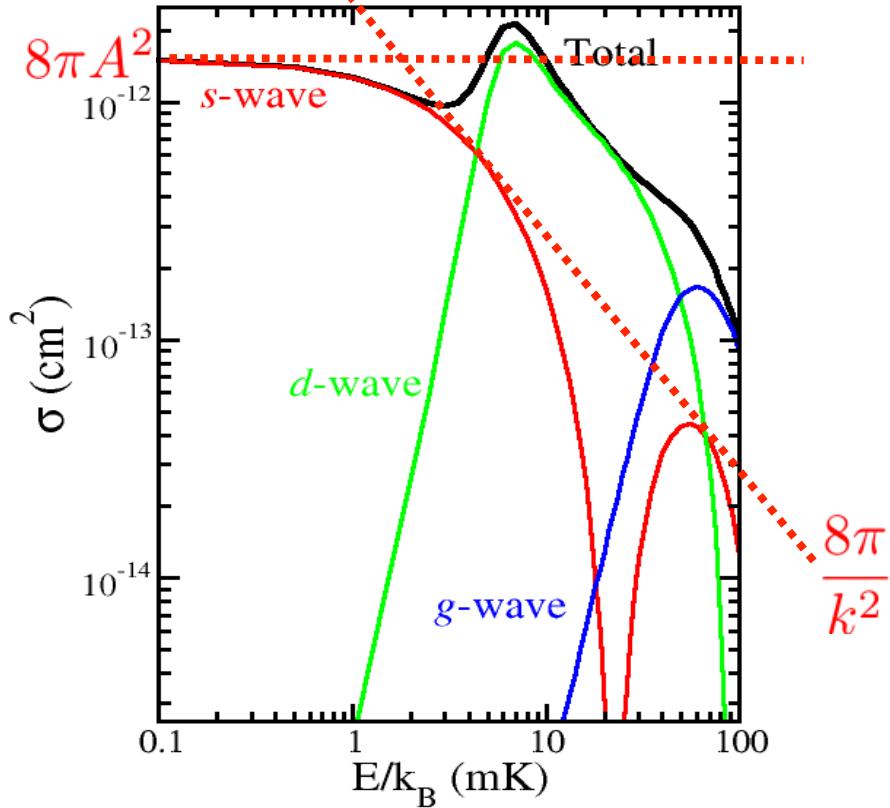
Many (even) partial waves

Threshold properties (elastic only)

$$\sigma(E) = \frac{4\pi}{k^2} \sin^2(kA) = 4\pi A^2 \text{ as } k \rightarrow 0$$

$(8\pi A^2 \text{ for identical bosons})$

Upper bound = 1 (unitarity limit)



$$\begin{aligned}\sigma(E) &= \frac{4\pi}{k^2} \propto \frac{1}{E} \\ &= 4\pi \left(\frac{\lambda}{2\pi} \right)^2\end{aligned}$$

Atomic and molecular collision rates

Standard chemical form from Mies, J. Chem. Phys. 51, 787, 798 (1969); see arXiv:0812.1233

$$\frac{dn_a}{dt} = -Kn_a n_b = -\frac{1}{\tau} n_a \quad \text{where} \quad \frac{1}{\tau} = Kn_b$$

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

Q_T = translational partition function

Λ_T = thermal de Broglie wavelength
of pair

$$f_D = \int_0^\infty \sum_{\ell m} (1 - |S(\ell m)|^2) e^{-E/(k_B T)} dE / (k_B T)$$

$$\frac{1}{\tau} = Kn_b = (n\Lambda_T^3) \frac{k_B T}{h} f_D$$

Phase Space Time scale
Space density Dynamics

Replace
 $1 - |S(\ell m)|^2$ by $|1 - S(\ell m)|^2$
for elastic collisions

Van der Waals potentials

Van der Waals potential

Write the Schrödinger equation in length and energy units of

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

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

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

The potential becomes $-\frac{16}{r^6} + \frac{\ell(\ell+1)}{r^2}$ in vdw units.

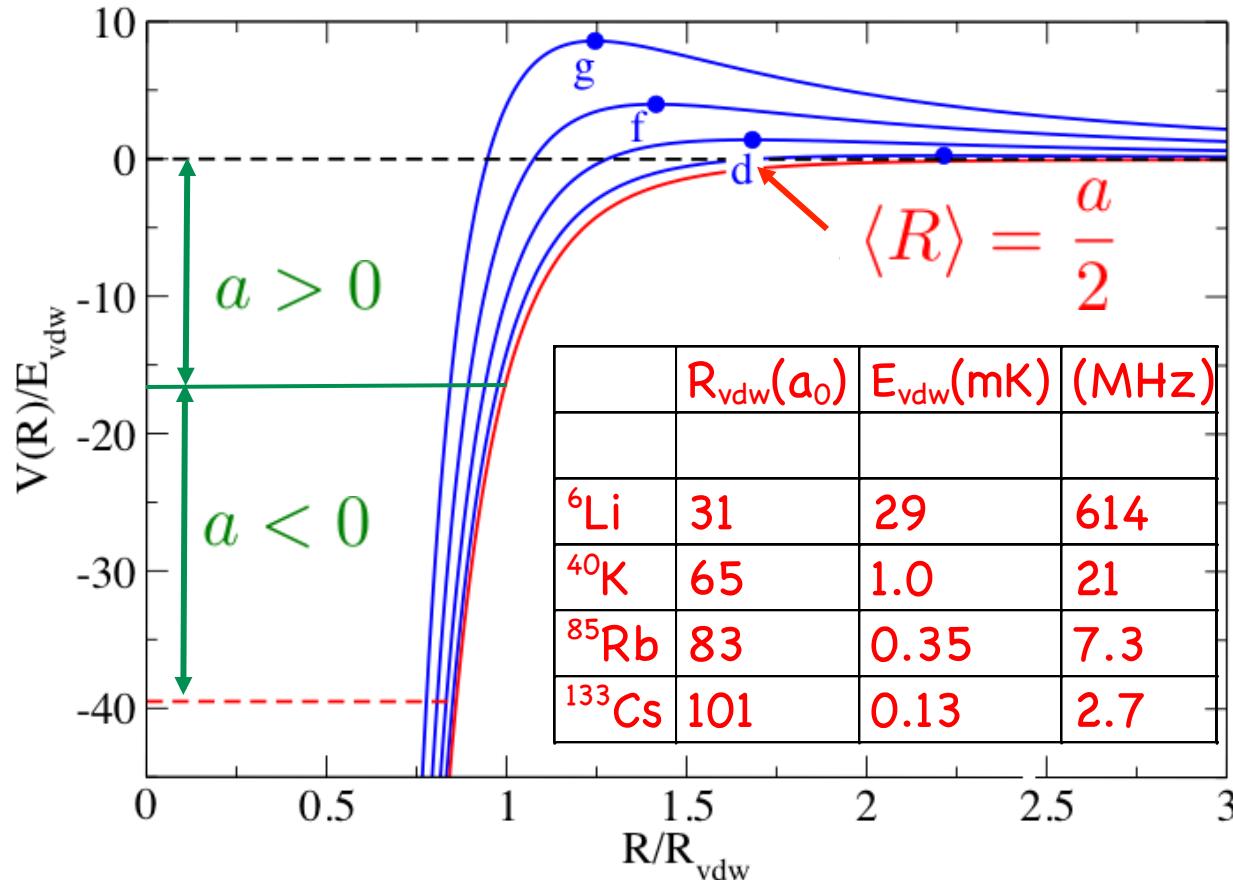
This potential has exact analytic solutions and many useful properties.

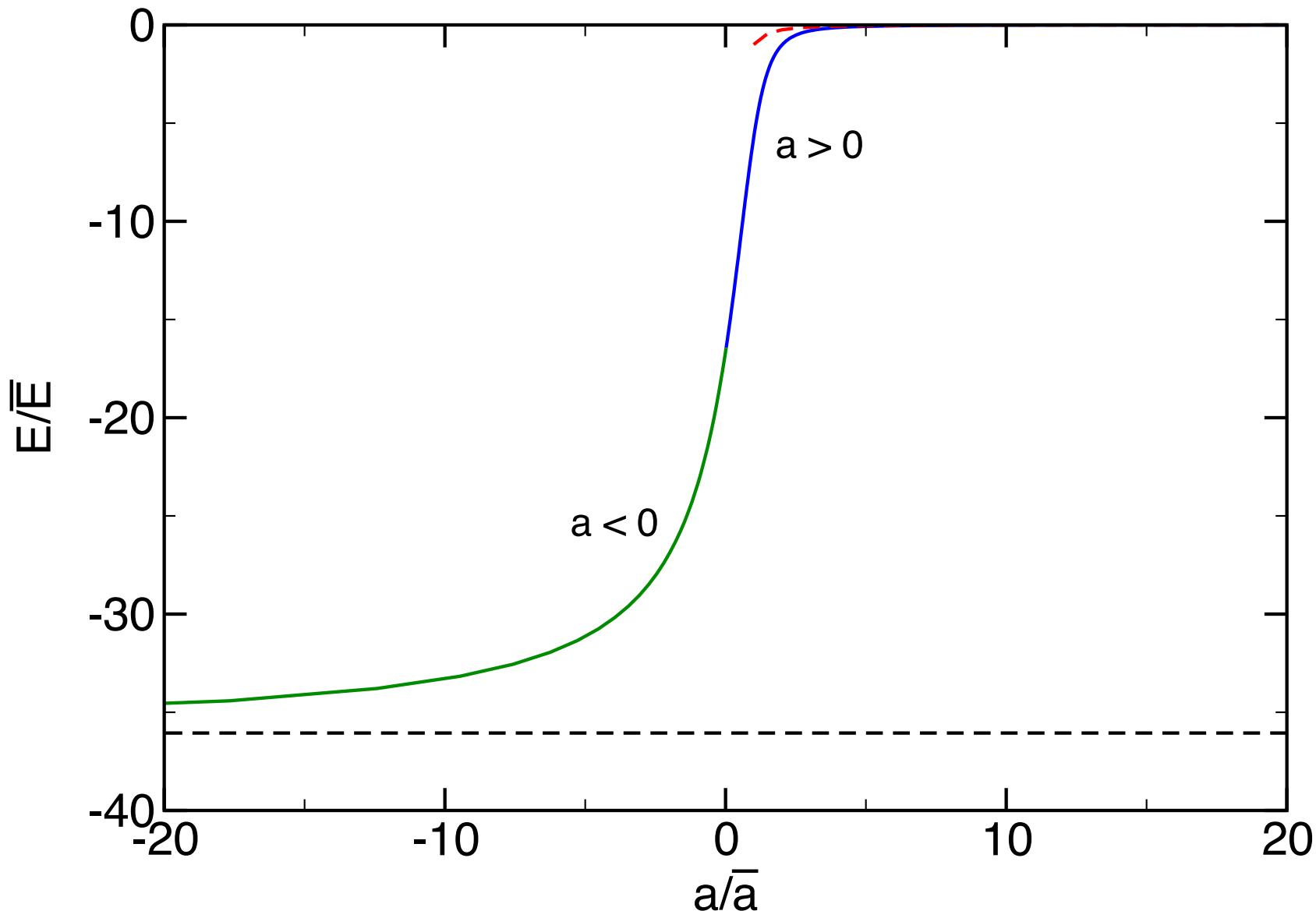
B. Gao, Phys. Rev. A 58, 1728, 4222 (1998) + series of papers.

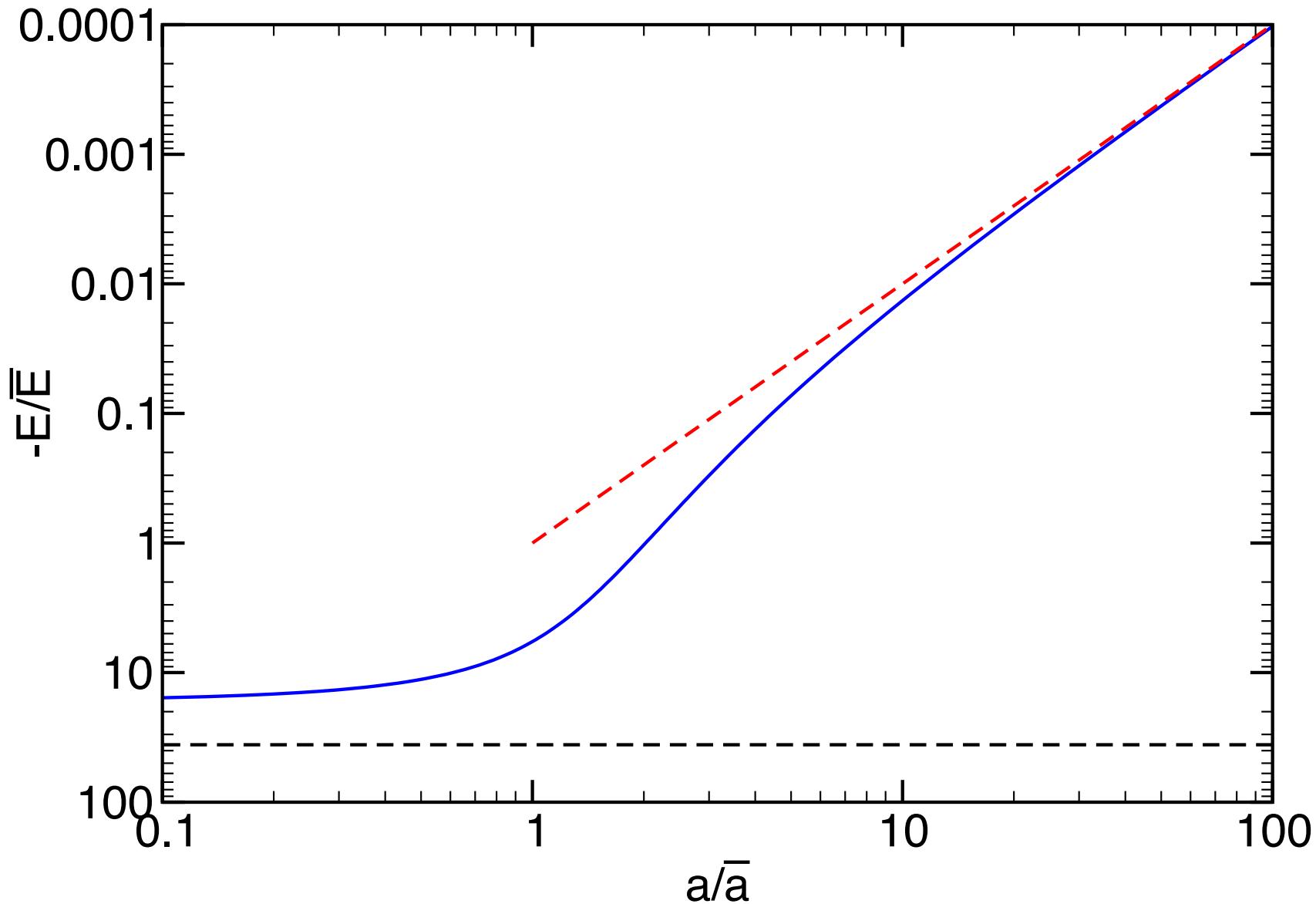
See Jones, et al., Rev. Mod. Phys. 78, 483 (2006)

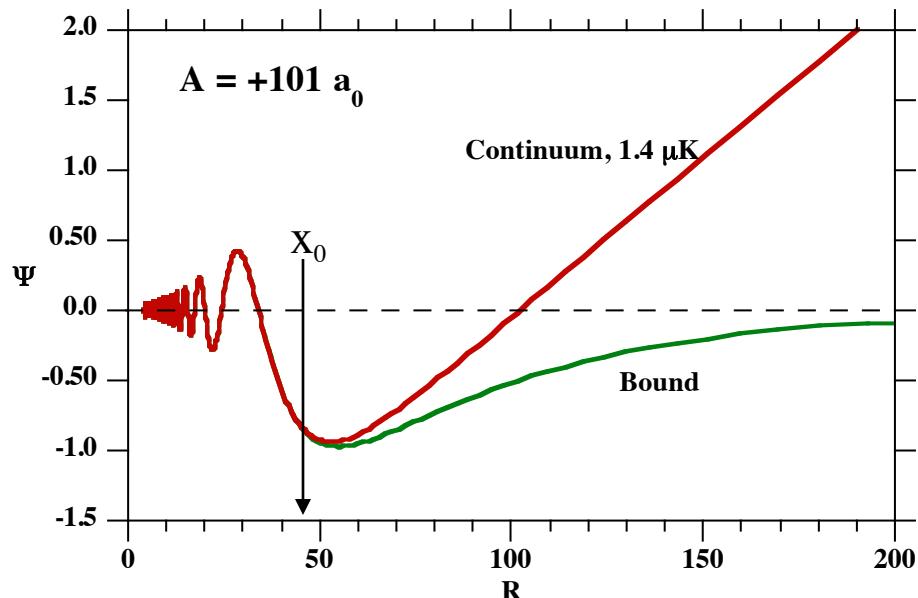
and Chin et al., Feshbach review

“Size” of vdW potential

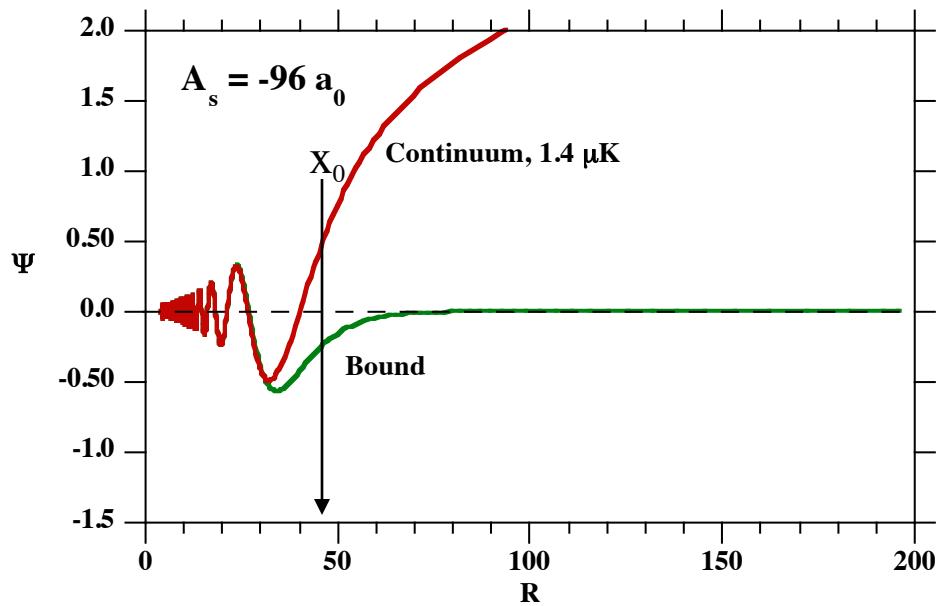




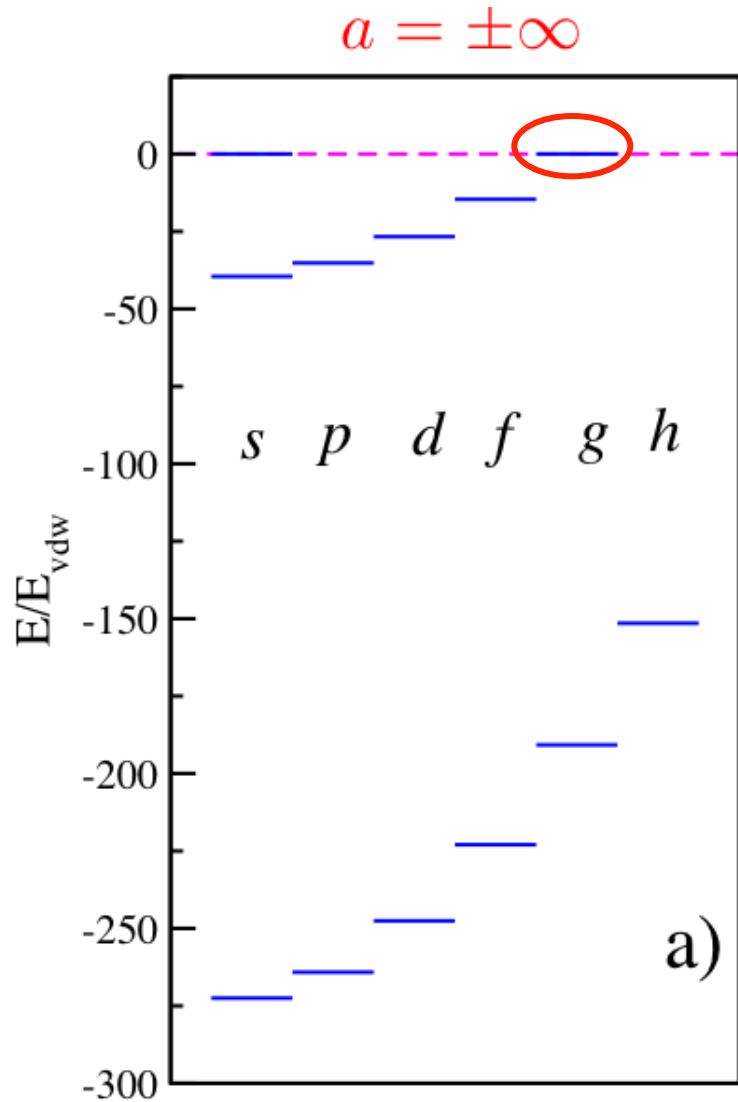




Scattering and last
bound state near
threshold
(normalized to same
value at small R)



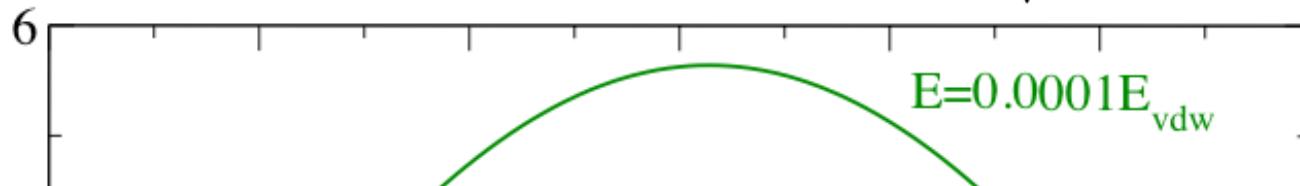
Bound states from van der Waals theory



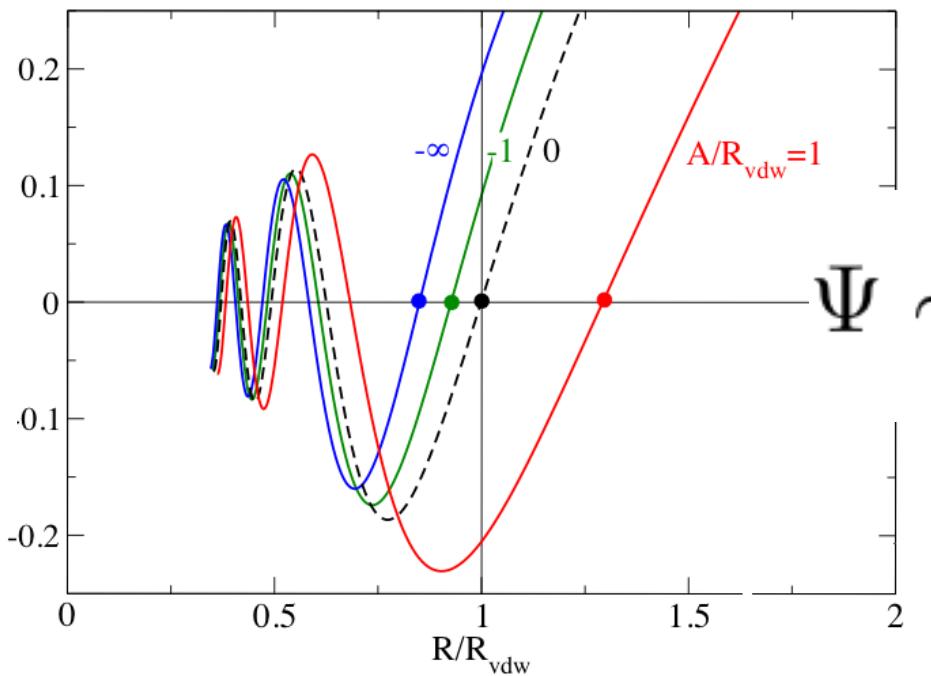
Adapted from Gao, Phys. Rev. A 62, 050702 (2000); Figure from Chin et al., review

Noninteracting atoms

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

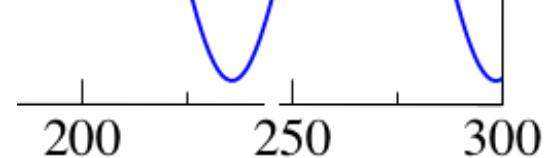


Interacting atoms



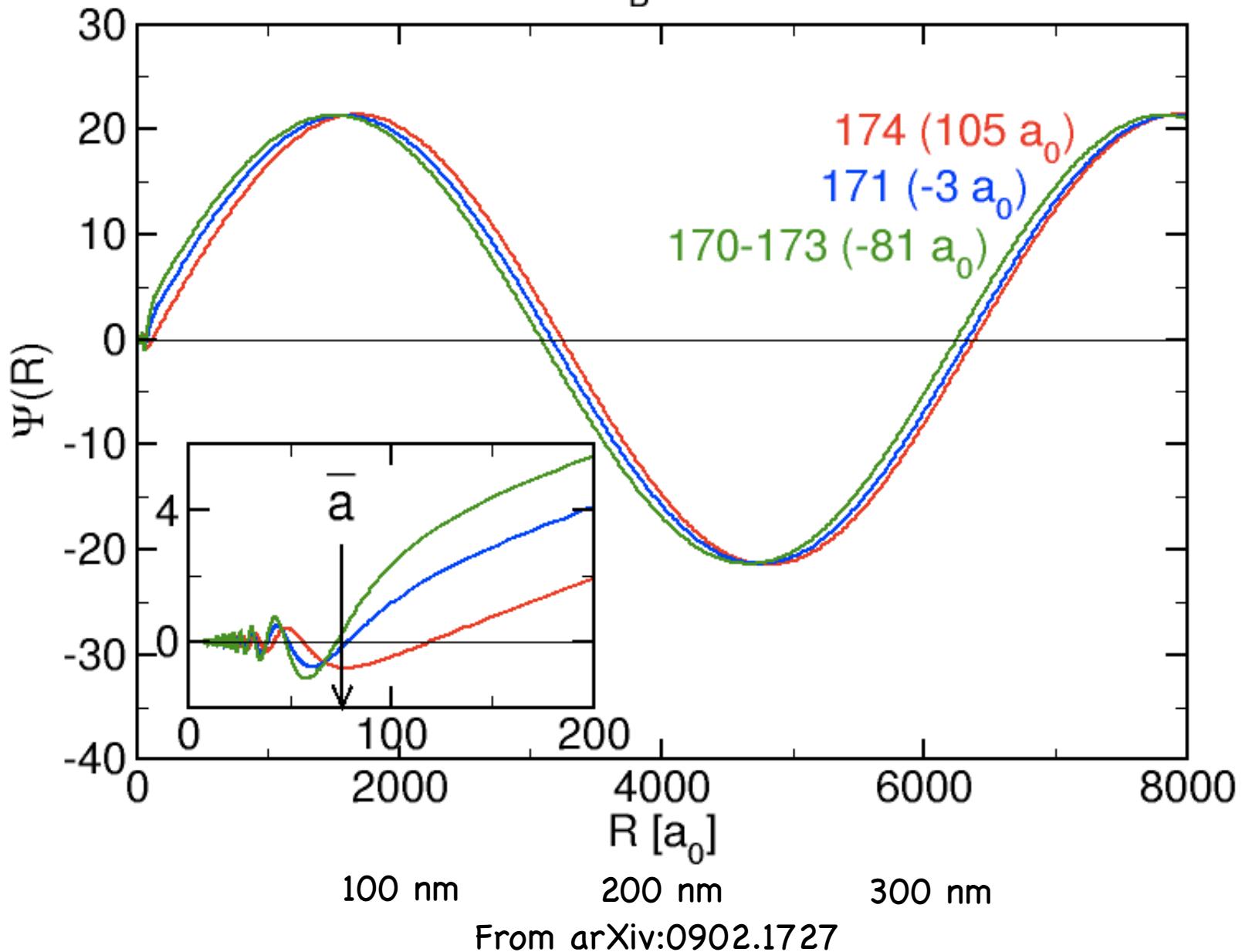
$$\Psi \sim$$

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



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

Yb + Yb $E/k_B = 1 \mu\text{K}$

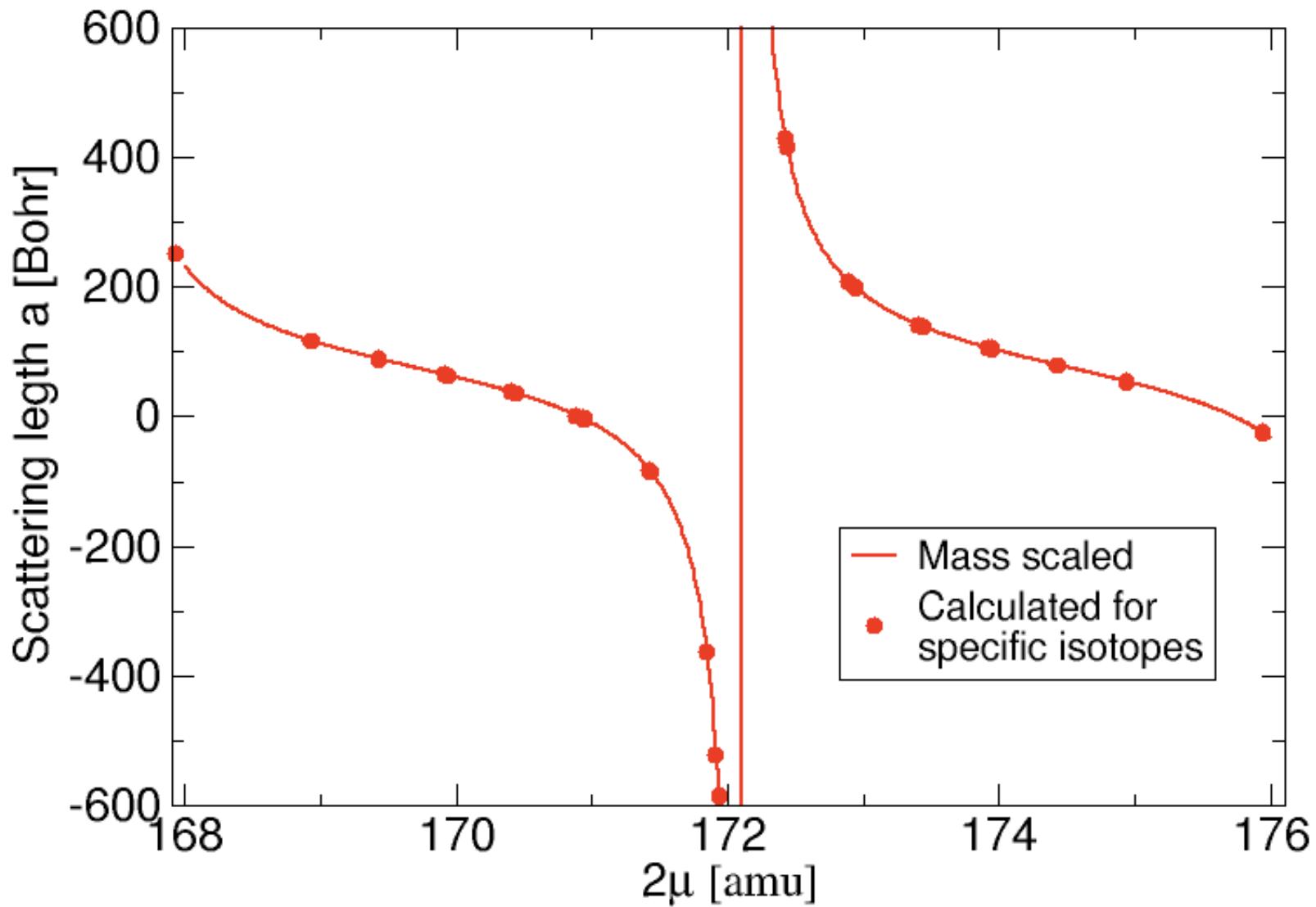


Scattering lengths for Yb ground state model (in a_0 units)

	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)

M. Kitagawa, K. Enomoto, K. Kasa, Y. Takahashi, R. Ciurylo, P. Naidon, P. Julienne,
 Phys. Rev. A 77, 012719 (2008)

Yb a versus reduced mass μ



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

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

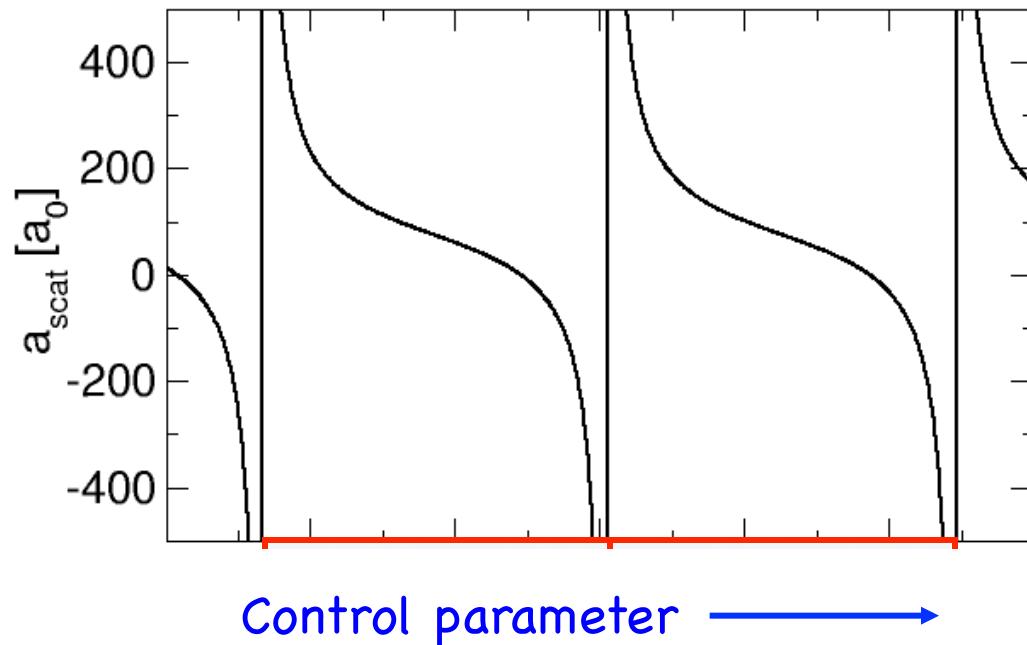
$$\Phi = \int_{r_{in}}^{\infty} \left(\frac{2\mu}{\hbar^2} (-V(R)) \right)^{1/2} dR$$

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

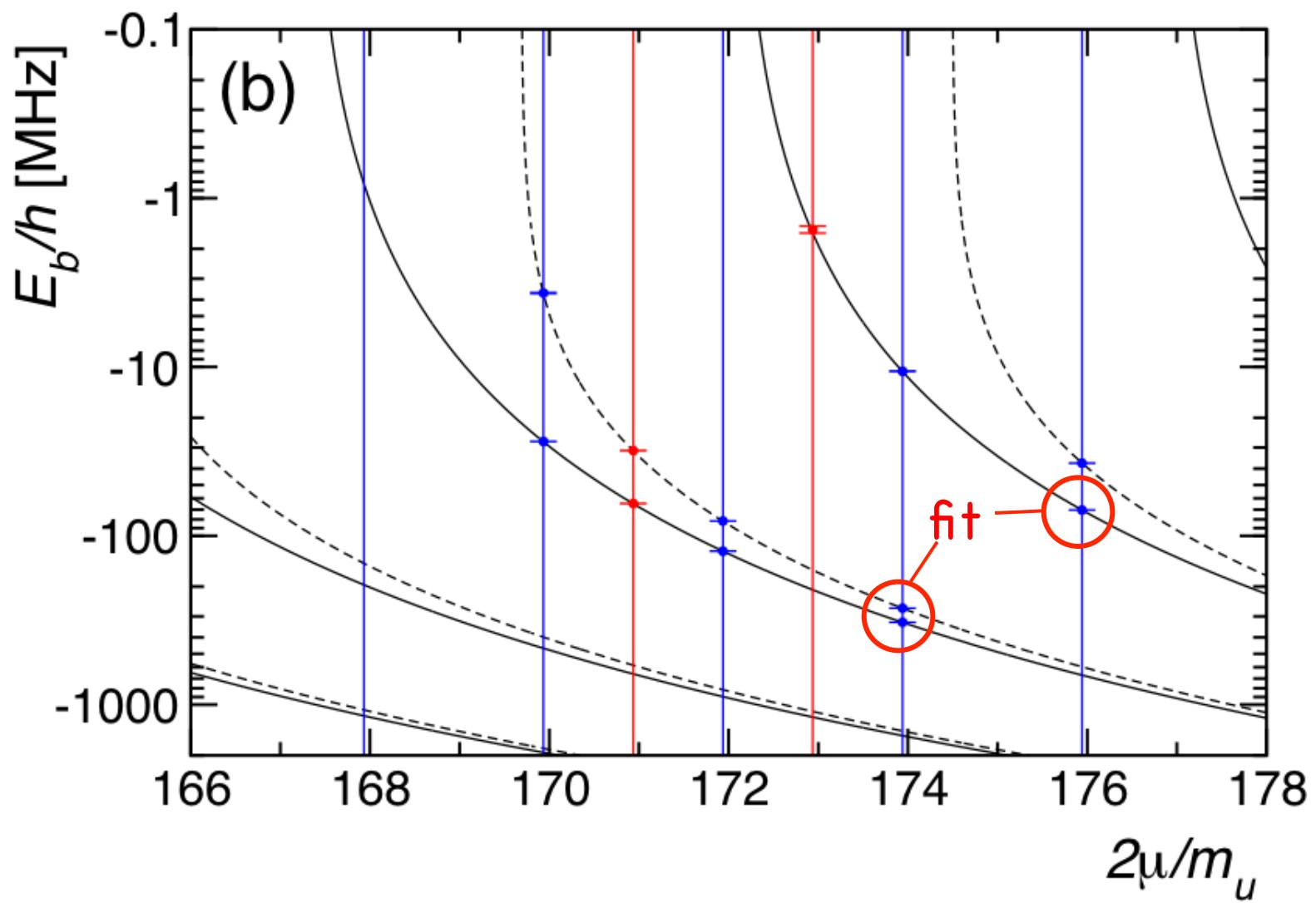
Simplest model:

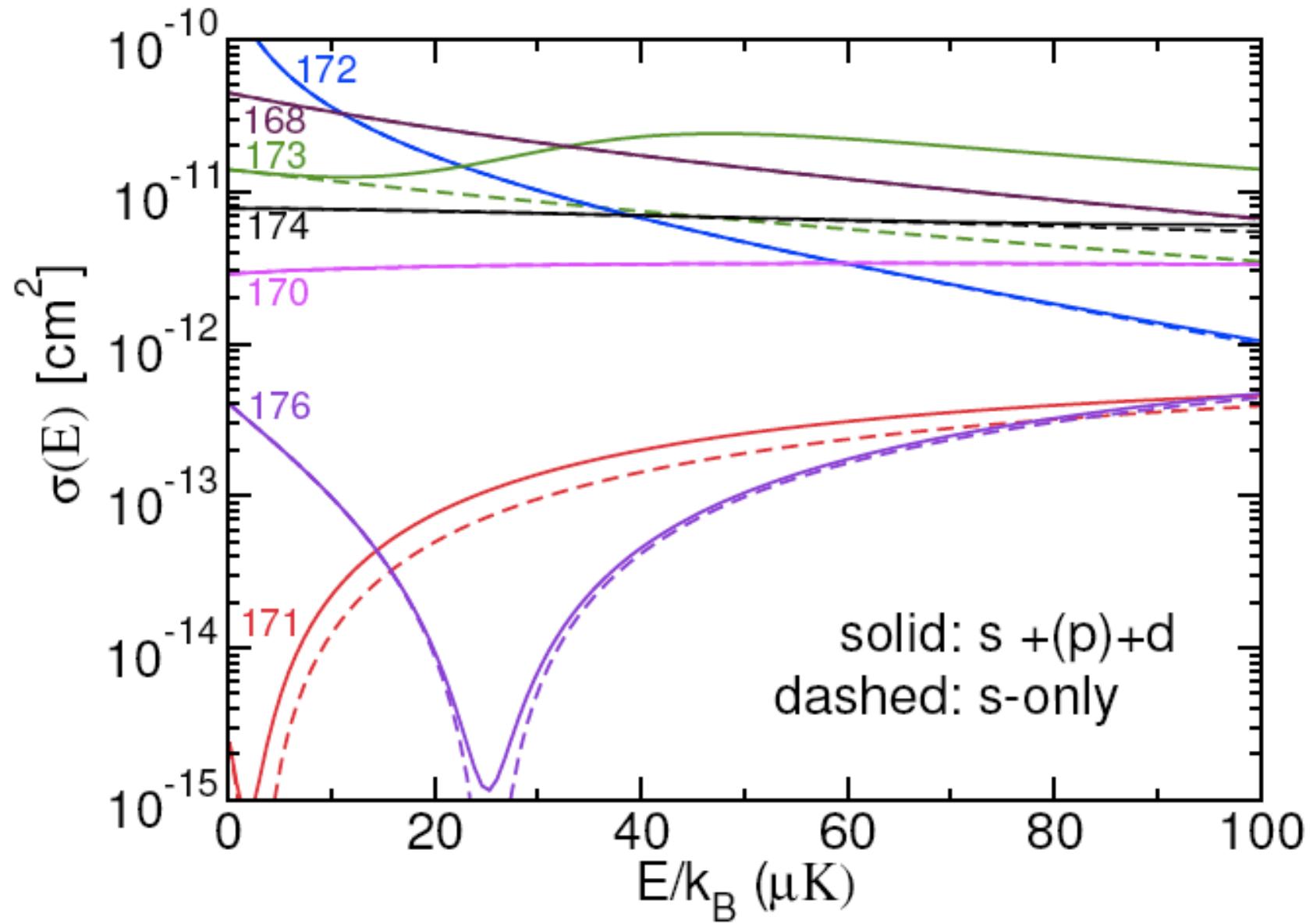
$$V(R) = -\frac{C_6}{R^6} \text{ for } R_{in} < R \leq \infty$$

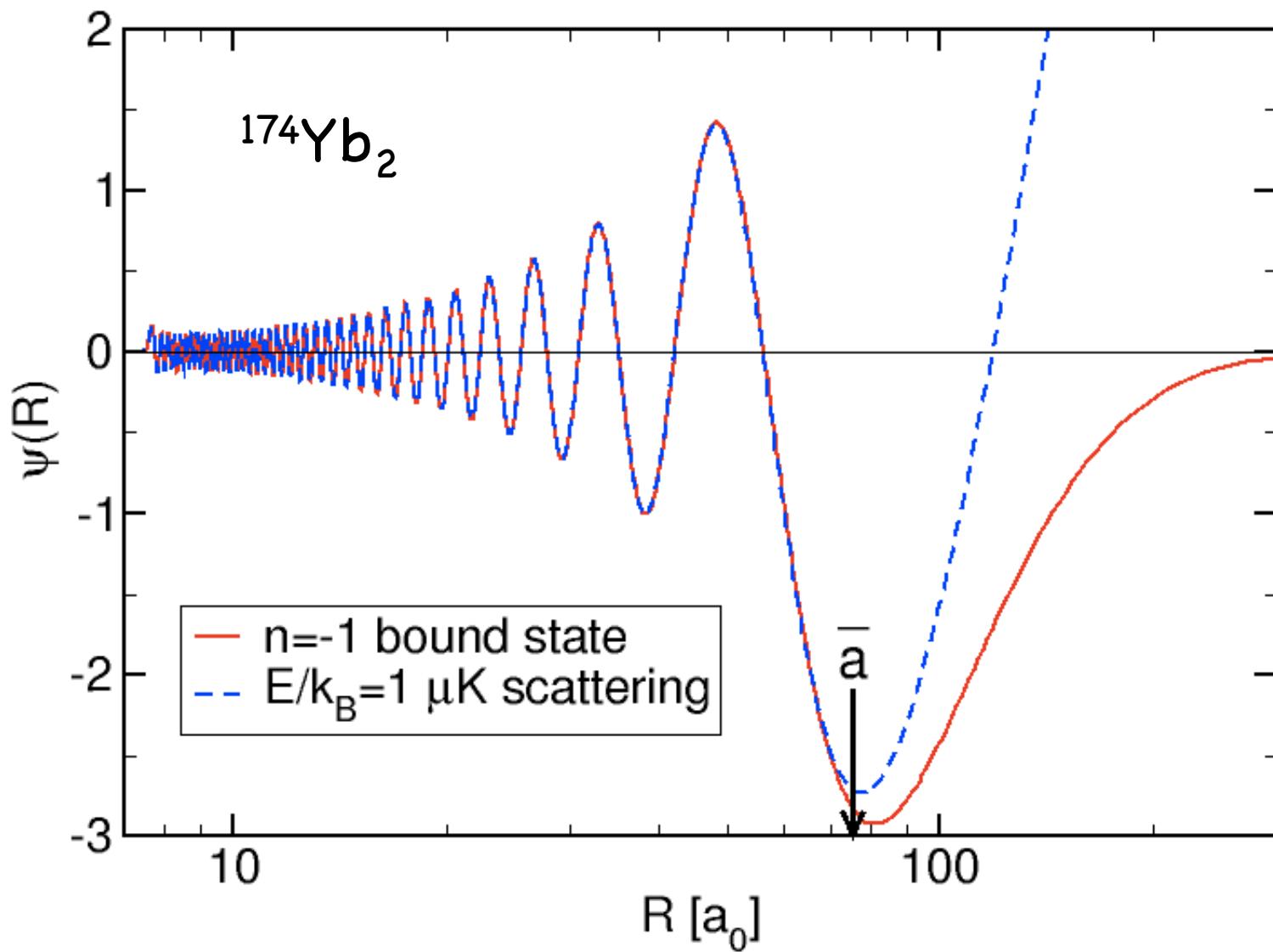
$$V(R) = \infty \text{ for } 0 < R \leq R_{in}$$



Last bound state energies versus mass
Solid: J=0
Dashed: J=2

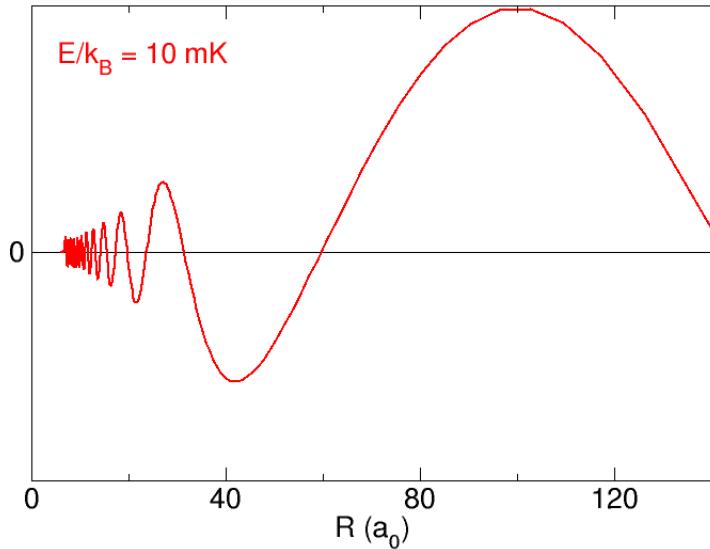






Semiclassical considerations

WKB phase-amplitude form: $\phi^{\text{WKB}}(R, E) = \alpha(R, E) \sin \beta(R, E)$



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

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

$$k(R, E) = \left(\frac{2\mu}{\hbar^2} (E - V(R)) \right)^{\frac{1}{2}} = \frac{2\pi}{\lambda(R, E)}$$

Validity criterion: $\frac{d\lambda(R, E)}{dR} \ll 1$

Semiclassical considerations continued

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

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

R_{vdw}

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

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

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

$$\lim_{E \gg E_{\text{vdw}}} C(E)^{-1} = 1$$

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

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

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

The End

ICAP 2014 Summer School, July 31, Williamsburg

Understanding cold atomic and molecular collisions

1. Feshbach resonances

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

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

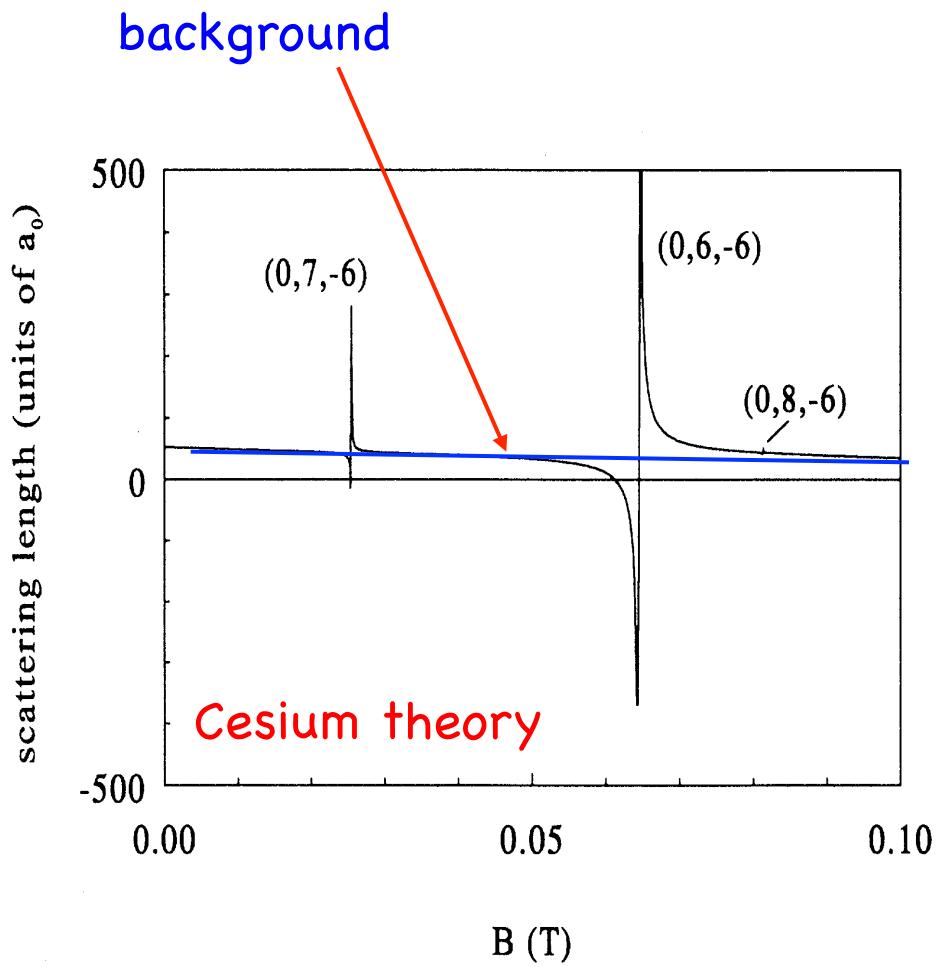
Supported by an AFOSR MURI

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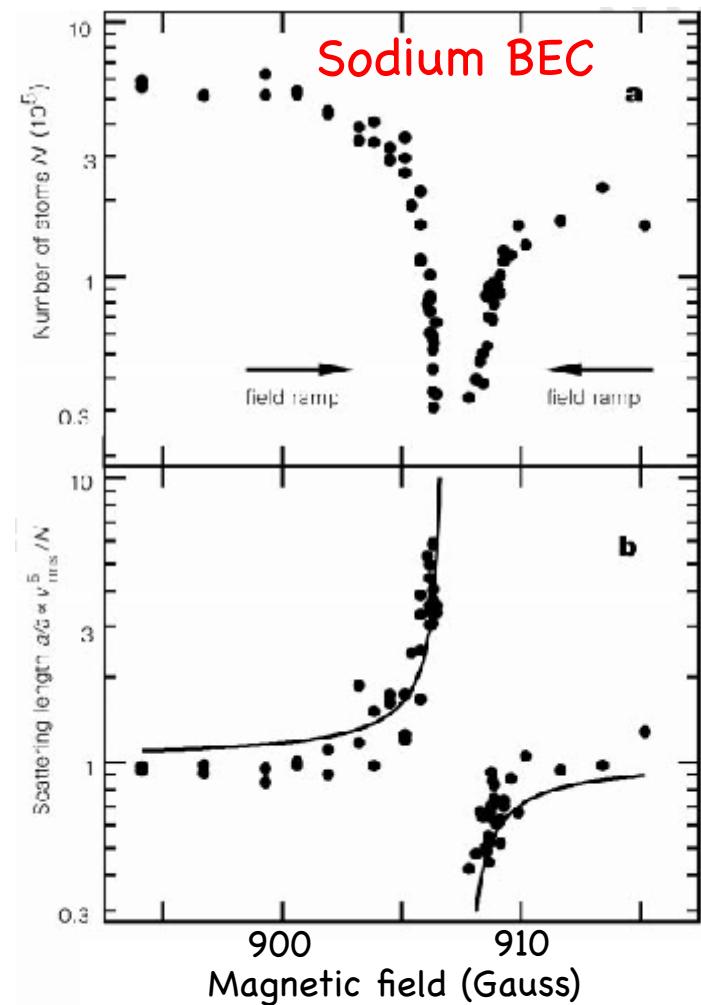


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Some examples of Feshbach resonances



E. Tiesinga *et al.*, Phys. Rev. A **47**, 4114 (1993)

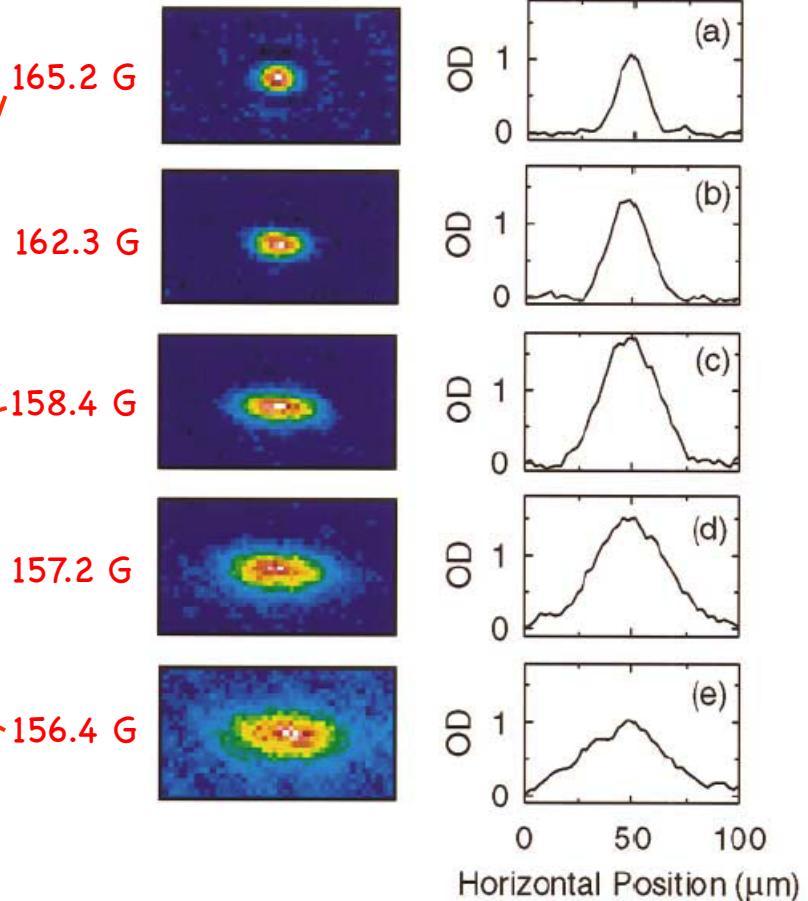
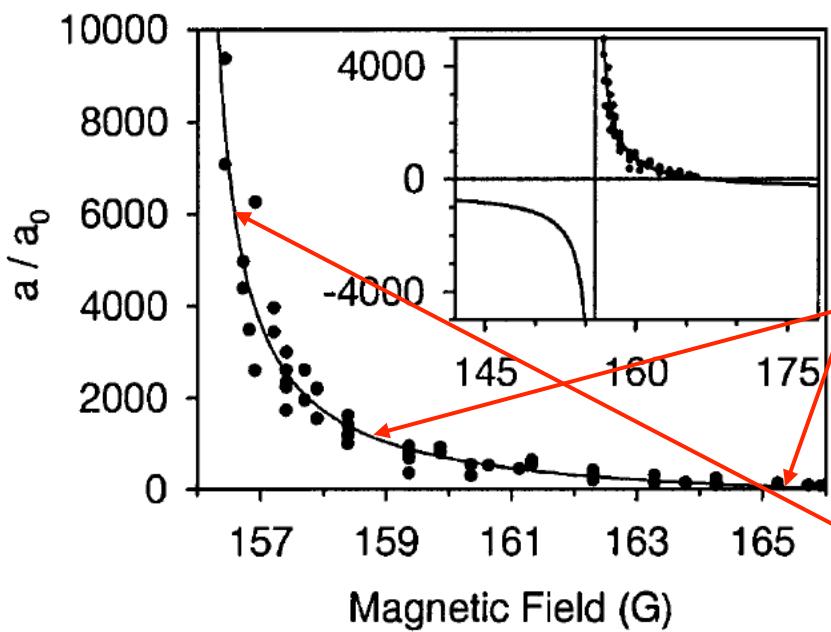


S. Inouye *et al*
Nature **392**, 141 (1998)

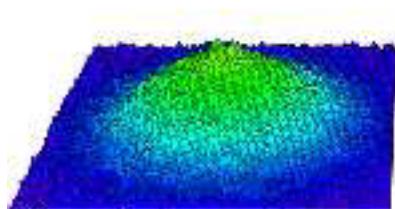
An example for $E \rightarrow 0$

Cornish, Claussen, Roberts, Cornell, Wieman,
Phys. Rev. Lett. 85, 1795 (2000)

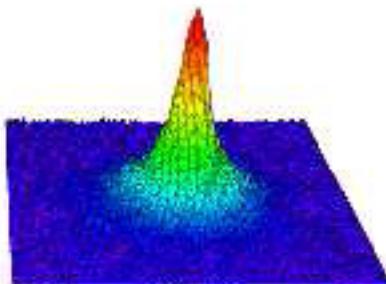
^{85}Rb BEC (below 15 nK)



Tunable scattering resonances used for



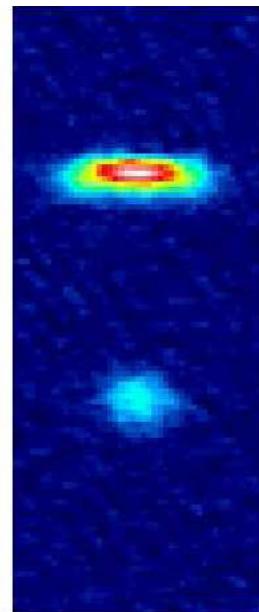
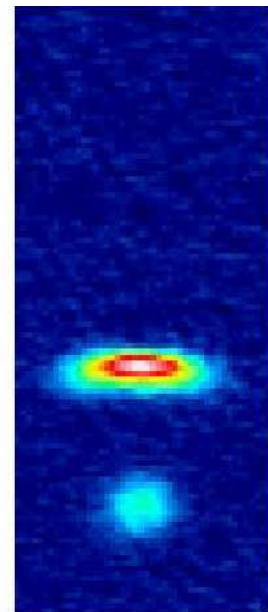
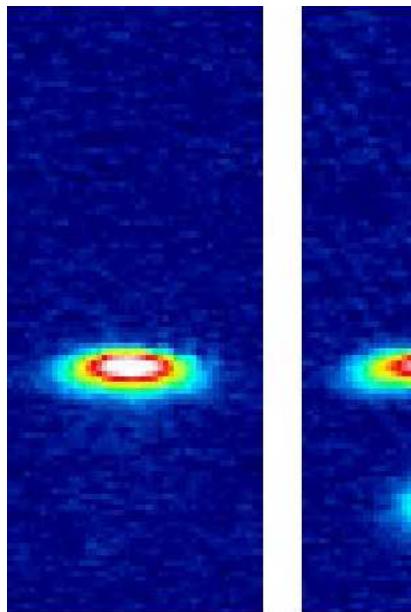
Thermal (250 nK)



BEC (79 nK)

Making $^{40}\text{K}_2$ molecules

Greiner, M., C. A. Regal, and D. S. Jin, 2003,
Nature (London) 426, 537.

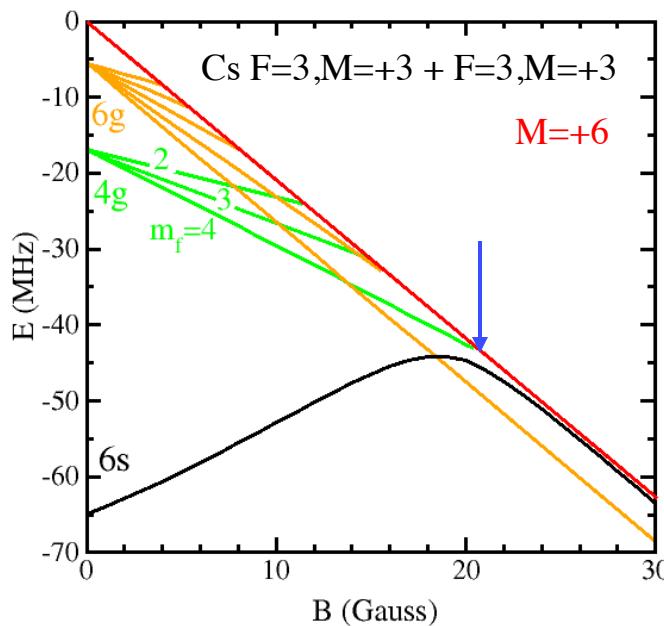
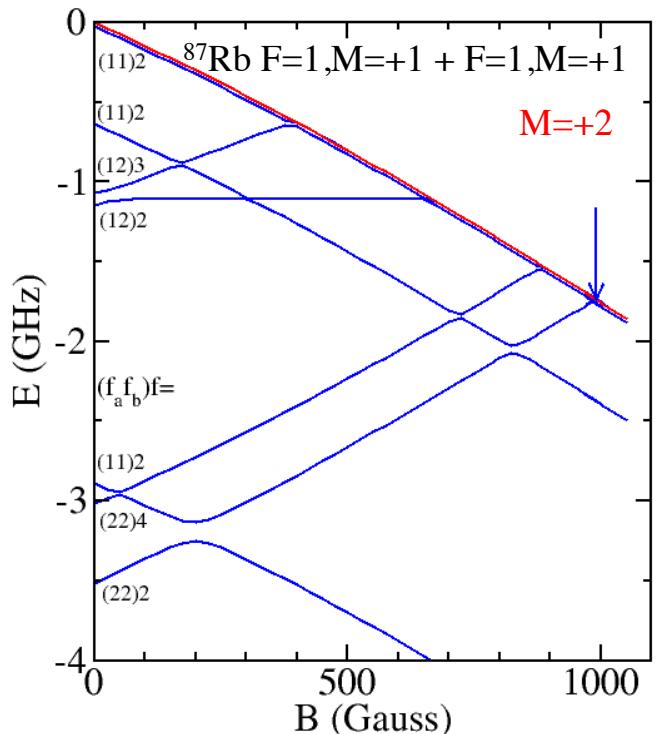
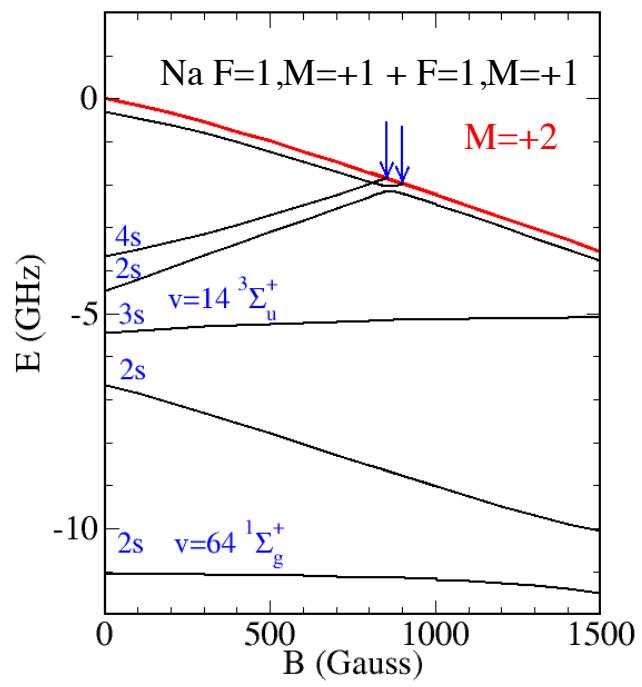
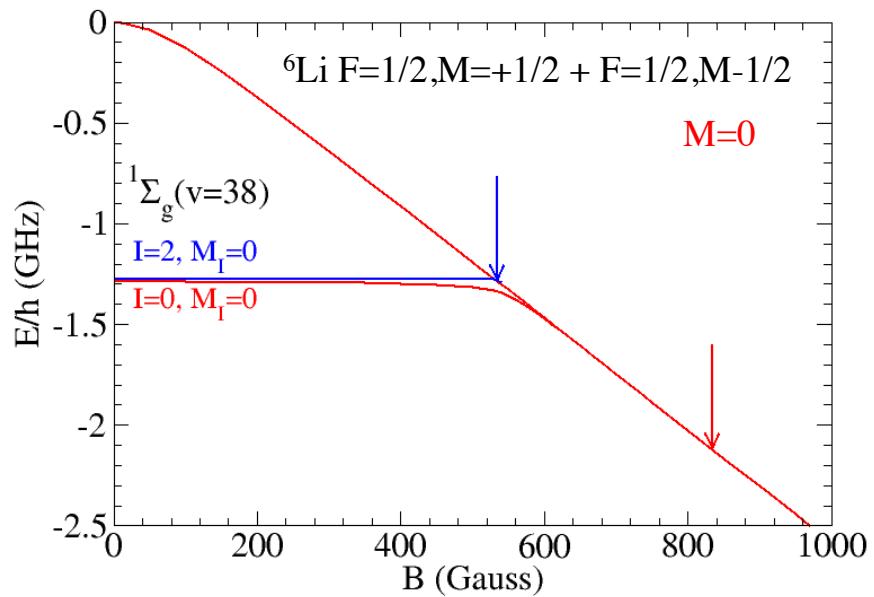


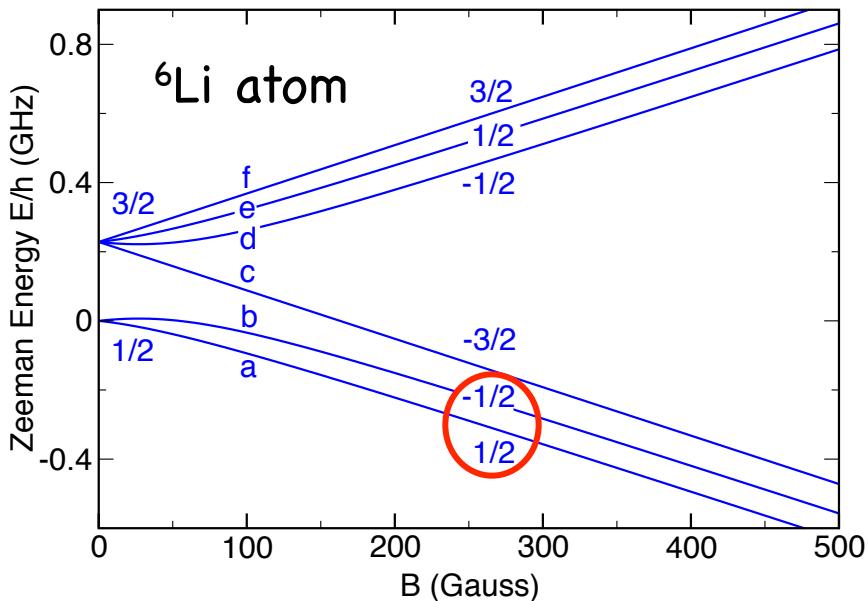
Making $^{133}\text{Cs}_2$ molecules

^{133}Cs atom cloud

$^{133}\text{Cs}_2$ molecule cloud

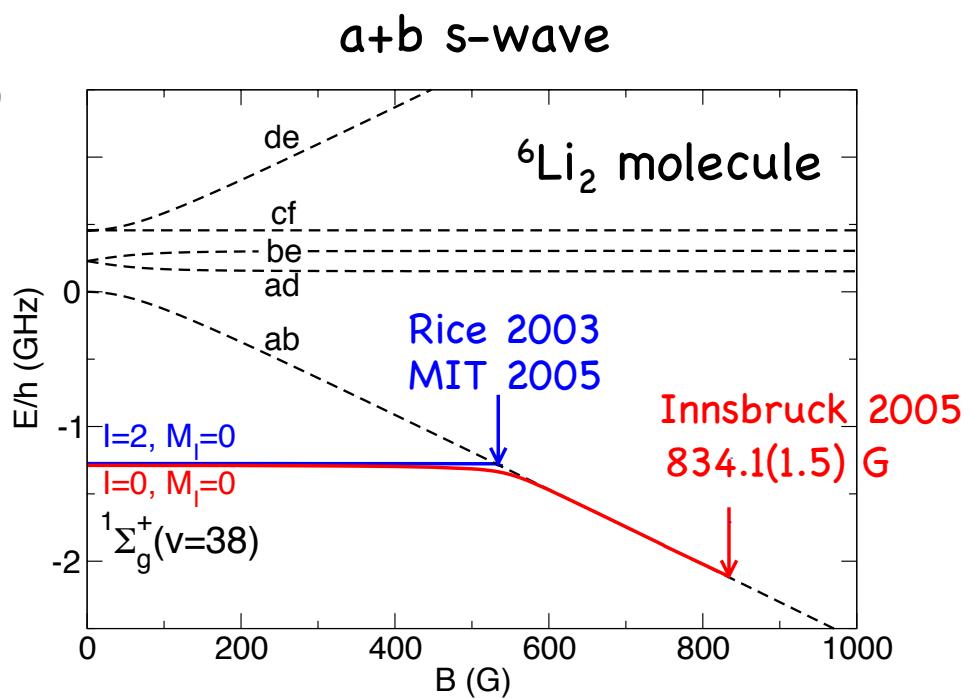
Herbig, J., T. Kraemer, M. Mark, T. Weber, C. Chin,
H.-C. Nagerl, and R. Grimm, 2003, Science 301, 1510.





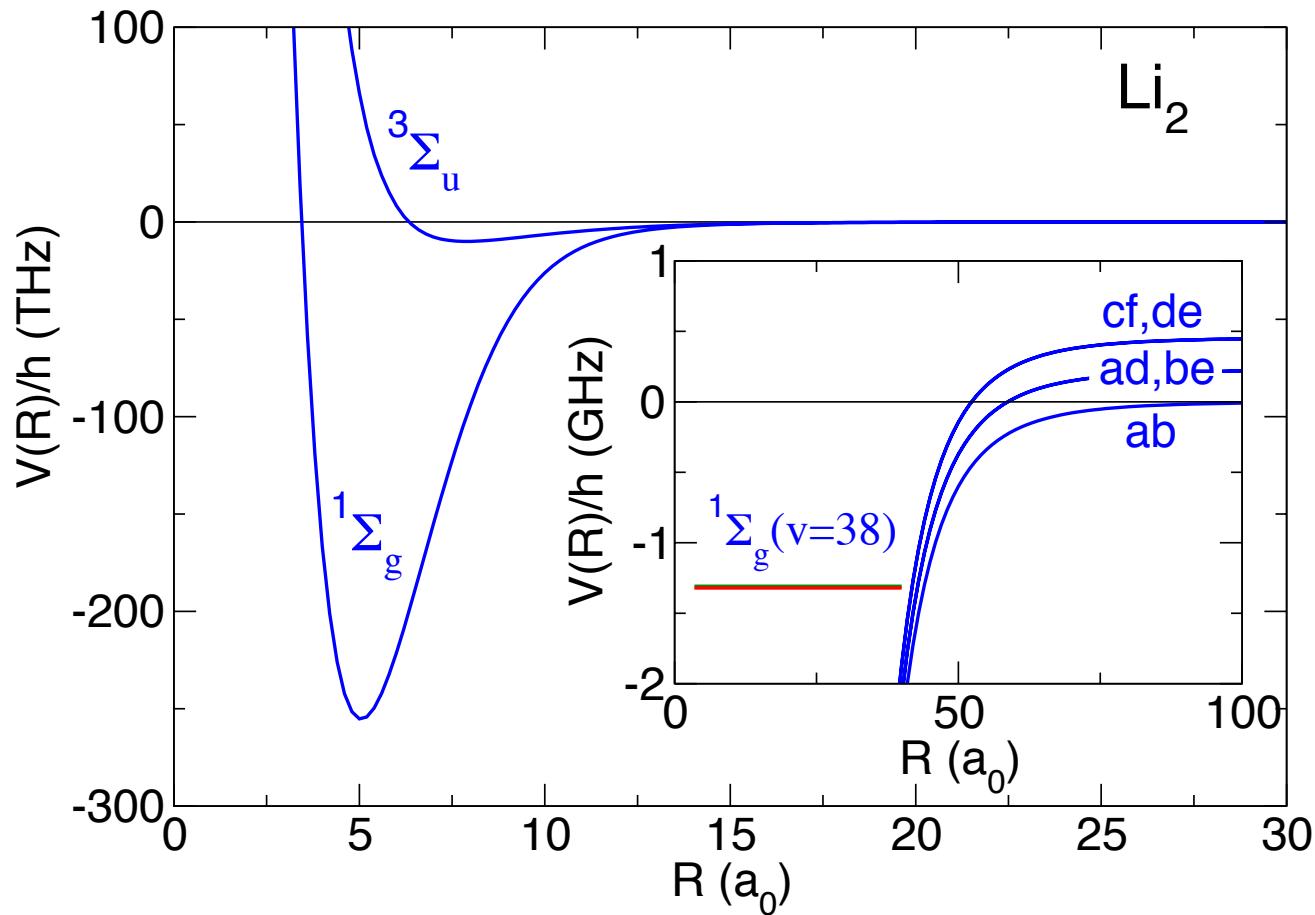
Molecular physics of Li+Li
is well-known

Quantum degenerate Fermi mixtures
BEC-BCS crossover
Strongly interacting gas
Equation of state

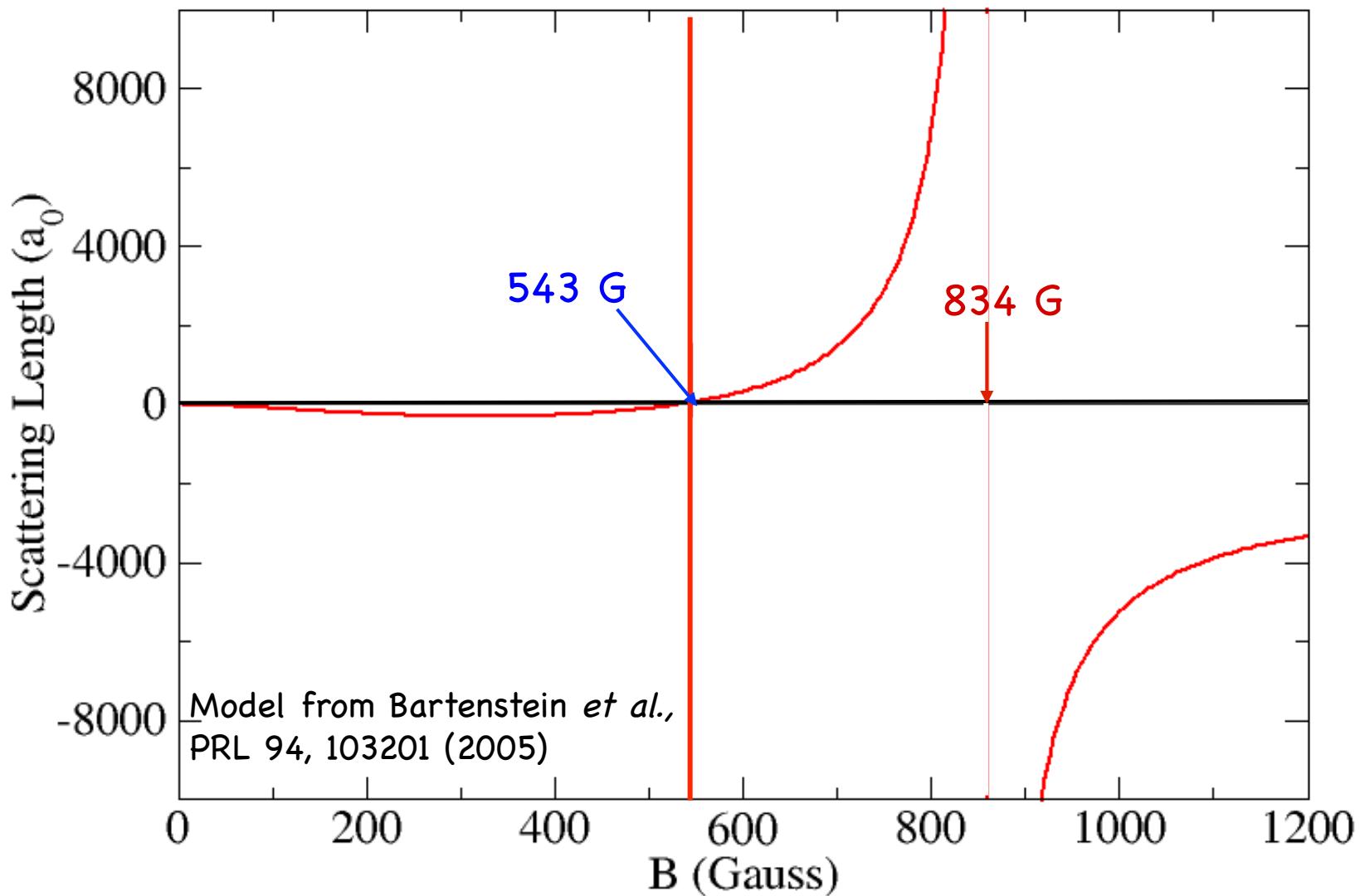


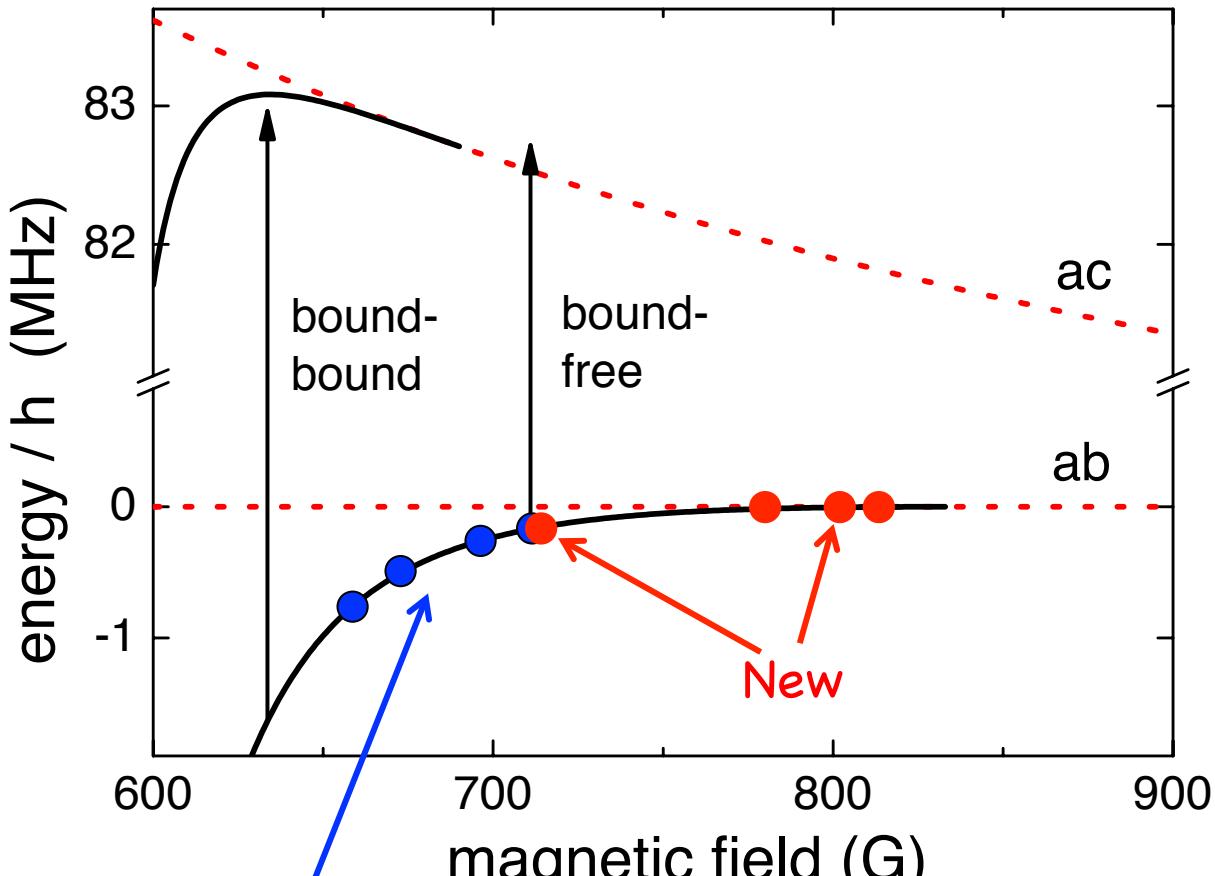
M. Bartenstein, et al., PRL 94, 103201(2005)

Coupled channels calculations based on accurately known potentials
All spin-dependent interactions treated in Hamiltonian
2 free parameters: S and T scattering lengths

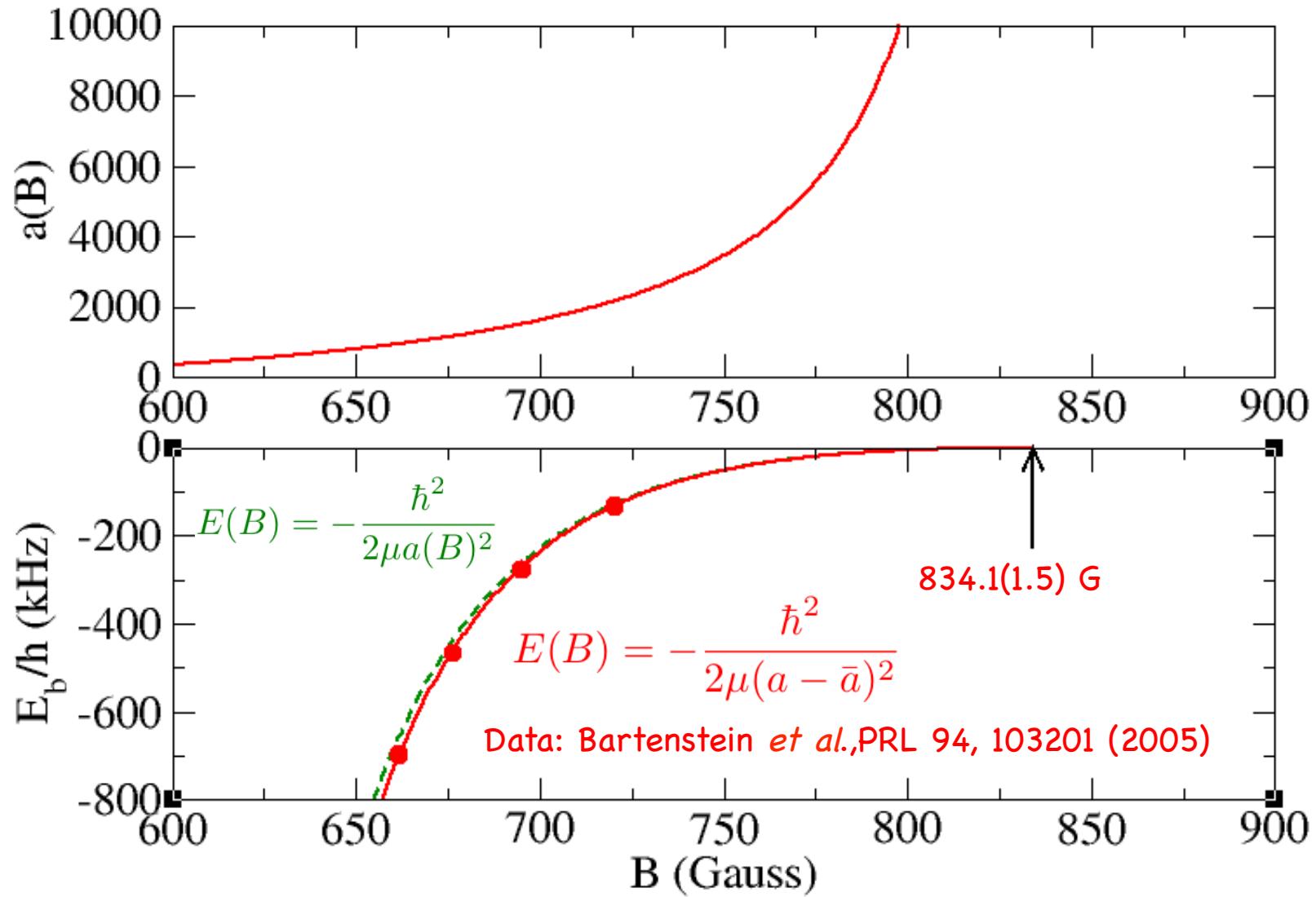


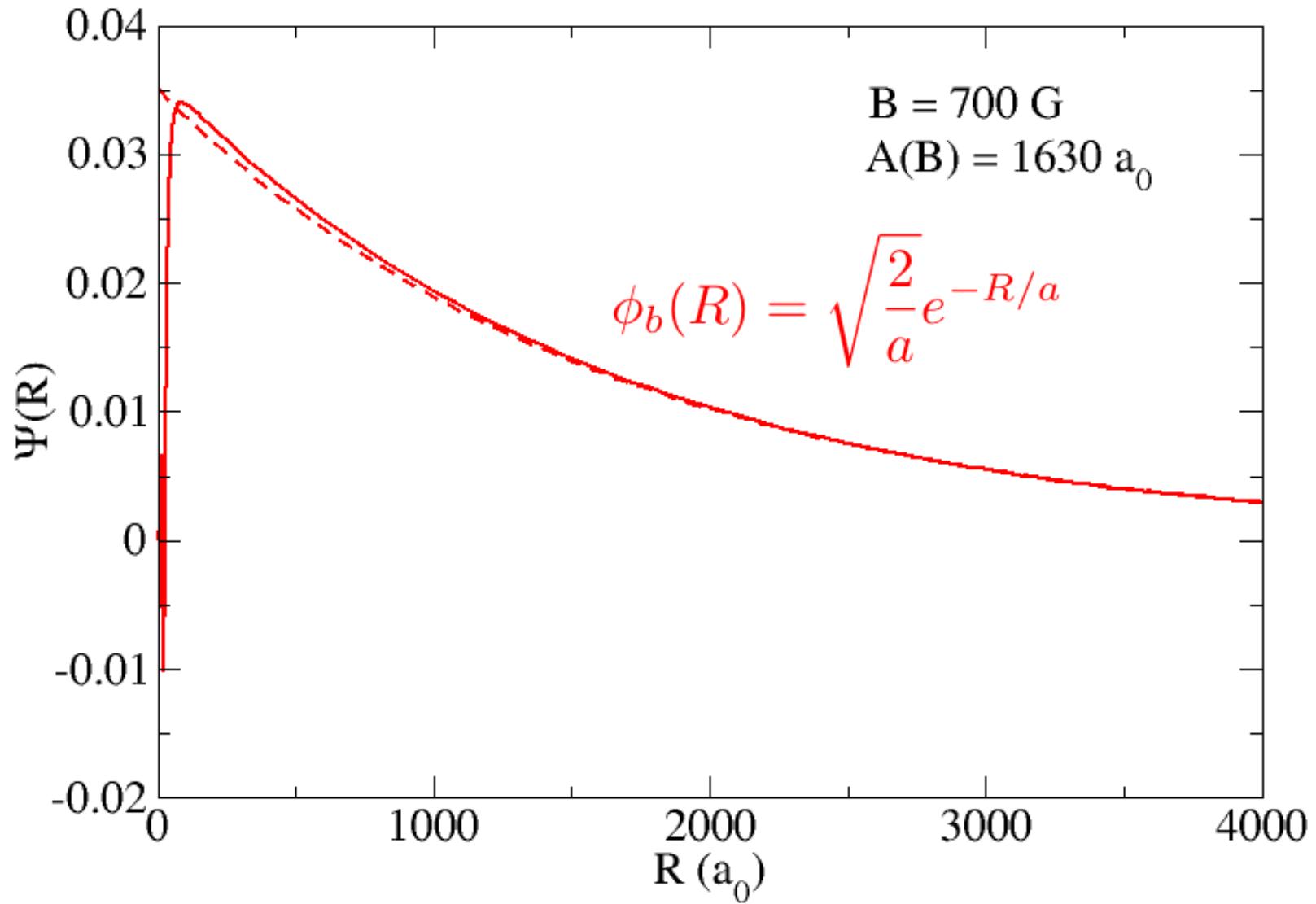
${}^6\text{Li } a+b$ Scattering Length vs. B





Bartenstein et al PRL (2005)





Long history of resonance scattering

O. K. Rice, J. Chem. Phys. 1, 375 (1933)

U. Fano, Nuovo Cimento 12, 154 (1935)

J. M. Blatt and V. F. Weisskopf, Theoretical Nuclear Physics (1952)

H. Feshbach, Ann. Phys. (NY) 5, 357 (1958); 19, 287 (1962)

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

Separation of system into:

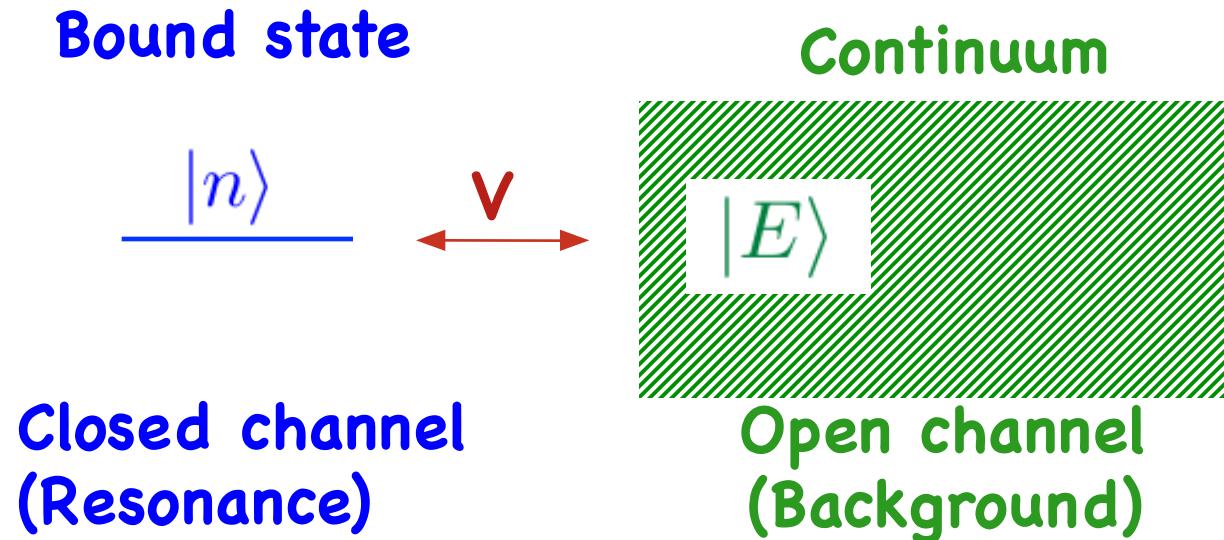
An (approximate) bound state

A scattering continuum

with some coupling between them

Resonant Scattering Picture

(following U. Fano, Phys. Rev. 124, 1866 (1961); see arXiv:0812.1486)



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

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

$\overbrace{\hspace{10em}}$ width

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

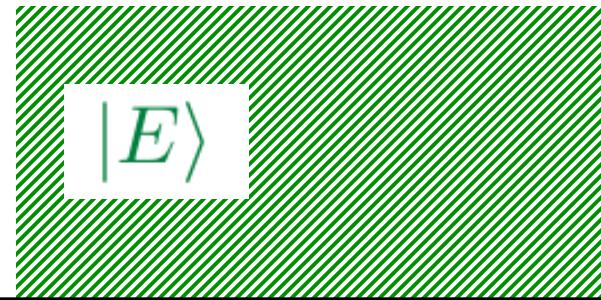
$\overbrace{\hspace{10em}}$ shift

$$\delta E_n = \int \frac{|\langle n|V|E'\rangle|^2}{E_n - E'} dE'$$

Threshold Resonant Scattering

$$E_n = \delta\mu(B - B_n)$$

∇



$E=0$

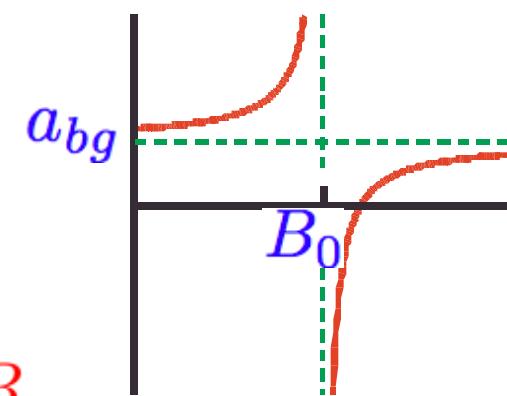
$$\eta(E, B) = \eta_{\text{bg}}(E) - \tan^{-1} \frac{\frac{1}{2}\Gamma(E)}{E - E_n - \delta E_n(E)}$$

As $E \rightarrow 0$ $\eta_{\text{bg}} = -ka_{\text{bg}}$

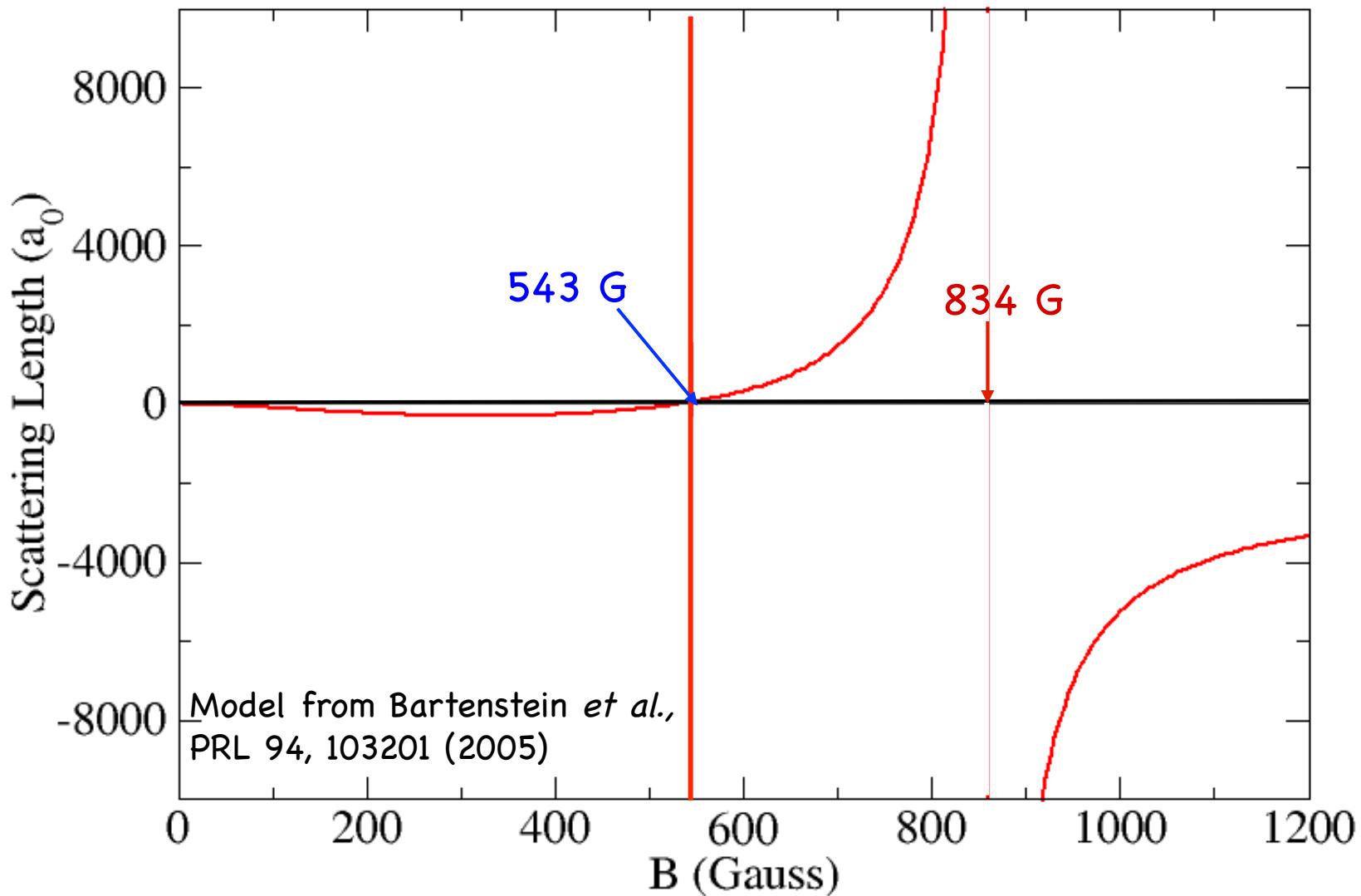
$$\frac{1}{2}\Gamma_n(E) = (ka_{\text{bg}}) \delta\mu \Delta_n$$

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

Shifted $B_0 = B_n + \delta B_n$

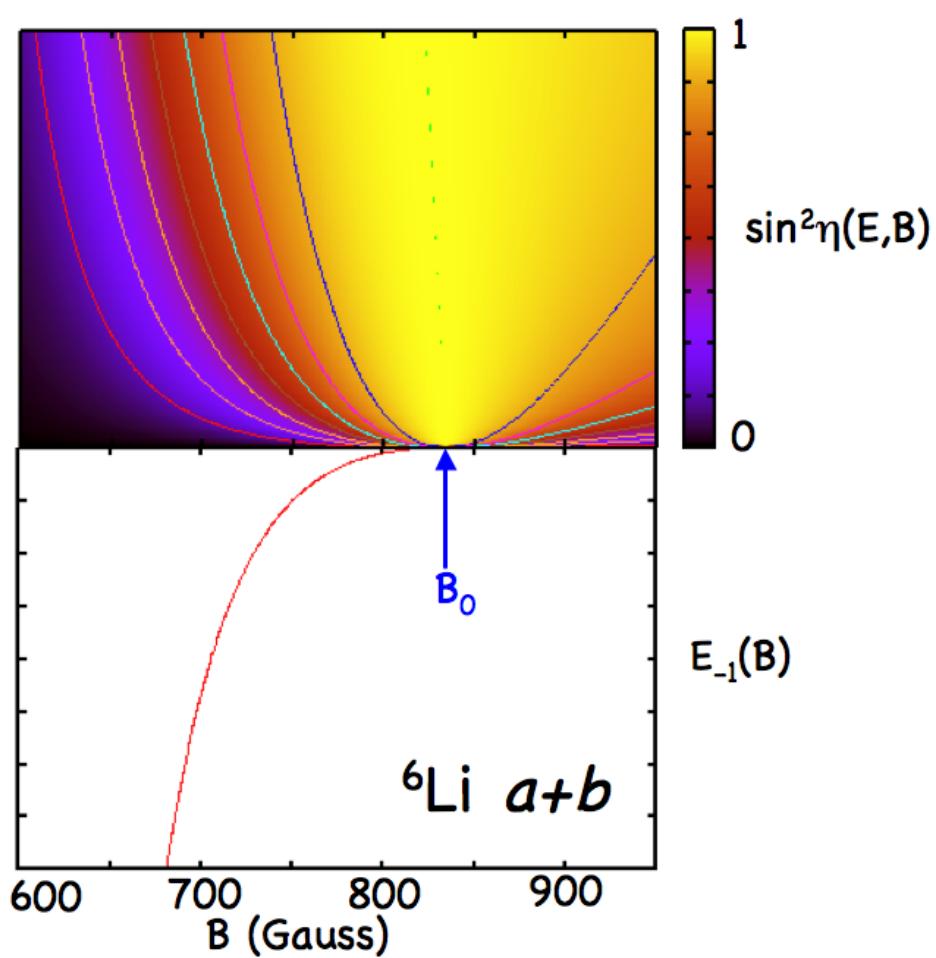
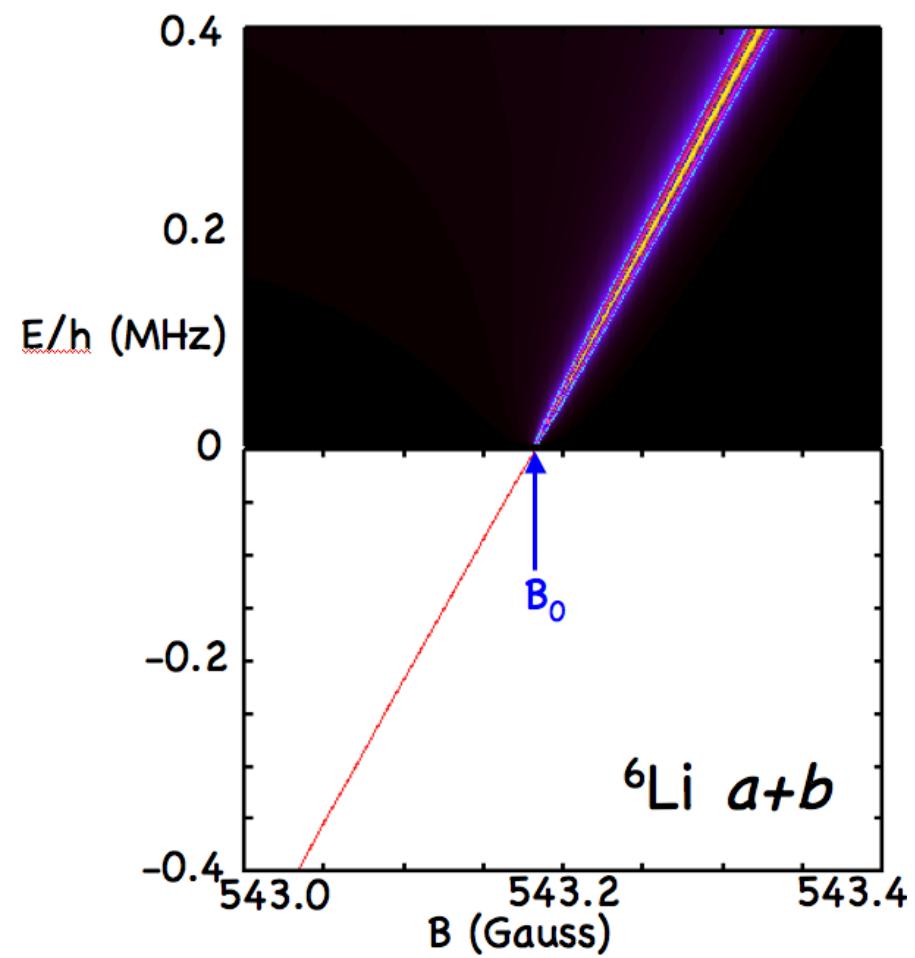


${}^6\text{Li}$ $a+b$ Scattering Length vs. B



Closed channel
dominated

Open channel
dominated



Classification of resonances by strength

$$\text{Resonance strength } s_{\text{res}} = \frac{a_{bg}}{\bar{a}} \frac{\delta\mu\Delta}{\bar{E}}$$

See Kohler et al, Rev. Mod. Phys. 78, 1311 (2006)

And Chin, Grimm, Julienne, Tiesinga, arXiv: 0812.1486

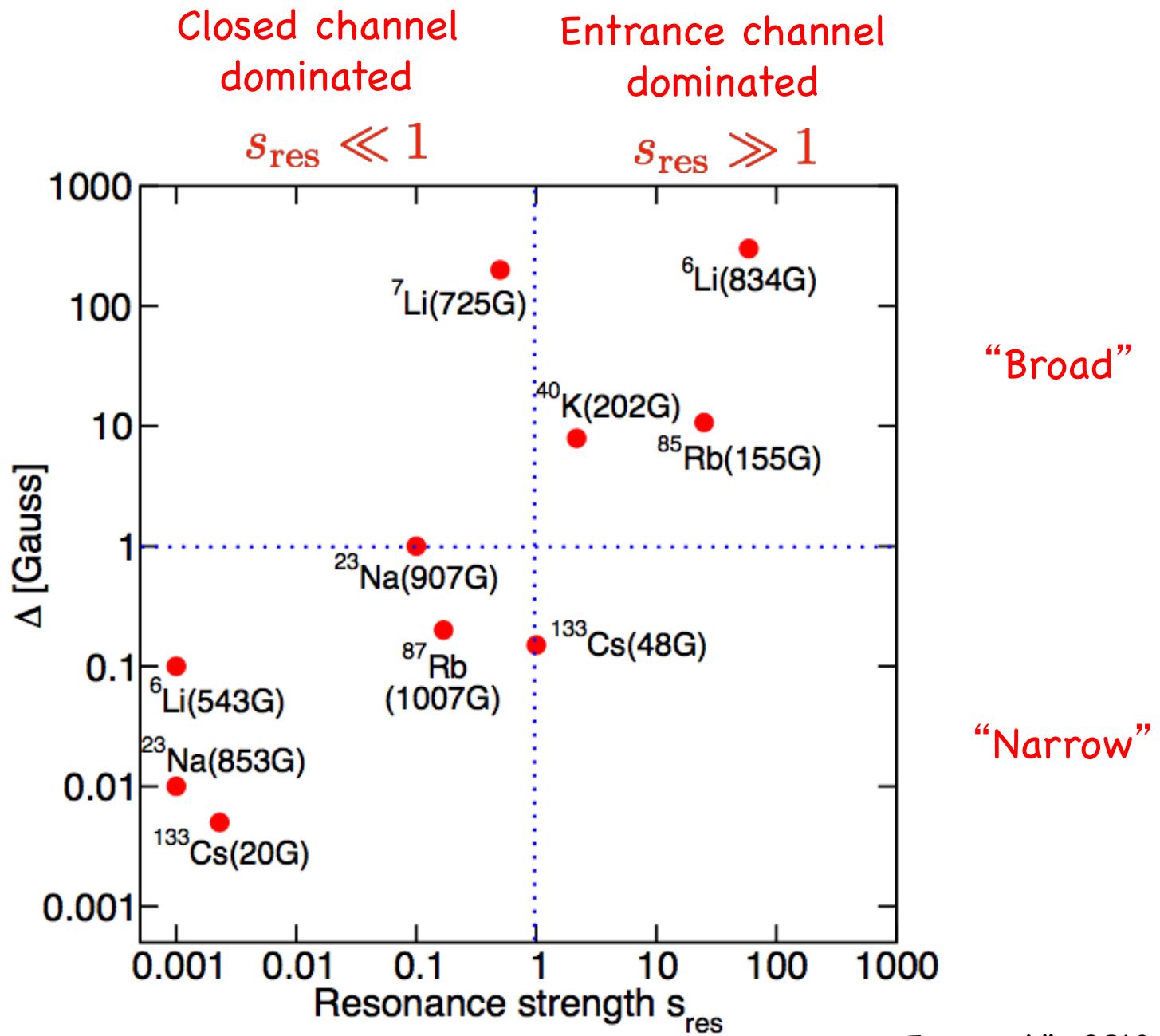
$$a(B) = a_{bg} \left(1 - \frac{\Delta}{B - B_0} \right)$$

For magnetically tunable resonances: $E_c = \delta\mu(B - B_c)$

Bound state norm Z as $E \rightarrow 0$ and $B \rightarrow B_0$

$$Z = \zeta^{-1} \left| \frac{B - B_0}{\Delta} \right|$$

$$\zeta = \frac{1}{2} s_{\text{res}} \frac{a_{bg}}{\bar{a}}$$



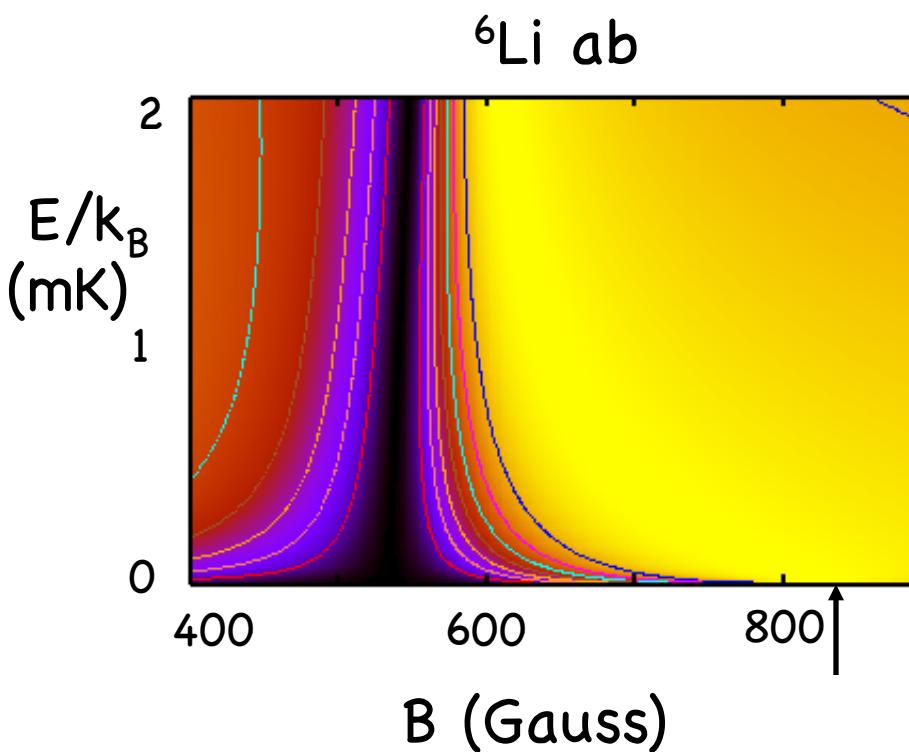
$$s_{\text{res}} = 59$$

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

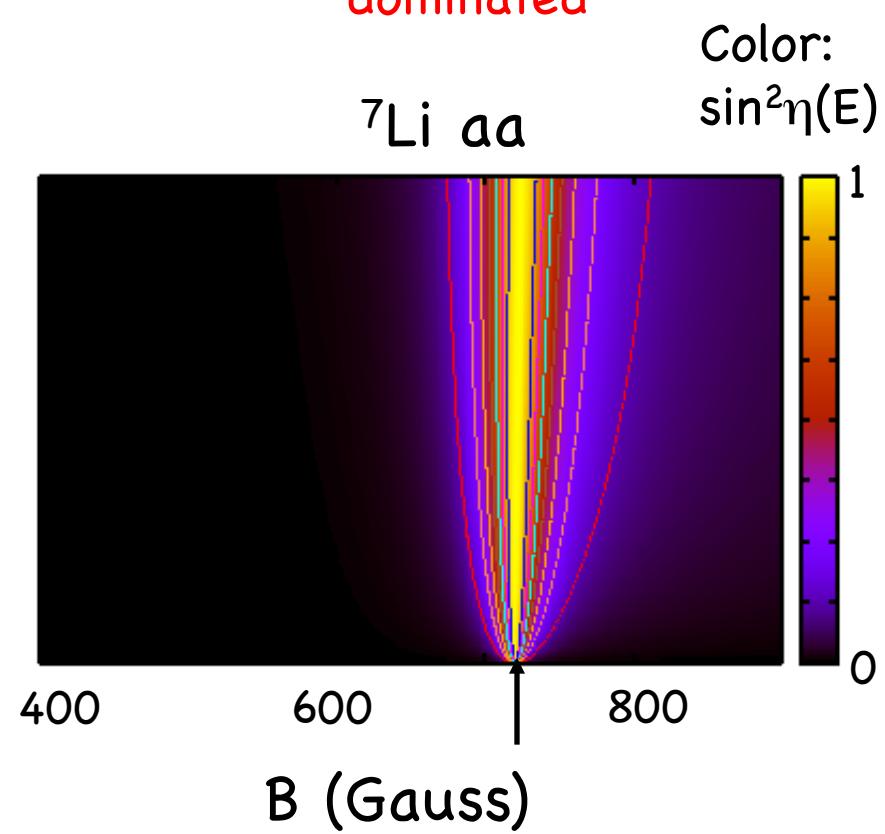
$$s_{\text{res}} = 0.61$$

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

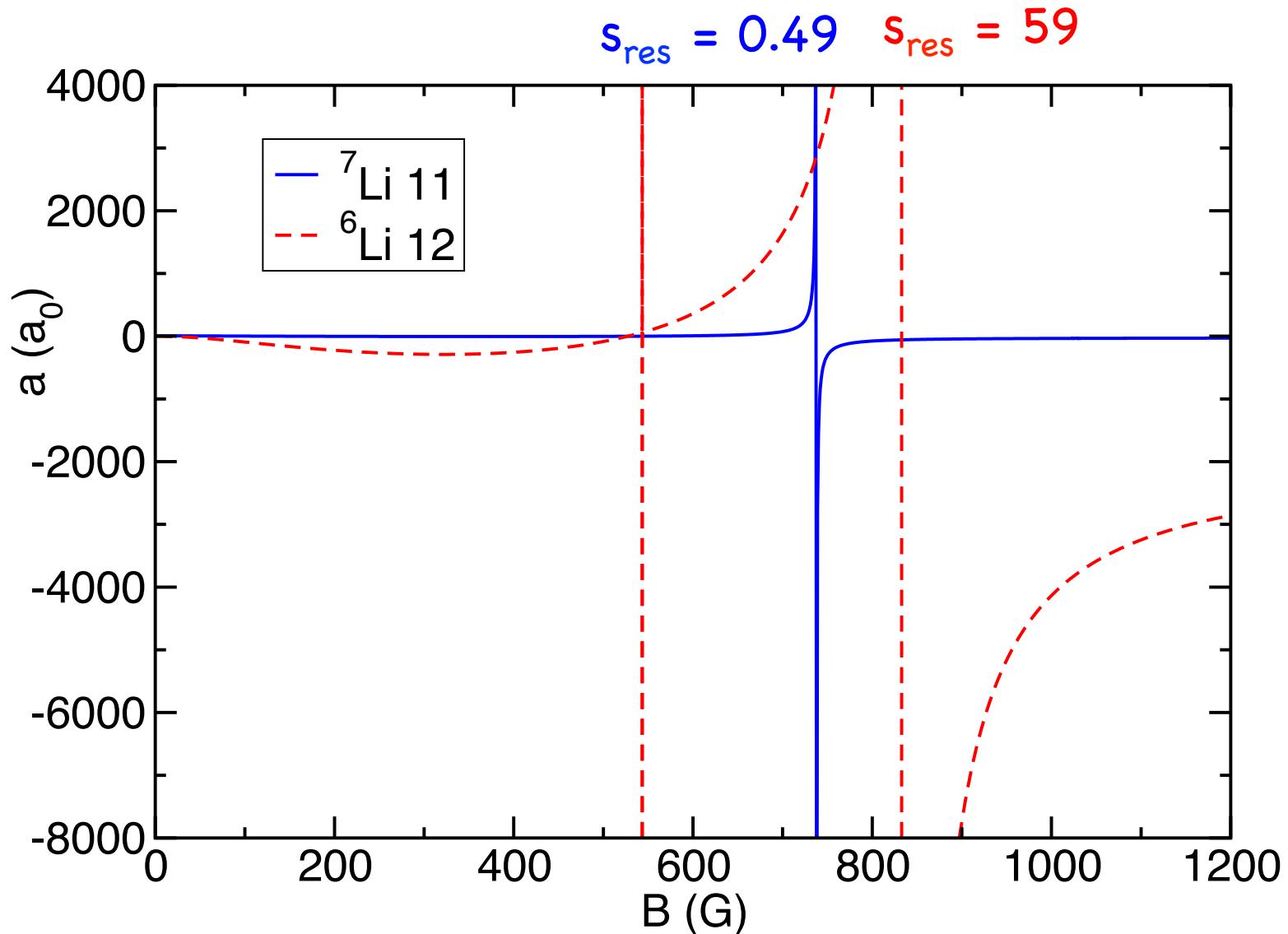
Entrance channel
dominated



Closed channel
dominated



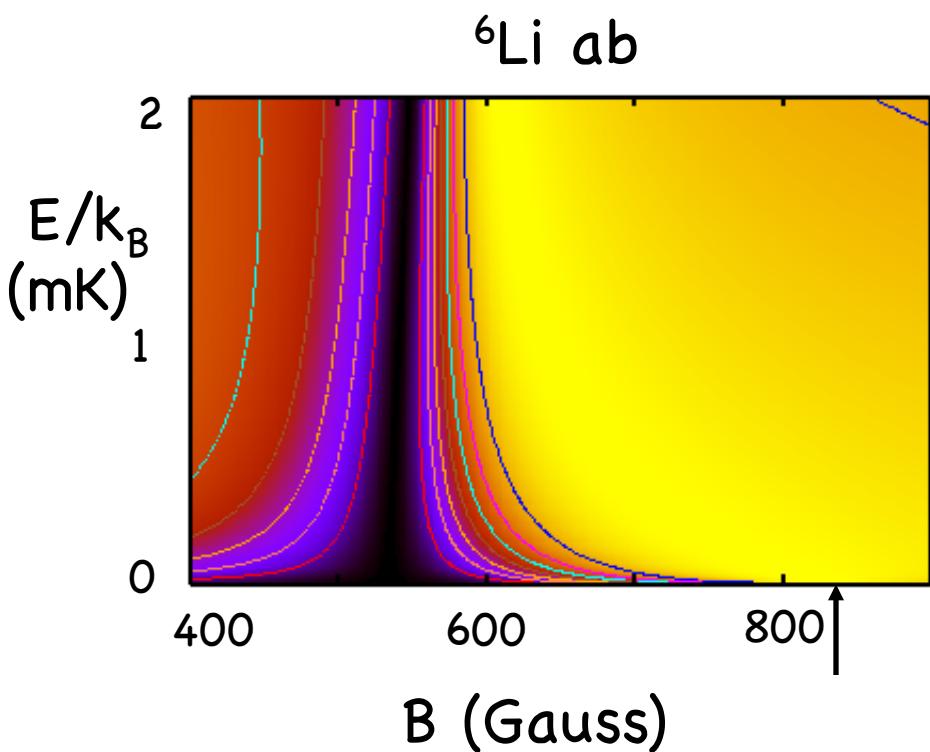
Color:
 $\sin^2 \eta(E)$



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

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

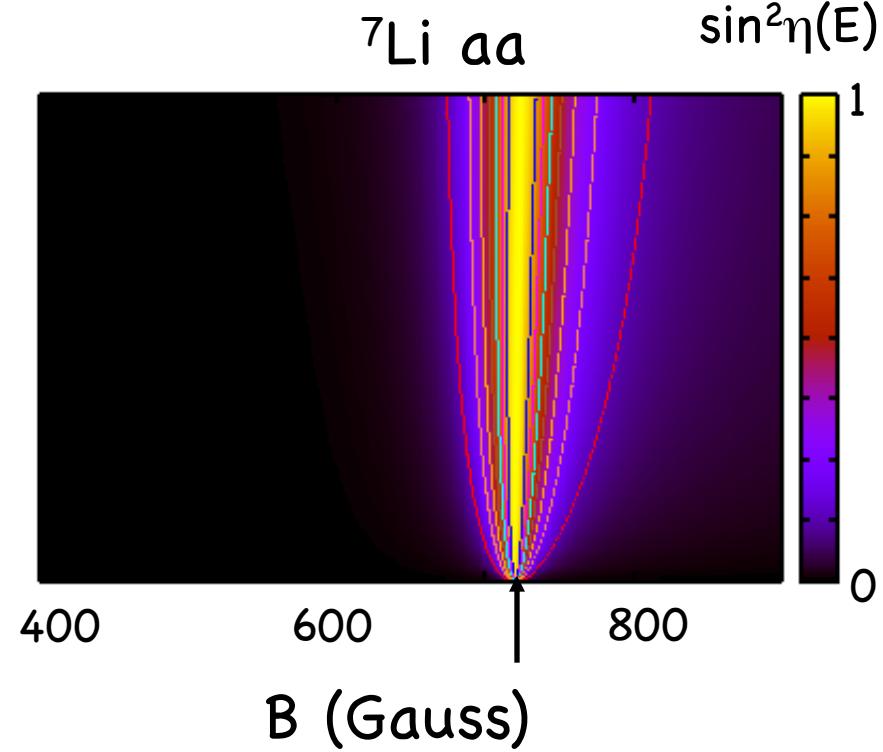
Entrance channel
dominated



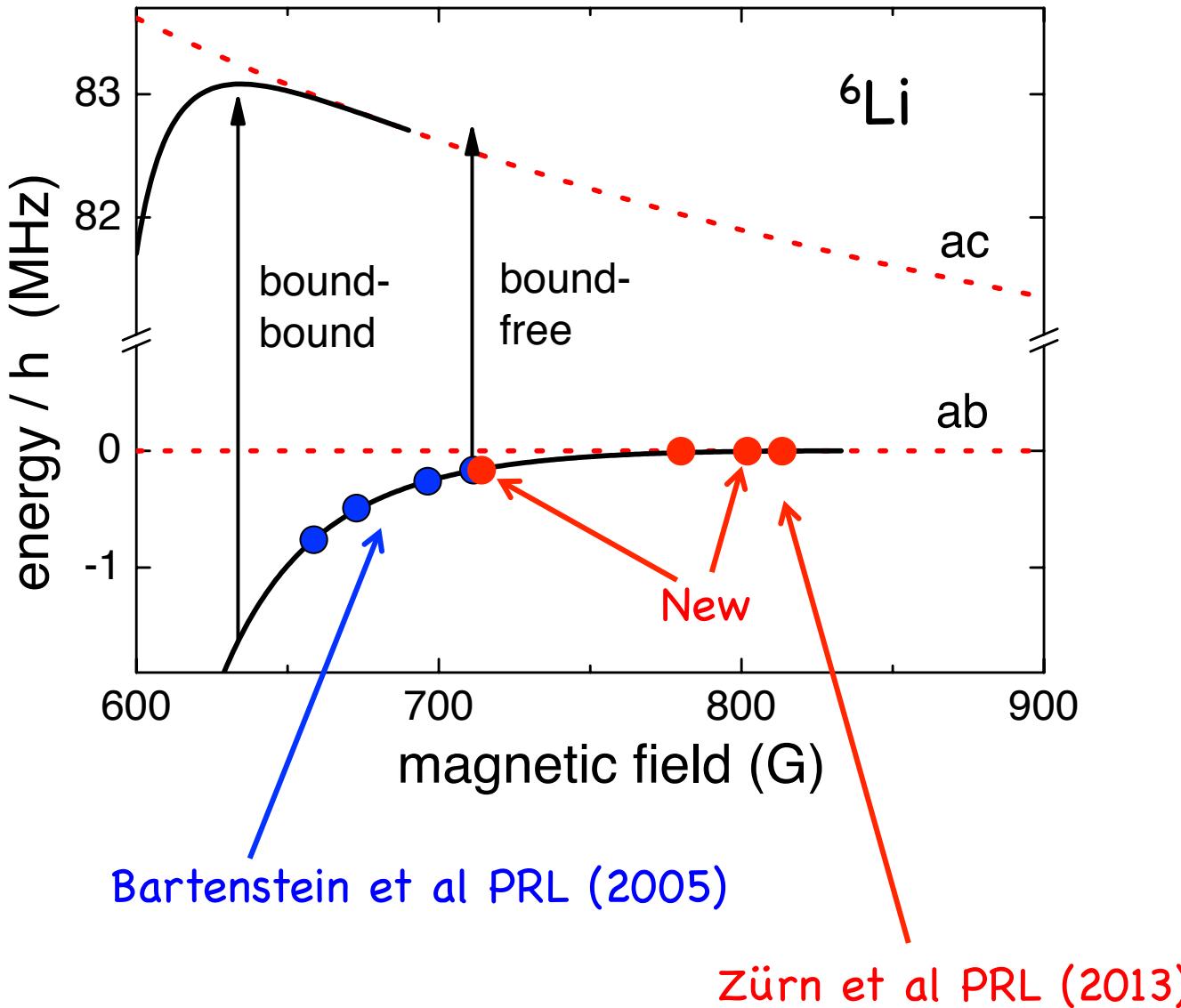
$$s_{\text{res}} = 0.61$$

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

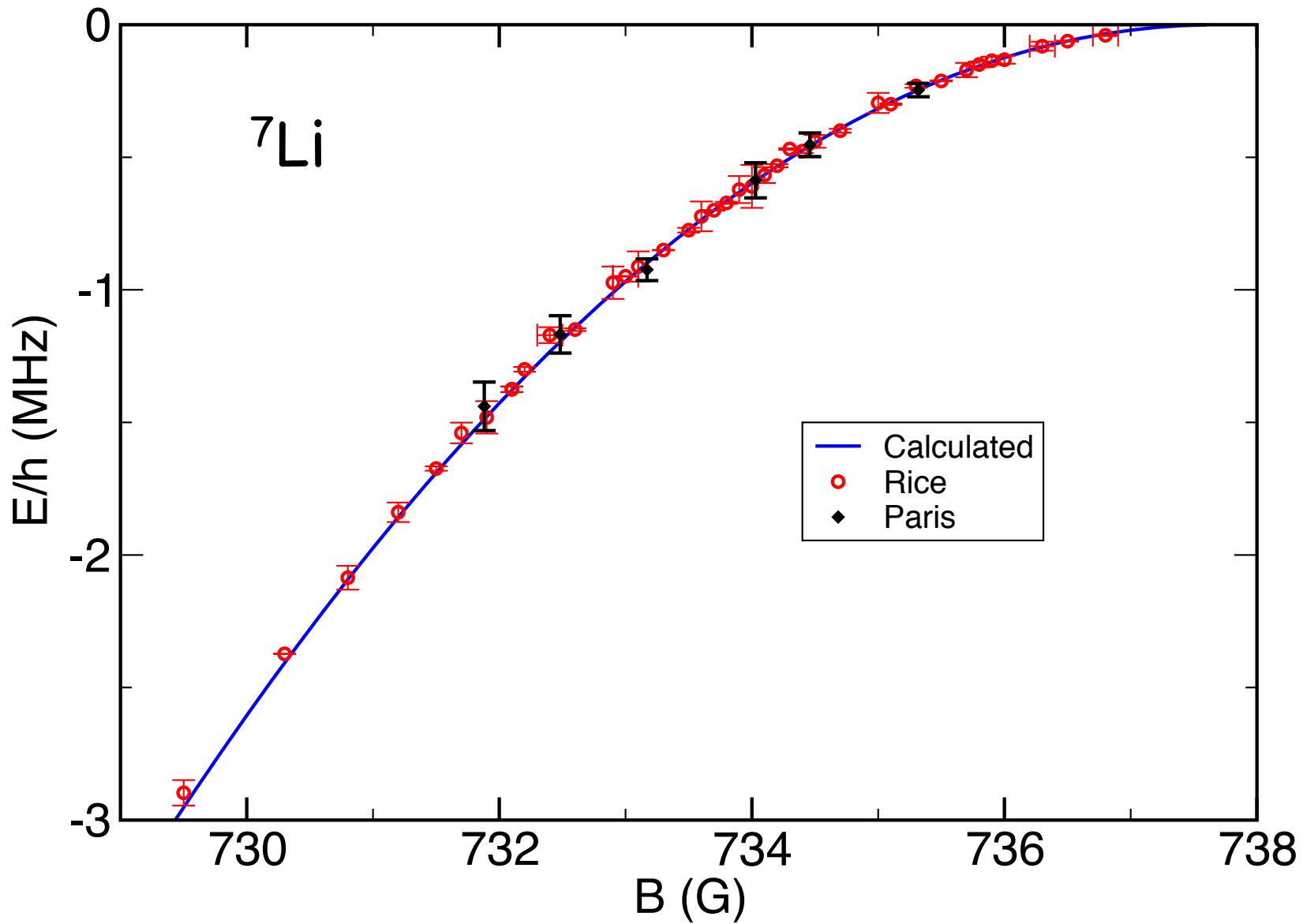
Closed channel
dominated



Color:
 $\sin^2 \eta(E)$



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



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

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

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

$$\epsilon^U r^2 = -1$$

$$\epsilon^U = -\frac{1}{r^2} \quad \text{Universal}$$

$$\epsilon^{GF} = -\frac{1}{(r-1)^2} \quad \text{Gribakin and Flambaum, PRA 48, 546 (1993)}$$

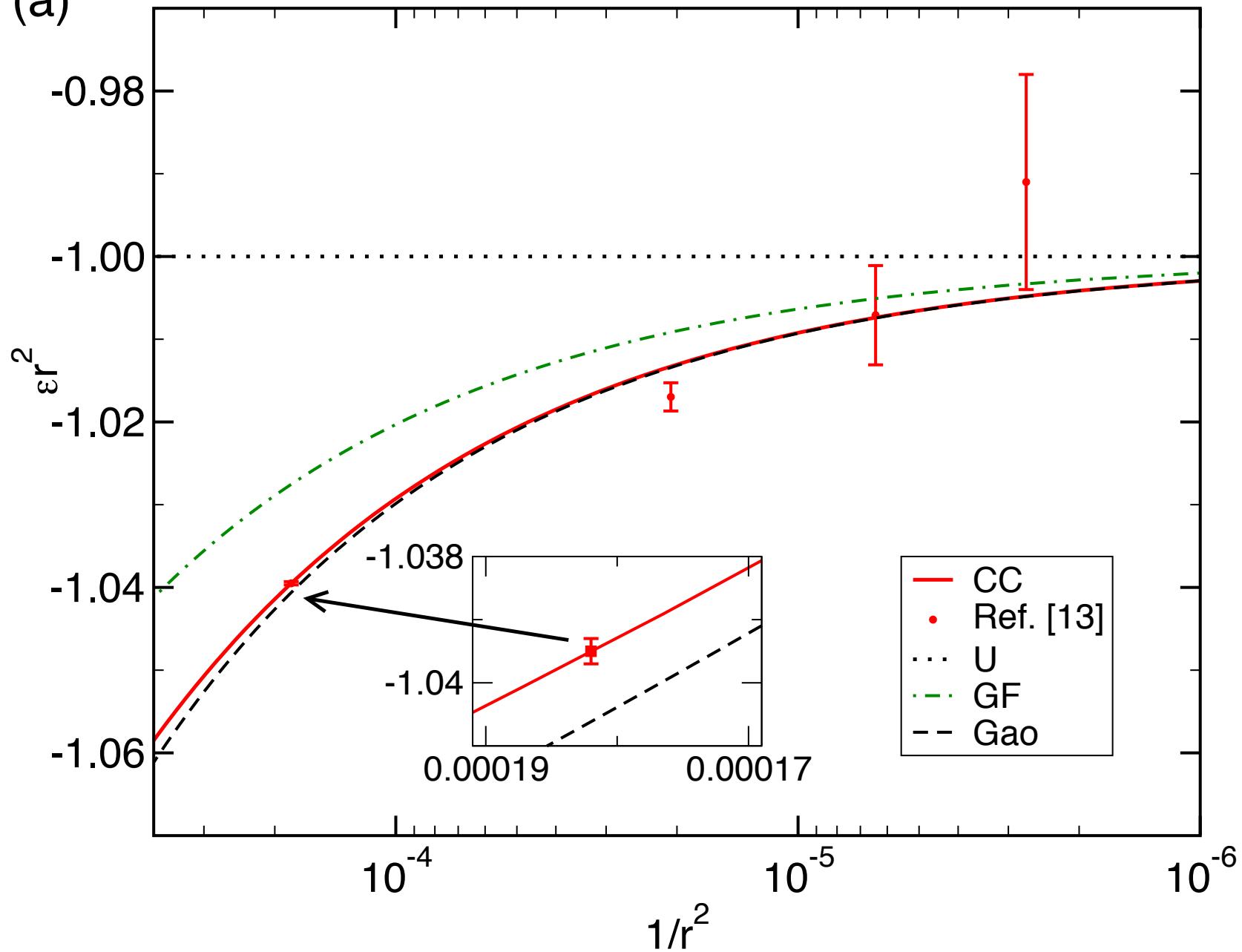
$$\epsilon^G = \epsilon^{GF} \left(1 + \frac{g_1}{r-1} + \frac{g_2}{(r-1)^2} \right)$$

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

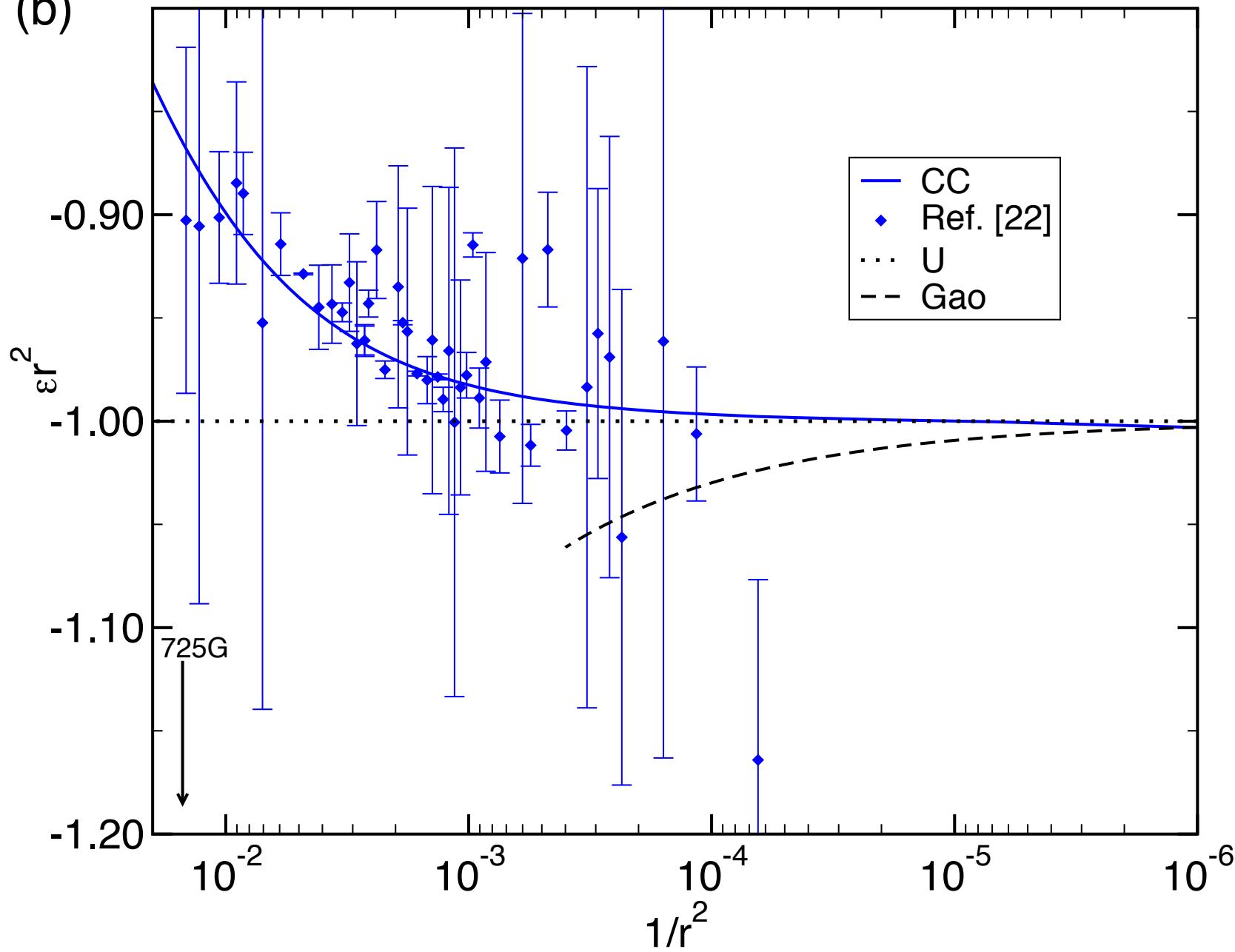
$$g_2 = (5/4)g_1^2 - 2 \approx -0.9468$$

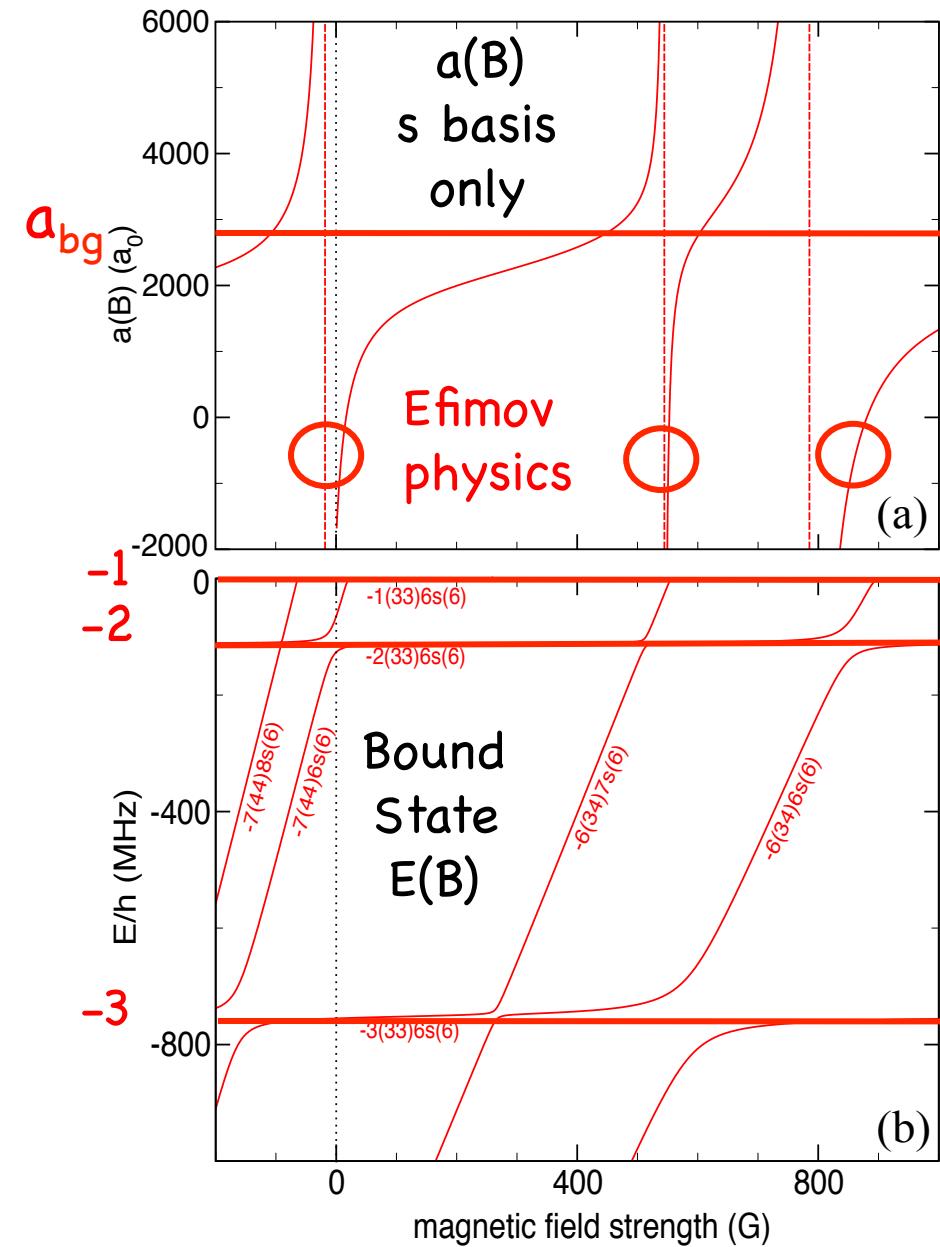
Gao, J. Phys. B 37, 4273 (2004)

(a)



(b)





The End