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1. Cold Collision Basics

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/

NIST

Joint Quantum Institute

Cold Collisions in Quantum Gases

"Good" -- Essential interactions for control and measurement
"Bad" -- Source of trapped atom loss, heating, and decoherence

Cold collisions can be quantitatively understood and controlled

Basic concepts, illustrated by examples, including current research.

Lecture 1: Basics.
- What is the scattering length?
- Cross sections and collision rates.
- Why is the long-range potential so important?

Lecture 2: Feshbach resonances
- A key to measurement and control.
- Field-tunable scattering properties.

Lecture 3: Other topics
- Universality: independence of short-range details.
- Confinement: role of reduced dimension.
- Chaotic collisons of complex atoms and molecules.

Complexity
Hot (chemical)
Short-range
Individuality

Simplicity
Cold (atoms)
Long-range
Universality

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

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

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

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

Two kinds of collision

Elastic--do not change internal state a + b --> a + b

- Thermalization
- Evaporation
- Mean field of BEC—scattering length*
- BEC-BCS crossover in Fermi gases*

  * For applications to quantum degenerate bose and fermi gases, see
  Dalfovo et al, Rev. Mod. Phys. 71, 463 (1999)
  Giorgini et al, Rev. Mod. Phys. 80, 1215 (2008)
- Equation of state
- Optical lattice shifts: U parameter of Hubbard models

Inelastic--change internal state a + b --> a' + b' + ΔE

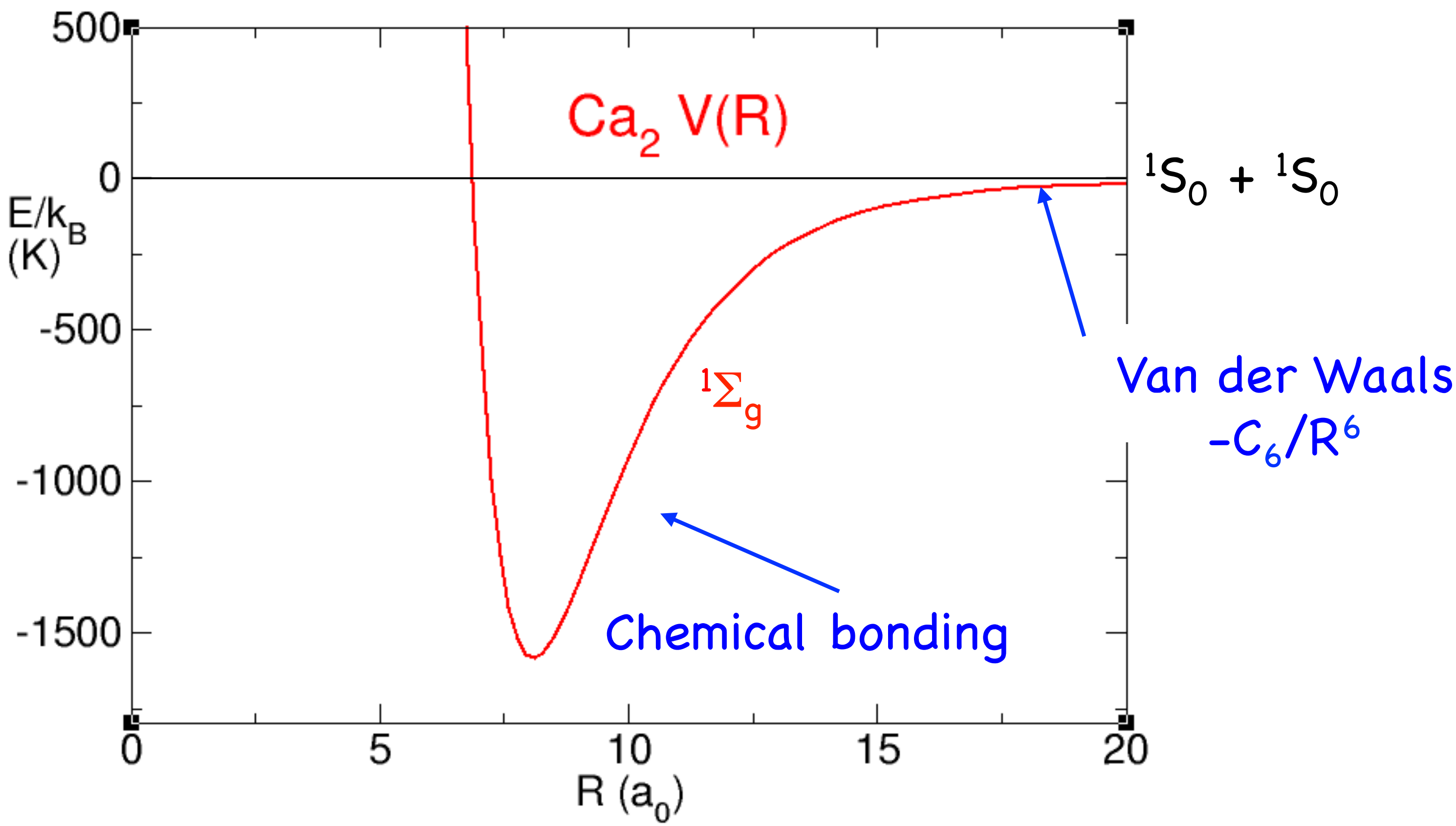
- Spin relaxation
- Loss of trapped atoms, gas lifetime
- Spinor condensates ($\Delta E=0$)
- Three-body, detect resonances
- Photoassociation
- Chemical reaction

Ca $4s^2\ ^1S_0$ atom

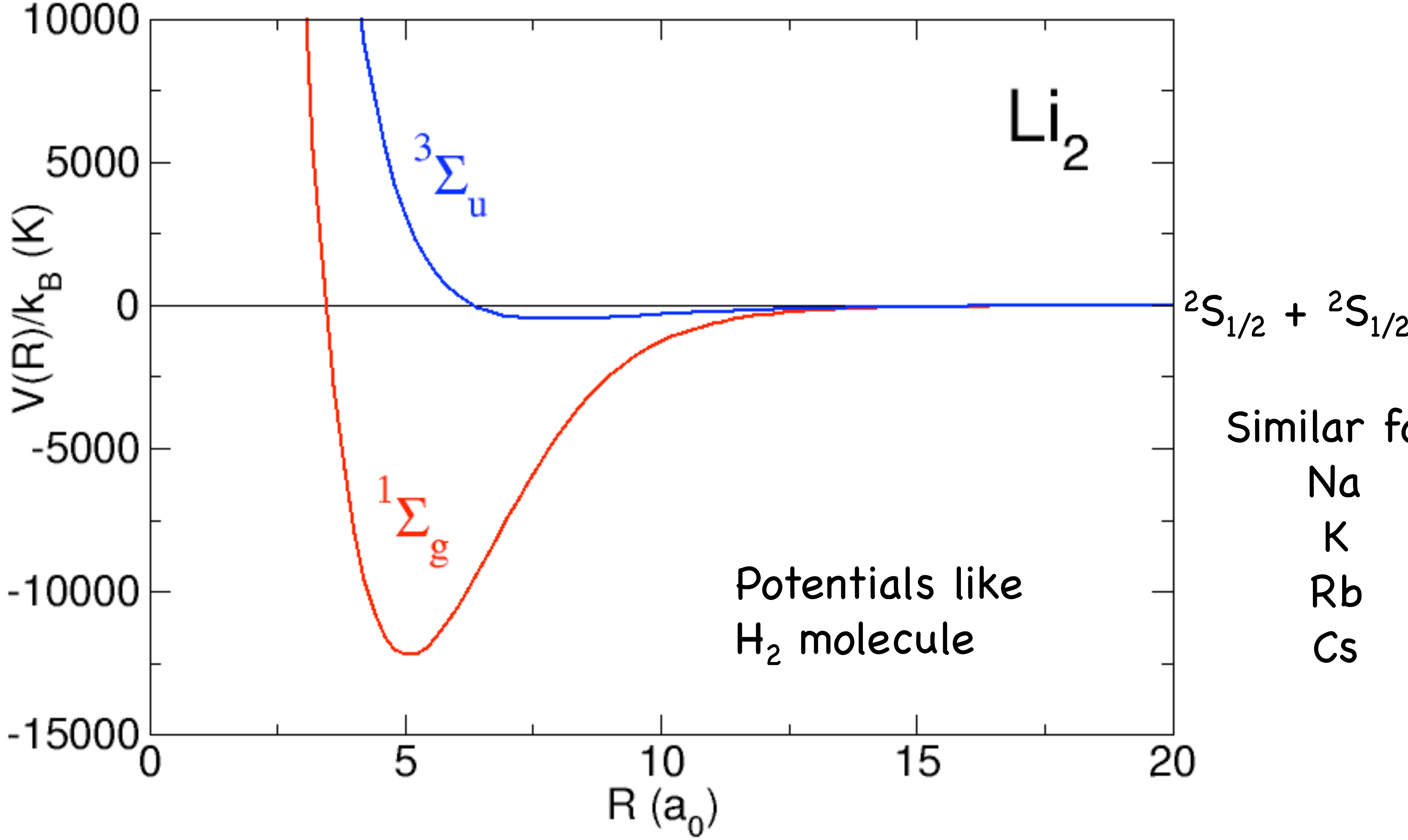
Spin degeneracy

Total angular momentum

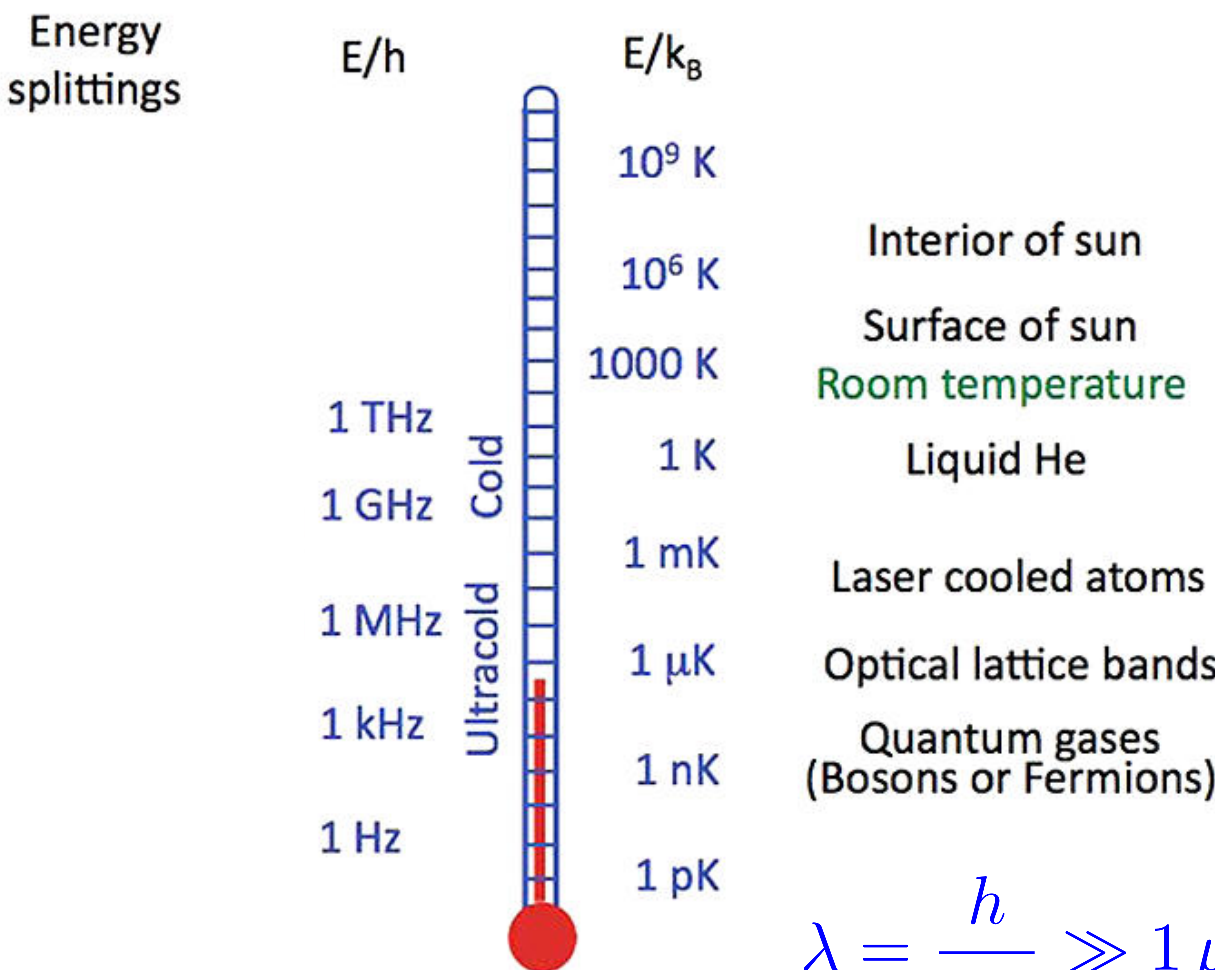
Born-Oppenheimer approximation => potential energy curve



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



Similar for
Na
K
Rb
Cs

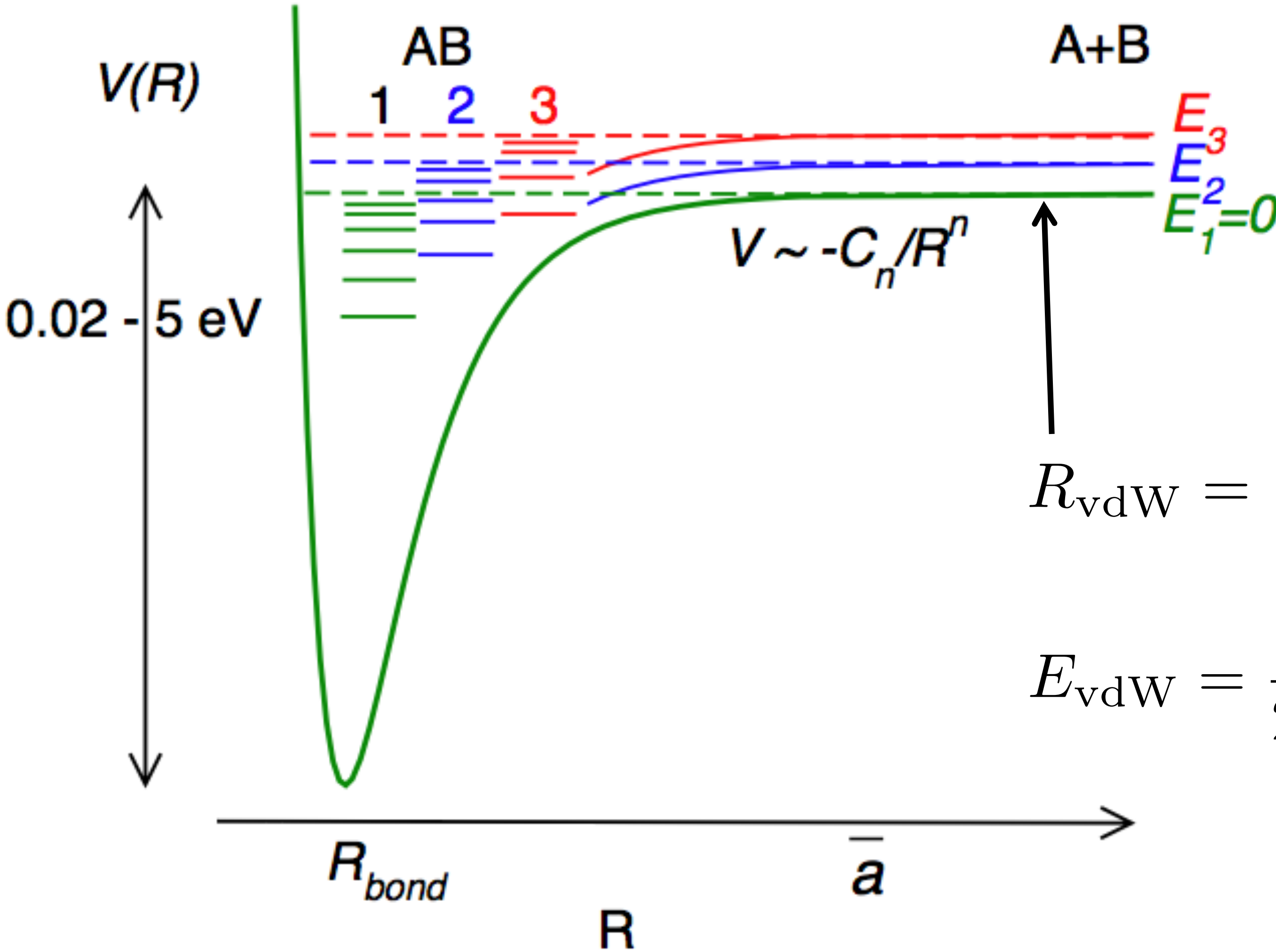


$$\lambda = \frac{h}{mv} \gg 1\,\mu m$$

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

>10 THz (1000K) 10 Ghz (K) 10 kHz (μK)

Short-range Long-range Separated



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

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

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... *s*–, *p*–, *d*–waves, ...

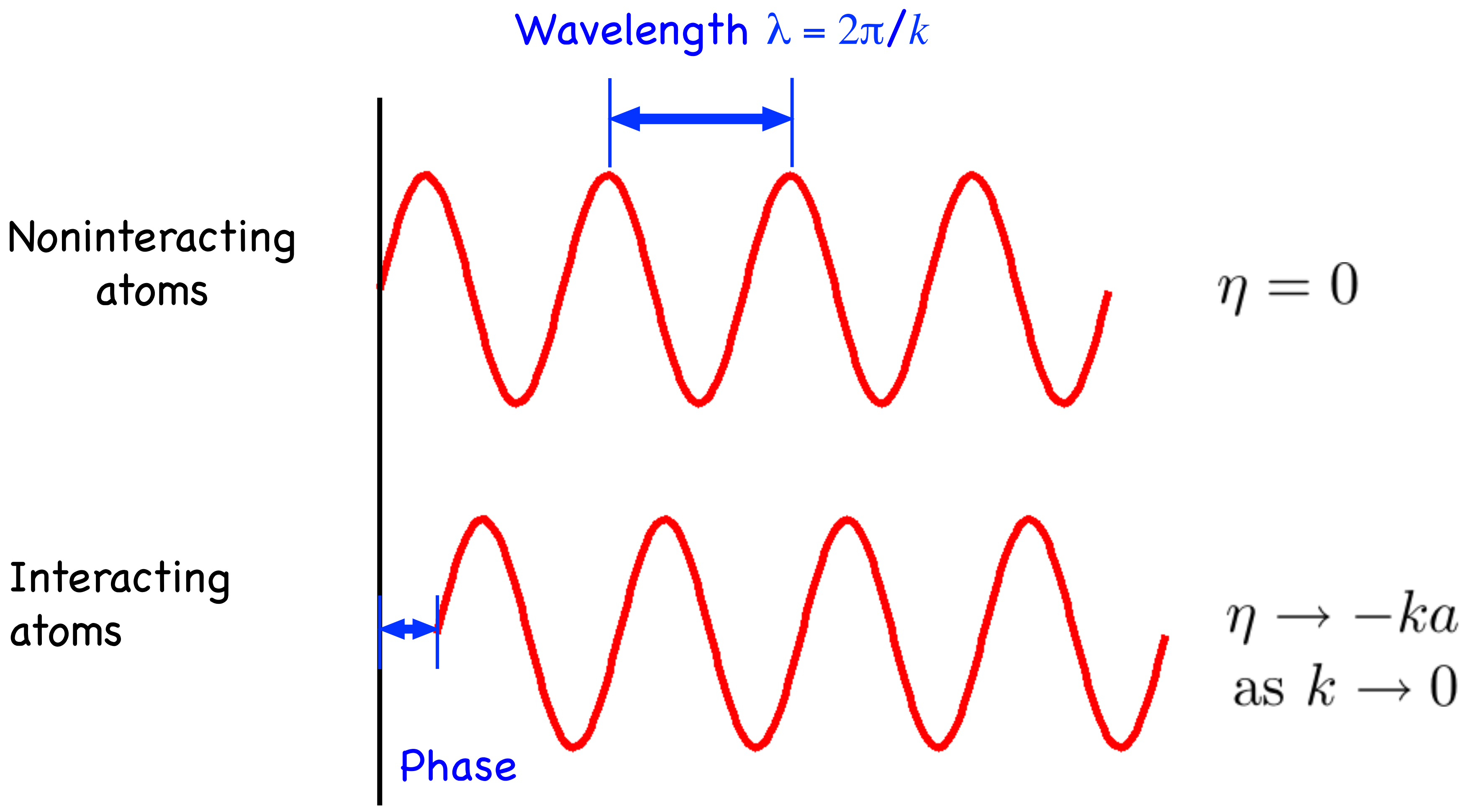
Potential energy: $V(R) + \dfrac{\hbar\ell(\ell+1)}{2\mu R^2}$ --> phase shift $\eta_\ell(E)$

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

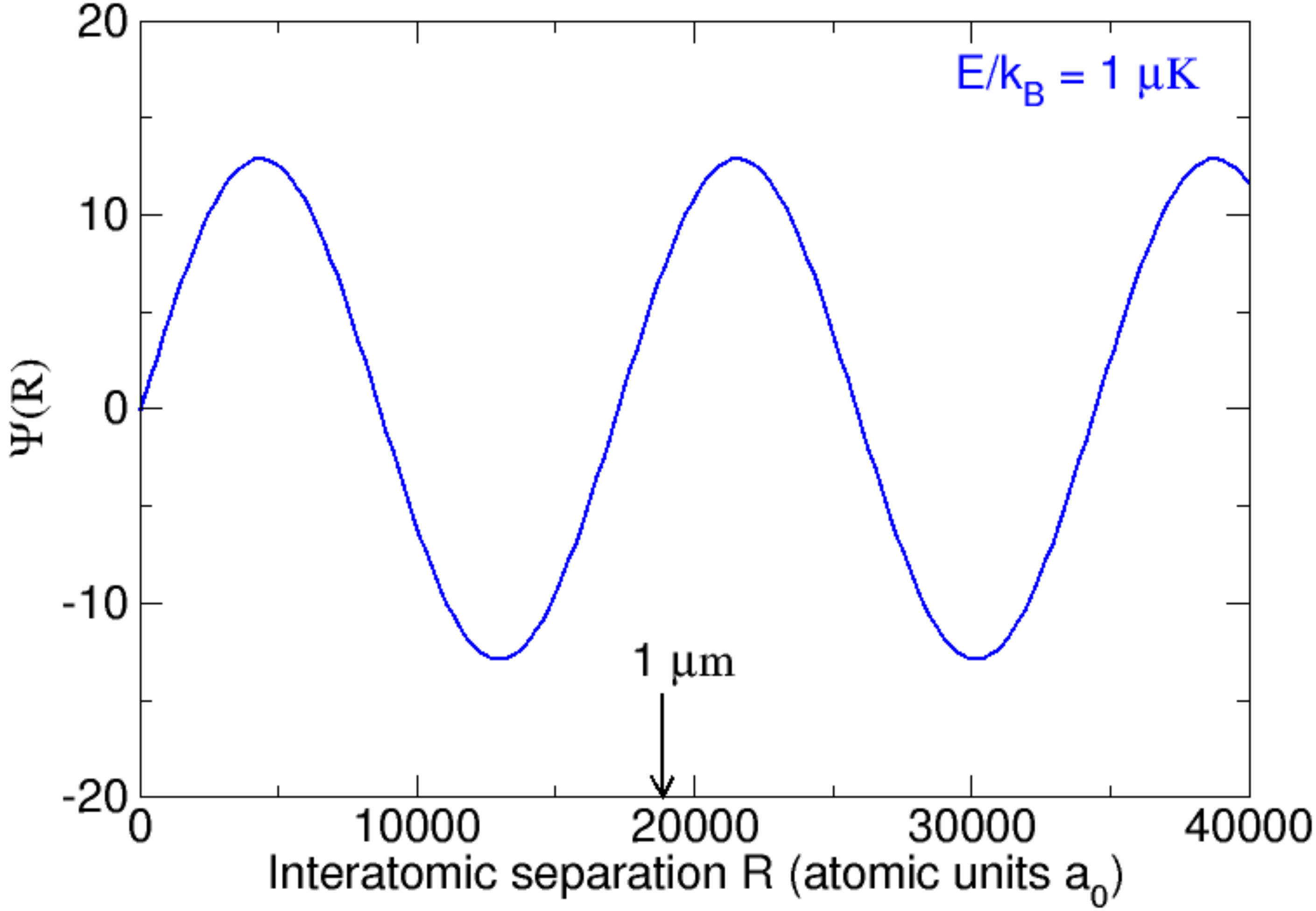
Solve Schrödinger equation for bound and scattering $\Psi(R,E)$
--> For E<0, bound states E_n
--> For E>0, scattering phases, amplitudes: S-matrix

s-wave scattering phase shift

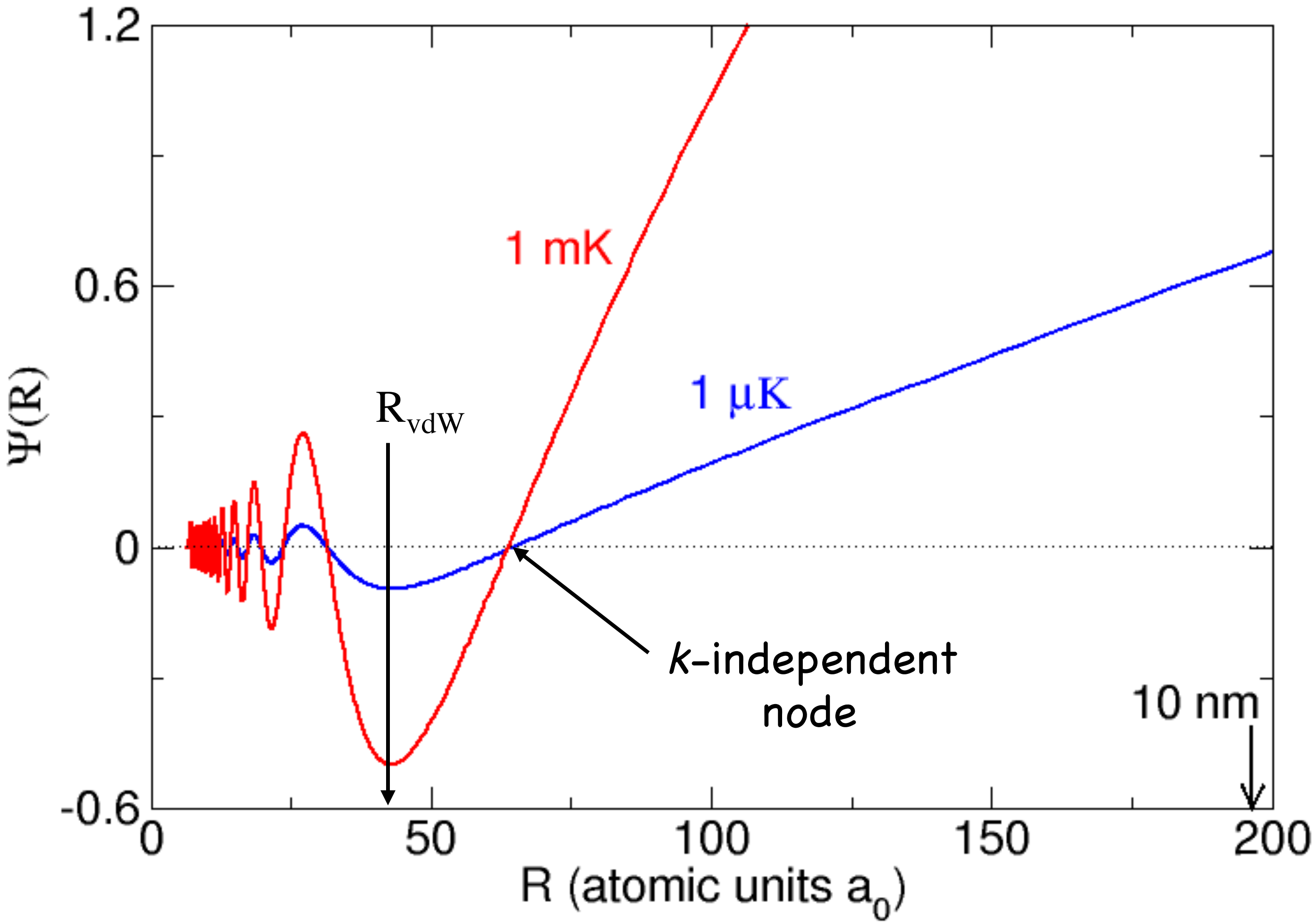
$$\Psi(R) \rightarrow \sin(kR + \eta)$$



Example with two Na atoms



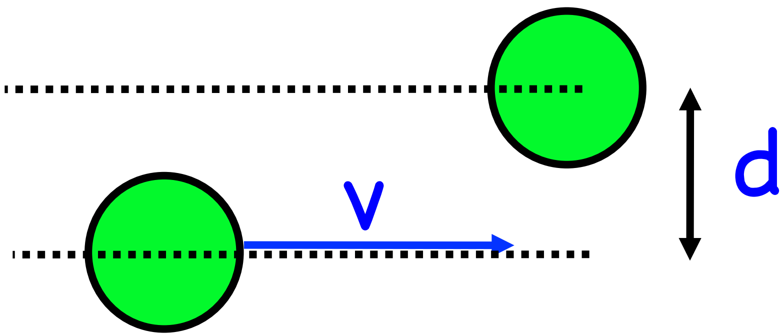
See Jones, Lett, Tiesinga, PSJ, Rev. Mod. Phys. 78, 483 (2006), Fig. 15



See Jones, Lett, Tiesinga, PSJ, Rev. Mod. Phys. 78, 483 (2006), Fig. 15

Cross section σ

Classical balls with distance of closest approach d (diameter)



define an area with $\sigma = \pi d^2$ (10^{-12} cm^2, d ≈ 5 nm)

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

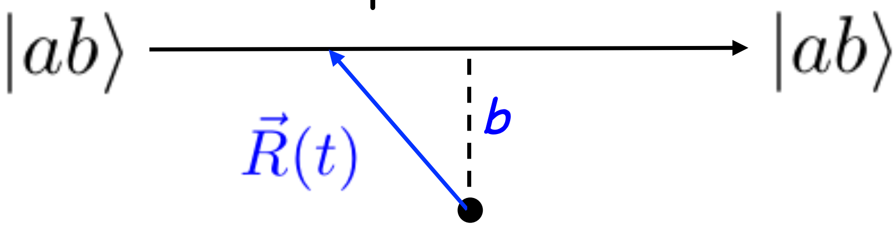
10^4 s^{-1}, BEC)

Rate constant $K = v\sigma$

Time between collisions = $1/\Gamma$ = $1/(Kn)$ ≈ 1s (MOT), 100μs (BEC)

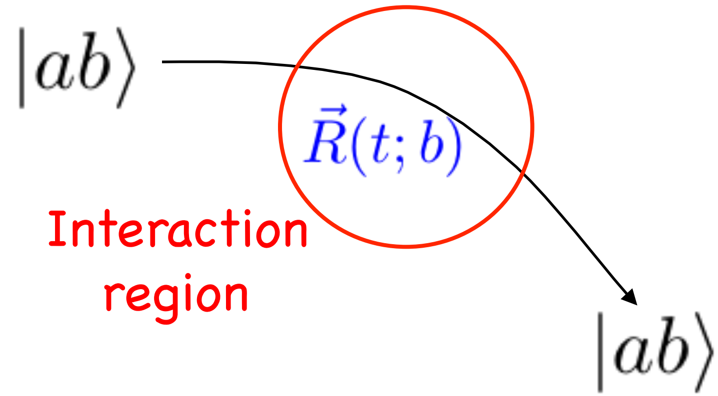
Classical picture

No potential

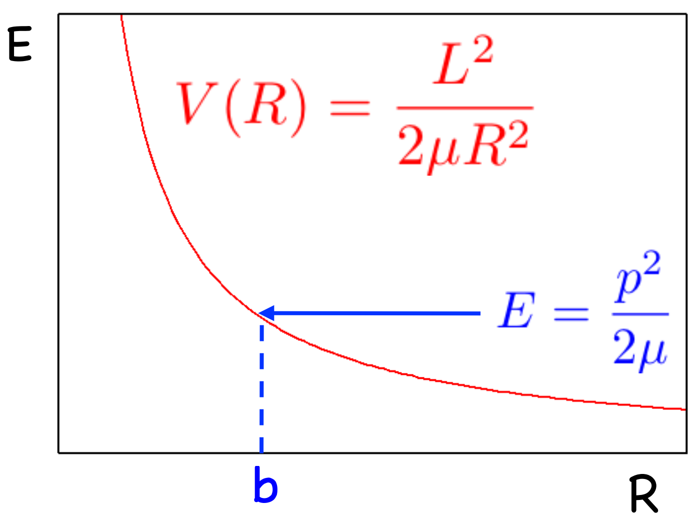


$$|\vec{L}| = |\vec{R} \times \vec{p}| = bp$$

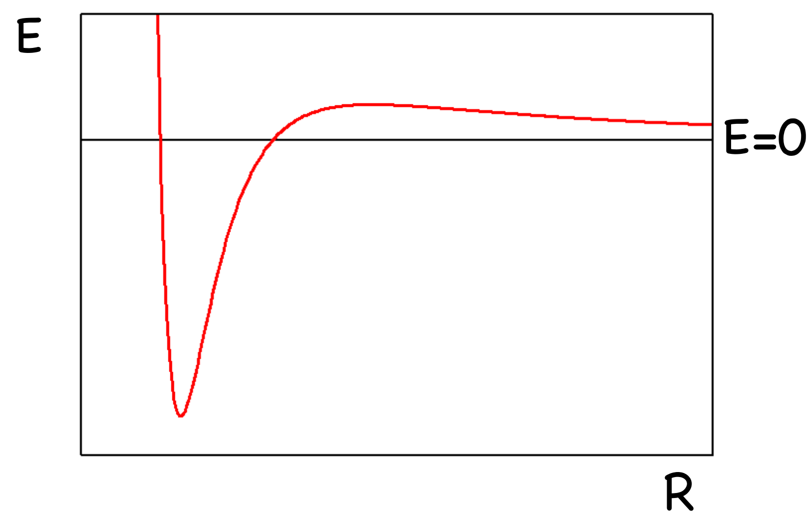
With potential



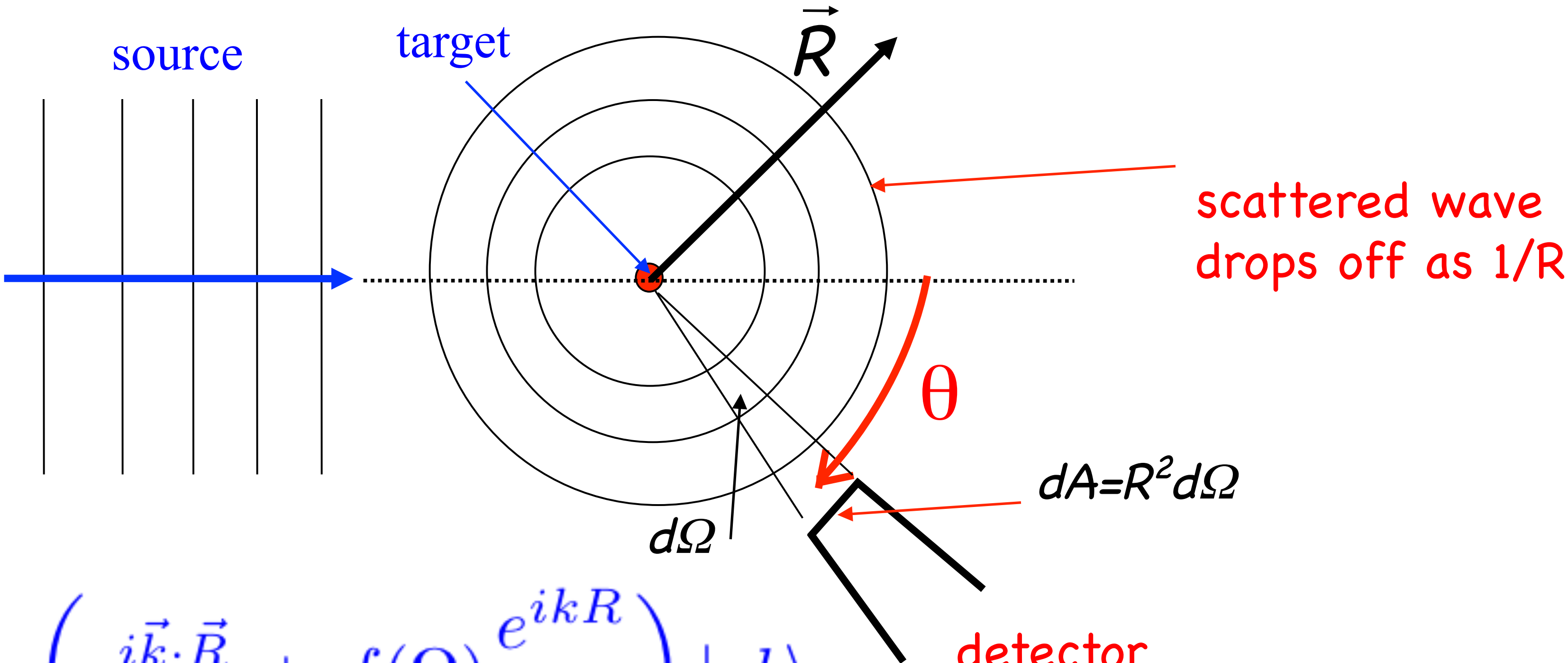
Centrifugal potential



Centrifugal barrier



Quantum scattering theory



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

scattering amplitude

$$\frac{\text{atoms/s scattered into } d\Omega}{\text{plane wave flux (atoms/cm}^2\text{/s)}} = \frac{d\sigma}{d\Omega} = |f(\Omega)|^2$$

$$\sigma_{\rm tot} = \int d\Omega \frac{d\sigma}{d\Omega}$$

cross section

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: $\dfrac{\sin\left(kR - \ell\frac{\pi}{2}\right)}{kR}$

When V(R) is present: $\dfrac{\sin\left(kR - \ell\frac{\pi}{2} + \eta_{\ell}(k)\right)}{kR}$

Collision cross section

Solve Schrödinger equation for each ℓ (isotropic case)

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:

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

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

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

General threshold laws in topical review: Sadeghpour et al, J. Phys. B 33, R93 (2000)

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

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

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

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

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 $\mathbf{H}\mathbf{\Psi}(R,E) = E\mathbf{\Psi}(R,E)$

Extract **S** from solution at large R >> R_{vdW}

Potential matrix $V_{\alpha\alpha'}(R)$

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

Isotropic (Born-Oppenheimer) V(R) does not change ℓ

Anisotropic (spin-dependent) potential changes ℓ

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

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

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

Complex scattering length *a–ib*

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

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

mean field $\frac{4\pi\hbar}{\mu} a(0) n$

loss rate $\frac{4\pi\hbar}{\mu} b(0) n$

Rate constants

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

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

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

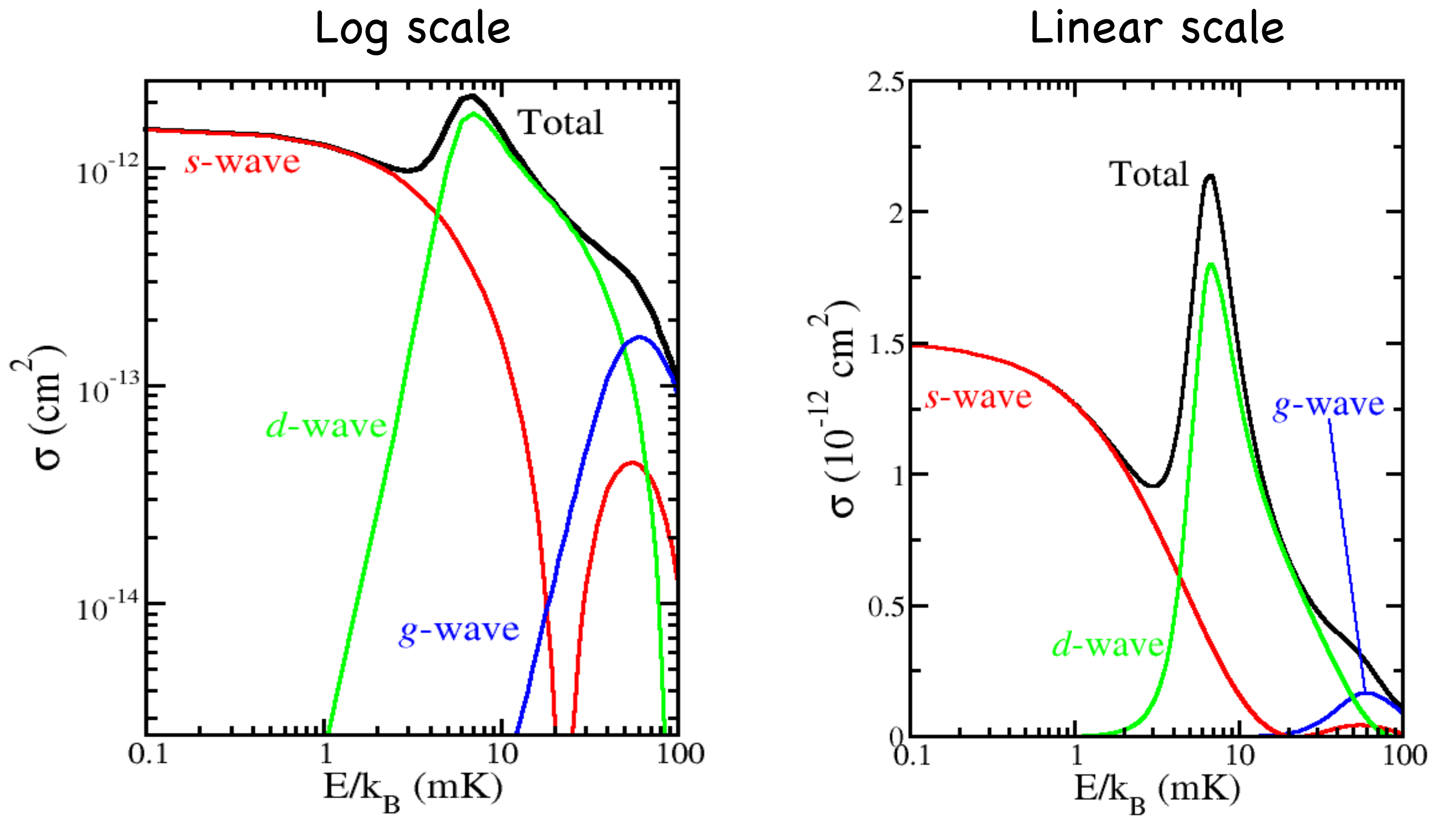
Typical values:

"Allowed" b ~ 10-100 a_0

"Forbidden" b << 1 a_0

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

Elastic cross section σ for like Na atoms



Many (even) partial waves

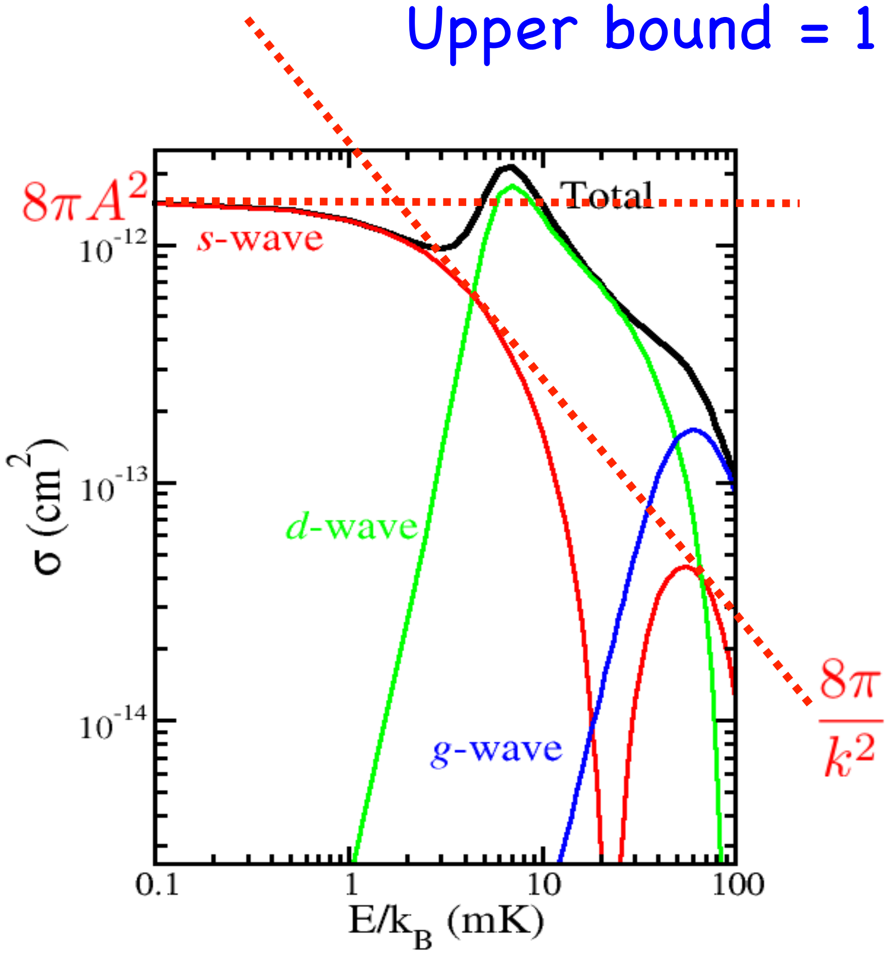
Threshold properties (elastic only)

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

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

Upper bound = 1 (unitarity limit)

$$\sigma(E) = \frac{4\pi}{k^2} \propto \frac{1}{E}$$



Atomic and molecular collision loss rates

Standard chemical form from Mies, J. Chem. Phys. 51, 787, 798 (1969); Faraday Disc. 142 (2009)

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

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

Q_T = translational partition function

Λ_T = thermal de Broglie wavelength of pair

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

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

Phase Space density — Time scale — Dynamics

Replace

$1 - |S(\ell m)|^2$ by $|1 - S(\ell m)|^2$

for elastic collisions

The long-range potential
Van der Waals case

Van der Waals potential

Write the Schrödinger equation in length and energy units of

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

or

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

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

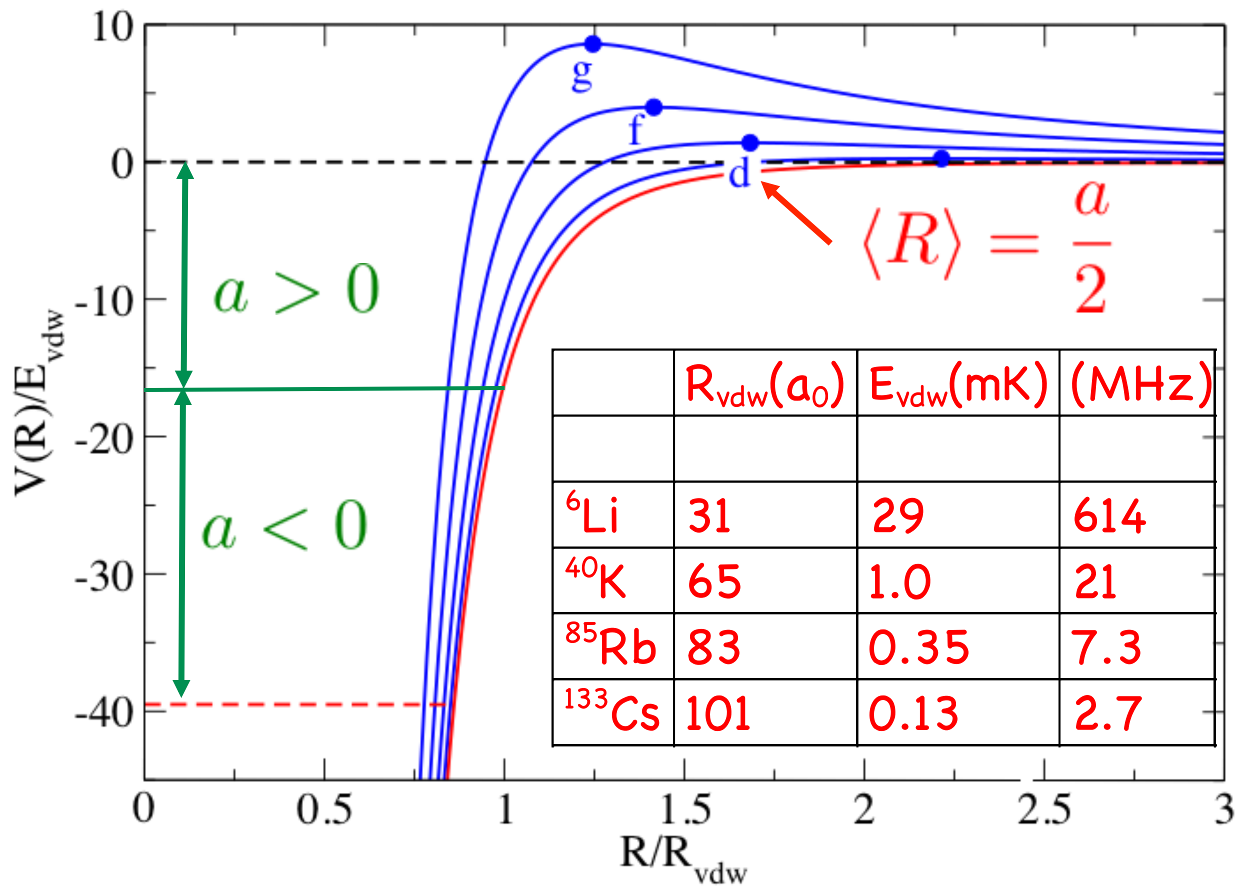
$$E_{\mathrm{vdw}} = \frac{\hbar^2}{2\mu R_{\mathrm{vdw}}^2}$$

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) Photoassociation
and Chin et al., Rev. Mod. Phys. 82, 1225 (2010) Feshbach resonances

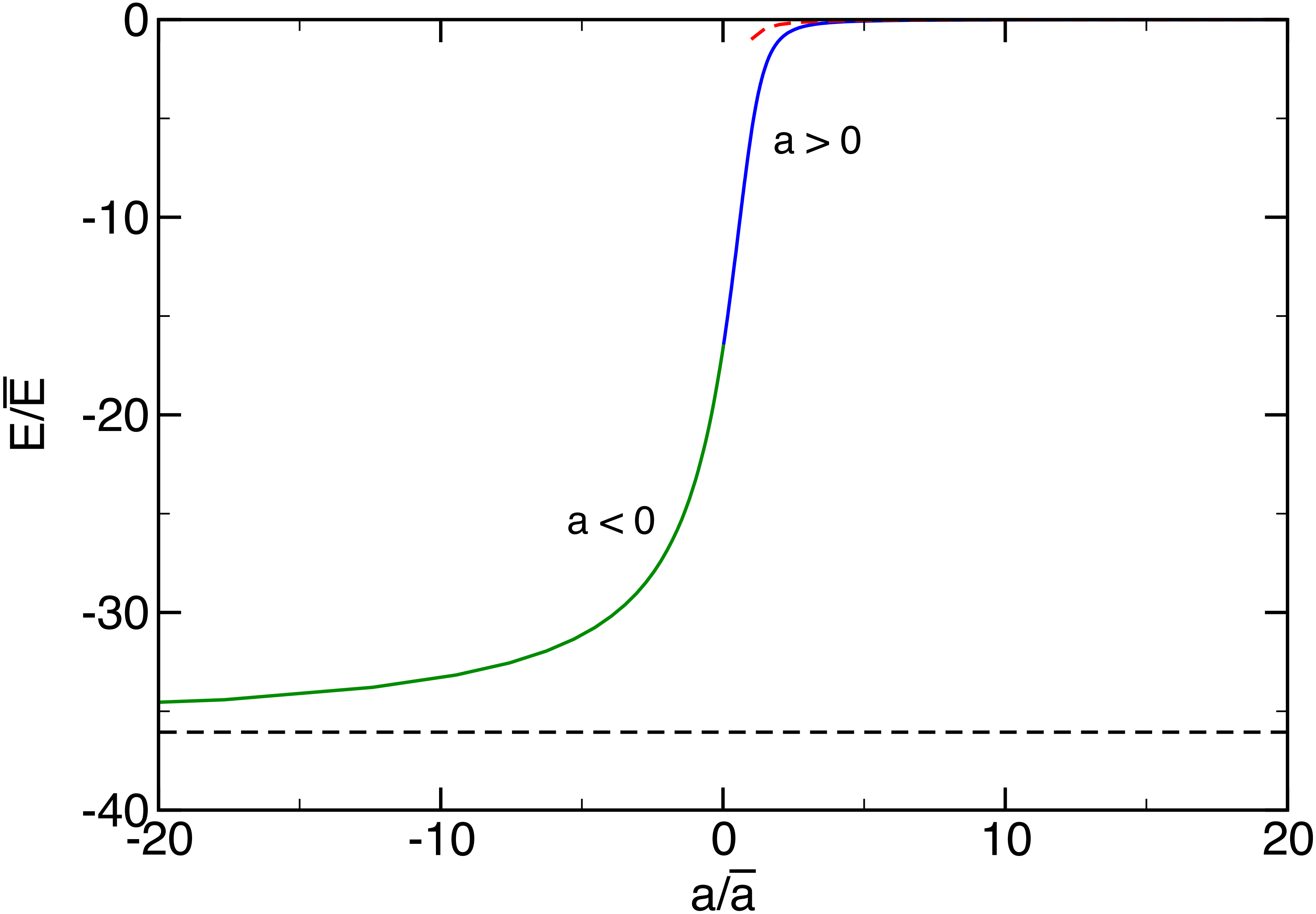
"Size" of vdW potential



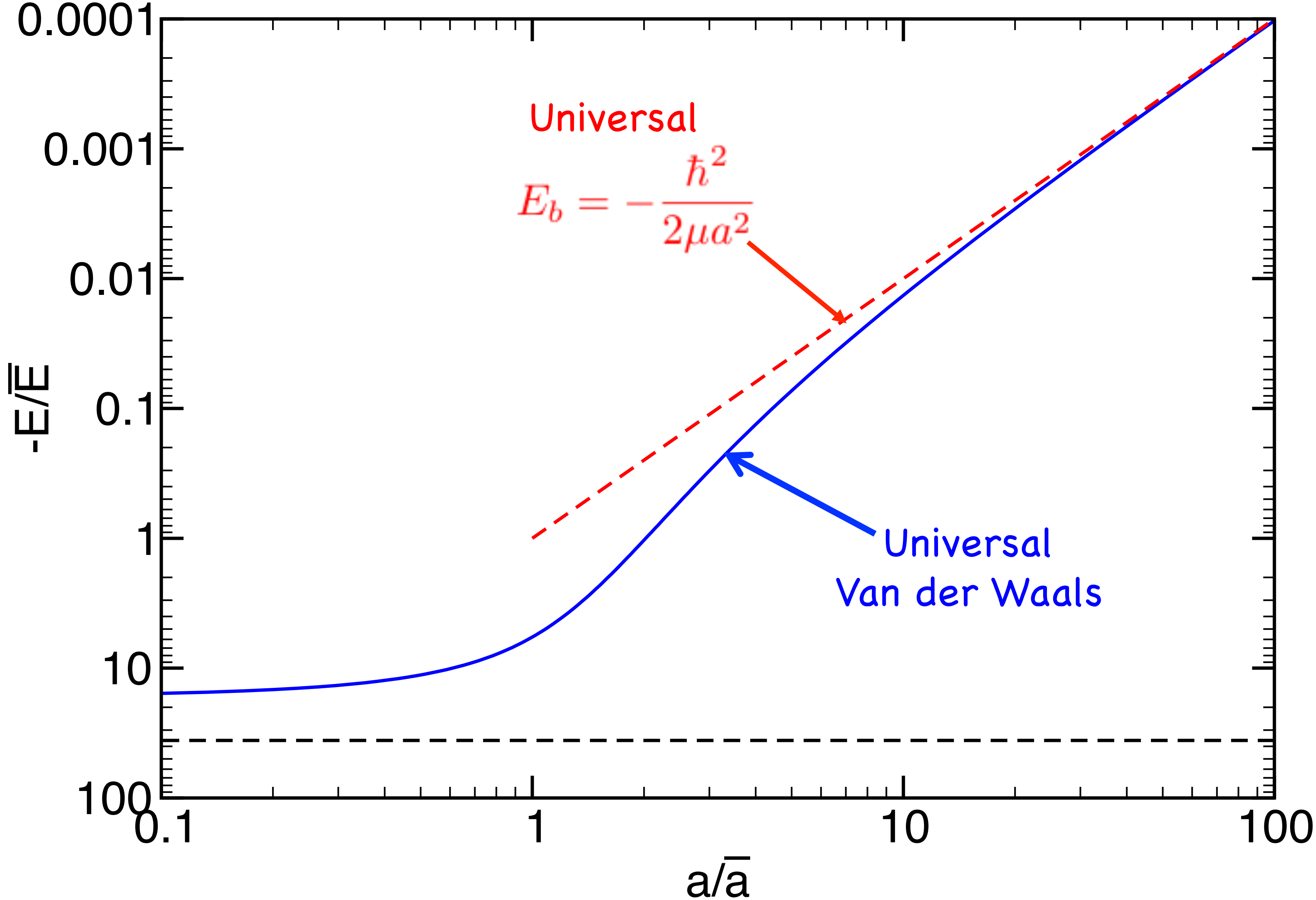
Universal

	$R_{vdw}(a_0)$	E_{vdw}(mK)	(MHz)
^{6}Li	31	29	614
^{40}K	65	1.0	21
^{85}Rb	83	0.35	7.3
^{133}Cs	101	0.13	2.7

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

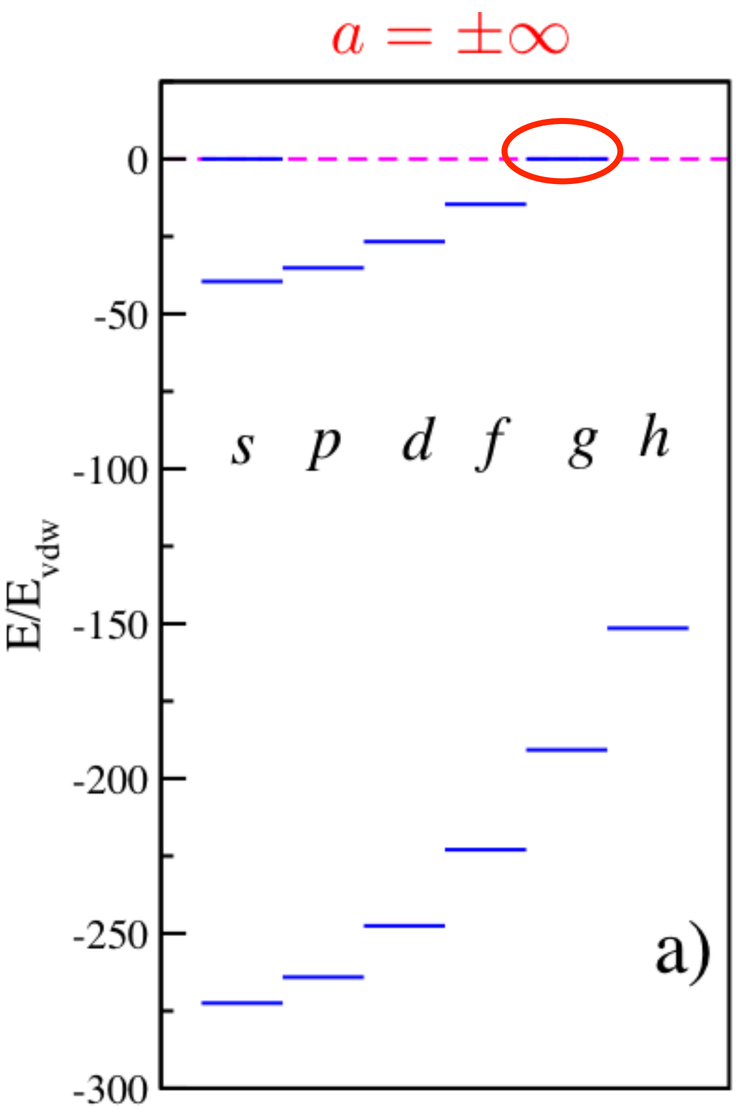


0
-10
-20
-30
-40
-20
-10
0
10
20
E/$\overline{E}$
a/$\overline{a}$
a > 0
a < 0



0.0001
0.001
0.01
0.1
1
10
100
0.1
1
10
100
-E/$\bar{E}$
a/$\bar{a}$
Universal
$E_b = -\frac{\hbar^2}{2\mu a^2}$
Universal
Van der Waals

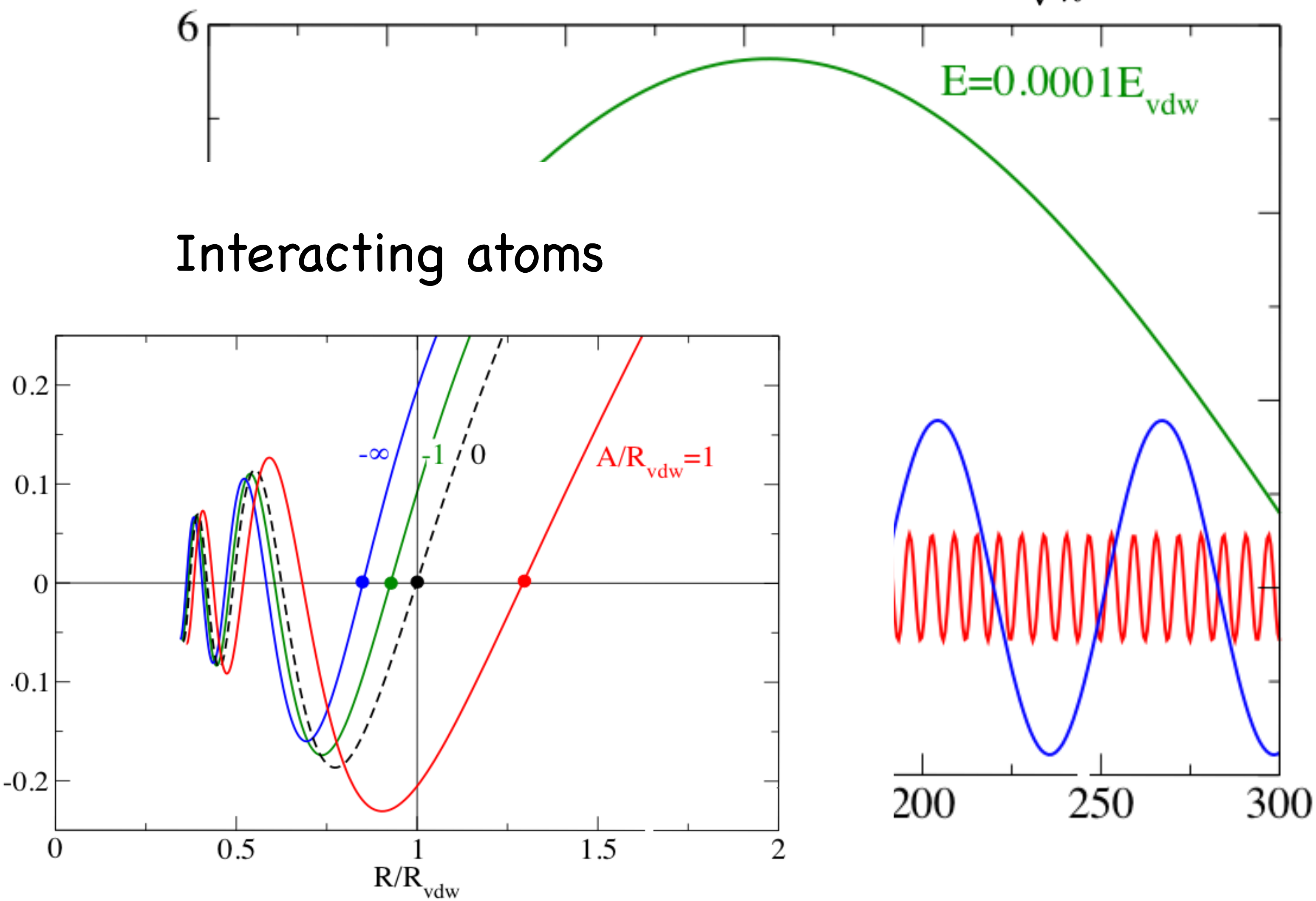
Bound states from van der Waals theory



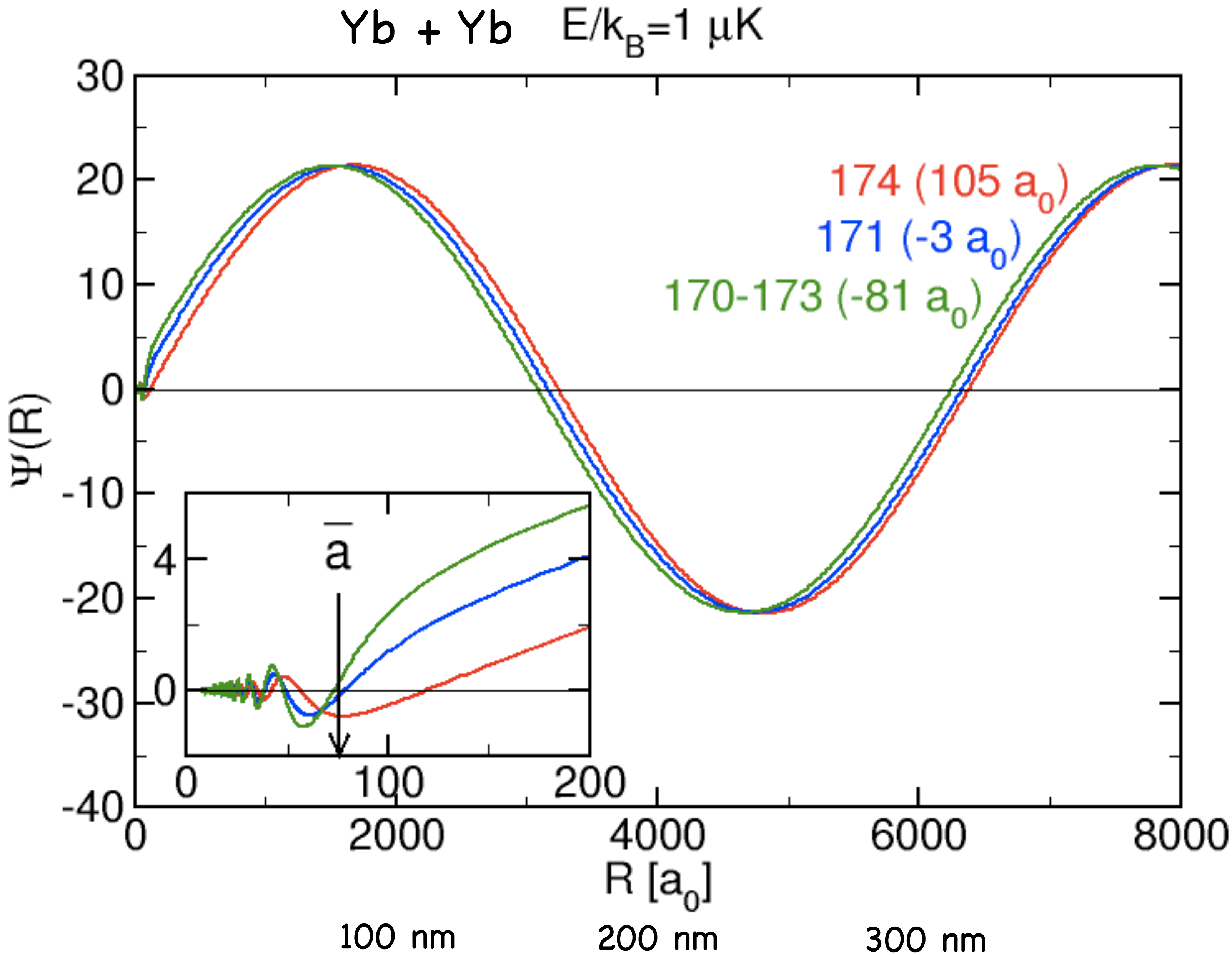
Adapted from Gao, Phys. Rev. A 62, 050702 (2000); Figure from Chin et al., review

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

Interacting atoms



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

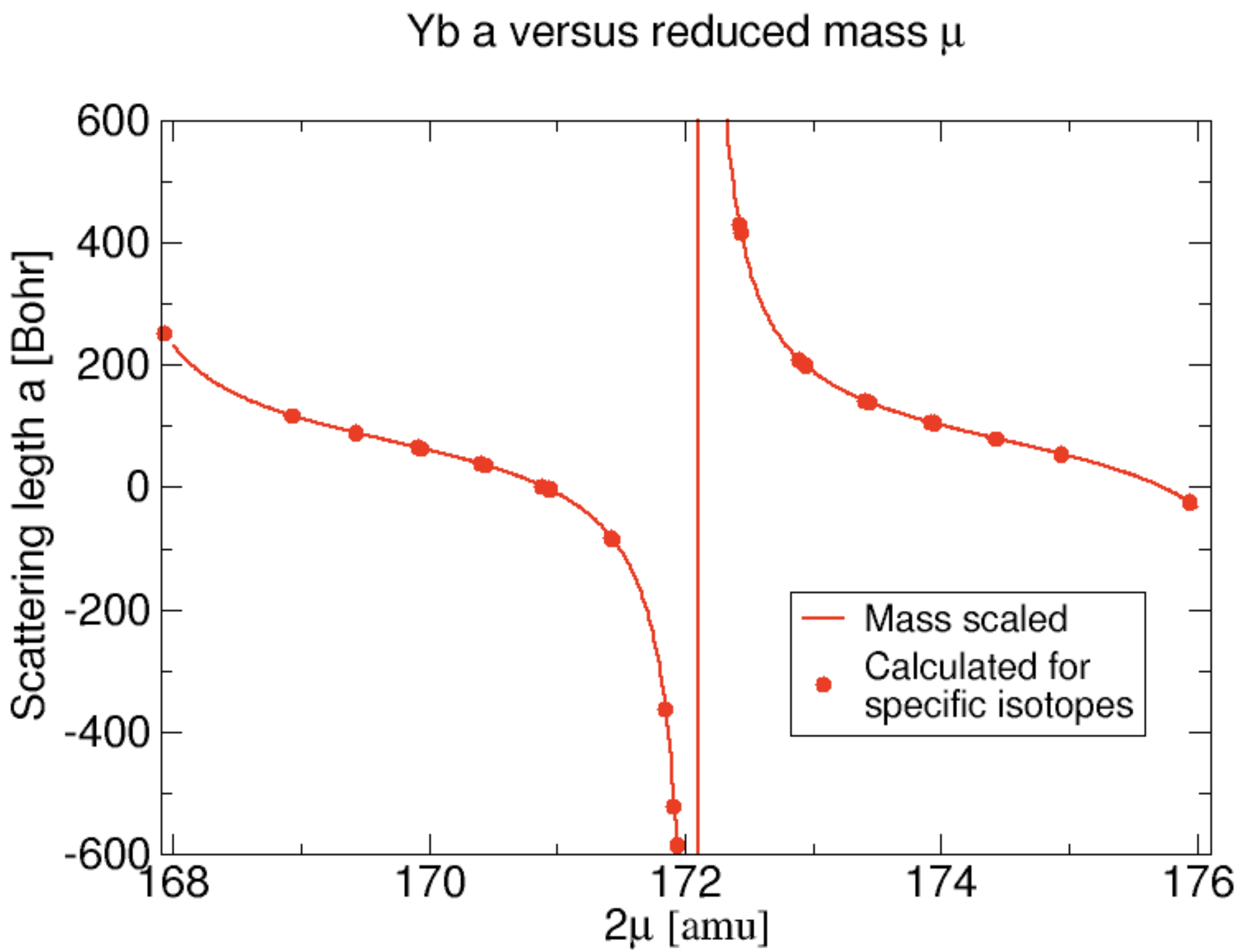


From Krems et al, Cold Molecules, Chapter 6, arXiv:0902.1727

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
Scattering legth a [Bohr]
600
400
200
0
-200
-400
-600
168
170
172
174
176
2μ [amu]
Mass scaled
Calculated for specific isotopes

Gribakin and Flambaum

Phys. Rev. A 48, 546 (1993)

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

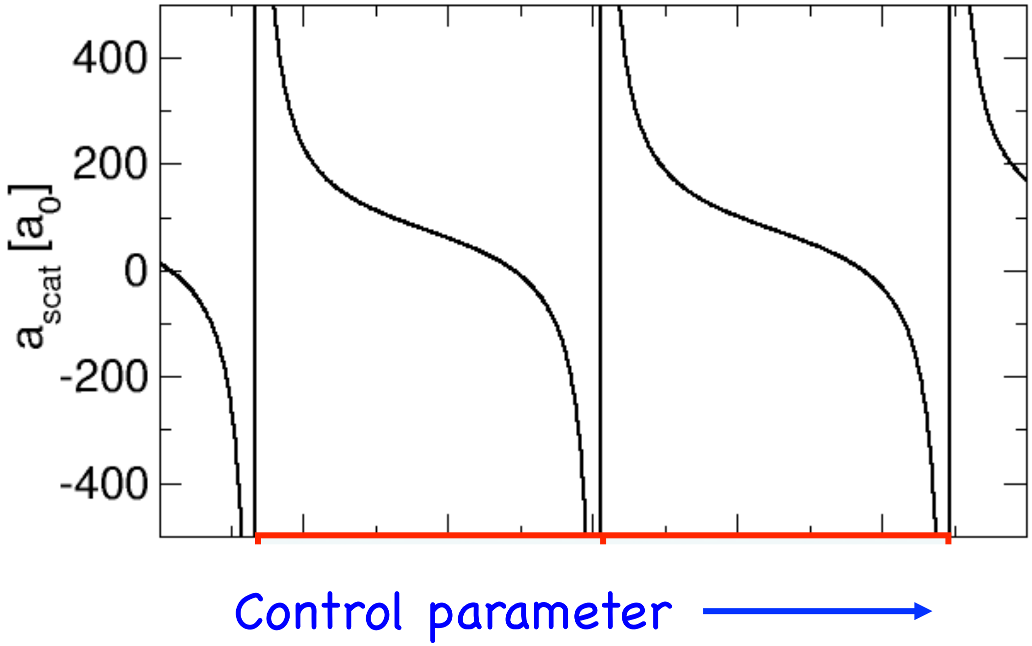
$$\Phi = \int_{r_{in}}^{\infty}\left(\frac{2\mu}{\hbar^2}(-V(R)\right)^{1/2} dR$$

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

Simplest model:

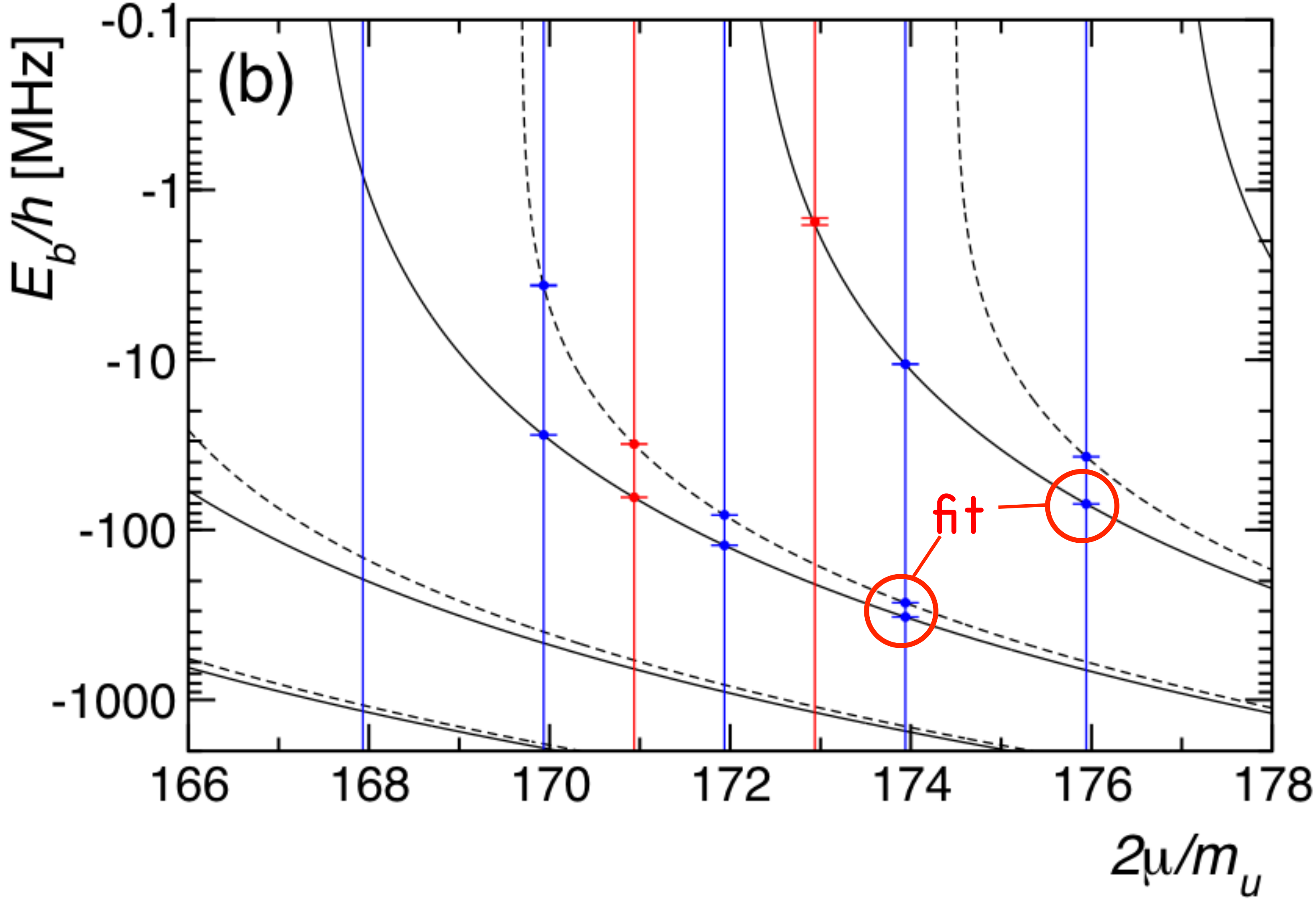
$$V(R) = -\frac{C_6}{R^6} \text{ for } R_{in} < R \leq \infty$$

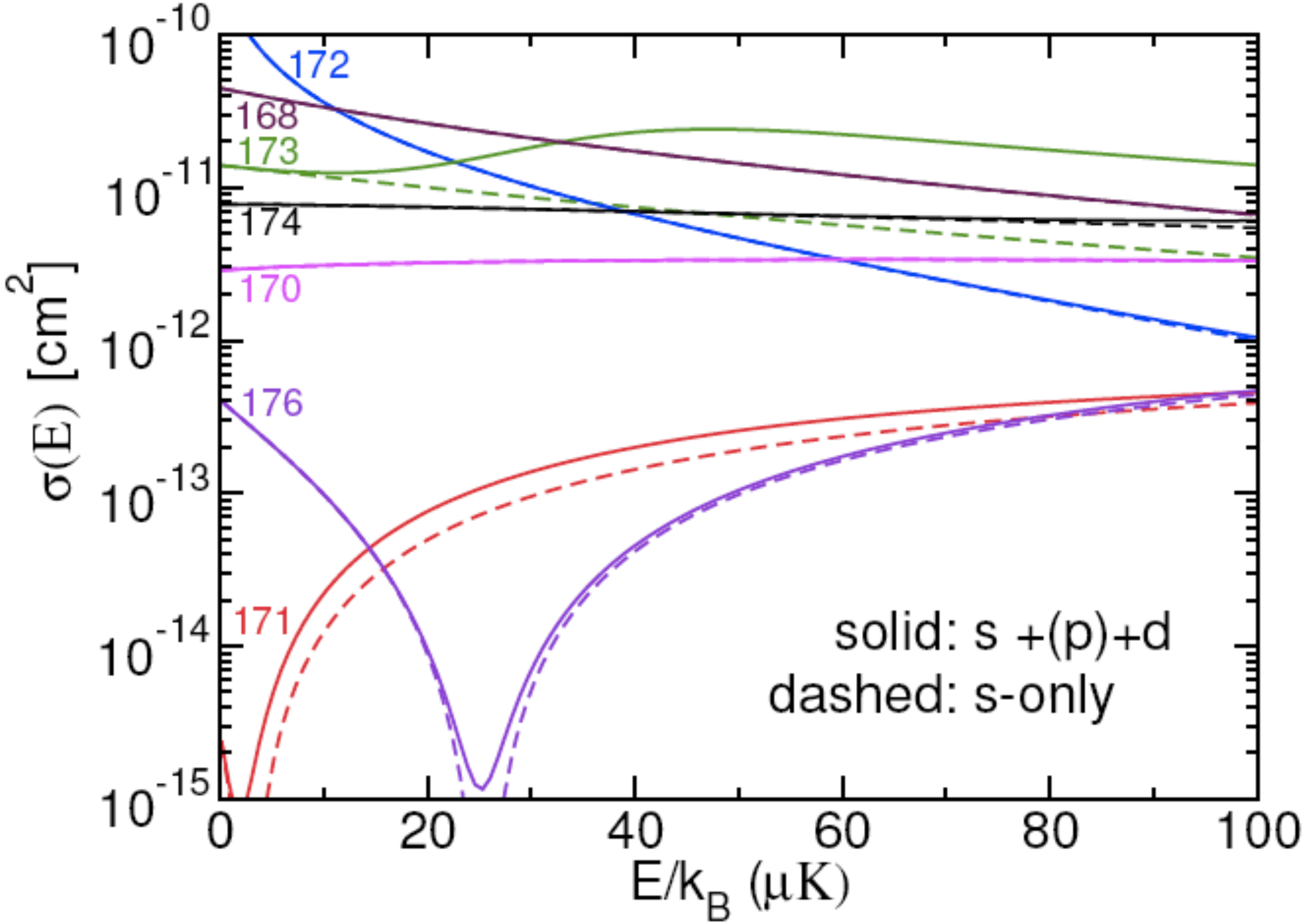
$$V(R) = \infty \text{ for } 0 < R \leq R_{in}$$

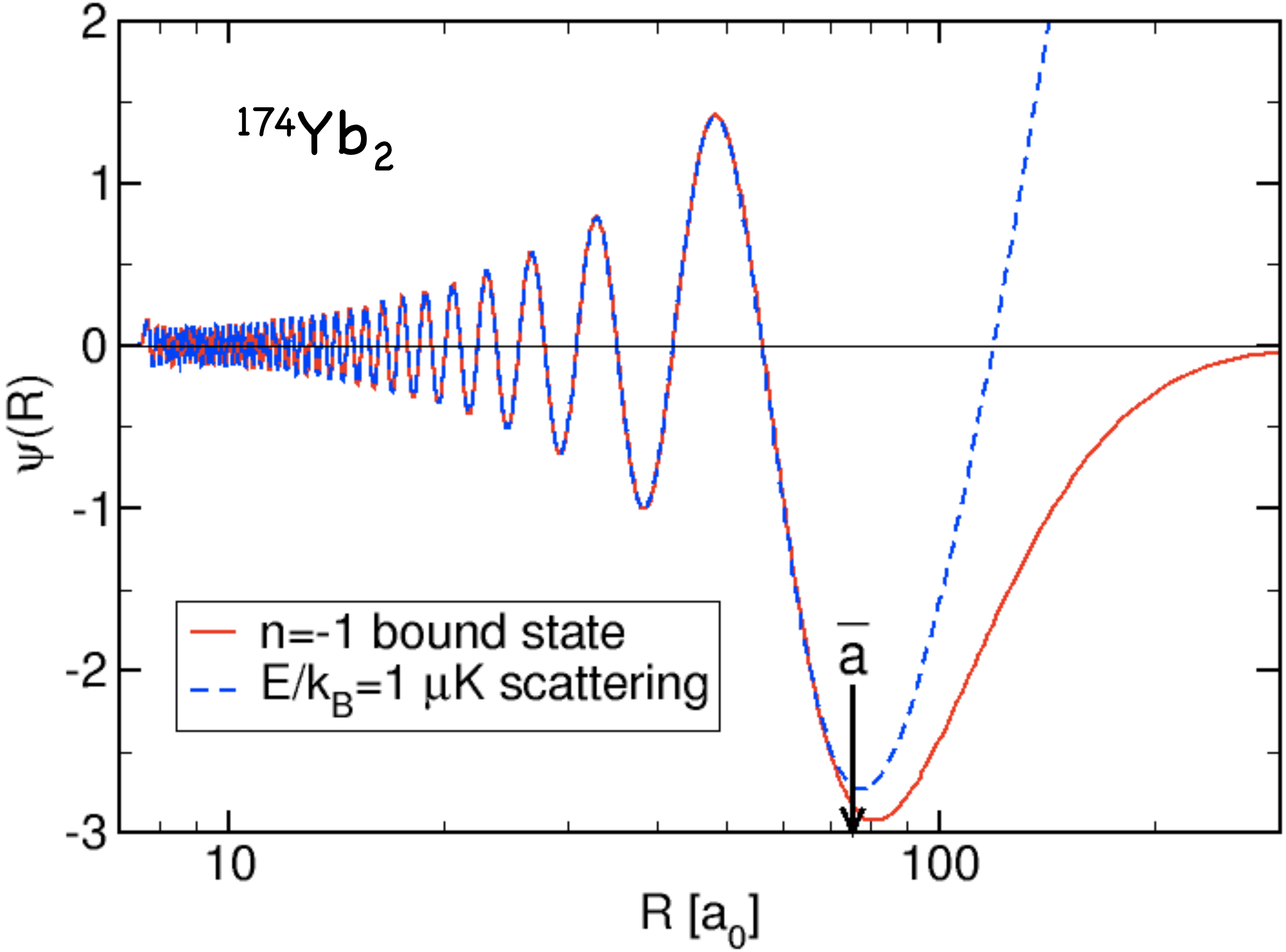


400
200
0
-200
-400
a_{scat} [a_0]
Control parameter

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



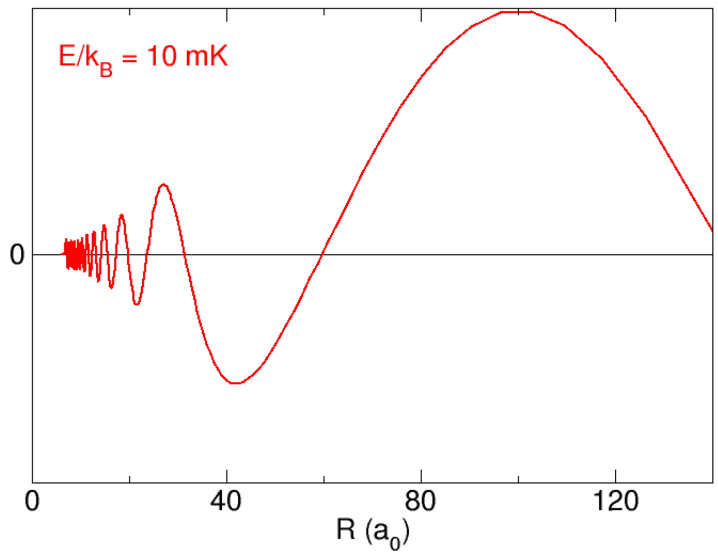

172
168
173
174
170
176
171
solid: s +(p)+d
dashed: s-only
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
0
20
40
60
80
100
$\sigma(E)$ [cm^2]
E/k_B (μK)



$^{174}Yb_2$
n=-1 bound state
E/k_B=1 μK scattering
$\bar{a}$
ψ(R)
R [a_0]
2
1
0
-1
-2
-3
10
100

Semiclassical considerations

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



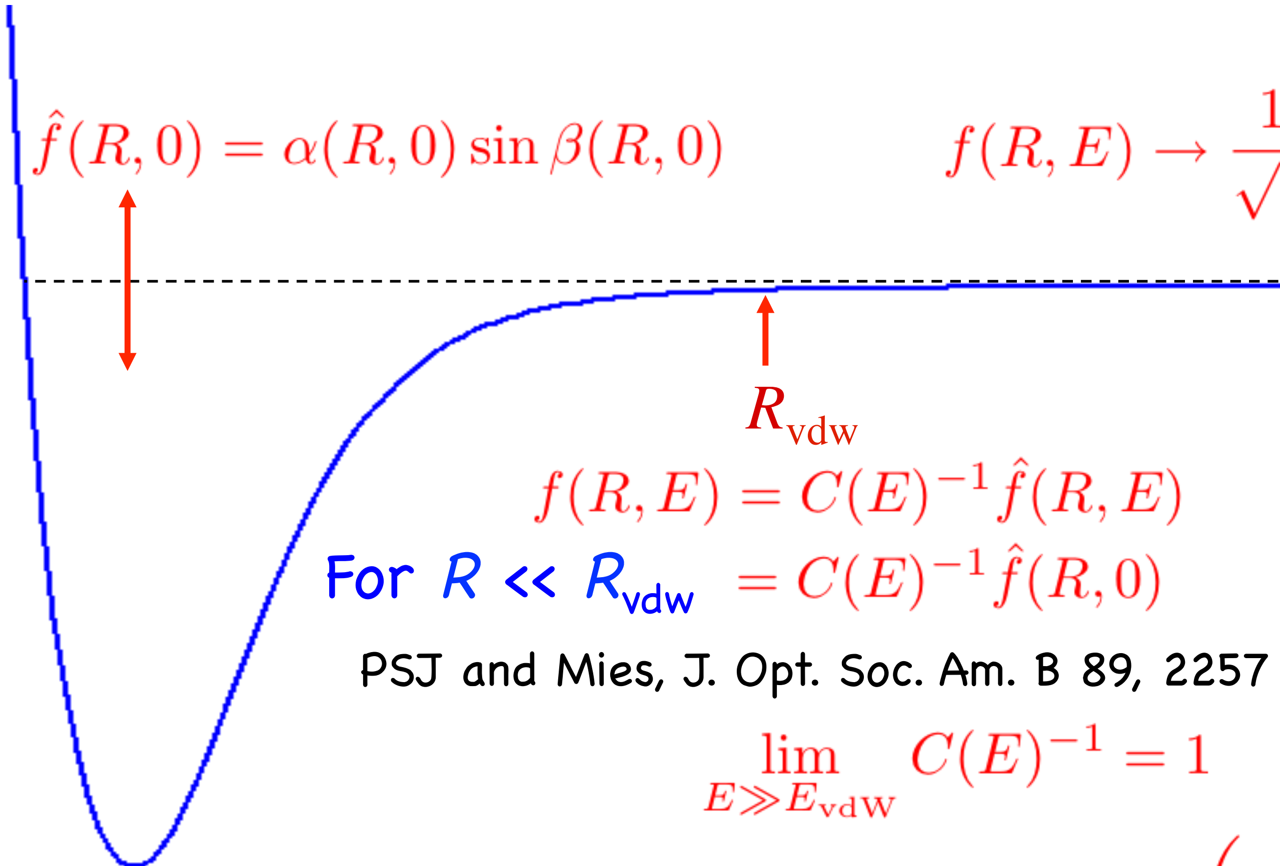
$$\alpha(R,E) = \frac{1}{k(R,E)^{\frac{1}{2}}}$$

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

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

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

Semiclassical considerations continued



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

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

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

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

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

$$\lim_{E \gg E_{\mathrm{vdW}}} C(E)^{-1} = 1$$

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

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

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

PSJ and Gao, Atomic Physics 20 (AIP), ICAP 2006, p. 261

PSJ and Mies, J. Opt. Soc. Am. B 6, 2257 (1989)

The End