ICAP Summer School 2006
University of Innsbruck

Cold Atomic and Molecular Collisions

1. Basics
2. Feshbach resonances
3. Photoassociation

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And many others, especially
Eite Tiesinga, Carl Williams, Pascal Naidon (NIST),
Thorsten Köhler (Oxford), Bo Gao (Toledo), Roman Ciurylo (Torun)

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.

- What is a scattering length, and why is it significant?

- Scattering resonances are a key to measurement and control.
  - Photoassociation
  - Magnetically tunable "Feshbach" resonances

- Collisions in tightly confining atom traps.

- Basic concepts, illustrated by examples.

Two kinds of collision

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

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

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

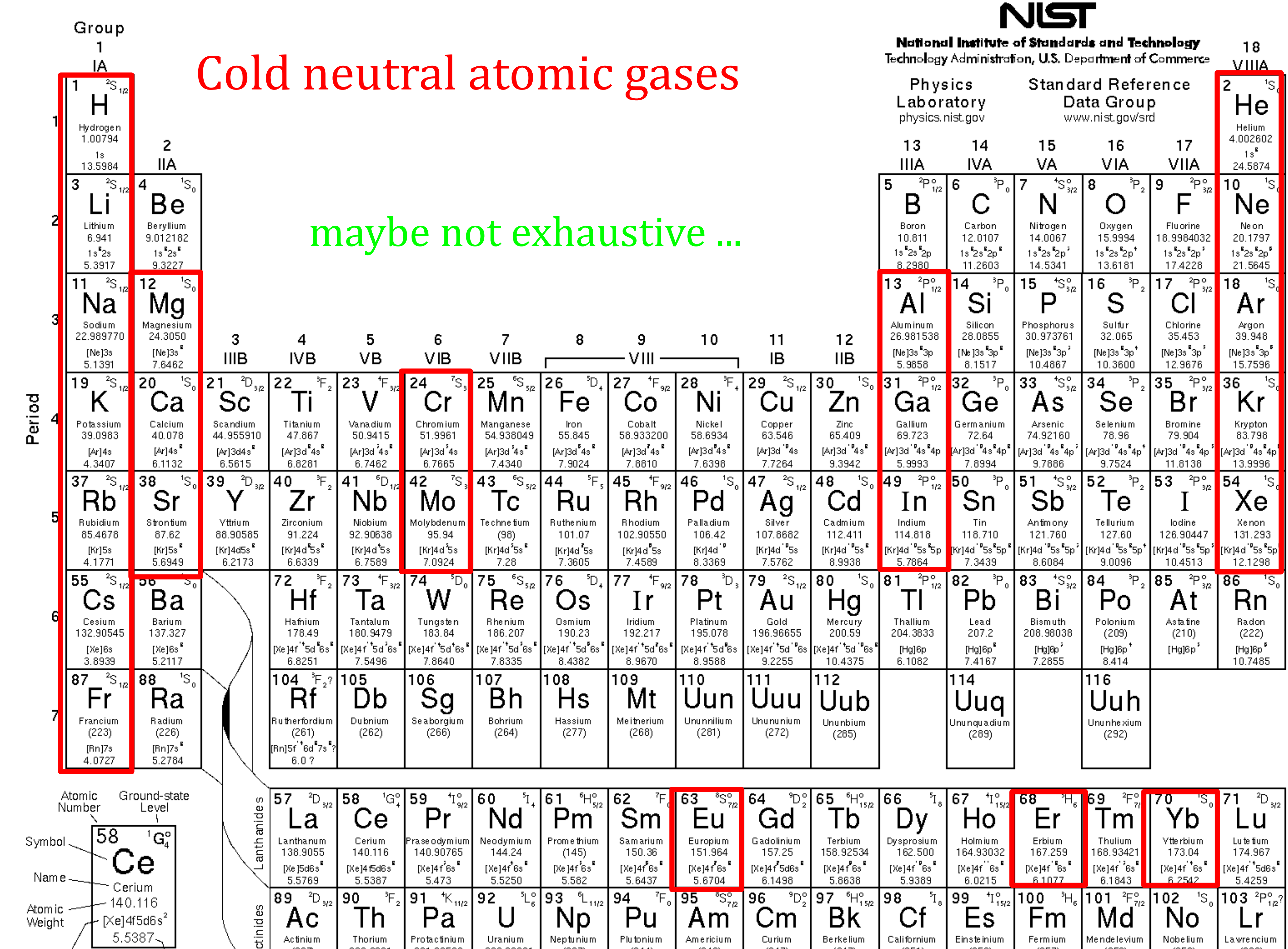
- Spin relaxation
- Photoassociation
- Loss of trapped atoms
- Decoherence
- Spinor condensates (ΔE=0)

Cold atomic and molecular collision basics

- Potential energy curves
  - Properties of the long range potential
  - Bound and scattering states
- Collision cross sections and rates
  - Partial waves and cross sections
  - Elastic and inelastic collisions
  - Threshold properties of collisions and bound states
  - Boson and fermion differences
- The effects of trap confinement on collisions
- How are molecular collisions different

Cold neutral atomic gases

maybe not exhaustive ...

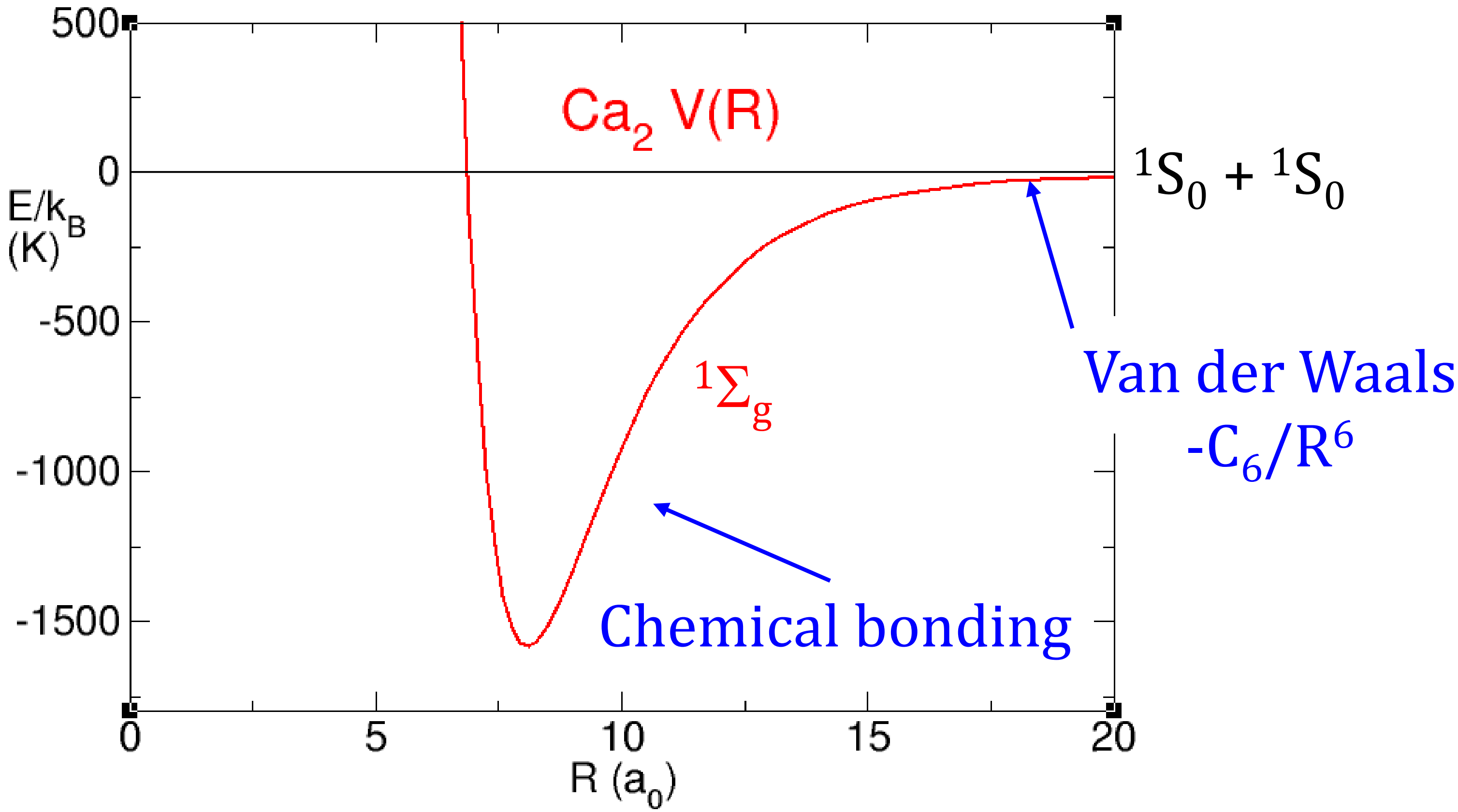


Ca $4s^2$ $^1S_0$ atom

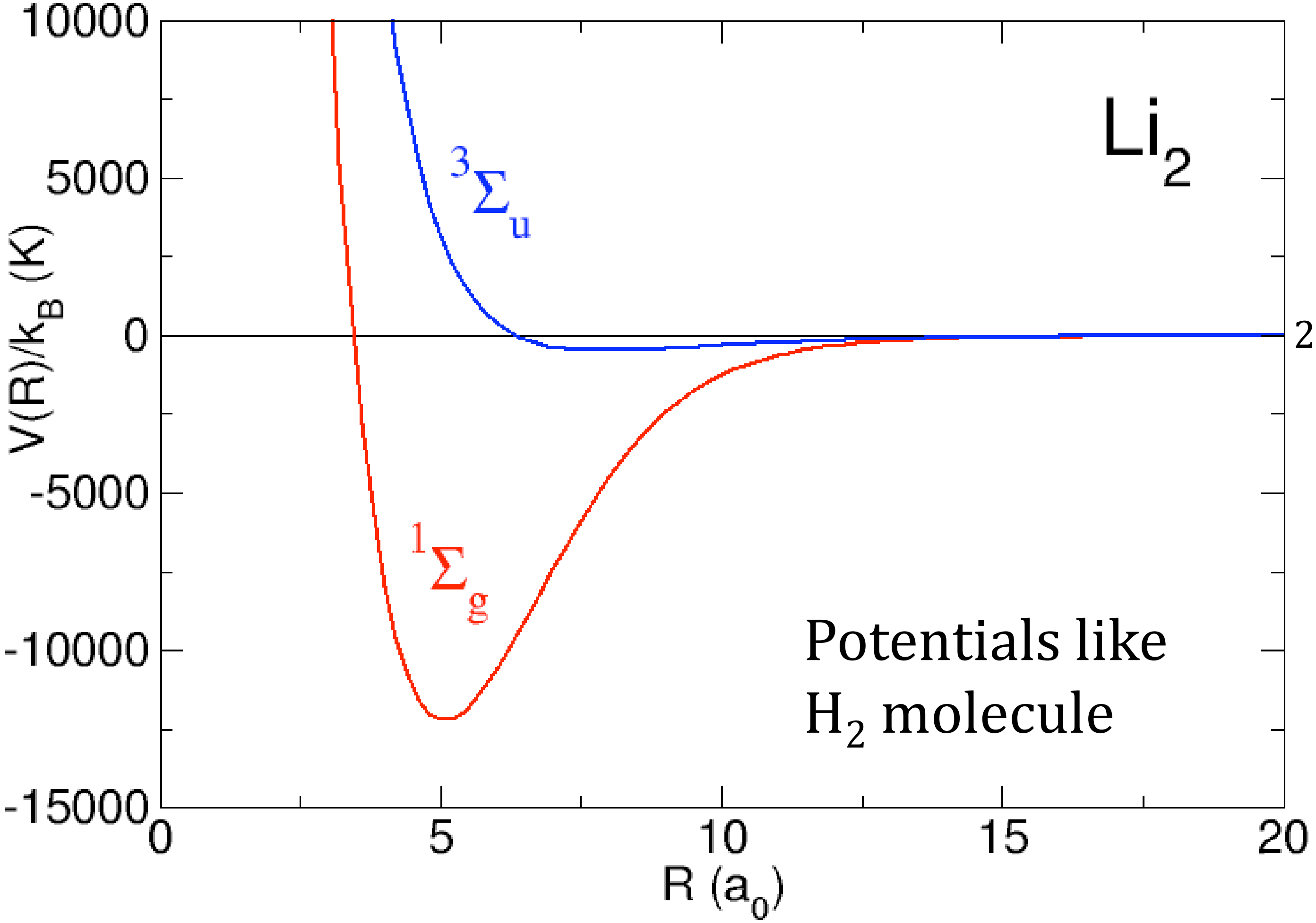
Spin degeneracy

Total angular momentum

Born-Oppenheimer approximation = potential energy curve

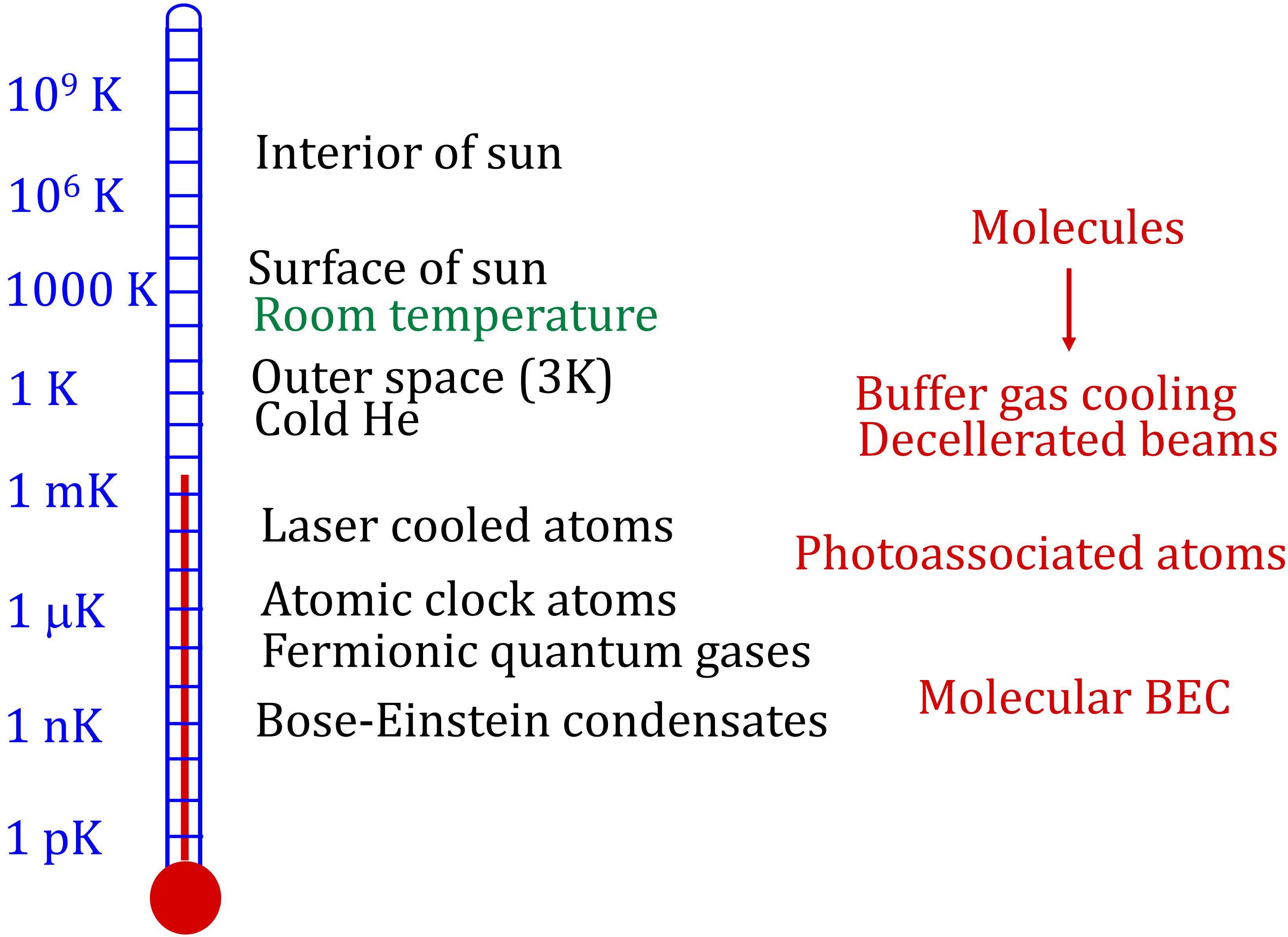


Li $1s^2 2s\ ^2S_{1/2}$ atom



$^2S_{1/2} + {}^2S_{1/2}$

Similar for
Na
K
Rb
Cs

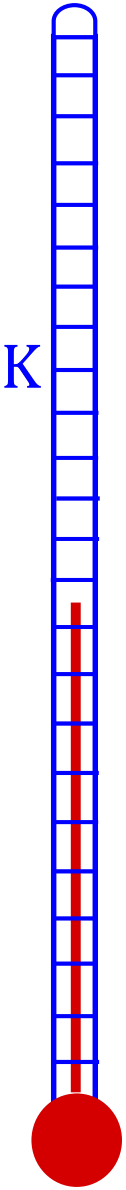


10^9 K
10^6 K
1000 K
1 K
1 mK
1 μK
1 nK
1 pK
Interior of sun
Surface of sun
Room temperature
Outer space (3K)
Cold He
Laser cooled atoms
Atomic clock atoms
Fermionic quantum gases
Bose-Einstein condensates
Molecules
Buffer gas cooling
Decellerated beams
Photoassociated atoms
Molecular BEC

momentum $p = \hbar k$

$\lambda = h/p$

^{6}Li x 0.2 for Cs



E/h	E/k_B	^{6}Li	
	10^9 K		
	10^6 K		
	1000 K	0.76 a_0	= 0.04 nm
	1 K	24 a_0	= 1.3 nm
21 MHz =	1 mK	760 a_0	= 40 nm
21 kHz =	1 μK	24000 a_0	= 1.3 μm
21 Hz =	1 nK	7.6×10^6 a_0	= 40 μm
	1 pK		

Characteristic Lengths

De Broglie wavelength	$\lambda = \frac{h}{p}$	$\sim 20000\ a_0$ (1 μm)
Van der Waals length	$x_0 = \frac{1}{2}\left(\frac{2\mu C_6}{\hbar^2}\right)^{1/4}$	30 - 100 a_0 (1.5 - 5 nm)
Chemical bond		< 20 a_0 (< 1nm)
Scattering length	A	$-\infty < A < \infty$
Trap size	$\left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}$	> 200000 a_0 (10 μm) Lattice: 1000 a_0 (50 nm)
Interparticle spacing	$n^{-1/3}$	2000 a_0 (100nm) at 10^{15}cm^{-3} 20000 a_0 (1000nm) at 10^{12}cm^{-3}

Collision of two atoms

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

Expand Ψ(R,E) in relative angular momentum basis lm.
l = 0, 1, 2… s-, p-, d-waves, …

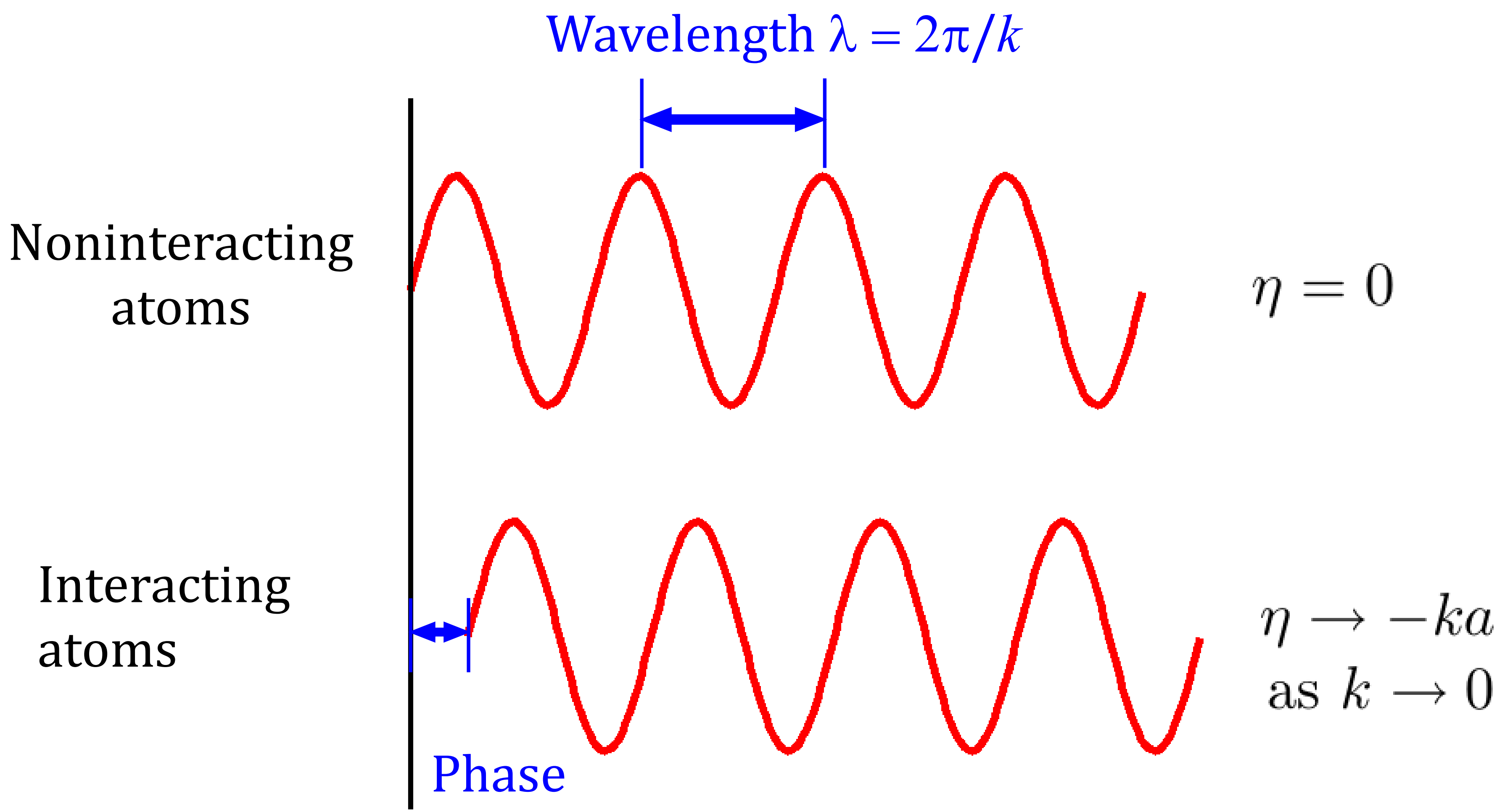
Potential energy: $V(R) + \frac{\hbar\ell(\ell+1)}{2\mu R^2}$ --> phase shift $\eta_\ell(E)$

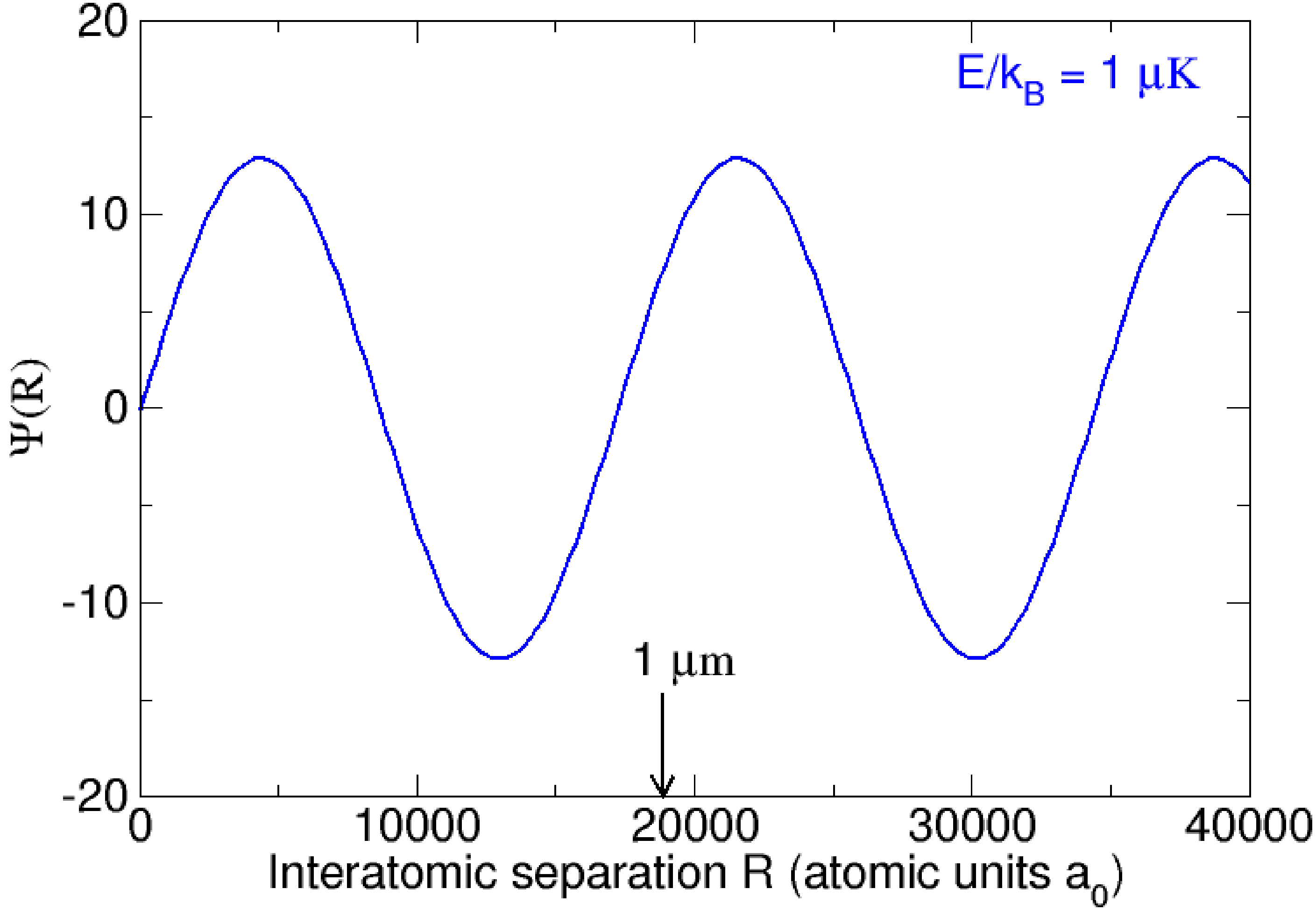
Neutral atoms (S-state): $V(R)$ --> $-C_6/R^6$ van der Waals

Solve Schrödinger equation for bound and scattering Ψ(R,E)
--> bound states E_n
--> scattering phases, amplitudes

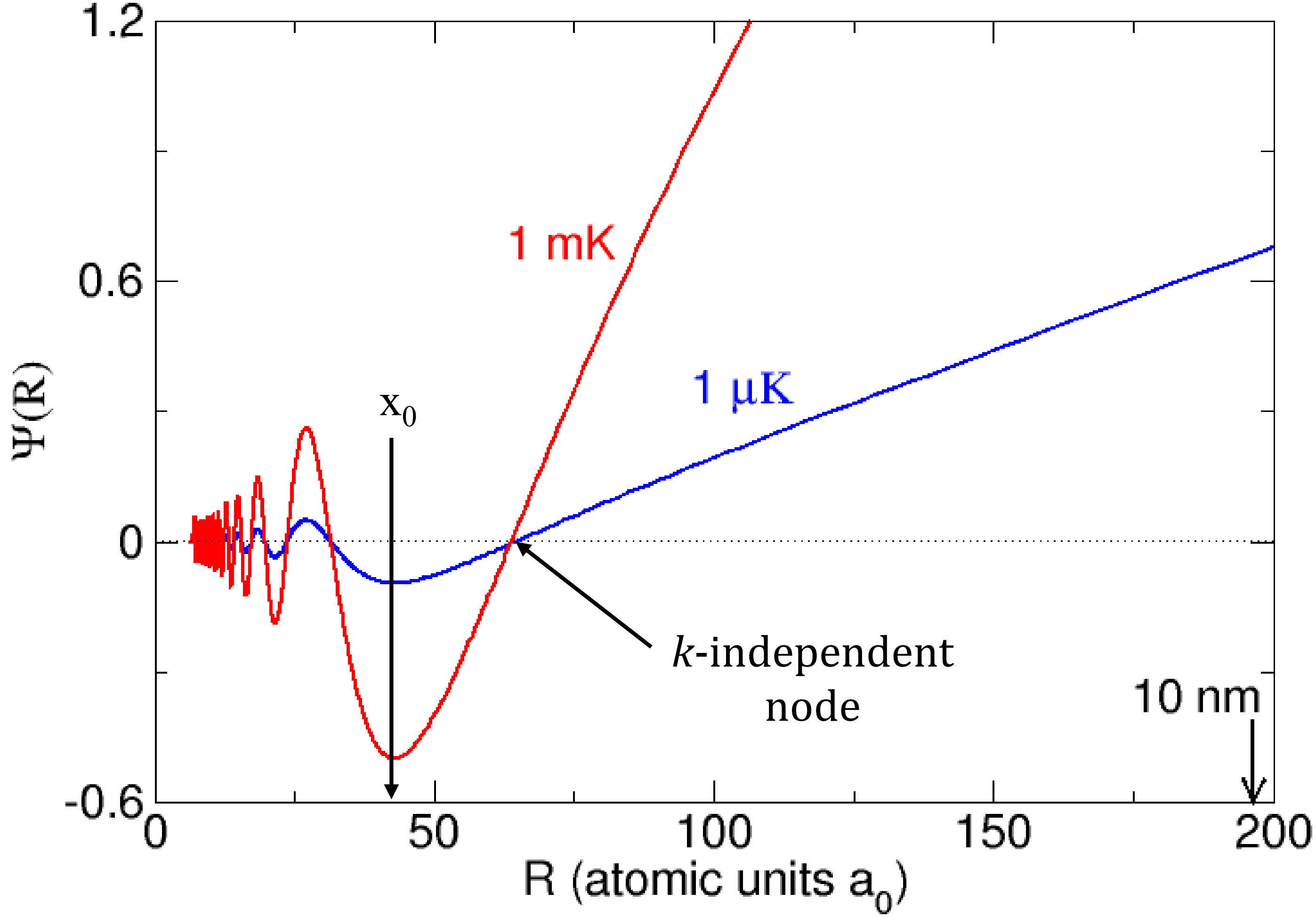
S-wave scattering phase shift

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





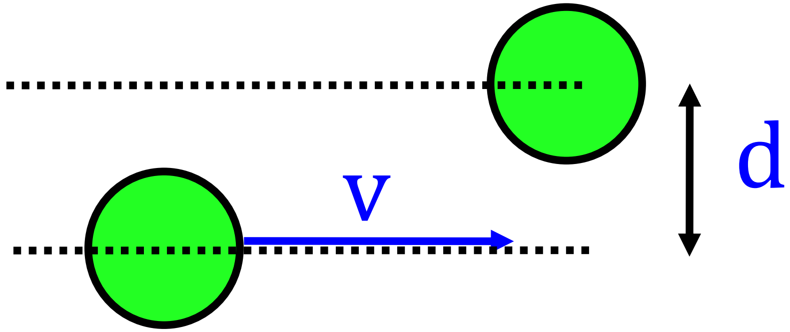
E/k_B = 1 μK
20
10
0
-10
-20
Ψ(R)
1 μm
0
10000
20000
30000
40000
Interatomic separation R (atomic units a_0)



1.2
0.6
0
-0.6
0
50
100
150
200
Ψ(R)
R (atomic units a0)
1 mK
1 μK
x0
k-independent node
10 nm

Cross section σ

Classical balls with distance of closest approach d (diameter)



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

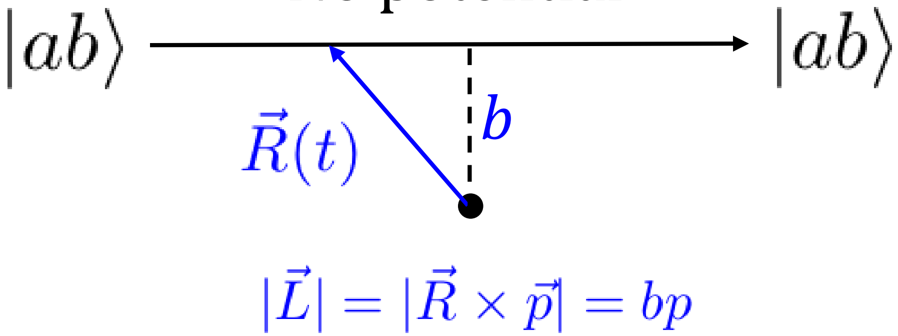
and a collision rate $\Gamma = nv\sigma$ (typical: 1 s^{-1}, MOT
10^4 s^{-1}, BEC)

Rate constant $K = v\ \sigma$

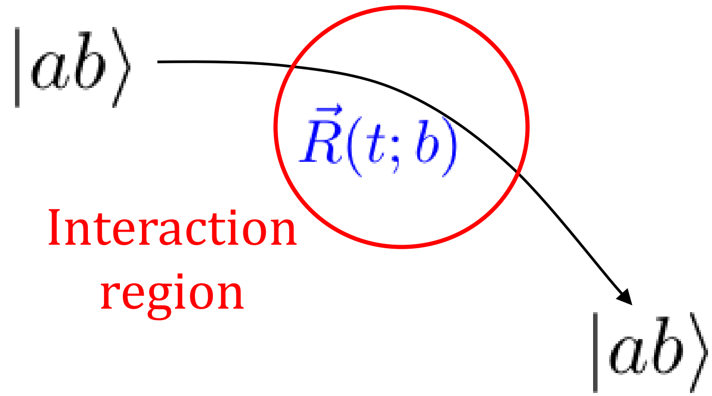
Time between collisions = $1/\Gamma$ = $1/(Kn) \approx$ 1s (MOT), 100μs (BEC)

Classical picture

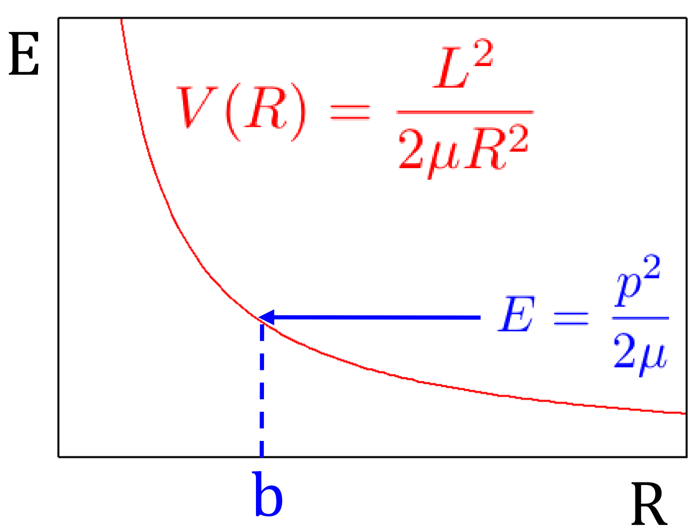
No potential



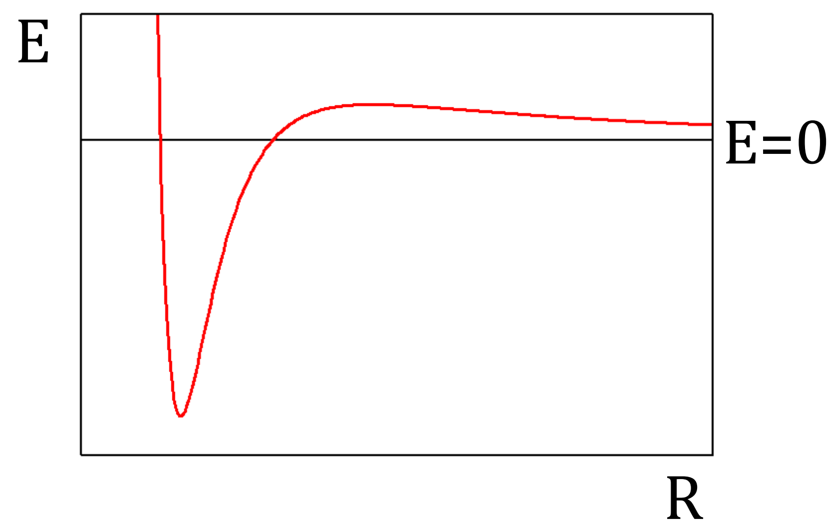
With potential



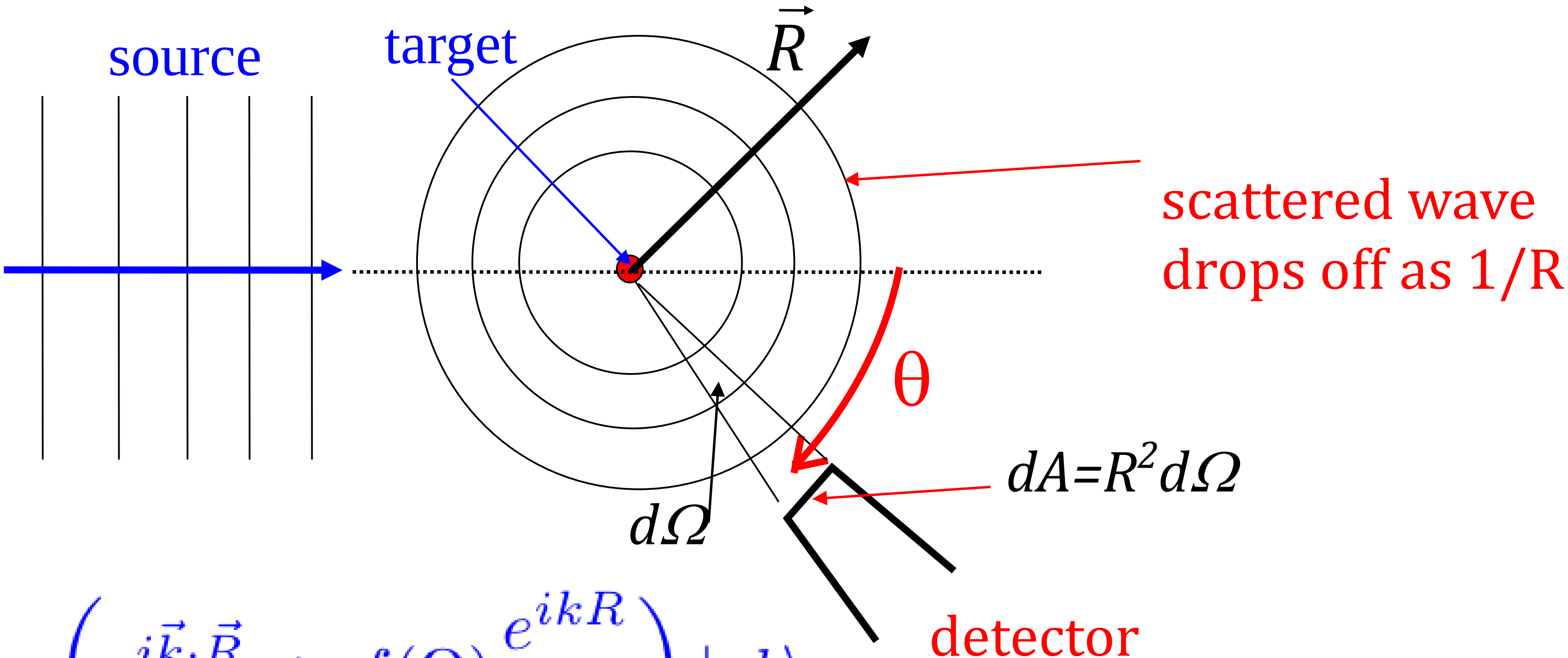
Centrifugal potential



Centrifugal barrier



Quantum scattering theory



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

cross section

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

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

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

where $j_\ell(kR) = \dfrac{\phi_\ell(R)}{kR} \rightarrow \dfrac{\sin\left(kR - \frac{\pi\ell}{2}\right)}{kR}$ as $R \rightarrow \infty$

an$\phi_\ell(R)$s a solution to the
radial Schrödinger equation

$$\frac{d^2\phi_\ell(R)}{dR^2} + \frac{2\mu}{\hbar^2}\left(E - \frac{\hbar^2\ell(\ell+1)}{2\mu R^2}\right)\phi_\ell(R) = 0$$

Centrifugal
potential

Add an interaction potential V(R)

$$e^{\vec{k}\cdot\vec{R}} \; + \; f(\Omega)\frac{e^{ikR}}{R} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^{\ell} Y^{*}_{\ell m}(\hat{k}) Y_{\ell,m}(\hat{R}) \frac{\phi_\ell^+(R)}{kR}$$

where $\phi_\ell^+(R)/(kR)$ represents a plane + scattered wave:

$$\frac{\phi_\ell^+(R)}{kR} \rightarrow \frac{\sin\left(kR - \frac{\pi\ell}{2} + \eta_\ell\right)}{kR} e^{i\eta_\ell} = j_\ell(kR) + f_\ell \frac{e^{ikR}}{R}$$

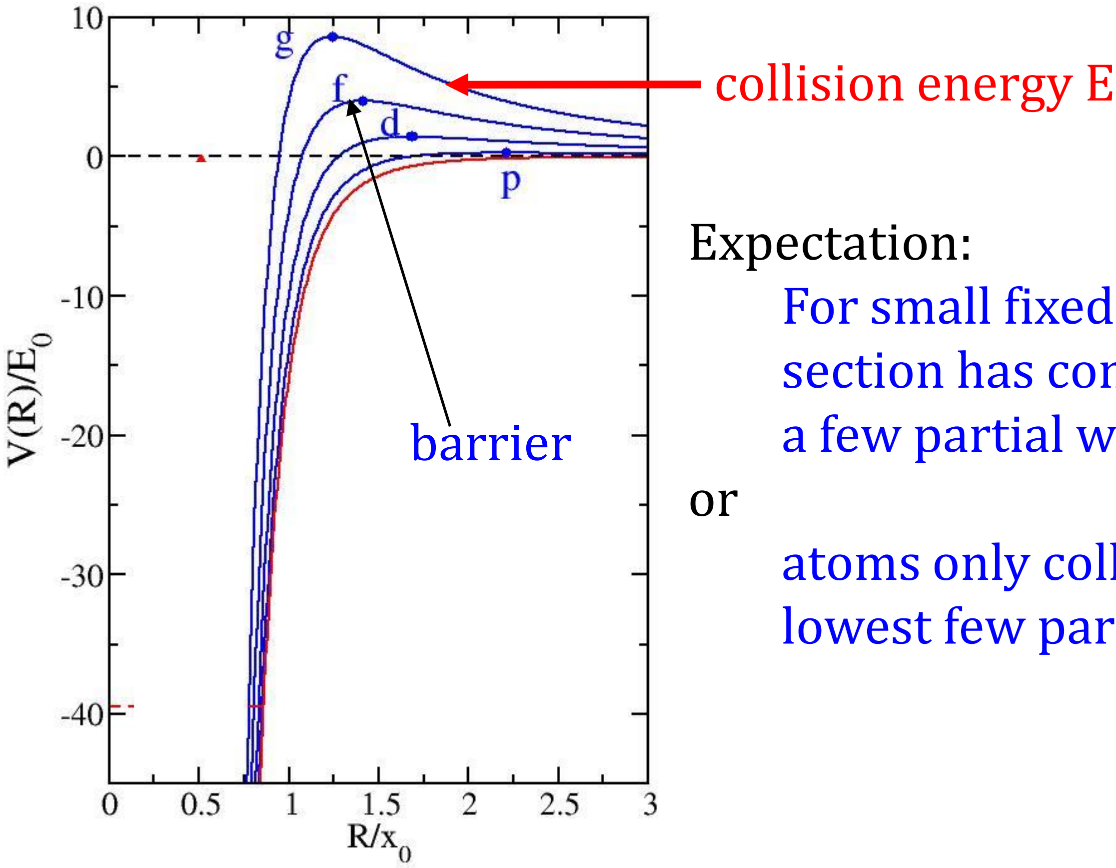
$$f_\ell = \frac{\sin\eta_\ell}{k} e^{i\left(\eta_\ell - \frac{\pi\ell}{2}\right)}$$

and $\phi_\ell^+(R)$ is a solution to the radial Schrödinger equation

$$\frac{d^2\phi_\ell^+(R)}{dR^2} + \frac{2\mu}{\hbar^2}\left(E - V(R) - \frac{\hbar^2\ell(\ell+1)}{2\mu R^2}\right)\phi_\ell^+(R) = 0$$

Centrifugal barrier

$$V(R) + \frac{\hbar^2 \ell(\ell+1)}{2\mu R^2}$$



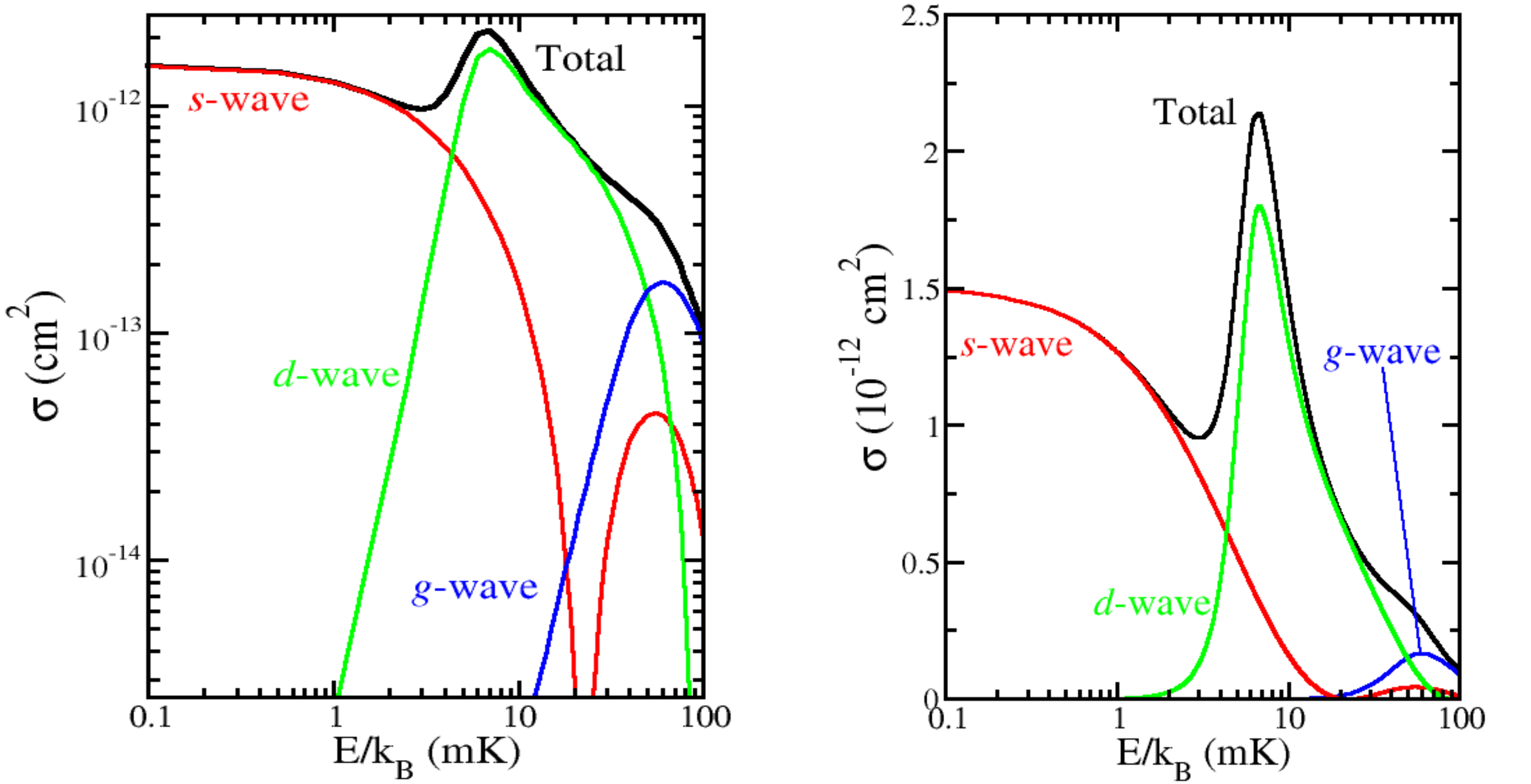
Expectation:

For small fixed E the cross section has contributions from a few partial waves

or

atoms only collide via the lowest few partial waves

Elastic cross section σ for like Na atoms



Many (even) partial waves

Identical particle collisions

Identical atoms in same internal state *a*:

Bosons: even ℓ only

Fermions: odd ℓ only

Identical atoms in *different* internal states *a,b*:

Boson, Fermions: even and odd ℓ

+1, boson

-1, fermion

$$\frac{1}{\sqrt{2}}\left(|ab\rangle e^{i\vec{k}_{ab}\cdot\vec{R}} + \delta_s |ba\rangle e^{-i\vec{k}_{ab}\cdot\vec{R}}\right)$$

$$= 4\pi \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} i^\ell Y^*_{\ell m}(\hat{k}) Y_{\ell,m}(\hat{R}) j_\ell(kR) \times \frac{|ab\rangle + \delta_s(-1)^\ell |ba\rangle}{\sqrt{2}}$$

See Stoof, Koelman and Verhaar, Phys. Rev. B 38, 4688 (1988).

Jim Burke's thesis http://jilawww.colorado.edu/pubs/thesis/burke/

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:

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

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

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

Threshold properties

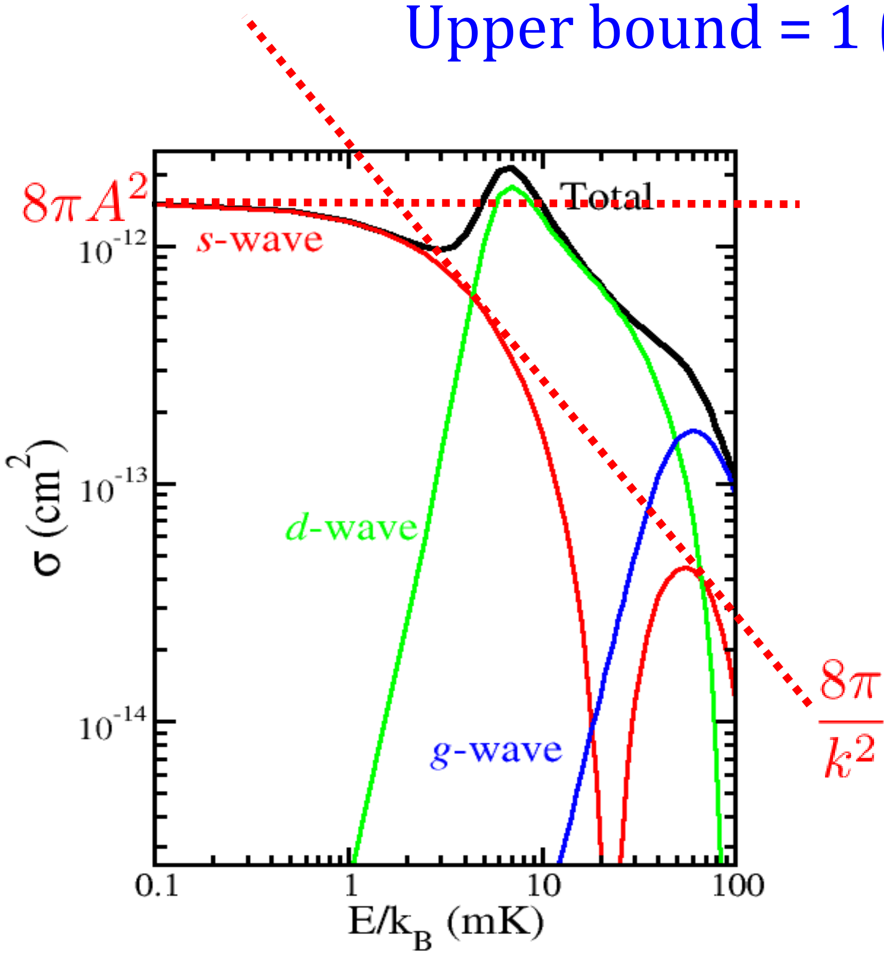
$$\sigma(E) = \frac{4\pi}{k^2}\sin^2(kA) = 4\pi A^2 \text{ as } k \to 0$$

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

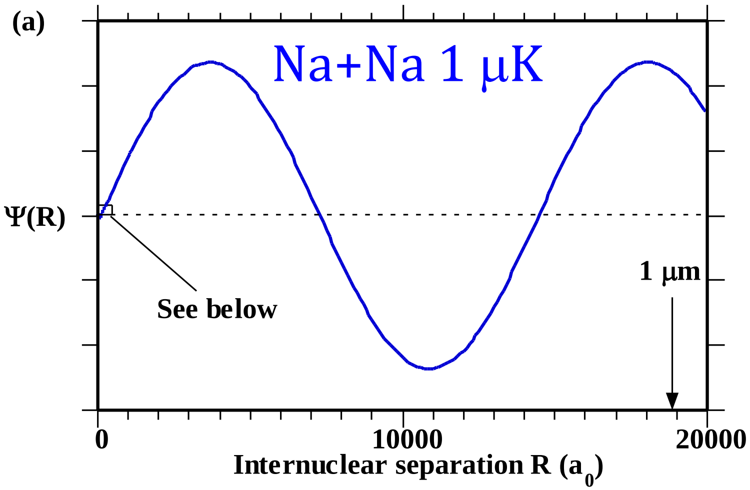
Upper bound = 1 (unitarity limit)

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

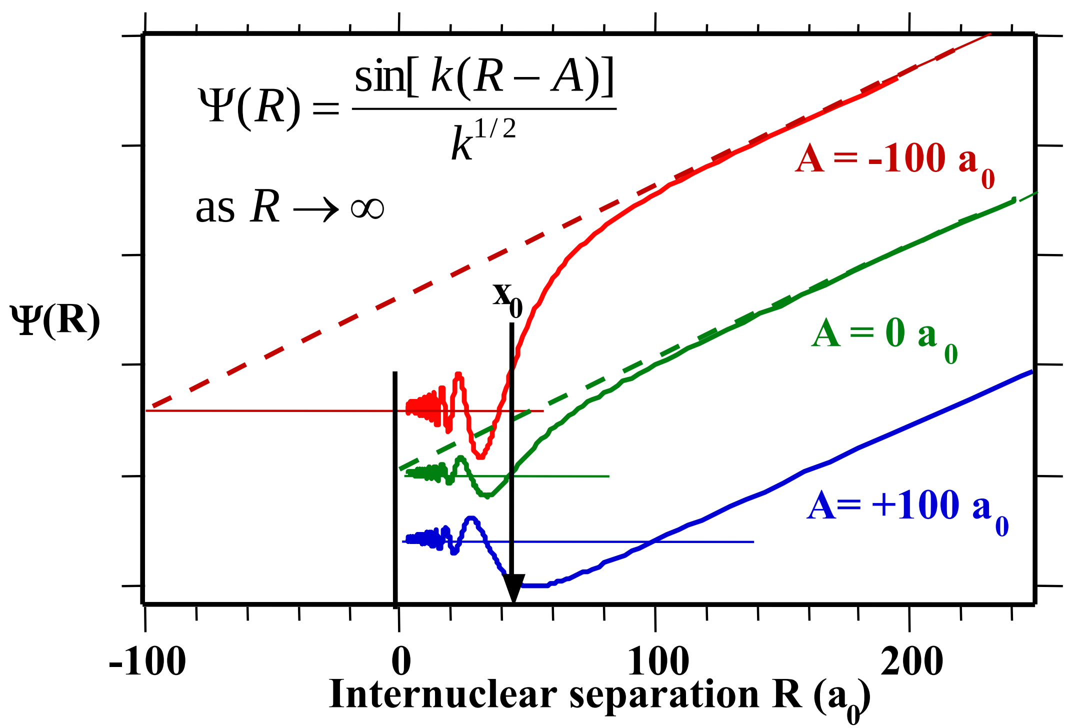
$$= 4\pi\left(\frac{\lambda}{2\pi}\right)^2$$



Interpretation of scattering length



3 different short-range potentials
with
3 different scattering lengths



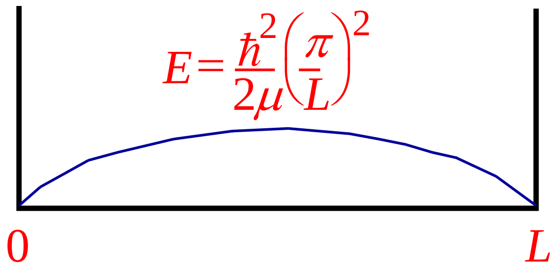
$$\hat{V} = \frac{4\pi\hbar^2}{m} A\delta(\vec{R})\frac{\partial}{\partial R}R$$

Huang and Yang, Phys. Rev. 105, 767 (1957)

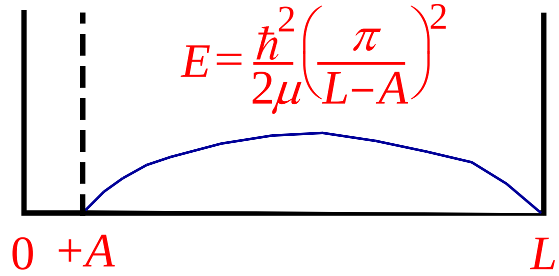
Also E. Fermi (1936), Breit (1947),
Blatt and Weisskopf (1952)

Particle (atom pair) in a box
μ = reduced mass

$$E = \frac{\hbar^2}{2\mu}\left(\frac{\pi}{L}\right)^2$$

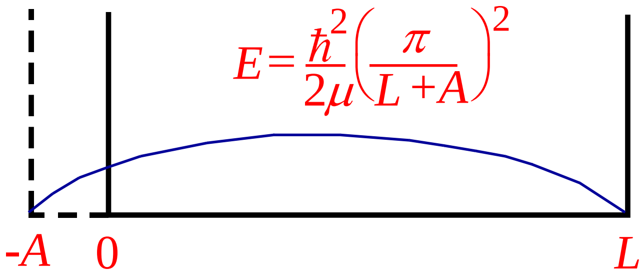


$$E = \frac{\hbar^2}{2\mu}\left(\frac{\pi}{L-A}\right)^2$$



Higher Energy

$$E = \frac{\hbar^2}{2\mu}\left(\frac{\pi}{L+A}\right)^2$$



Lower Energy

$$\Delta E = \frac{\hbar^2}{2\mu}\left[\left(\frac{\pi}{L \mp A}\right)^2 - \left(\frac{\pi}{L}\right)^2\right] \longrightarrow \frac{\pm A}{mL^3}$$

ΔE per particle for N pairs $\longrightarrow \dfrac{N}{L^3}\,\dfrac{\pm A}{m}$

A word about normalization

Energy-normalized: $$\phi_\ell(R,E) \to \left(\frac{2\mu}{\pi\hbar^2}\right)^{\frac{1}{2}} \frac{\sin\left(kR - \frac{\pi\ell}{2} + \eta_\ell\right)}{k^{\frac{1}{2}}}$$

Thus $$\int_0^\infty \phi_\ell(R,E)\phi_\ell(R,E')dR = \delta(E-E')$$

e.g., energy width from Fermi Golden Rule matrix element:

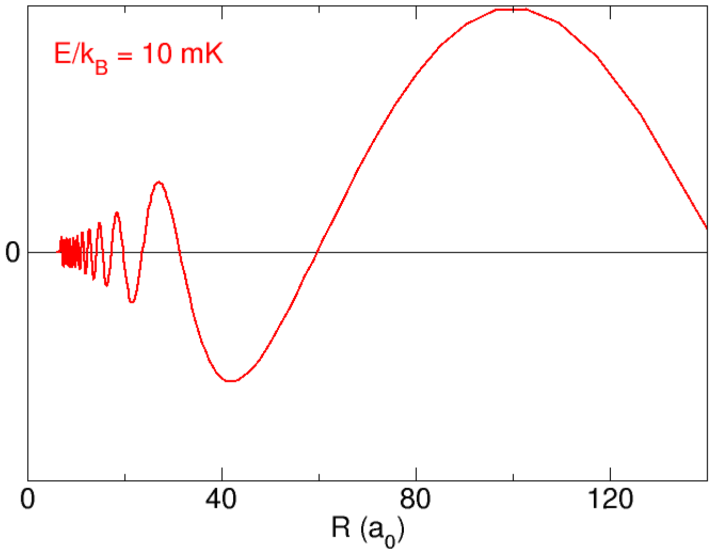
$$\Gamma(E) = 2\pi \left|\langle n|H|\phi_\ell(R,E)\rangle\right|^2$$

Also, "classical time" normalization: $$\left(\frac{2\mu}{\pi\hbar^2}\right)^{\frac{1}{2}} \frac{1}{k^{\frac{1}{2}}} = \frac{2}{(hv)^{\frac{1}{2}}}$$

Probability in *dR* proportional to time in *dR*: $$dt = \frac{dR}{v}$$

More semiclassical considerations

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



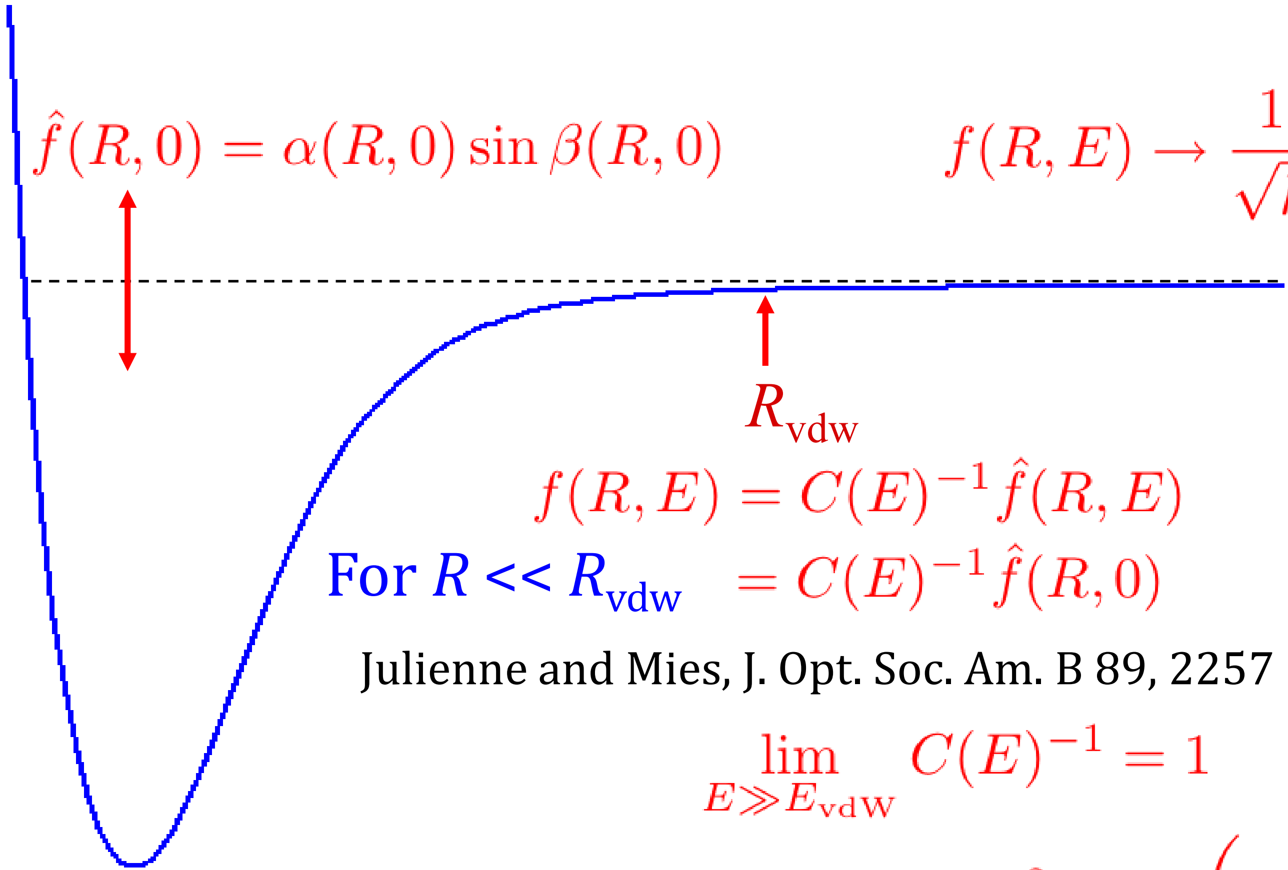
$$\alpha(R,E) = \frac{1}{k(R,E)^{\frac{1}{2}}}$$

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

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

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

Semiclassical considerations continued



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

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

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

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

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

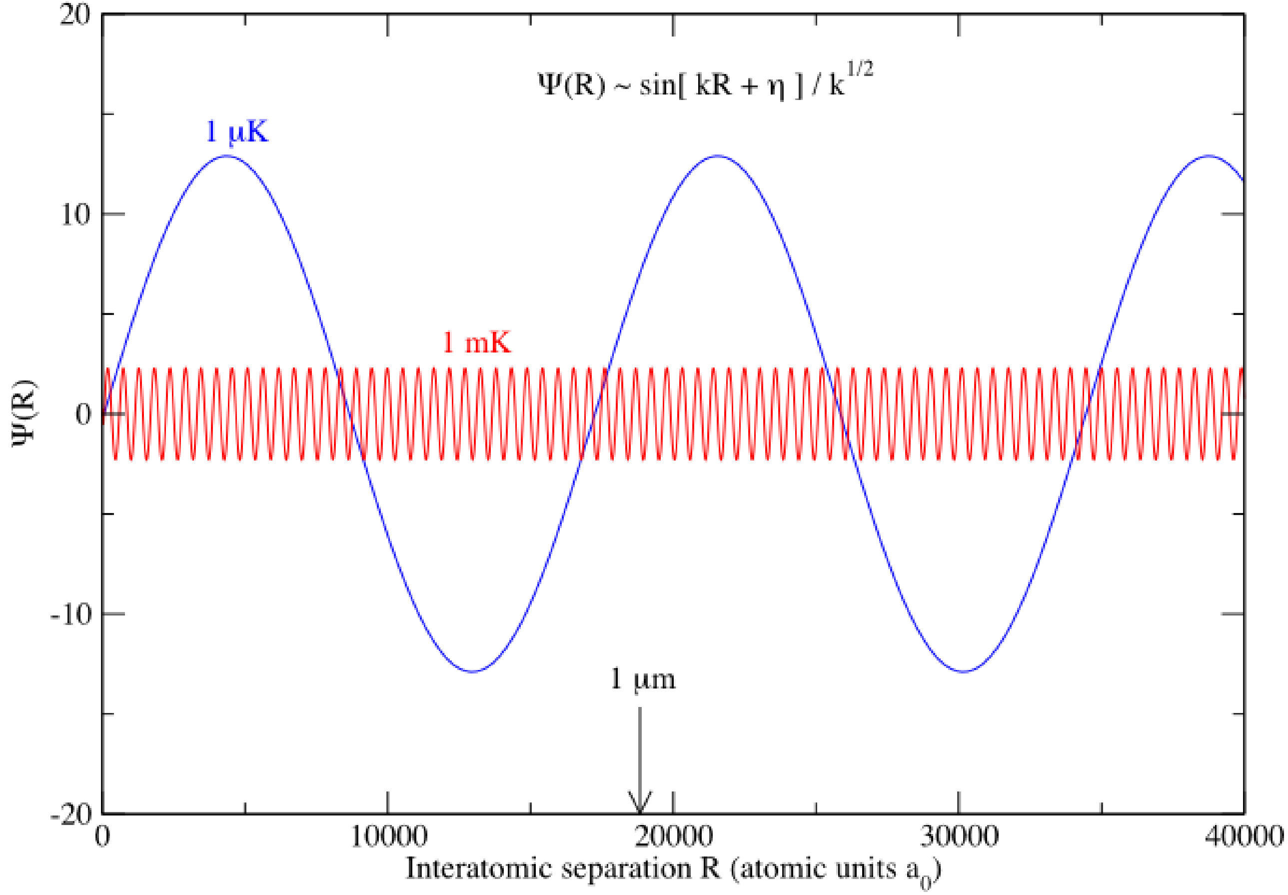
$$\lim_{E \gg E_{\text{vdW}}} C(E)^{-1} = 1$$

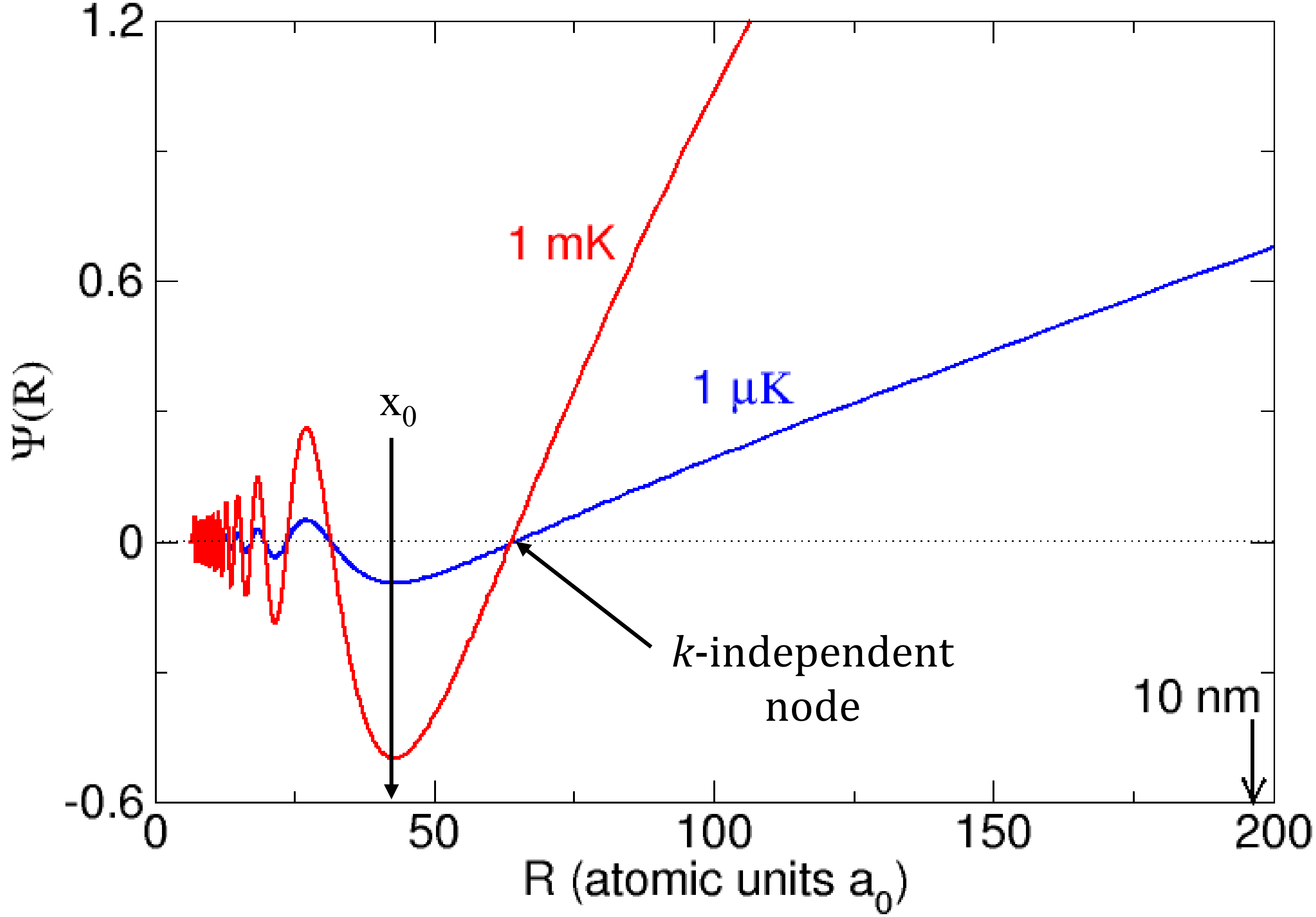
$$\lim_{E \to 0} C(E)^{-2} = k\bar{a}\left(1 + \left(\frac{a}{\bar{a}} - 1\right)^2\right)$$

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

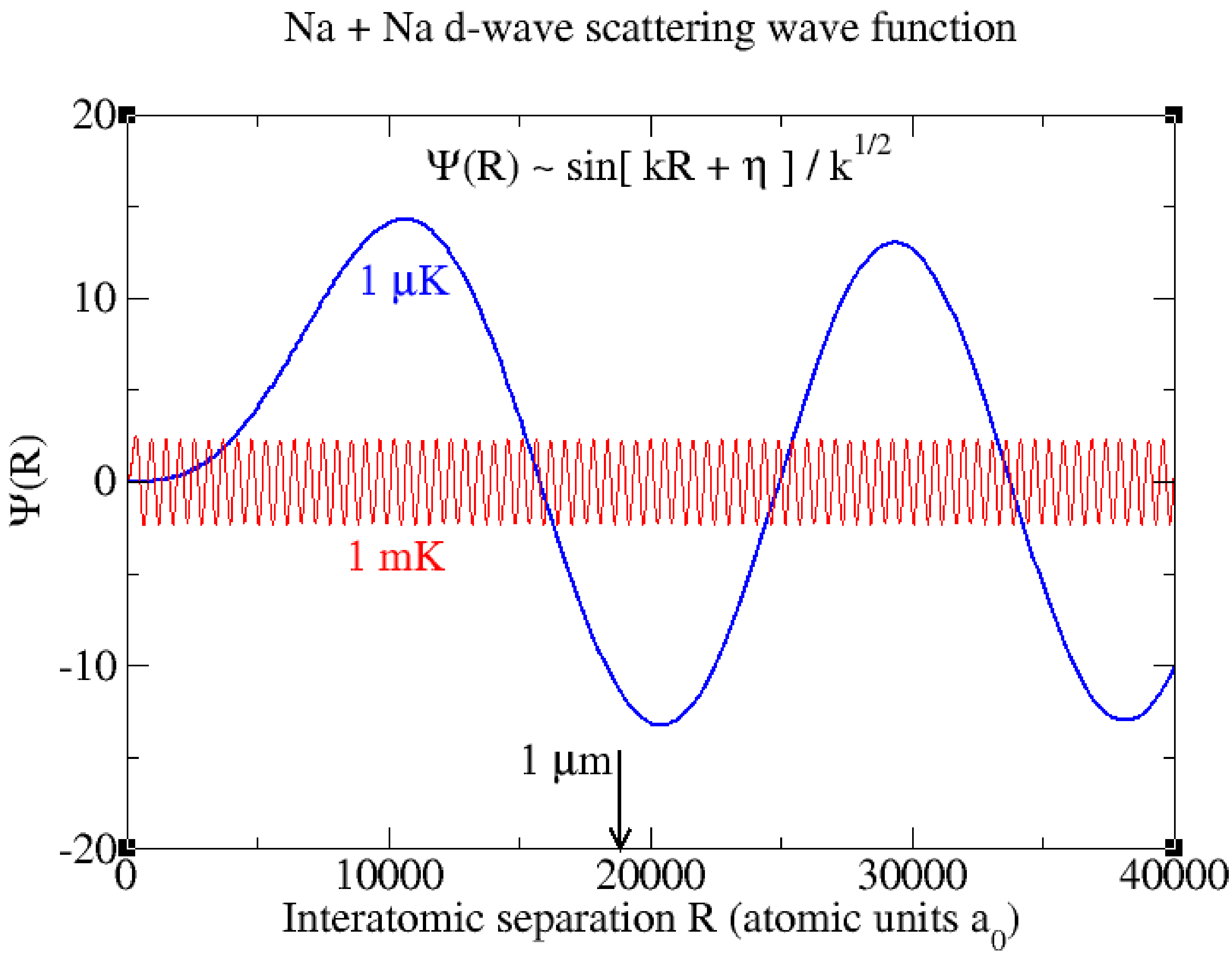
$$\beta(R,E) = \int_{R_t}^{R} k(R',E)dR' + \frac{\pi}{4}$$

Na + Na s-wave scattering wave function



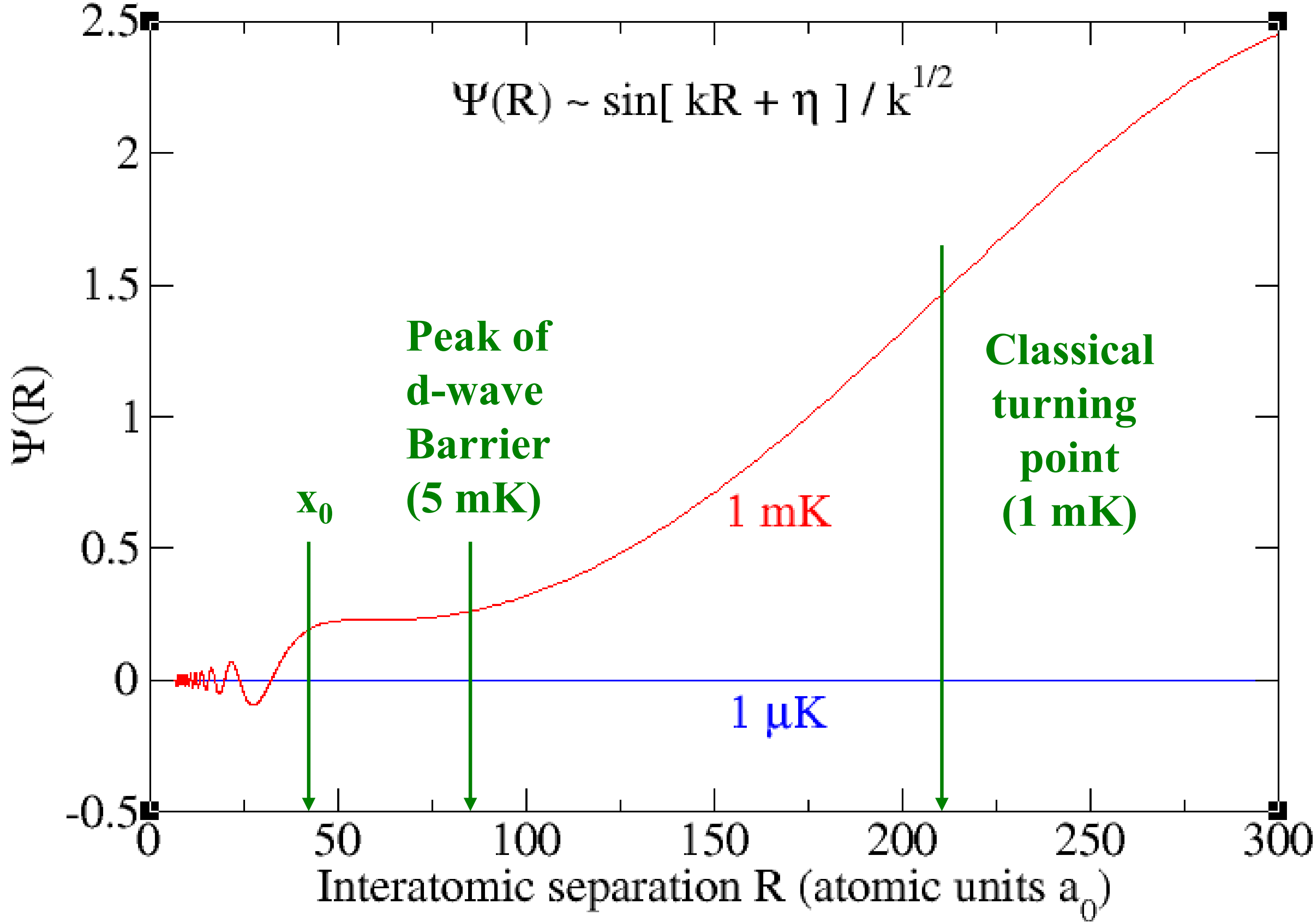


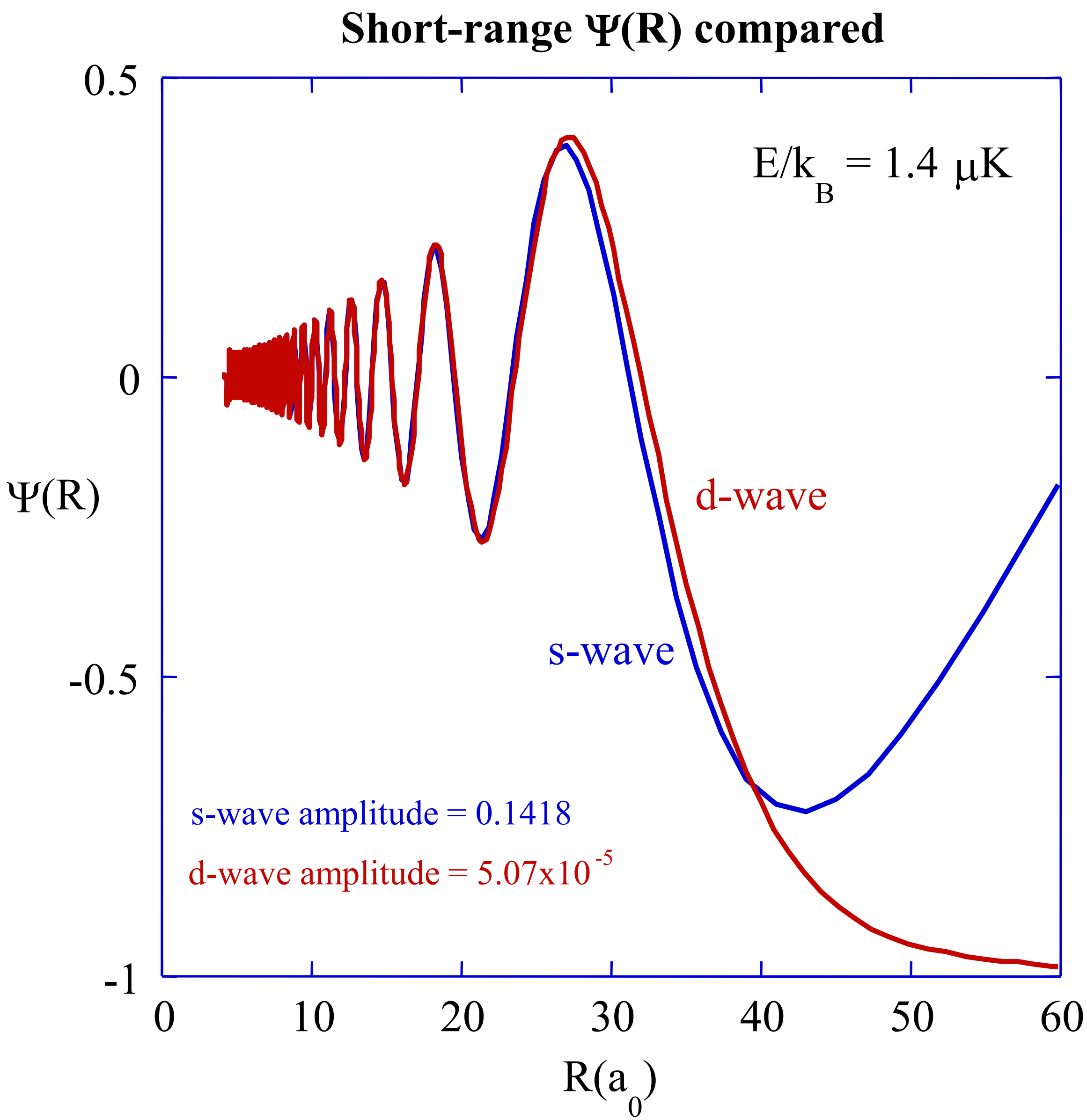
1.2
0.6
0
-0.6
Ψ(R)
1 mK
1 μK
x0
k-independent
node
10 nm
0
50
100
150
200
R (atomic units a0)



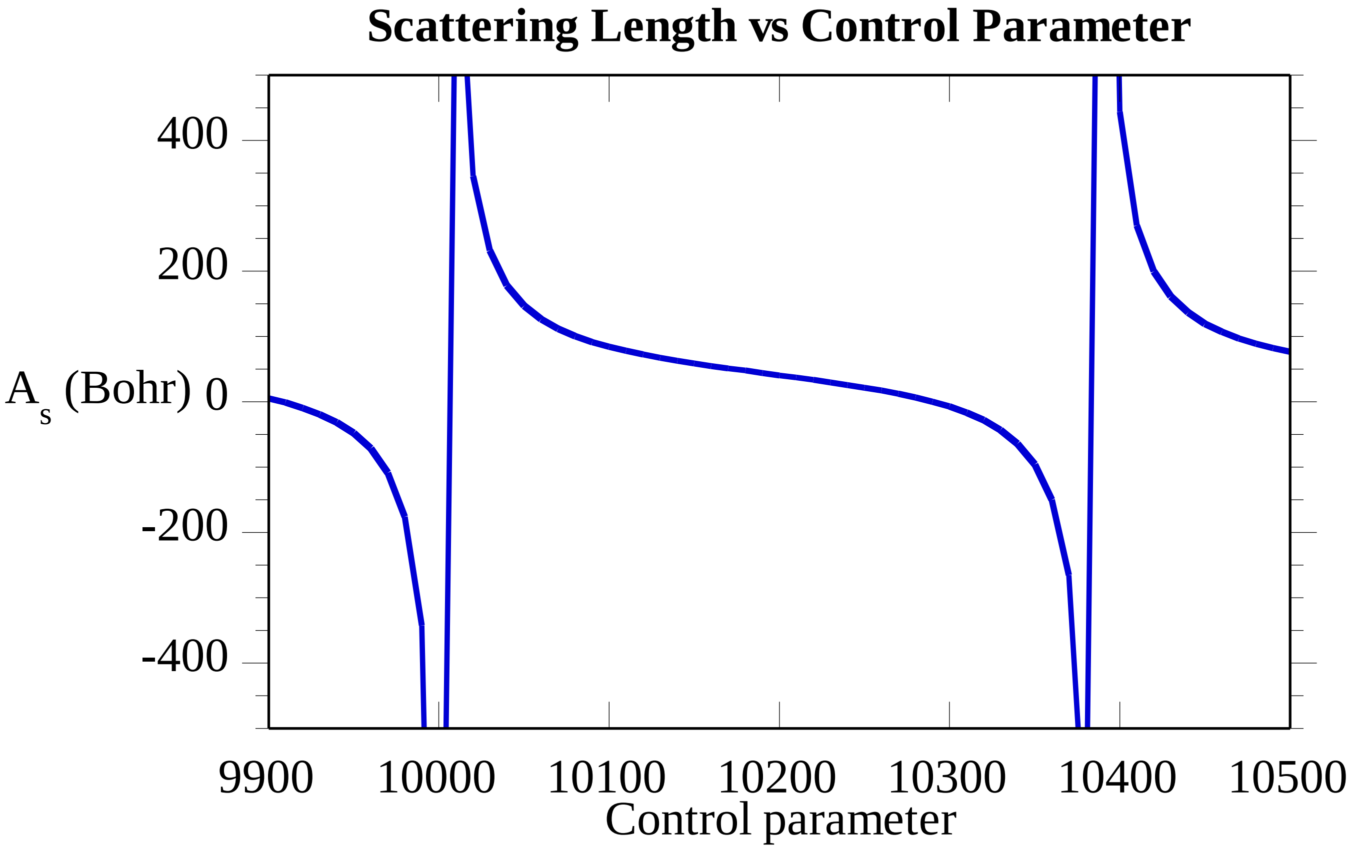
Na + Na d-wave scattering wave function
Ψ(R) ~ sin[kR + η] / k^1/2
1 μK
1 mK
1 μm
Ψ(R)
20
10
0
-10
-20
0
10000
20000
30000
40000
Interatomic separation R (atomic units a0)

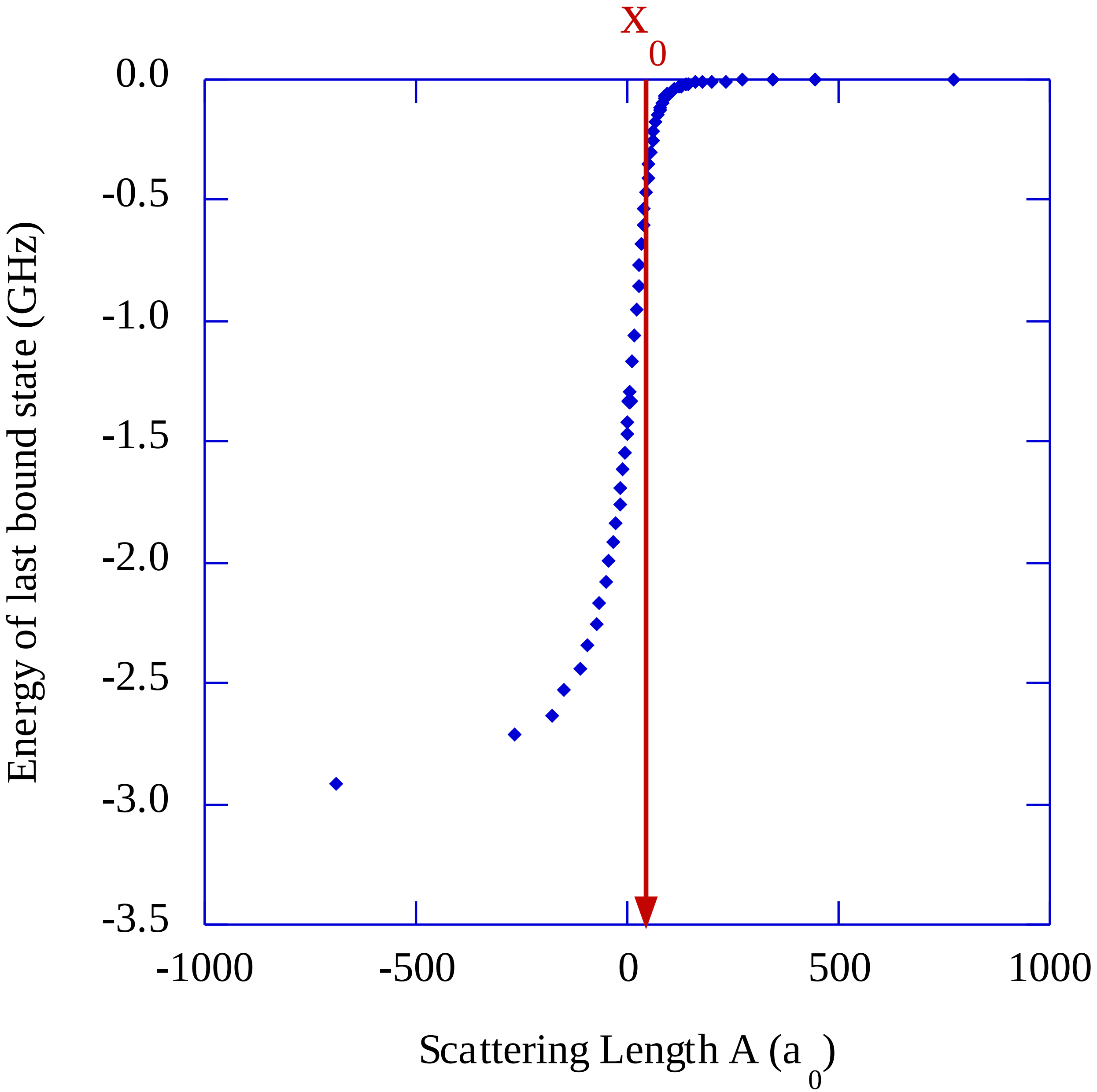
Na + Na d-wave scattering wave function



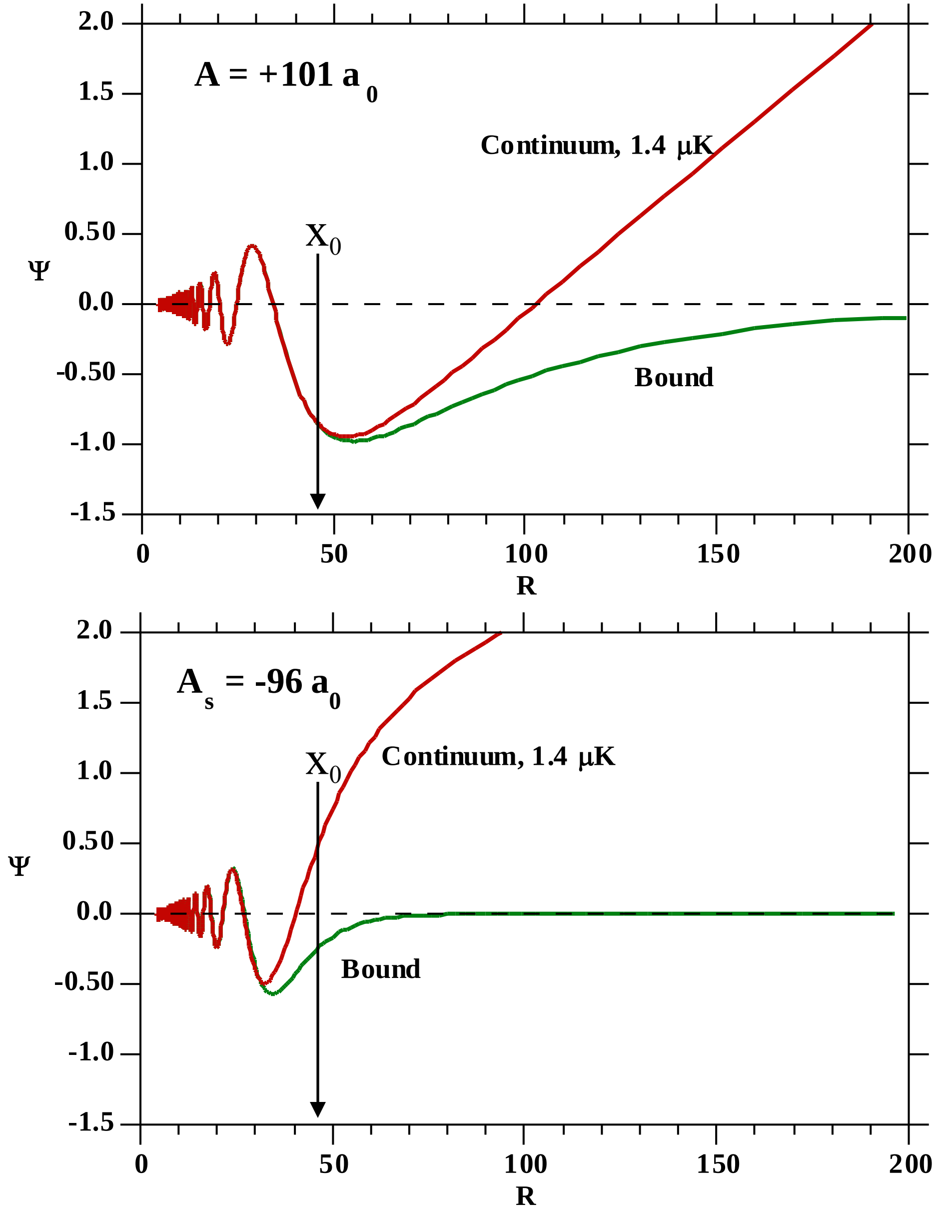


Short-range Ψ(R) compared
0.5
0
-0.5
-1
Ψ(R)
E/k_B = 1.4 μK
d-wave
s-wave
s-wave amplitude = 0.1418
d-wave amplitude = 5.07x10^-5
0
10
20
30
40
50
60
R(a_0)


Scattering Length vs Control Parameter
400
200
A_s (Bohr) 0
-200
-400
9900
10000
10100
10200
10300
10400
10500
Control parameter



X
0
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
-3.0
-3.5
-1000
-500
0
500
1000
Energy of last bound state (GHz)
Scattering Length A (a
0
)



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

Van der Waals potential

Write the Schrödinger equation in length and energy units of

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

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

The potential becomes $-\dfrac{16}{r^6} + \dfrac{\ell(\ell+1)}{r^2}$

This potential has exact analytic solutions and many useful properties.

B. Gao, Phys. Rev. A 58, 1728, 4222 (1998) + series of papers.
See Lett, Jones, Tiesinga, Julienne, Rev. Mod. Phys. 78, 483 (2006).

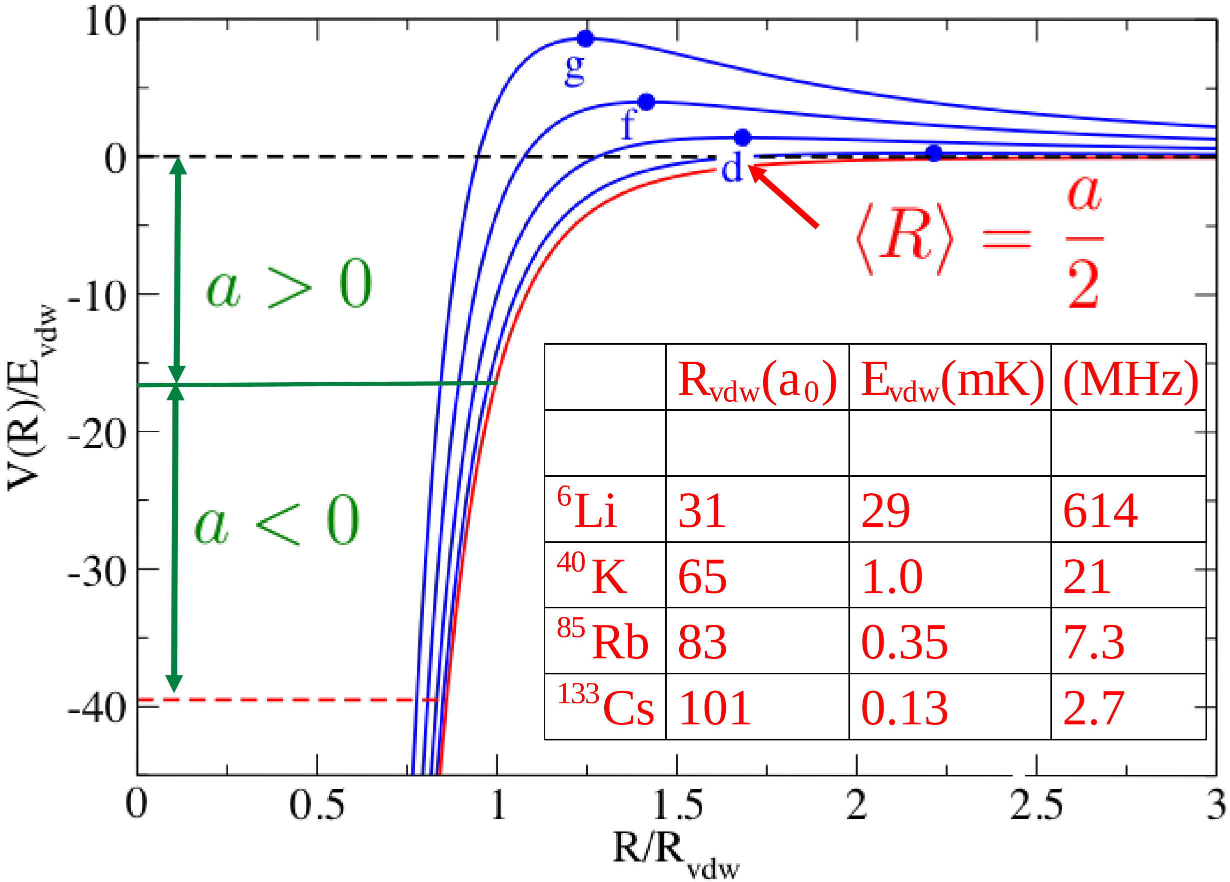
“Size” of potential V(R)

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

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

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

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

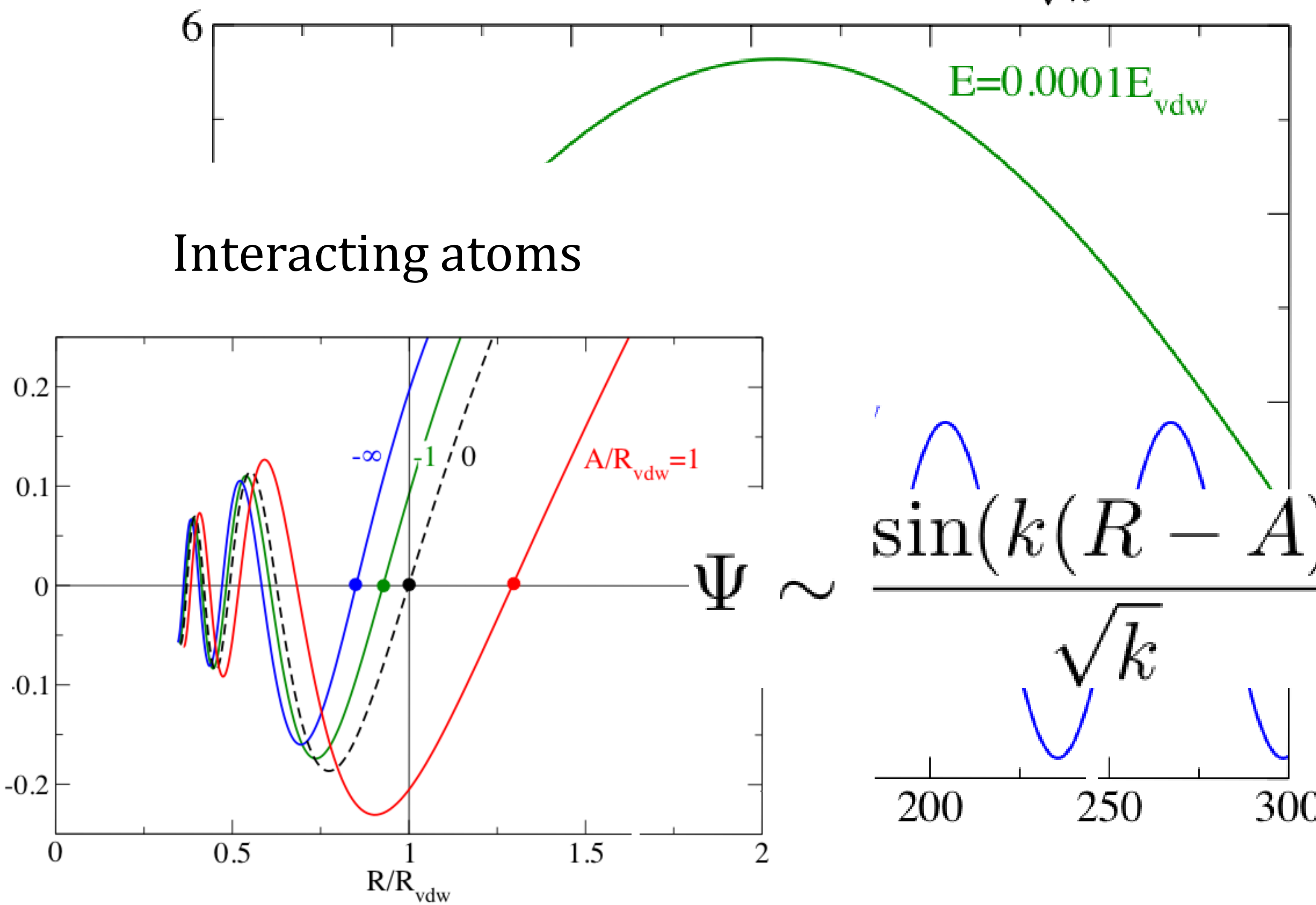


	$R_{\rm vdw}(a_0)$	$E_{\rm vdw}$(mK)	(MHz)
^{6}Li	31	29	614
^{40}K	65	1.0	21
^{85}Rb	83	0.35	7.3
^{133}Cs	101	0.13	2.7

Noninteracting atoms

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

Interacting atoms



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