

ICAP Summer School 2006
University of Innsbruck

Cold Atomic and Molecular Collisions

- 1. Basics***
- 2. Feshbach resonances***
- 3. Photoassociation***

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Atomic Physics Division
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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 $a + b \rightarrow a + b$

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

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

- Spin relaxation
- Photoassociation
- Loss of trapped atoms
- Decoherence
- Spinor condensates ($\Delta E=0$)

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 ...

<div> <div>Group</div> <div>1</div> <div>IA</div> </div> <div> <div>1</div> <div>¹S_{1/2}</div> <div>H</div> <div>Hydrogen</div> <div>1.00794</div> <div>1s</div> <div>13.5984</div> </div> <div> <div>2</div> <div>¹S₀</div> <div>Be</div> <div>Beryllium</div> <div>9.012182</div> <div>1s²2s</div> <div>9.3227</div> </div>																	
<div> <div>3</div> <div>²S_{1/2}</div> <div>Li</div> <div>Lithium</div> <div>6.941</div> <div>1s²2s</div> <div>5.3917</div> </div> <div> <div>4</div> <div>¹S₀</div> <div>Na</div> <div>Sodium</div> <div>22.989770</div> <div>[Ne]3s</div> <div>5.1391</div> </div>																	
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<div> <div>19</div> <div>⁴S_{3/2}</div> <div>K</div> <div>Potassium</div> <div>39.0983</div> <div>[Ar]4s</div> <div>4.3407</div> </div> <div> <div>20</div> <div>¹S₀</div> <div>Ca</div> <div>Calcium</div> <div>40.078</div> <div>[Ar]4s</div> <div>6.1132</div> </div>																	
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<div> <div>72</div> <div>³F₂</div> <div>Hf</div> <div>Hafnium</div> <div>178.49</div> <div>[Xe]4f¹⁴5d²6s²</div> <div>6.8251</div> </div> <div> <div>73</div> <div>³F_{3/2}</div> <div>Ta</div> <div>Tantalum</div> <div>180.9479</div> <div>[Xe]4f¹⁴5d³6s²</div> <div>7.5496</div> </div>																	
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NIST

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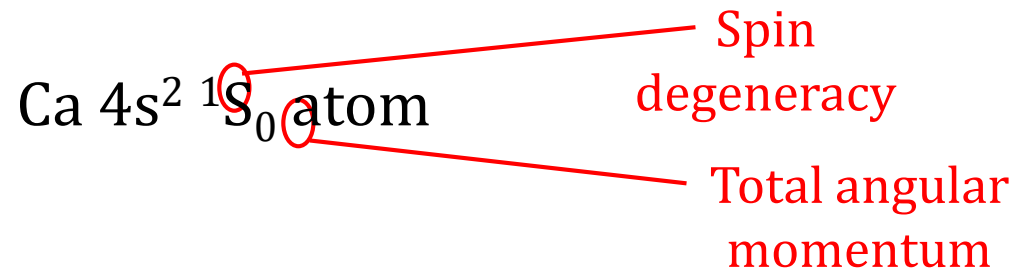
18
VIII A

2
¹S₀
He
Helium
4.002602
1s²
24.5874

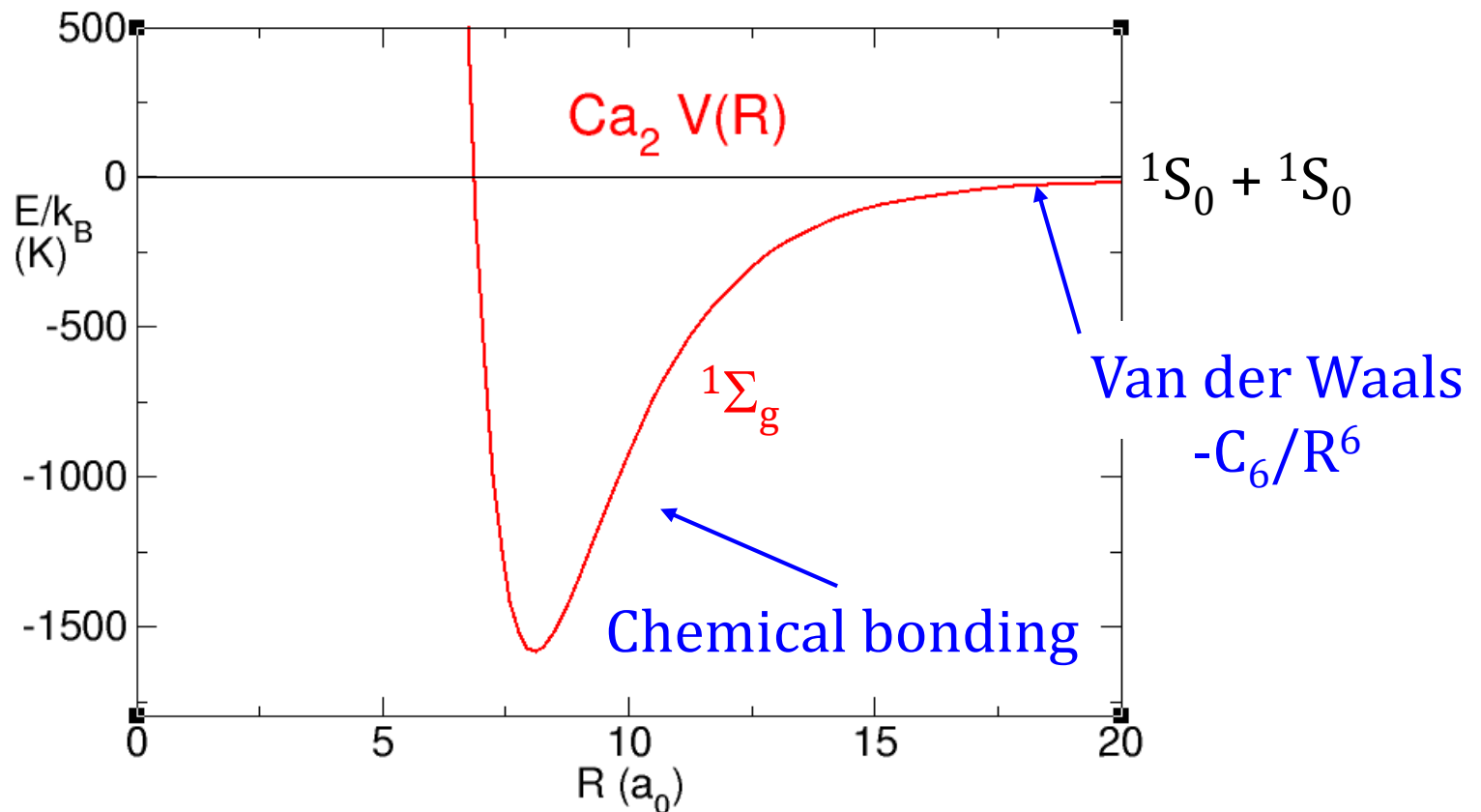
5 ² P _{1/2} B Boron 10.811 1s ² 2s ² 2p 8.2980	6 ³ P ₀ C Carbon 12.0107 1s ² 2s ² 2p 11.2603	7 ³ S _{1/2} N Nitrogen 14.0067 1s ² 2s ² 2p 14.5341	8 ³ P ₂ O Oxygen 15.9994 1s ² 2s ² 2p 13.6181	9 ³ P ₂ F Fluorine 18.9984032 1s ² 2s ² 2p 17.4228	10 ¹ S ₀ Ne Neon 20.1797 1s ² 2s ² 2p 21.5645
13 ² P _{1/2} Al Aluminum 26.981538 [Ne]3s ² 3p 5.9858	14 ³ P ₀ Si Silicon 28.0855 [Ne]3s ² 3p 8.1517	15 ³ S _{1/2} P Phosphorus 30.973761 [Ne]3s ² 3p 10.4867	16 ³ P ₂ S Sulfur 32.065 [Ne]3s ² 3p 10.3600	17 ³ P ₂ Cl Chlorine 35.453 [Ne]3s ² 3p 12.9676	18 ¹ S ₀ Ar Argon 39.948 [Ne]3s ² 3p 15.7596
31 ² P _{1/2} Ga Gallium 69.723 [Ar]3d ¹⁰ 4s ¹ 4p 5.9993	32 ³ P ₀ Ge Germanium 72.64 [Ar]3d ¹⁰ 4s ¹ 4p 7.8994	33 ³ S _{1/2} As Arsenic 74.92160 [Ar]3d ¹⁰ 4s ¹ 4p 9.7886	34 ³ P ₂ Se Selenium 78.96 [Ar]3d ¹⁰ 4s ¹ 4p 9.7524	35 ³ P ₂ Br Bromine 79.904 [Ar]3d ¹⁰ 4s ¹ 4p 11.8138	36 ¹ S ₀ Kr Krypton 83.798 [Ar]3d ¹⁰ 4s ¹ 4p 13.9996
49 ² P _{1/2} In Indium 114.818 [Kr]4d ¹⁰ 5s ¹ 5p 5.7864	50 ³ P ₀ Sn Tin 118.710 [Kr]4d ¹⁰ 5s ¹ 5p 7.3439	51 ³ S _{1/2} Sb Antimony 121.760 [Kr]4d ¹⁰ 5s ¹ 5p 8.6084	52 ³ P ₂ Te Tellurium 127.60 [Kr]4d ¹⁰ 5s ¹ 5p 9.0096	53 ³ P ₂ I Iodine 126.90447 [Kr]4d ¹⁰ 5s ¹ 5p 10.4513	54 ¹ S ₀ Xe Xenon 131.293 [Kr]4d ¹⁰ 5s ¹ 5p 12.1298
81 ² P _{1/2} Tl Thallium 204.3833 [Hg]6p 6.1082	82 ³ P ₀ Pb Lead 207.2 [Hg]6p 7.4167	83 ³ S _{1/2} Bi Bismuth 208.98038 [Hg]6p 7.2655	84 ³ P ₂ Po Polonium (209) [Hg]6p 8.414	85 ³ P ₂ At Astatine (210) [Hg]6p 8.414	86 ¹ S ₀ Rn Radon (222) [Hg]6p 10.7485

Atomic Number
Ground-state Level
Symbol
Name
Atomic Weight

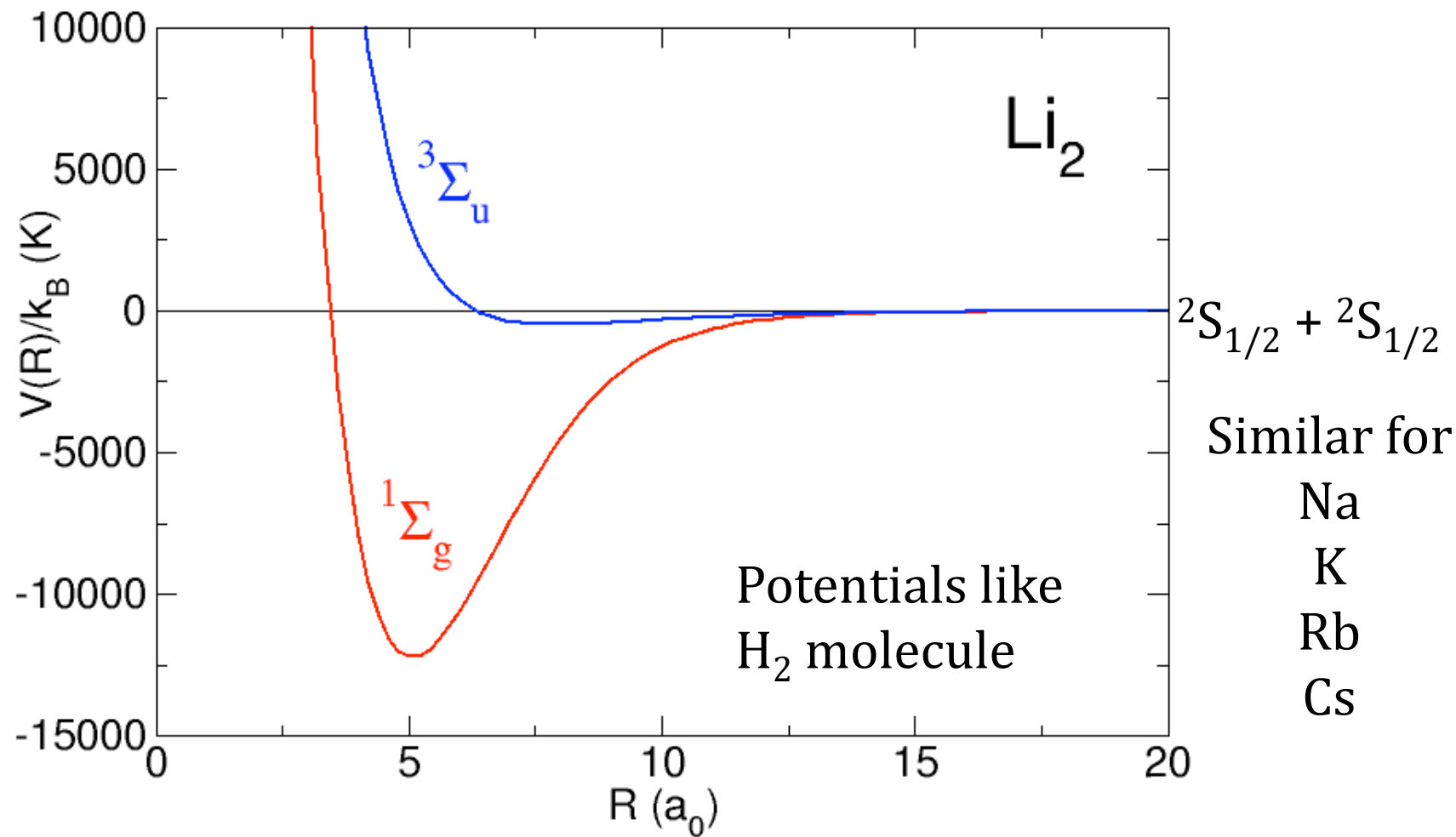
58
¹G₄
Ce
Cerium
140.116

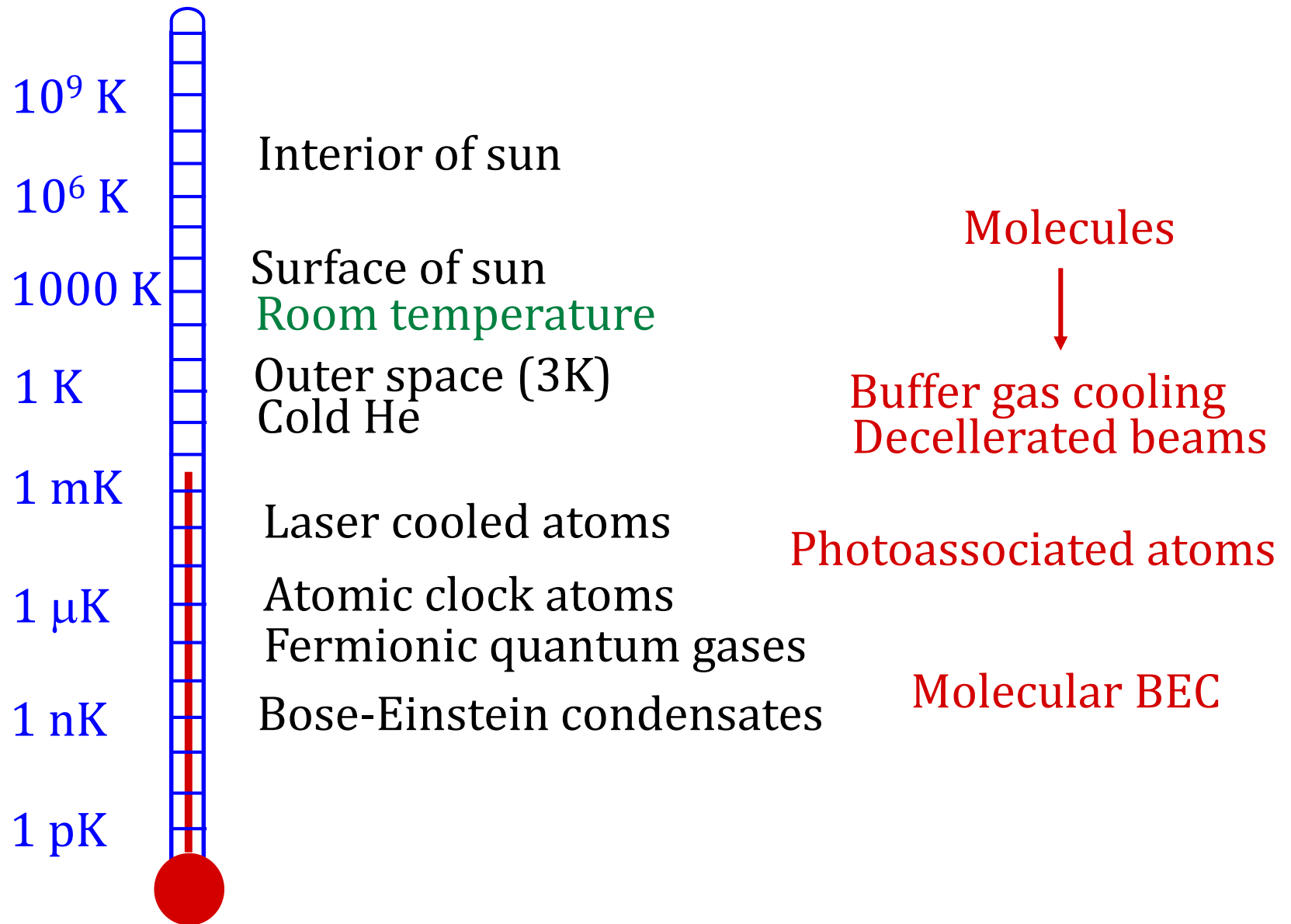


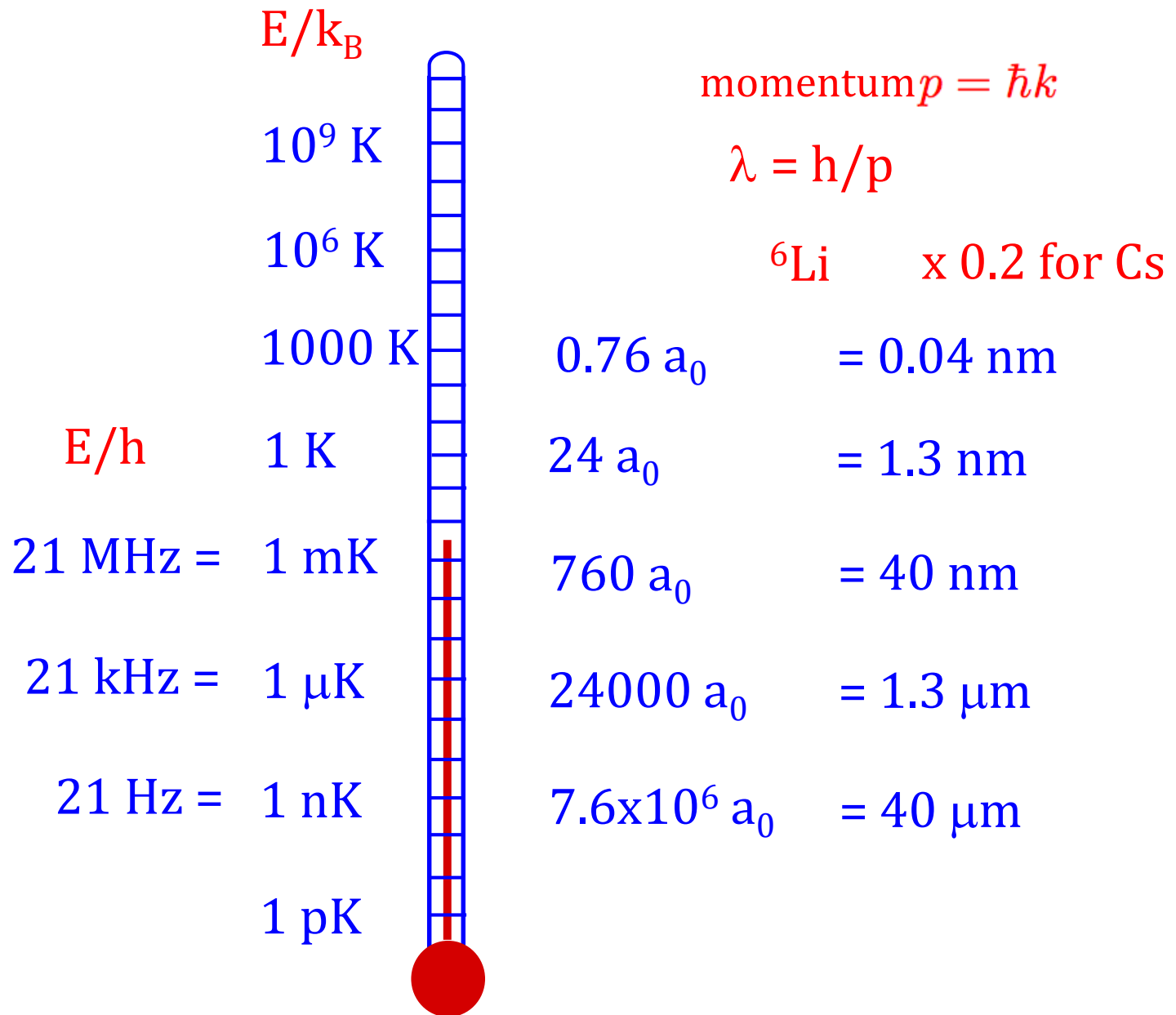
Born-Oppenheimer approximation = potential energy curve



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







Characteristic Lengths

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

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: $V(R) + \frac{\hbar^2 l(l+1)}{2\mu R^2} \rightarrow$ phase shift $\eta_l(E)$

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

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

\rightarrow bound states E_n

\rightarrow scattering phases, amplitudes

S-wave scattering phase shift

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

Wavelength $\lambda = 2\pi/k$

Noninteracting
atoms

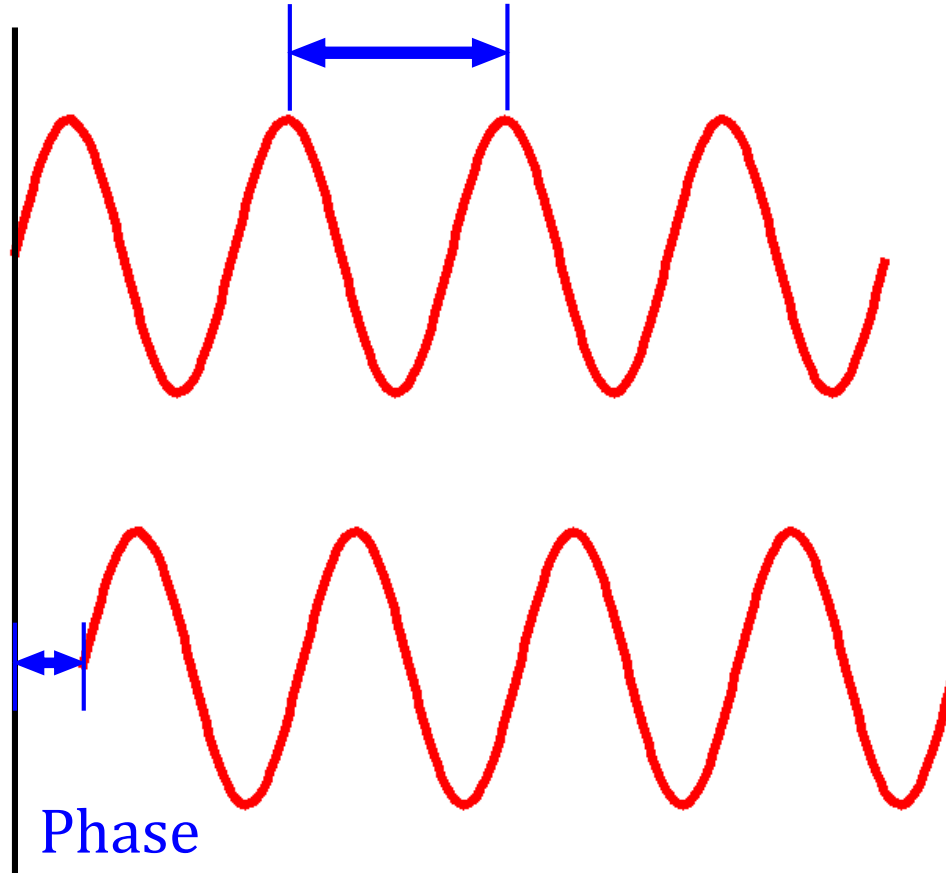
$$\eta = 0$$

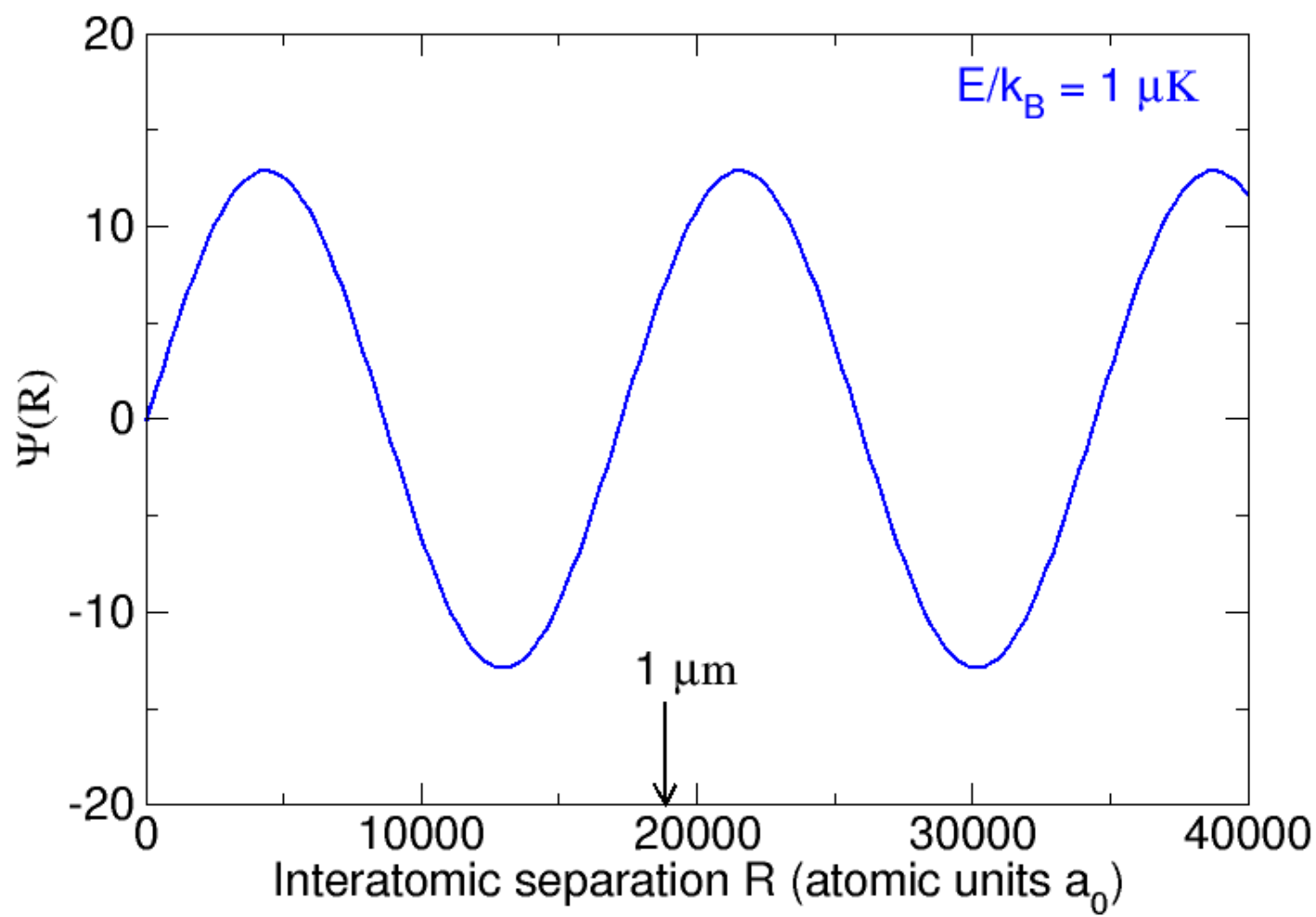
Interacting
atoms

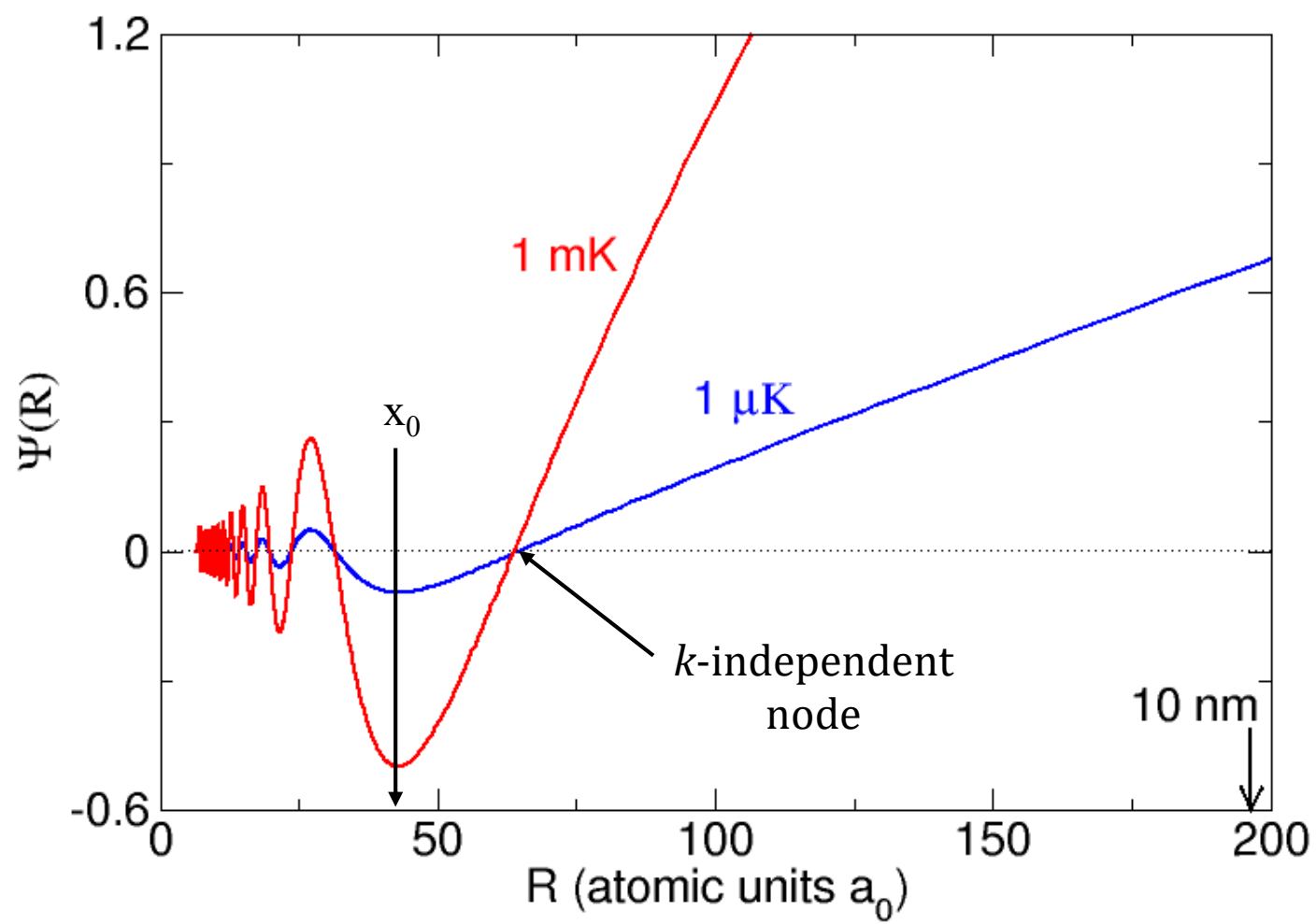
$$\eta \rightarrow -ka$$

as $k \rightarrow 0$

Phase

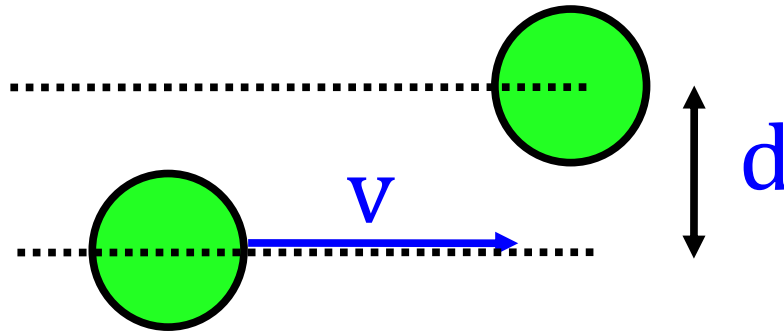






Cross section σ

Classical balls with distance of closest approach d (diameter)



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

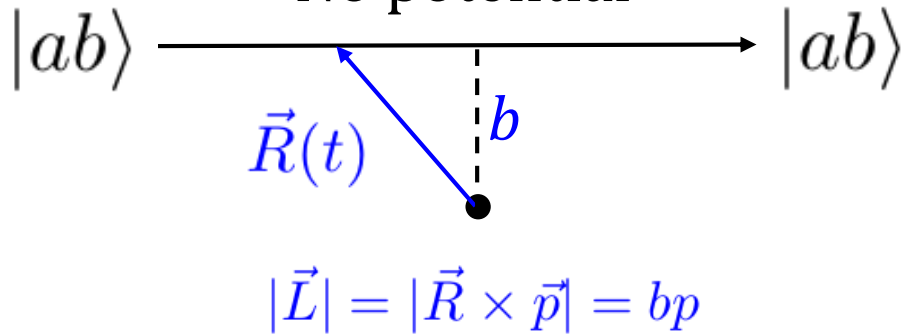
and a collision rate $\Gamma = n v \sigma$ (typical: 1 s^{-1} , MOT
 10^4 s^{-1} , BEC)

Rate constant $K = v \sigma$

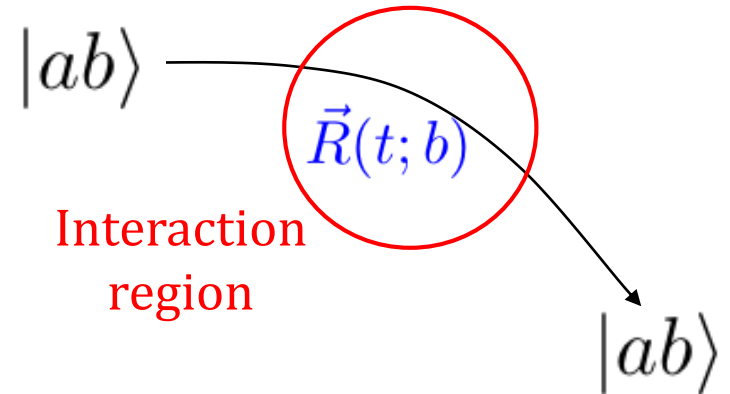
Time between collisions = $1/\Gamma = 1/(Kn) \approx 1 \text{ s}$ (MOT), $100 \mu\text{s}$ (BEC)

Classical picture

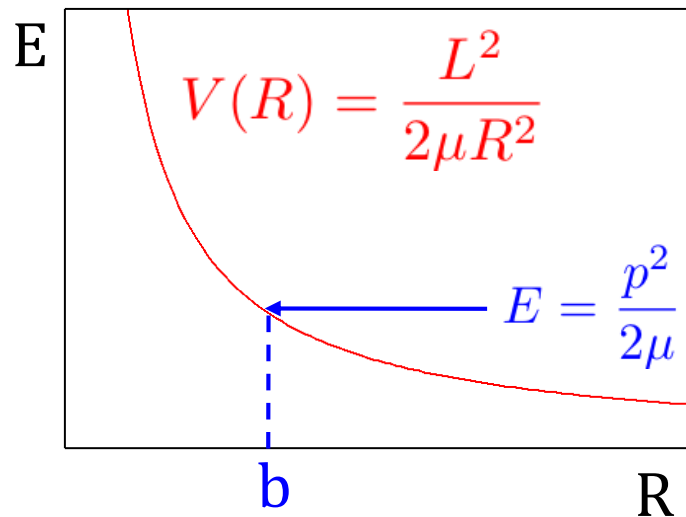
No potential



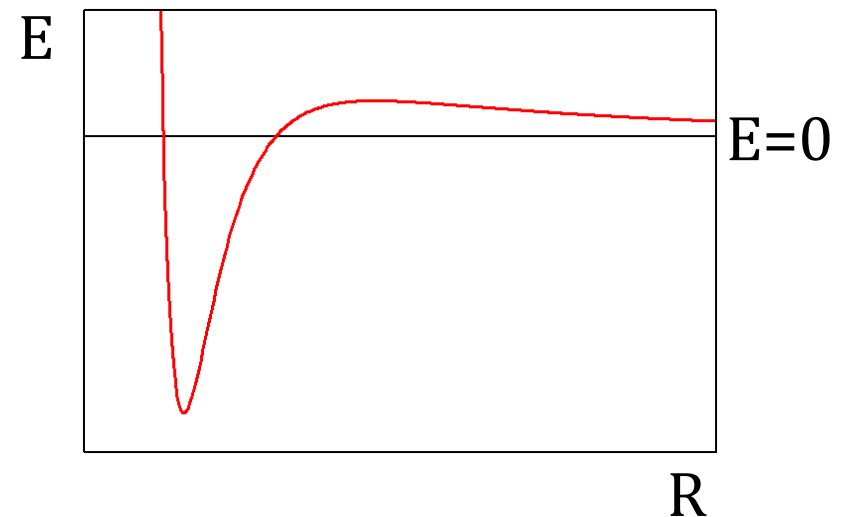
With potential



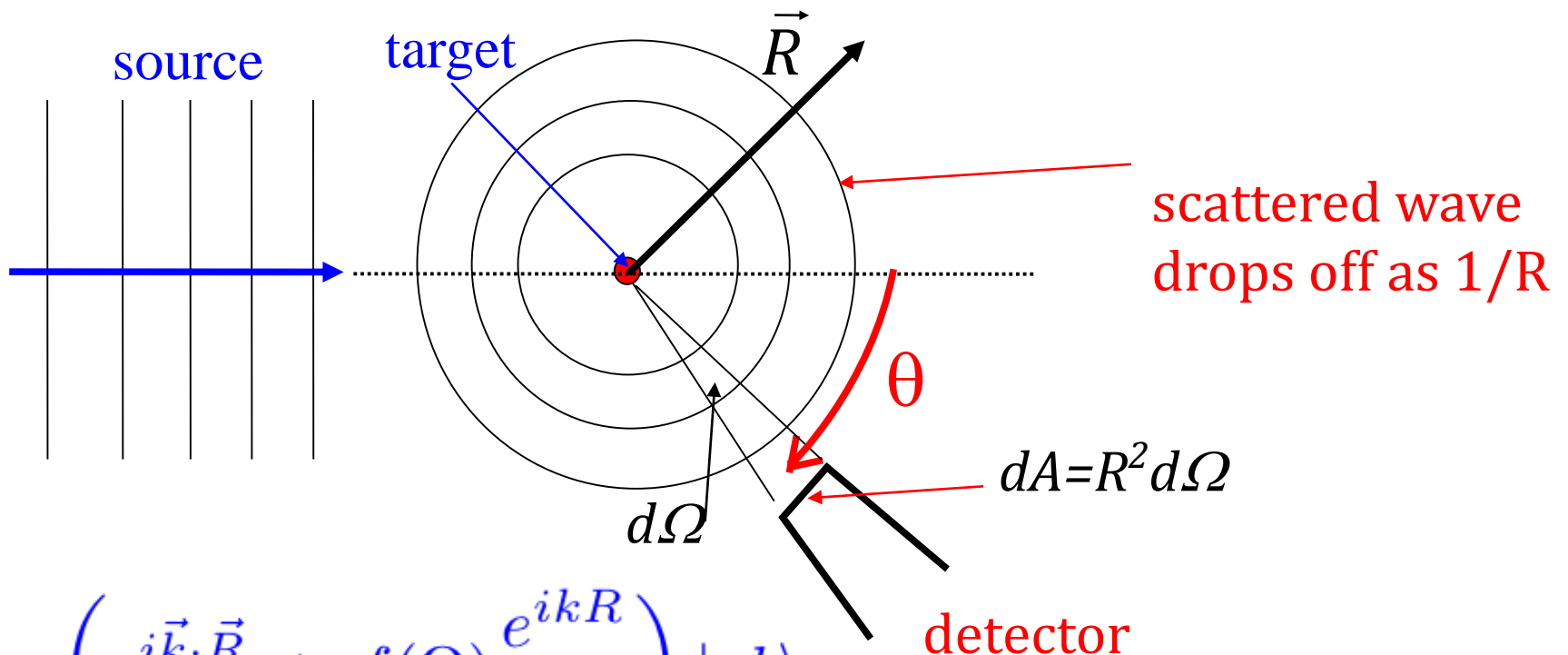
Centrifugal potential



Centrifugal barrier



Quantum scattering theory



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

atoms/s scattered flux into $d\Omega$

plane wave flux (atoms/cm²/s)

cross section

$$= \frac{d\sigma}{d\Omega} = |f(\Omega)|^2$$

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

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

an $\phi_{\ell}(R)$ is a solution to the
radial Schrödinger equation

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

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:

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

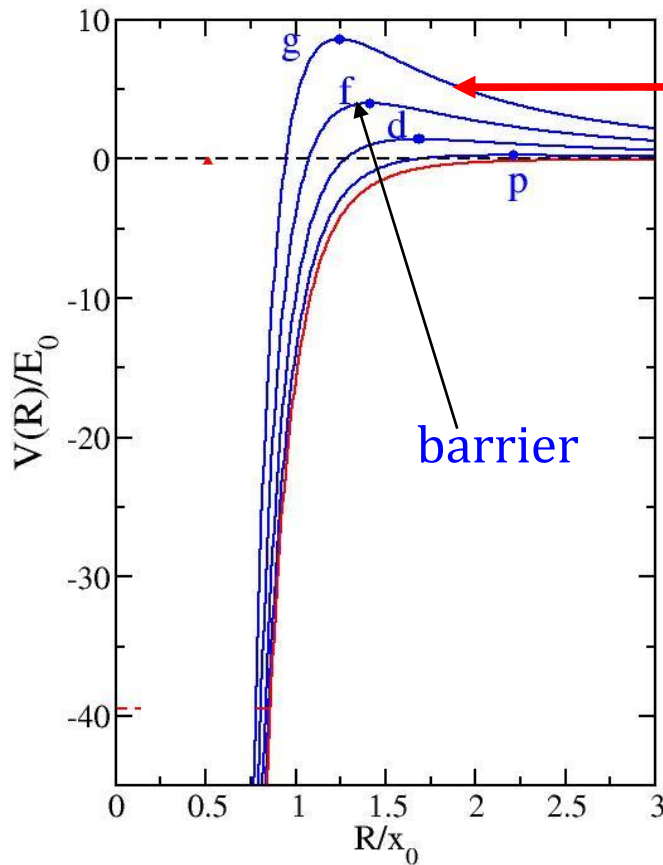
and $\phi_{\ell}^{+}(R)$ is a solution to the radial Schrödinger equation

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

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

Centrifugal barrier

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



collision energy E

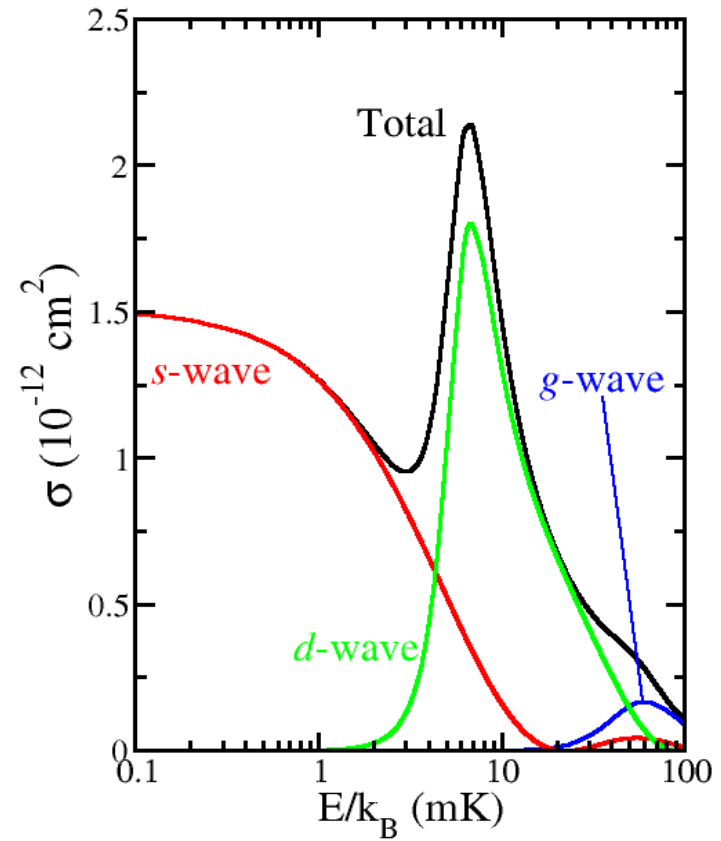
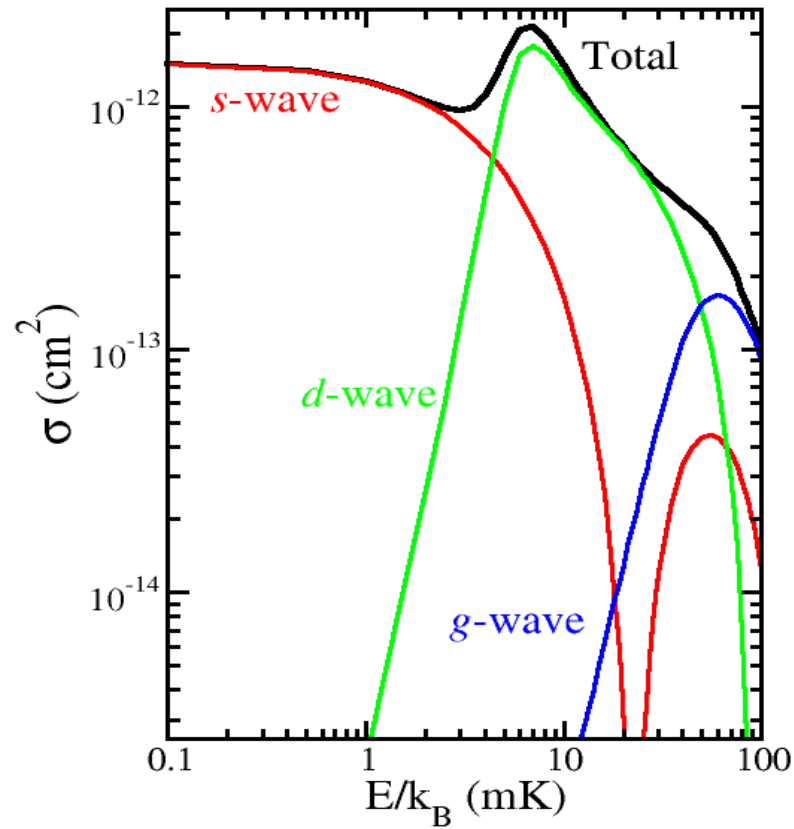
Expectation:

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

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

$+1, \text{ boson}$
 $-1, \text{ fermion}$

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

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:

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

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

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

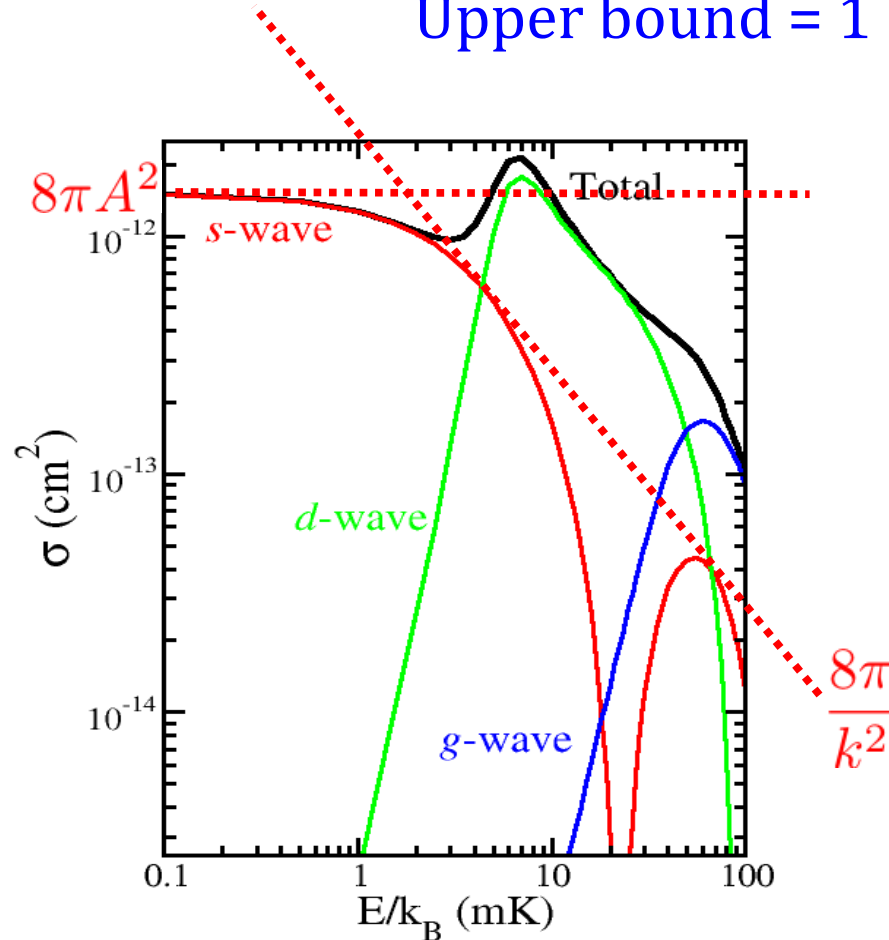
Threshold properties

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

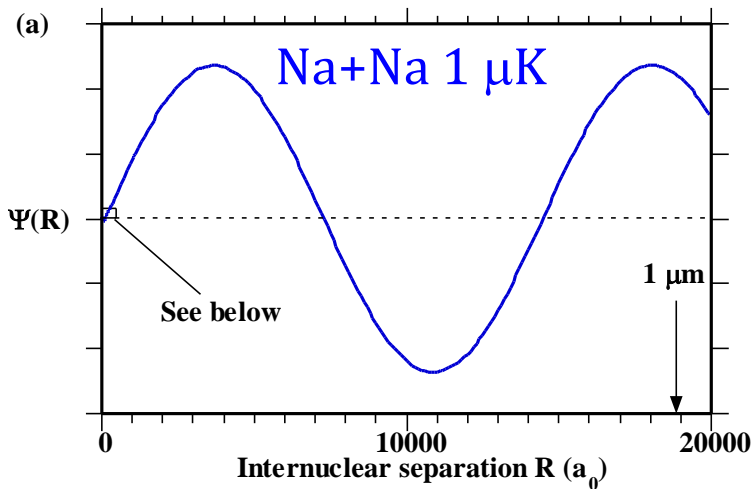
(8πA² for identical bosons)

Upper bound = 1 (unitarity limit)

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



Interpretation of scattering length

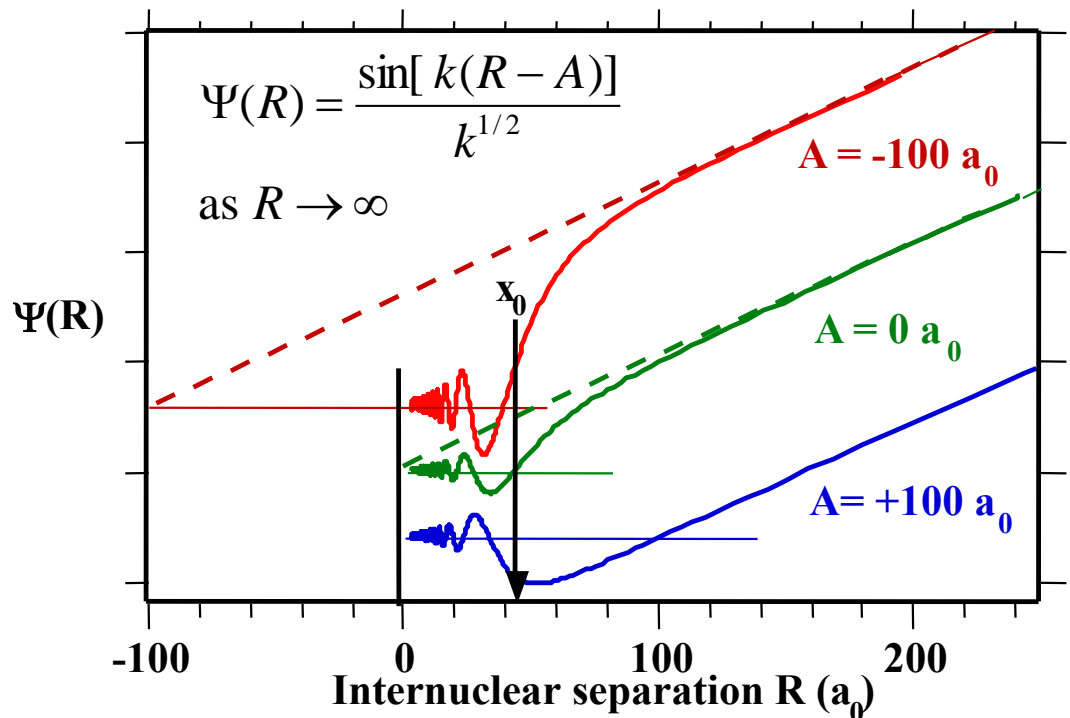


$$\hat{V} = \frac{4\pi\hbar^2}{m} A \delta(\vec{R}) \frac{\partial}{\partial R} R$$

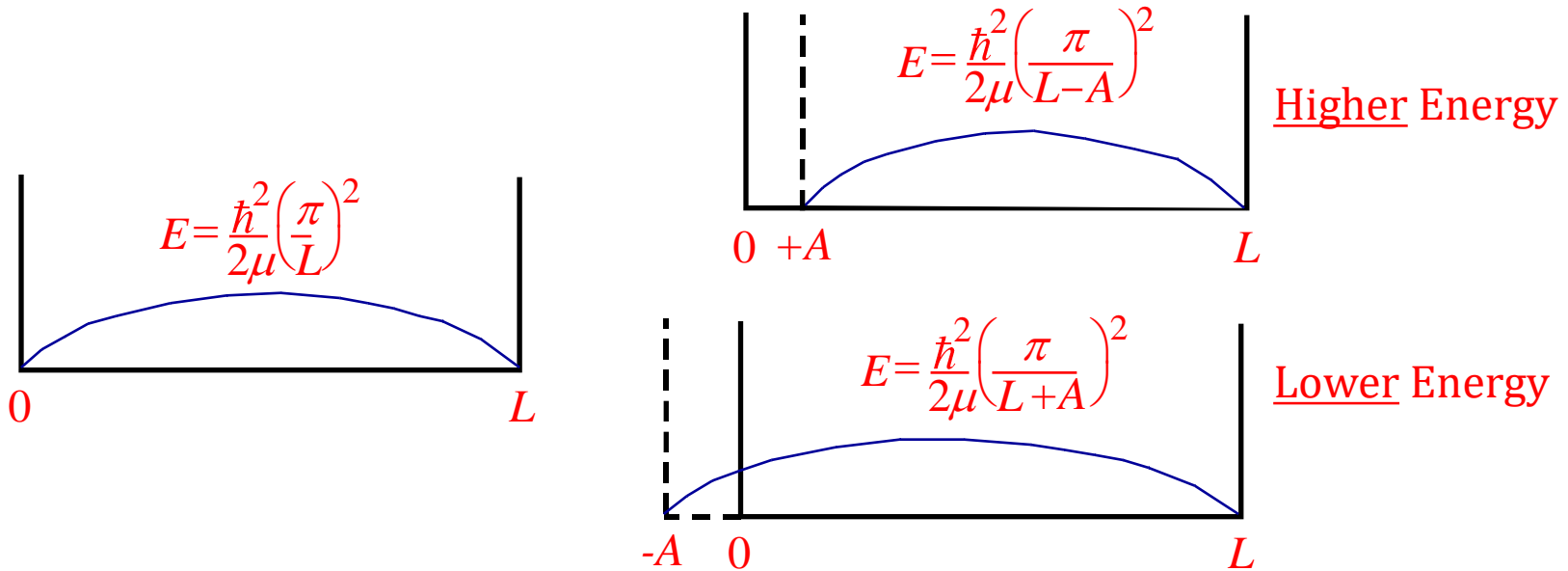
Huang and Yang, Phys. Rev. 105, 767 (1957)

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

3 different short-range potentials
with
3 different scattering lengths



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



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

$$\Delta E \text{ per particle for } N \text{ pairs} \longrightarrow \frac{N}{L^3} \frac{\pm A}{m}$$

A word about normalization

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

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:

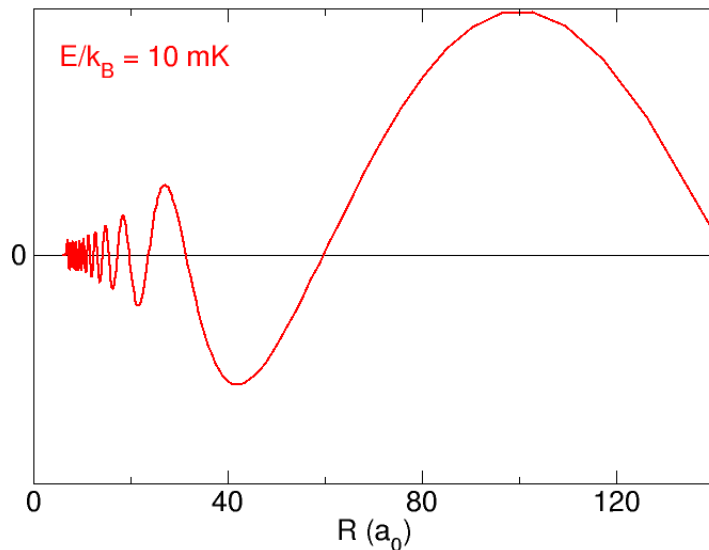
$$\Gamma(E) = 2\pi |\langle n|H|\phi_\ell(R, E)\rangle|^2$$

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



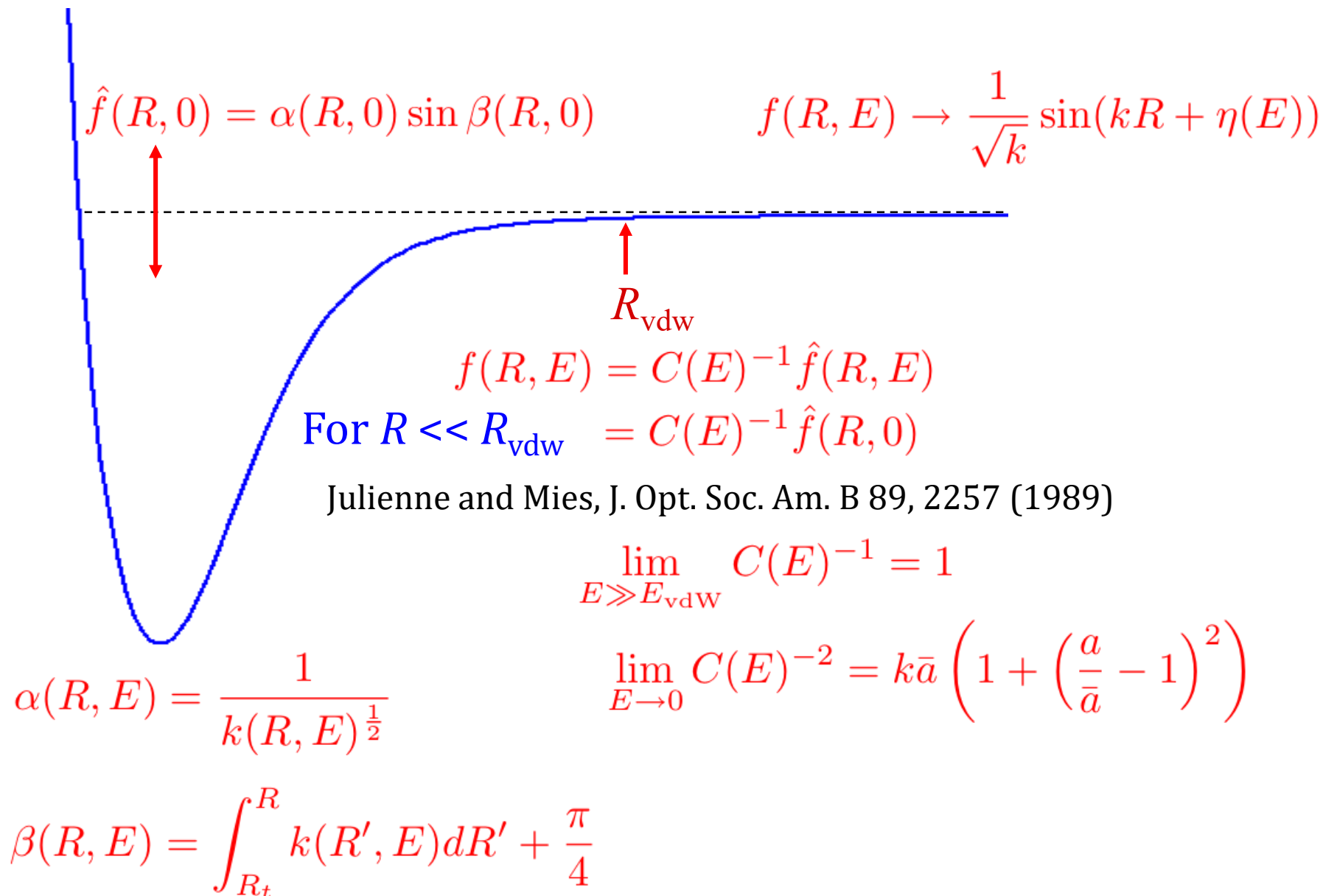
$$\alpha(R, E) = \frac{1}{k(R, E)^{\frac{1}{2}}}$$

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

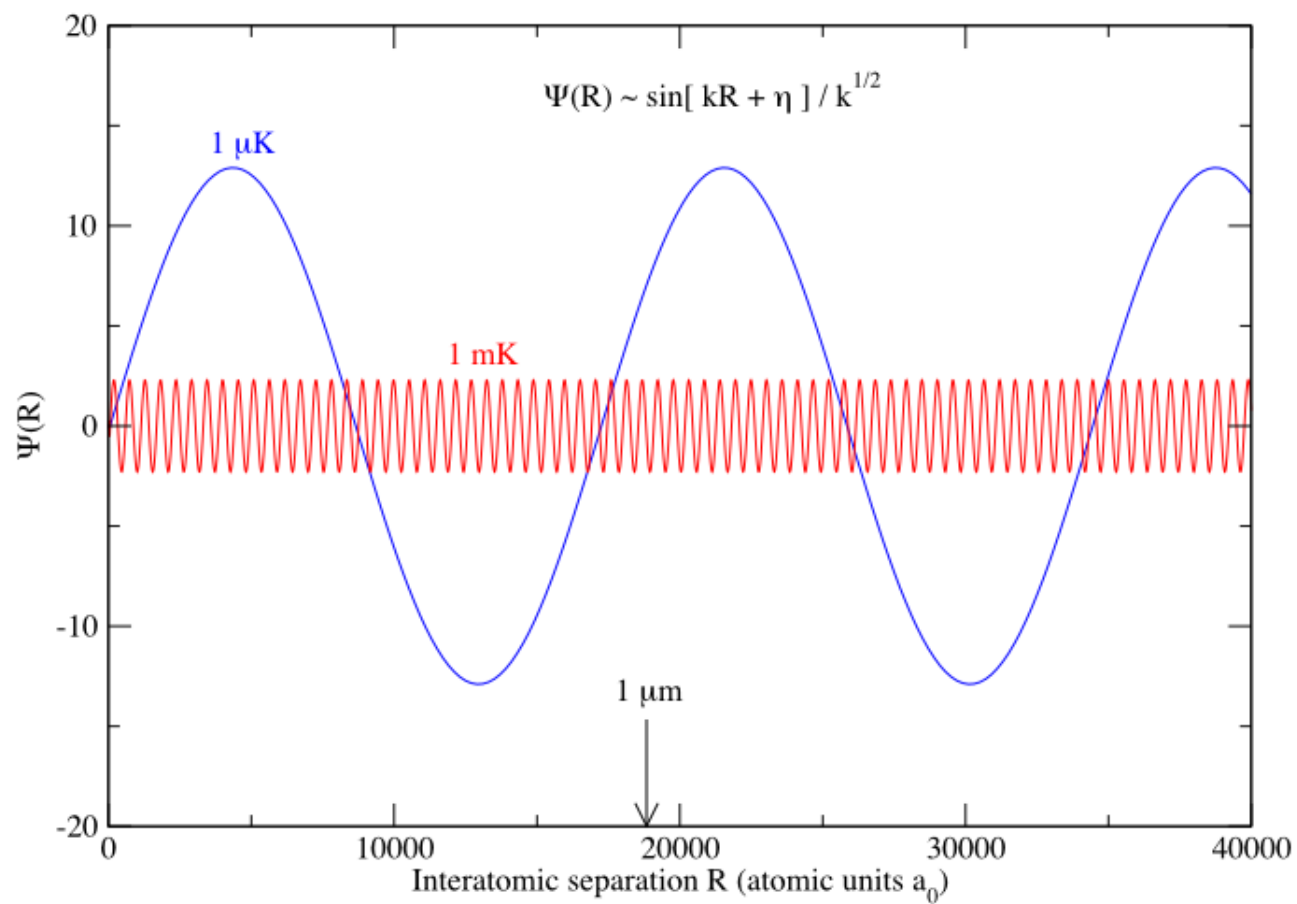
$$k(R, E) = \left(\frac{2\mu}{\hbar^2} (E - V(R)) \right)^{\frac{1}{2}} = \frac{2\pi}{\lambda(R, E)}$$

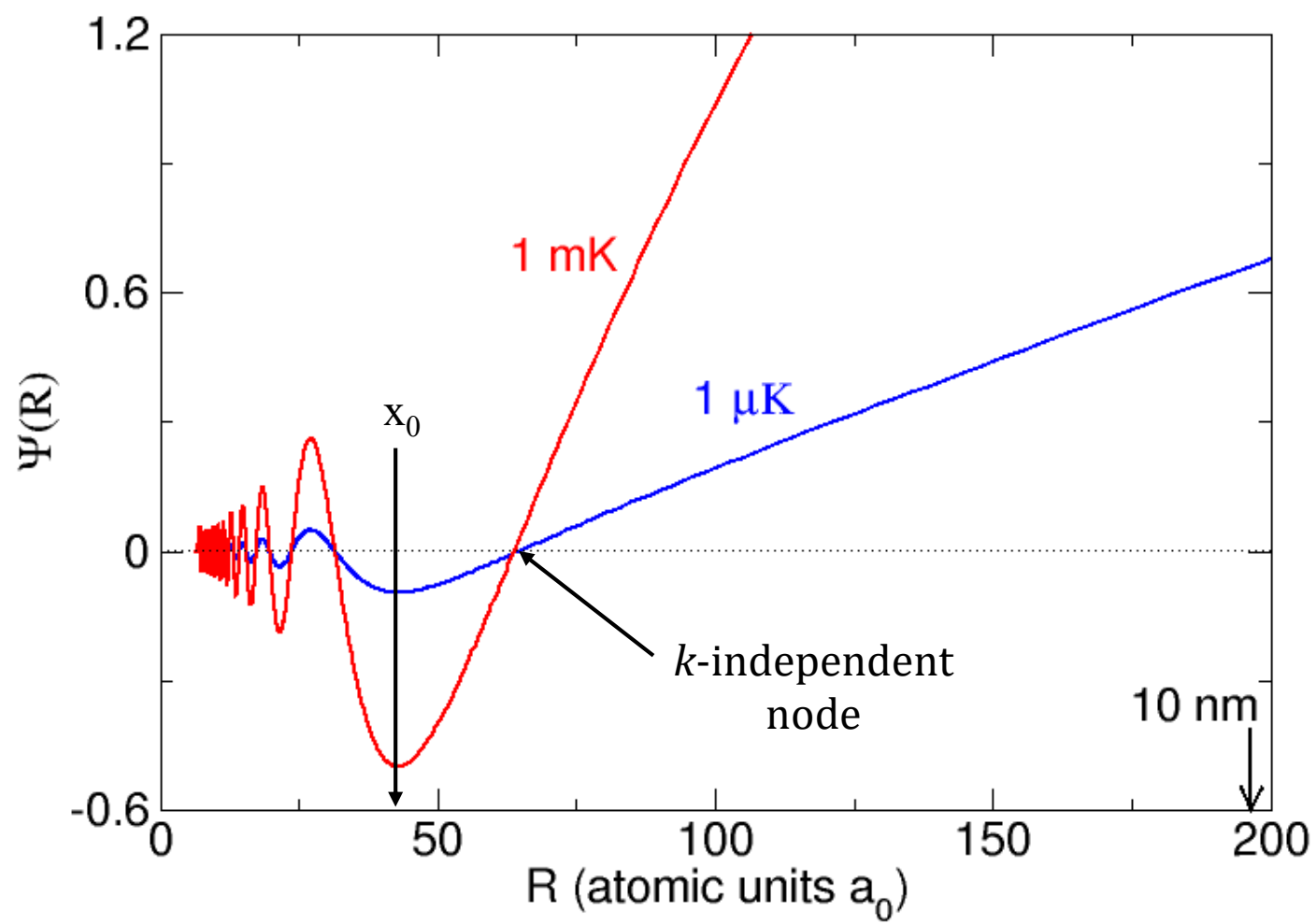
Validity criterion: $\frac{d\lambda(R, E)}{dR} \ll 1$

Semiclassical considerations continued

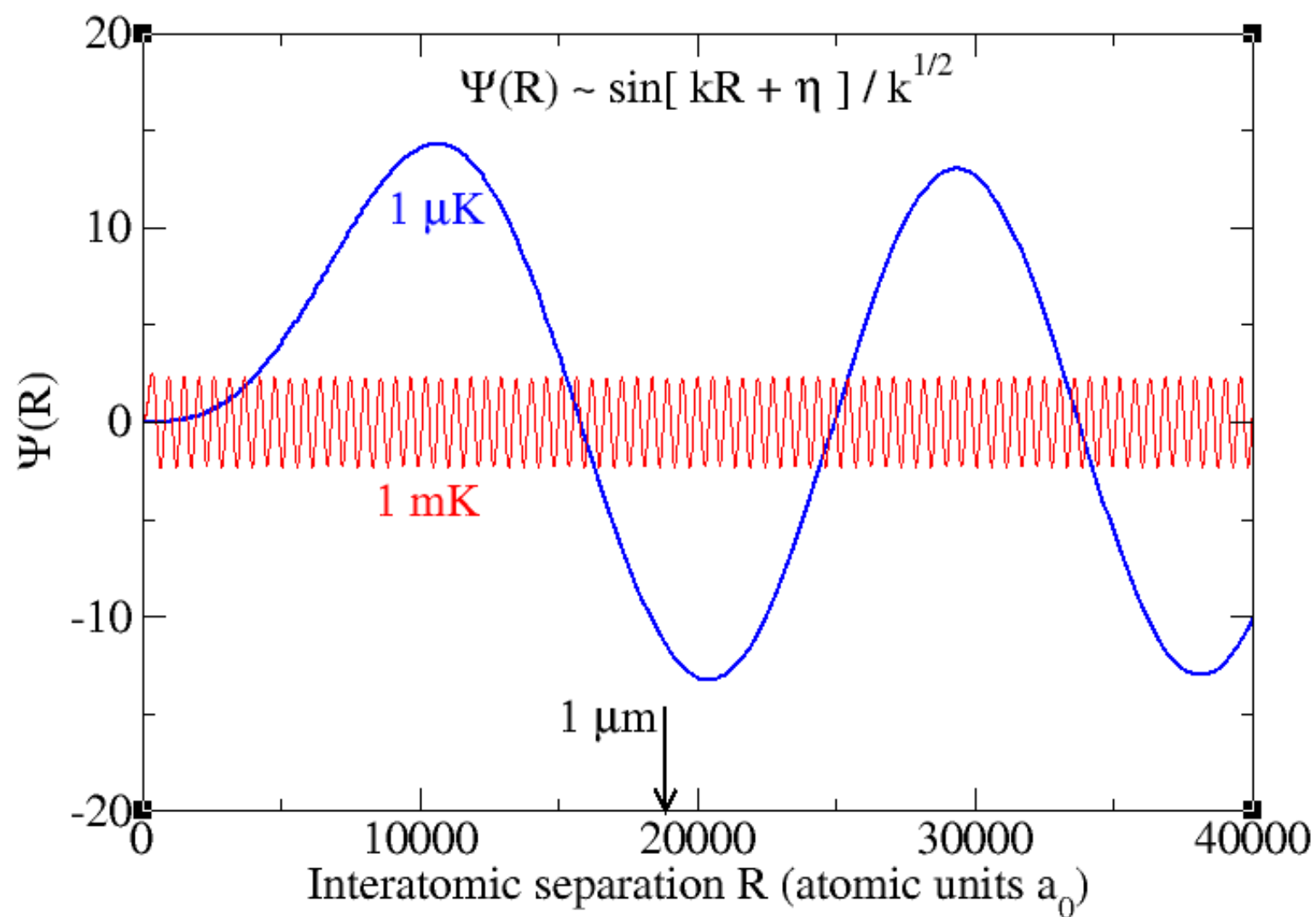


Na + Na s-wave scattering wave function

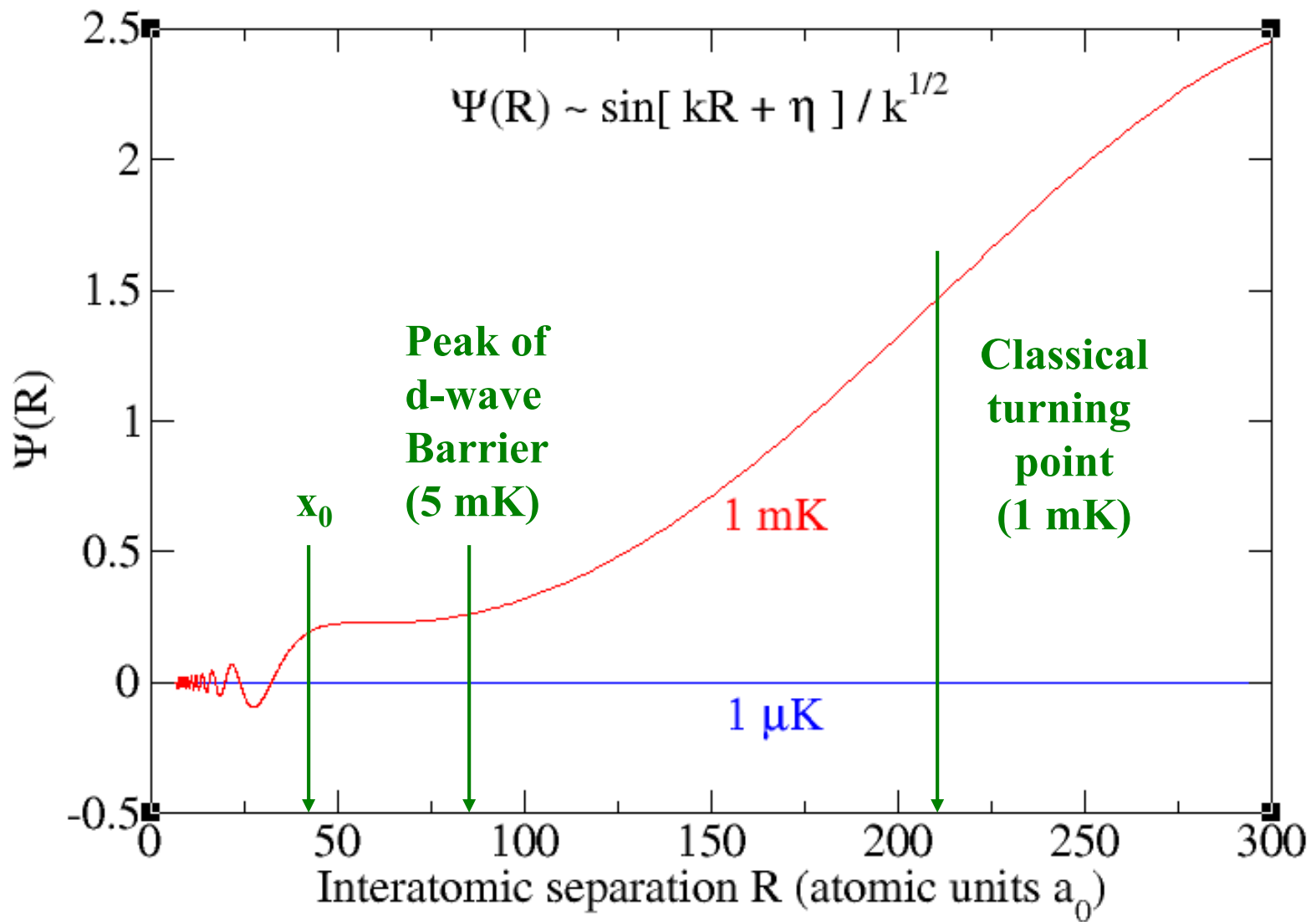




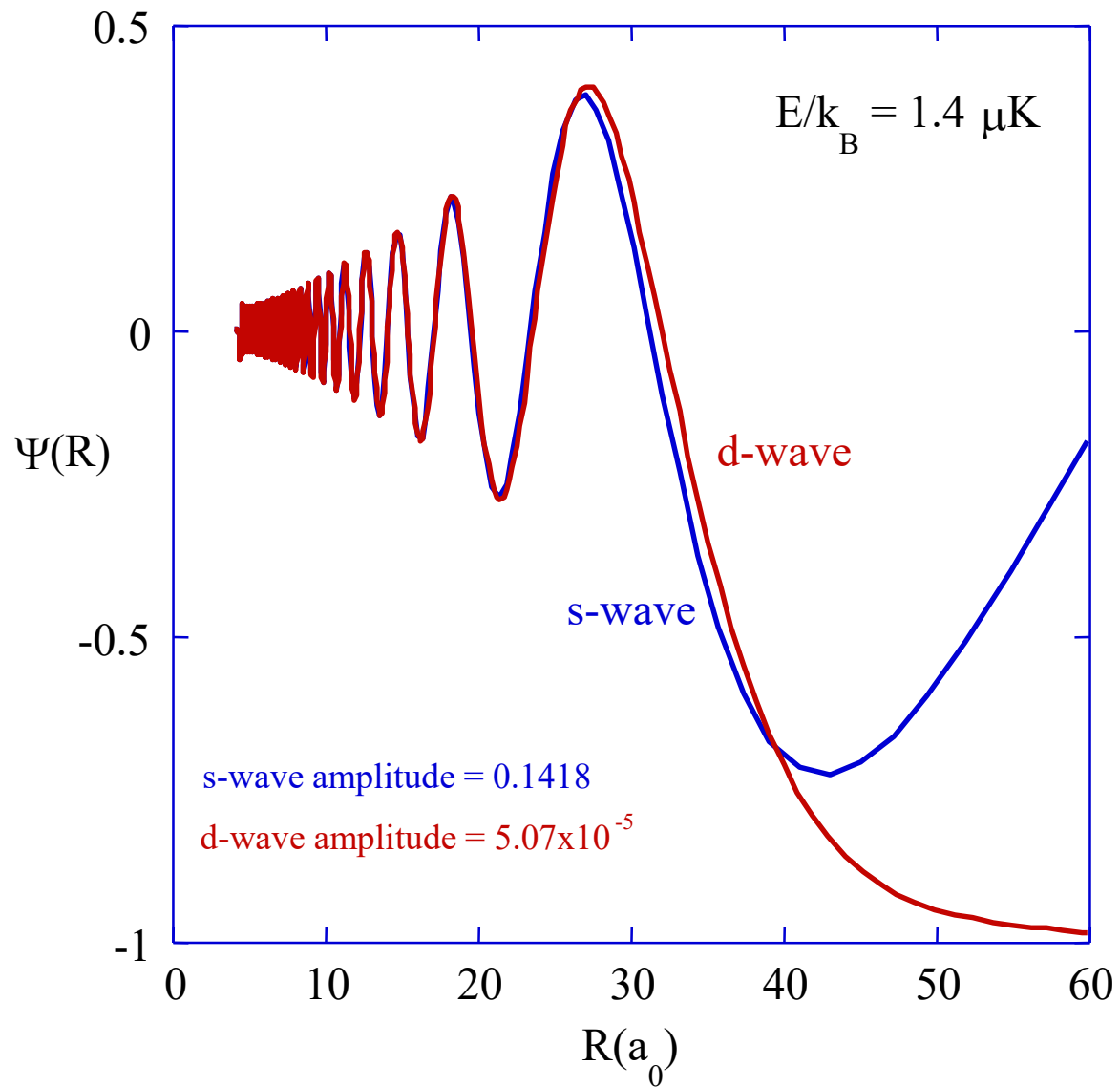
Na + Na d-wave scattering wave function



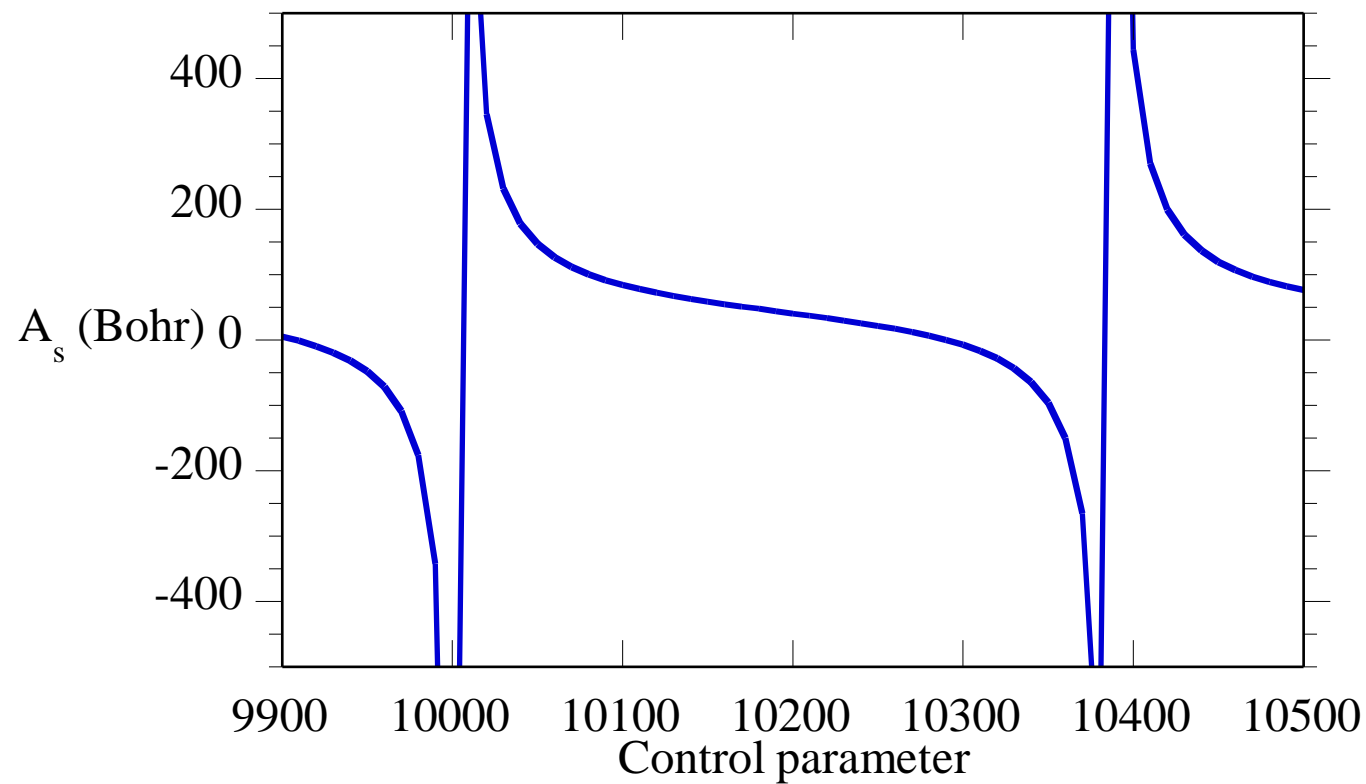
Na + Na d-wave scattering wave function

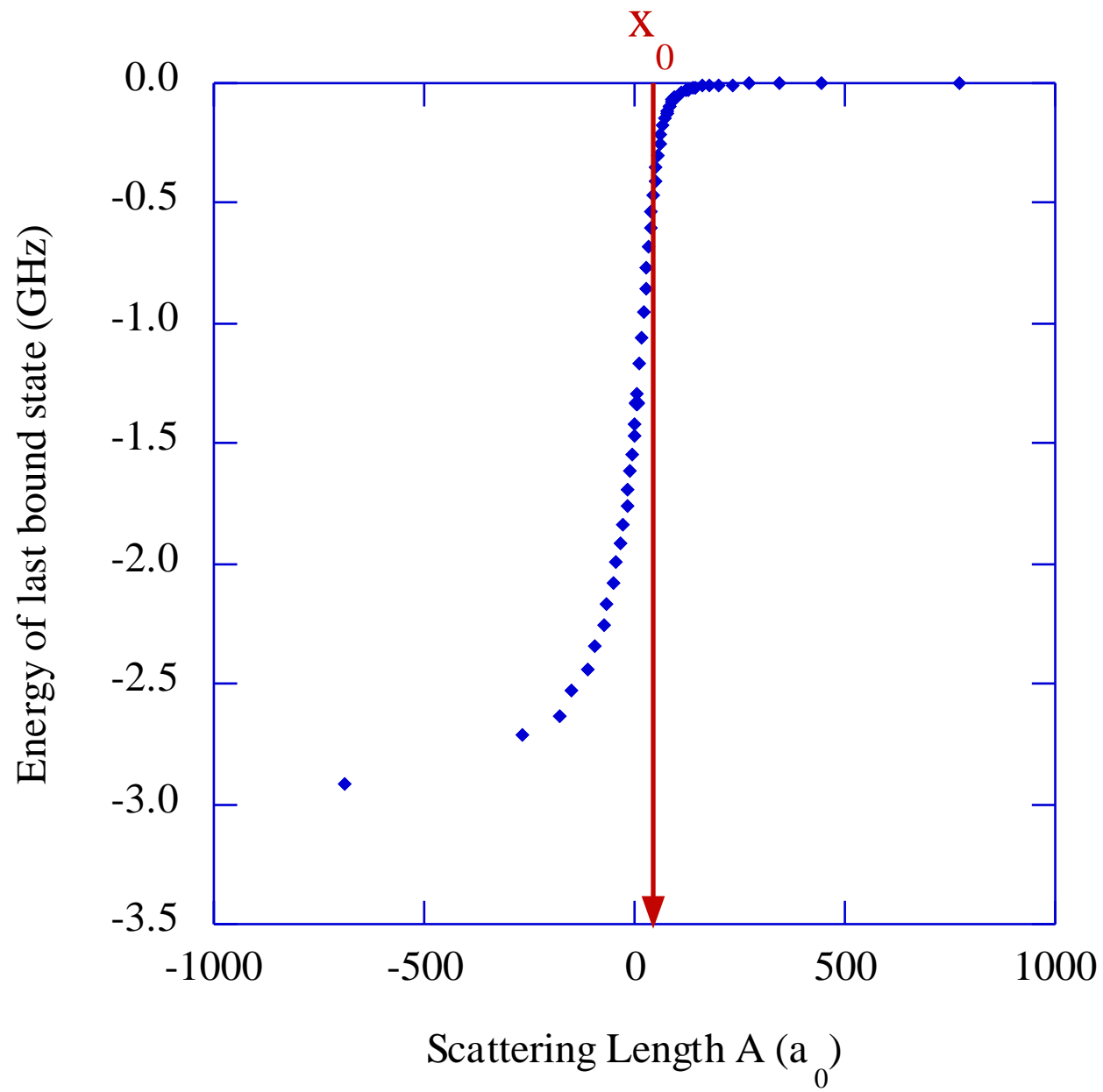


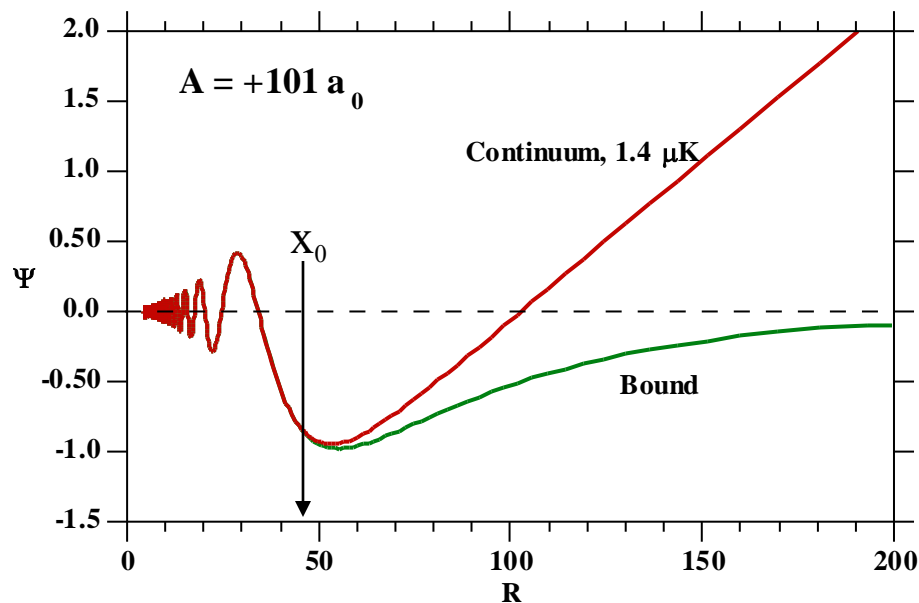
Short-range $\Psi(R)$ compared



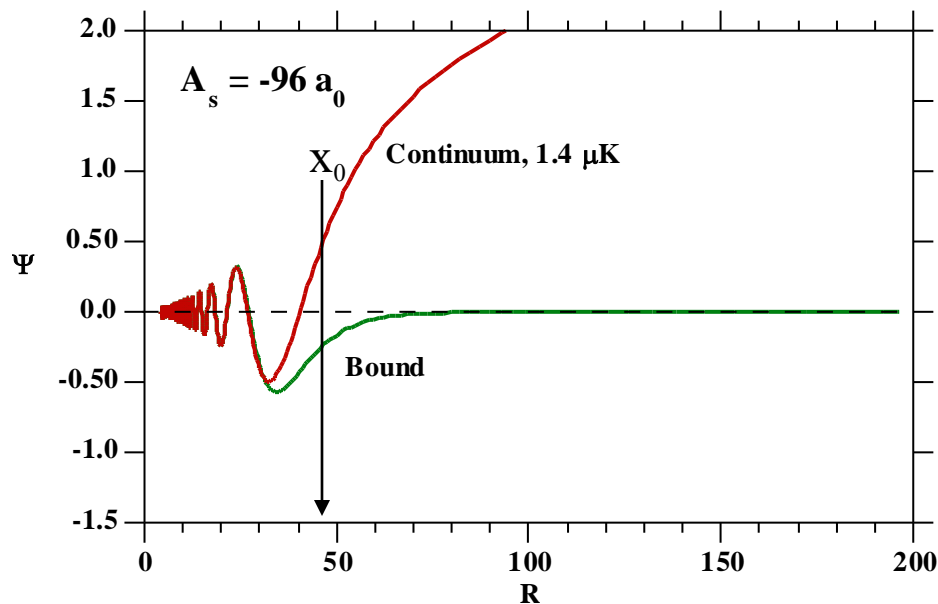
Scattering Length vs Control Parameter







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

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

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

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

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).

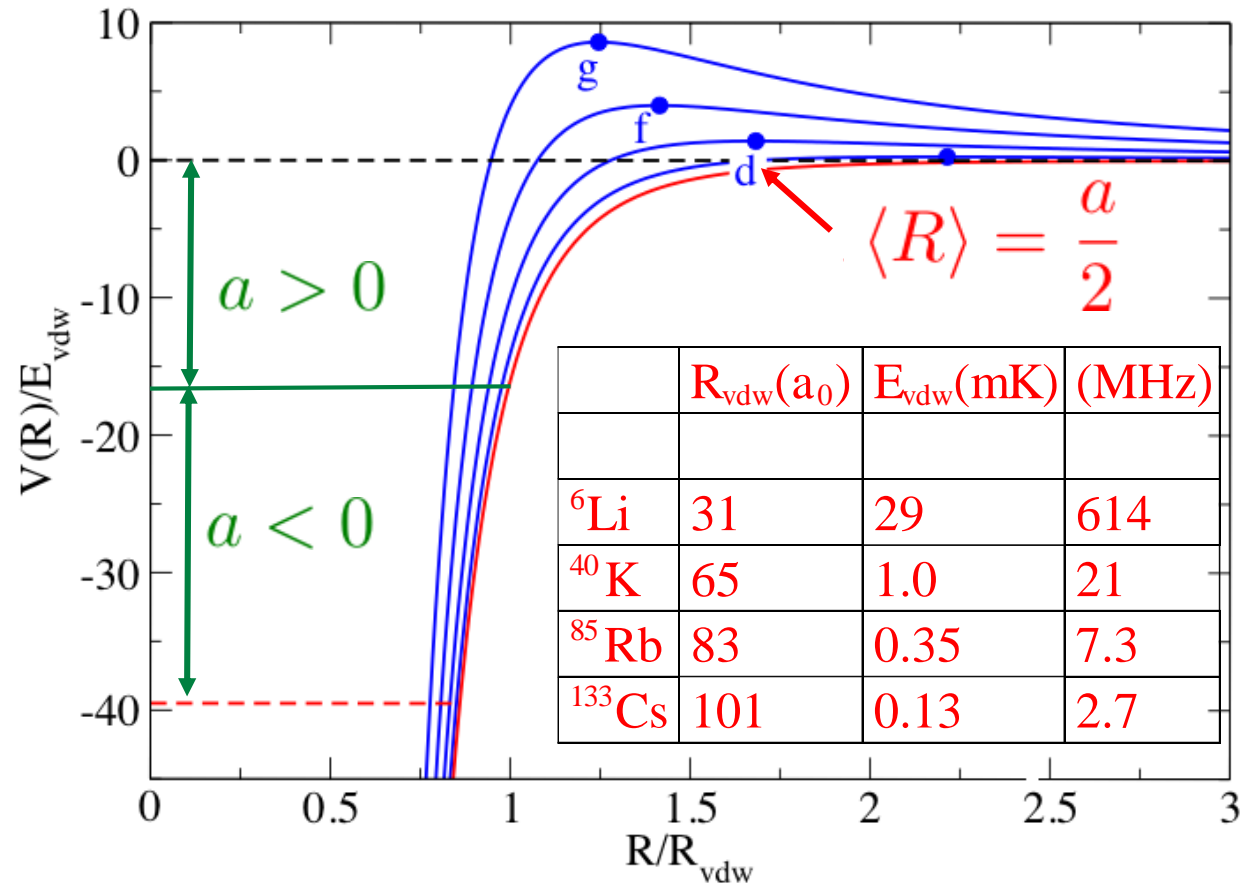
“Size” of potential V(R)

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

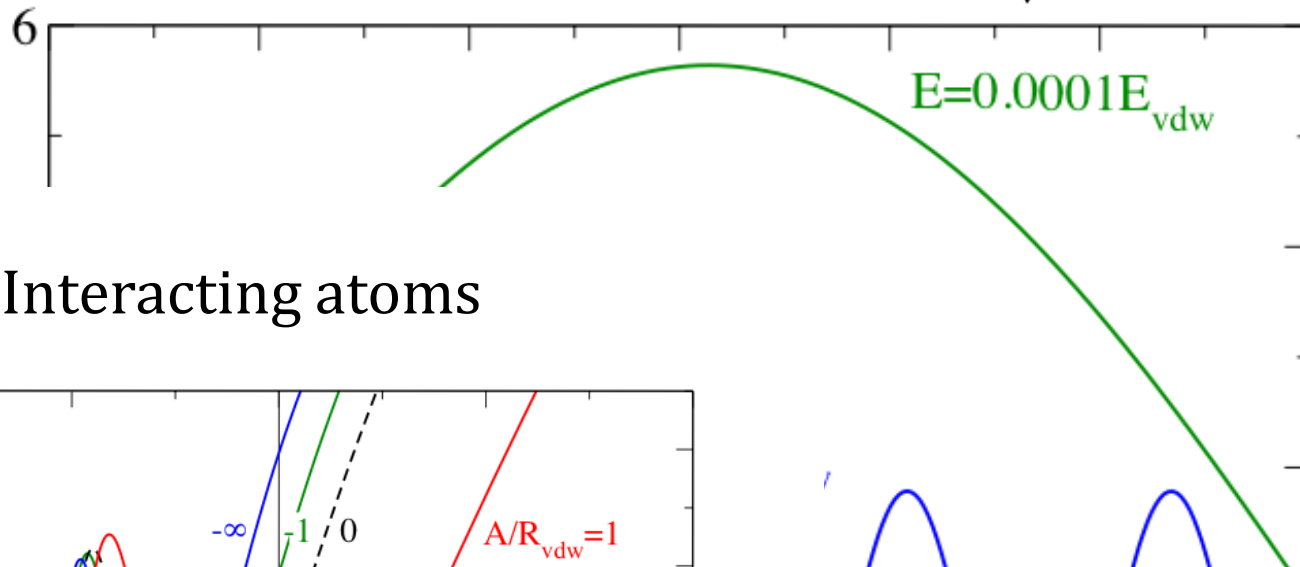
$$\bar{a} = \frac{\Gamma(3/4)}{\Gamma(5/4)} R_{\text{vdW}} = 0.956 R_{\text{vdW}}$$

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

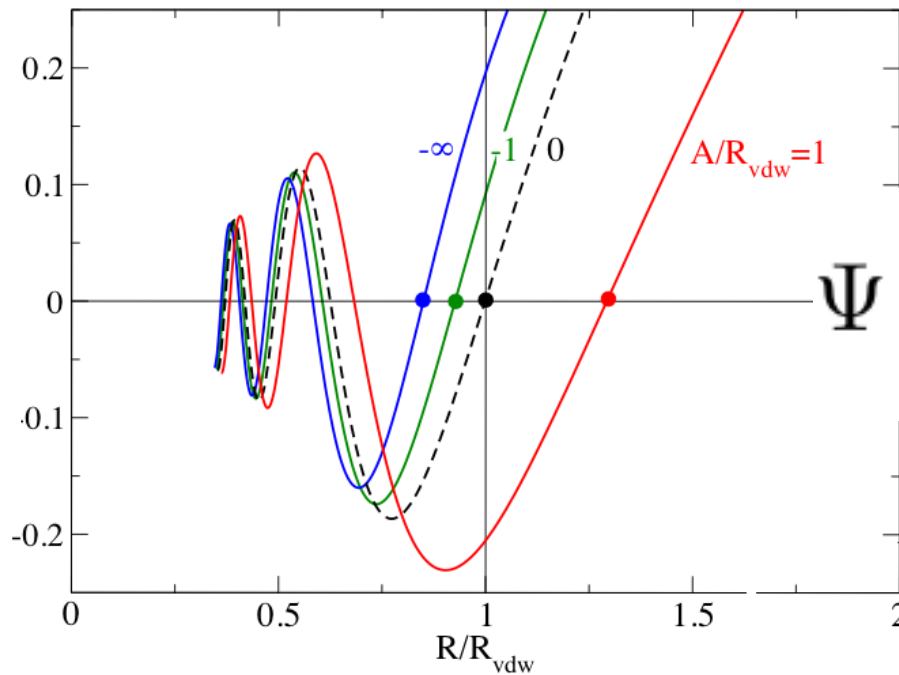
$$E_{\text{vdw}} = \frac{\hbar^2}{2\mu R_{\text{vdw}}^2}$$



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



Interacting atoms



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

A zoomed-in plot of the wavefunction Ψ versus R/R_{vdw} for interacting atoms, showing the oscillatory behavior for negative energies. The x-axis ranges from 200 to 300, and the y-axis ranges from -0.2 to 0.2. The plot shows several peaks and troughs, with the peaks reaching $\Psi \approx 0.15$ and the troughs reaching $\Psi \approx -0.15$.