2010 European Conference on Trapped Ions
19-24 September 2010, Redworth Hall, County Durham, UK

Cold Collisions of Atoms, Molecules, and Ions

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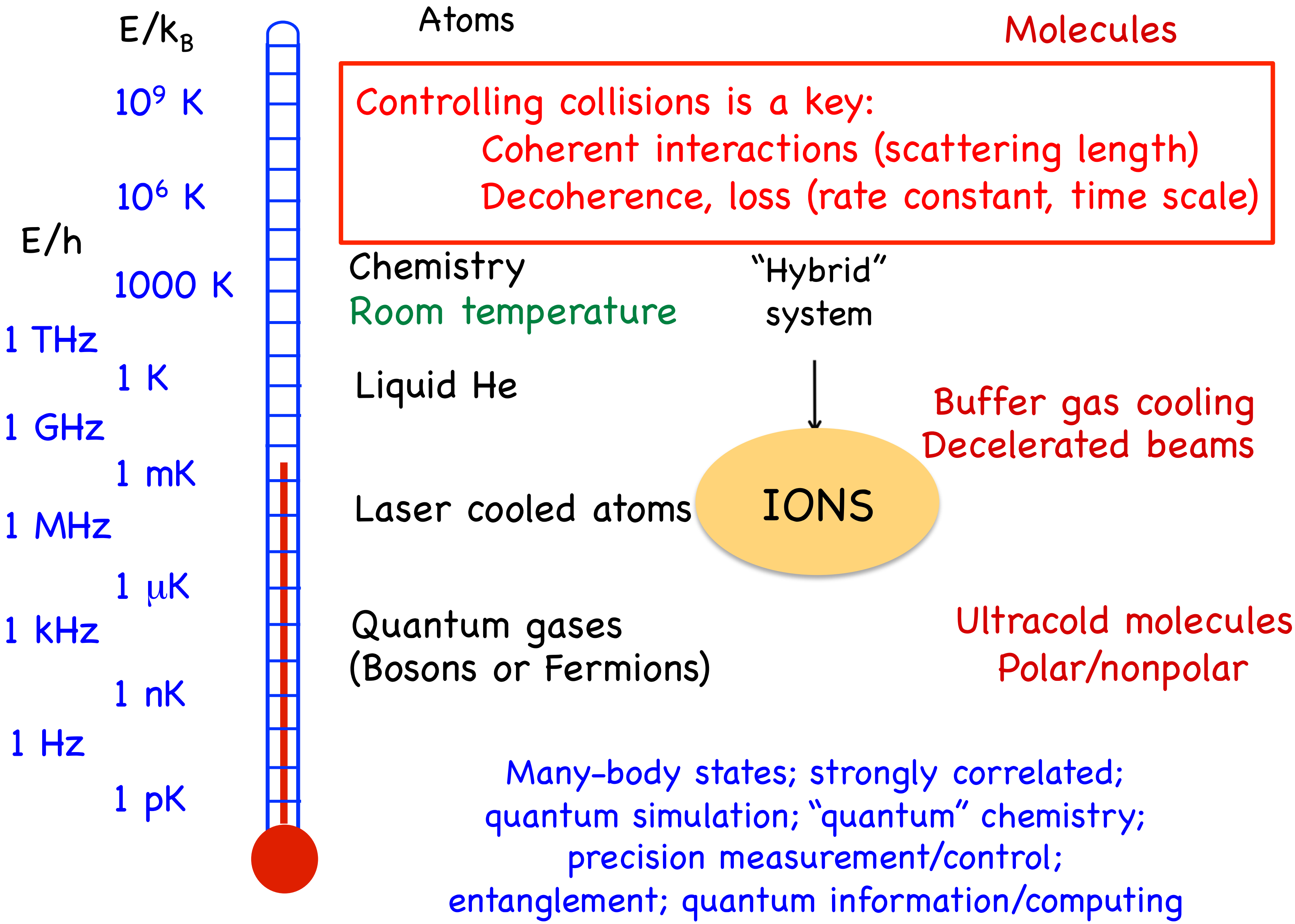


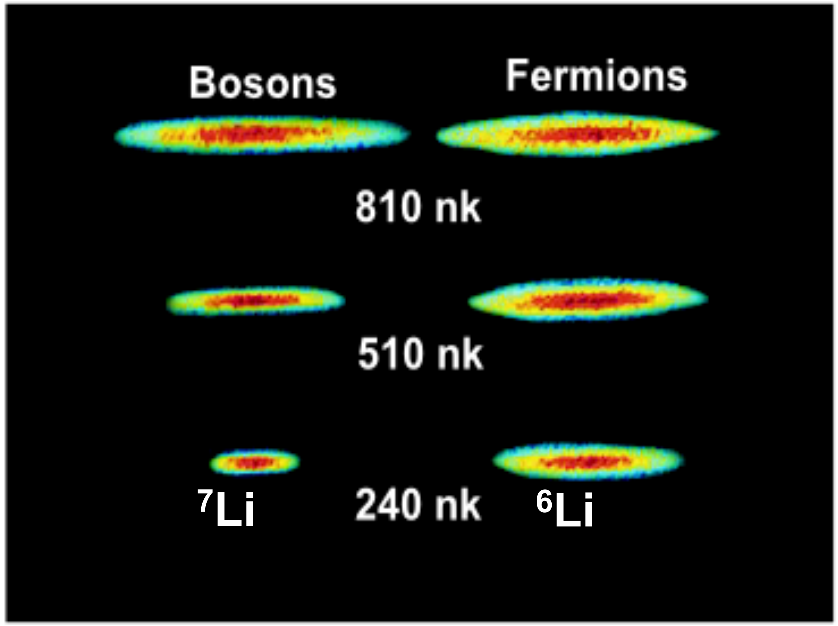
E/k_B
10^9 K
10^6 K
E/h
1000 K
1 THz
1 K
1 GHz
1 mK
1 MHz
1 μK
1 kHz
1 nK
1 Hz
1 pK
Atoms
Molecules
Controlling collisions is a key:
Coherent interactions (scattering length)
Decoherence, loss (rate constant, time scale)
Chemistry
Room temperature
"Hybrid" system
Liquid He
Buffer gas cooling
Decelerated beams
Laser cooled atoms
IONS
Quantum gases (Bosons or Fermions)
Ultracold molecules
Polar/nonpolar
Many-body states; strongly correlated;
quantum simulation; "quantum" chemistry;
precision measurement/control;
entanglement; quantum information/computing

Outline

1. Atoms/molecules review
   (5 slides)

2. A consistent treatment of atom/molecule/ion collisions
   (12 slides)

3. Example calculations on $Na + Ca^+$
   (6 slides)



Truscott, Strecker, McAlexander, Partridge, Hulet, *Science* **291**, 2570 (2001)

Theory of Bose-Einstein condensation in trapped gases

Franco Dalfovo and Stefano Giorgini

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Reviews of Modern Physics, Vol. 71, No. 3, April 1999

Theory of ultracold atomic Fermi gases

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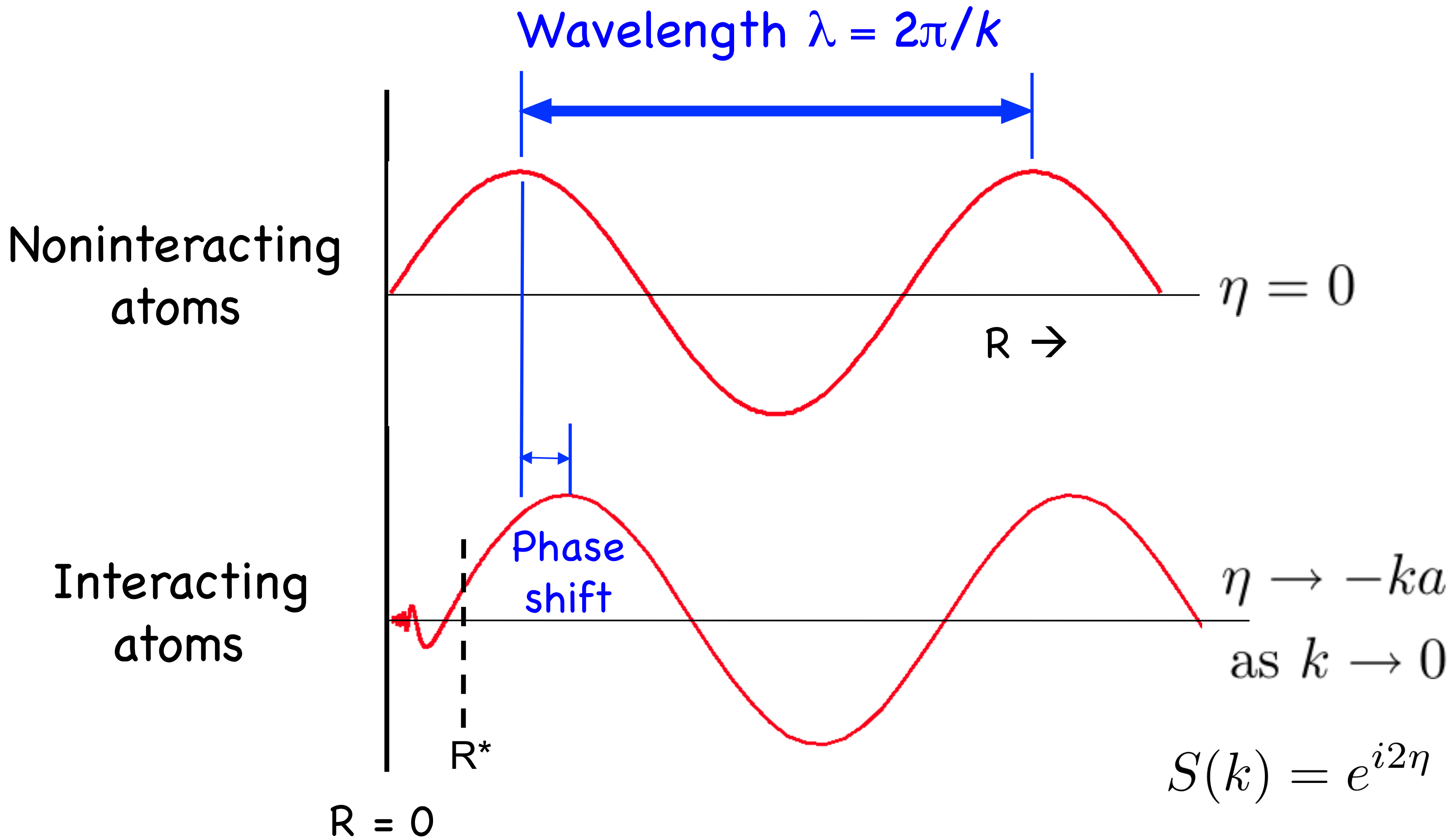
REVIEWS OF MODERN PHYSICS, VOLUME 80, OCTOBER–DECEMBER 2008

Interactions: $g = 4\pi \frac{\hbar^2}{m} a$

a = s-wave scattering length

s-wave scattering phase shift

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



REVIEWS OF MODERN PHYSICS, VOLUME 82, APRIL–JUNE 2010

Feshbach resonances in ultracold gases

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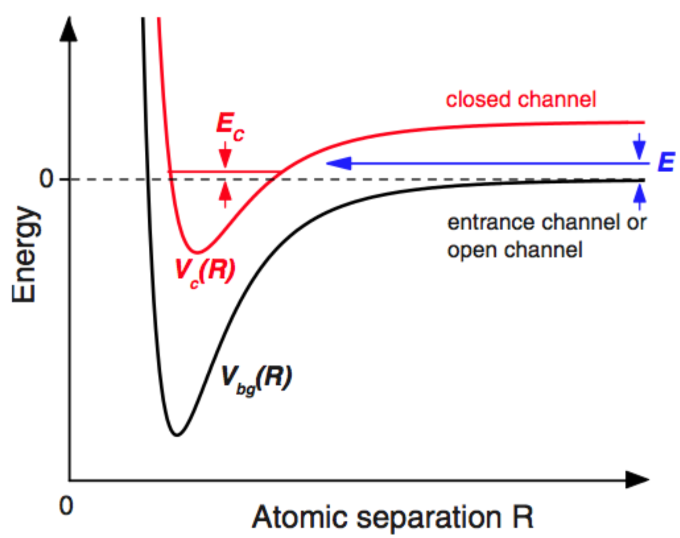
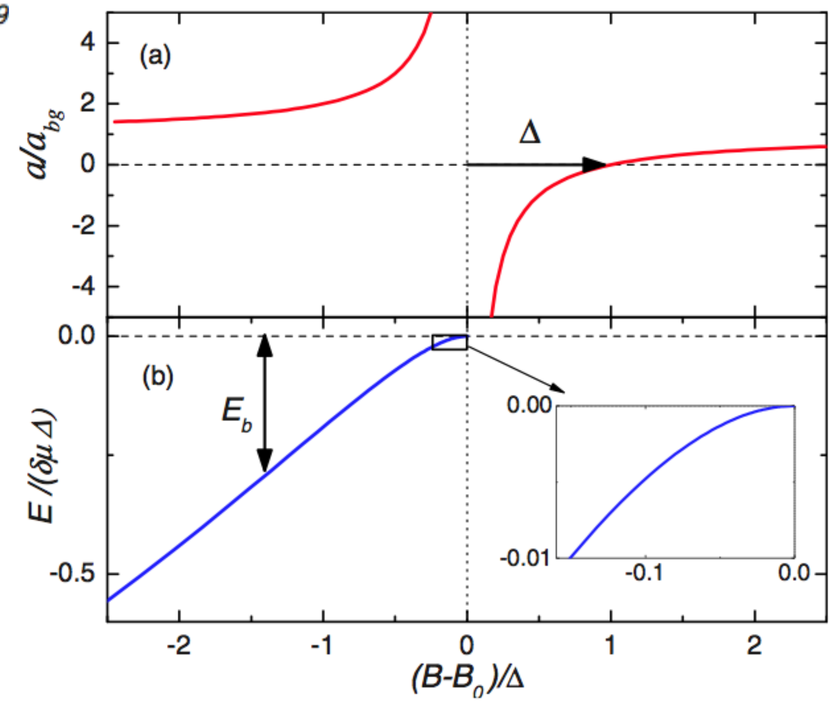
Resonances in atom-ion collisions

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





A High Phase-Space-Density Gas of Polar Molecules

SCIENCE VOL 322 10 OCTOBER 2008

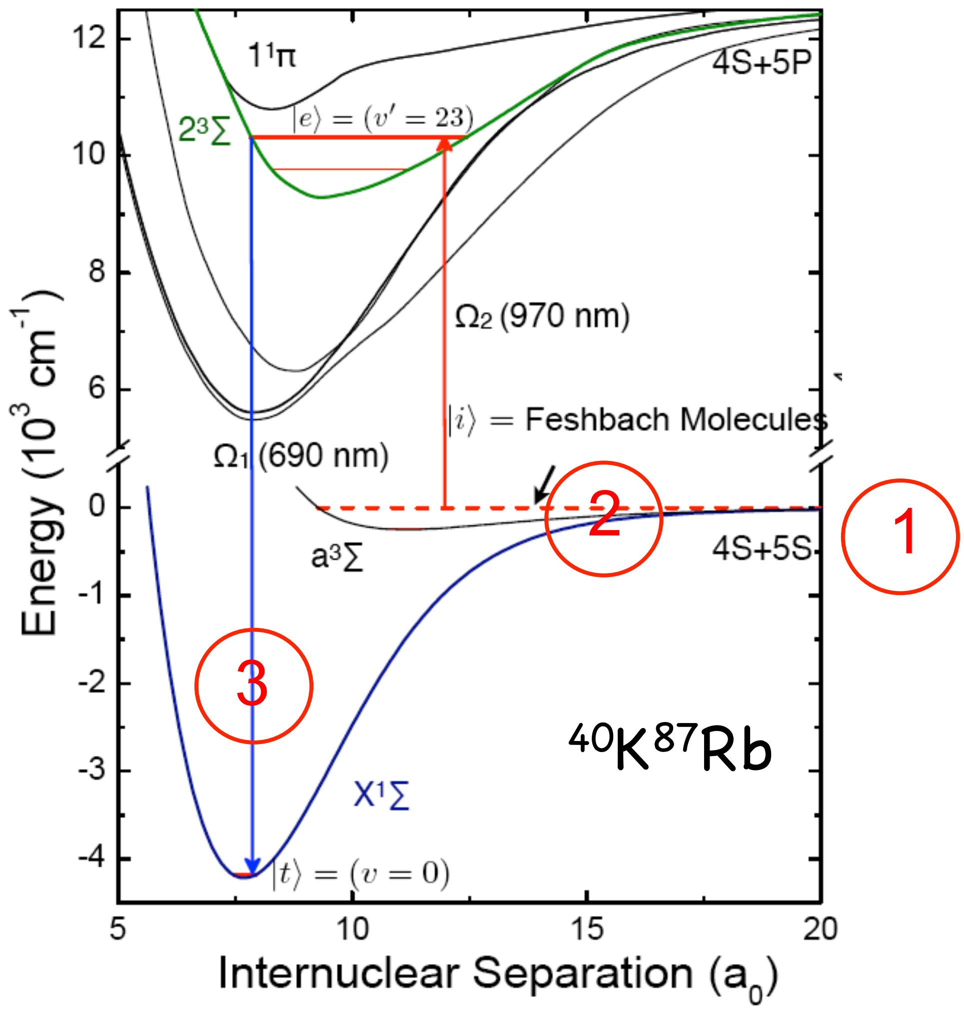
K.-K. Ni,[1*] S. Ospelkaus,[1*] M. H. G. de Miranda,[1] A. Pe'er,[1] B. Neyenhuis,[1] J. J. Zirbel,[1] S. Kotochigova,[2] P. S. Julienne,[3] D. S. Jin,[1†] J. Ye[1†]

40000 $^{40}K^{87}Rb$ molecules
v=0, J=0, single spin level
200 to 800 nK
Density ≈ 10^{12} cm^{-3}

1. Prepare mixed atomic gas

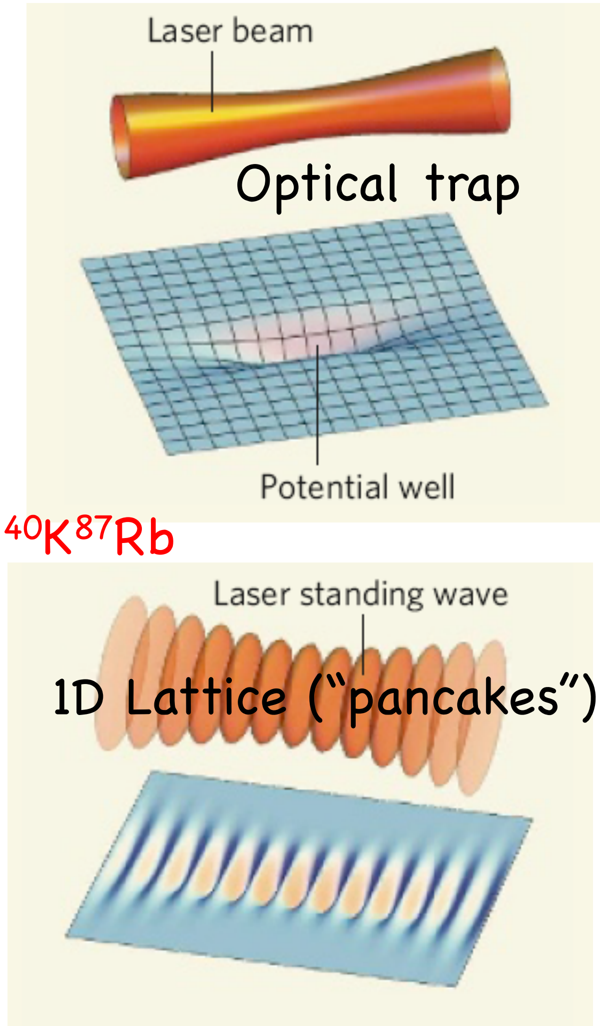
2. Magneto-association to Feshbach molecule

3. Optically switch to v=0 ground state

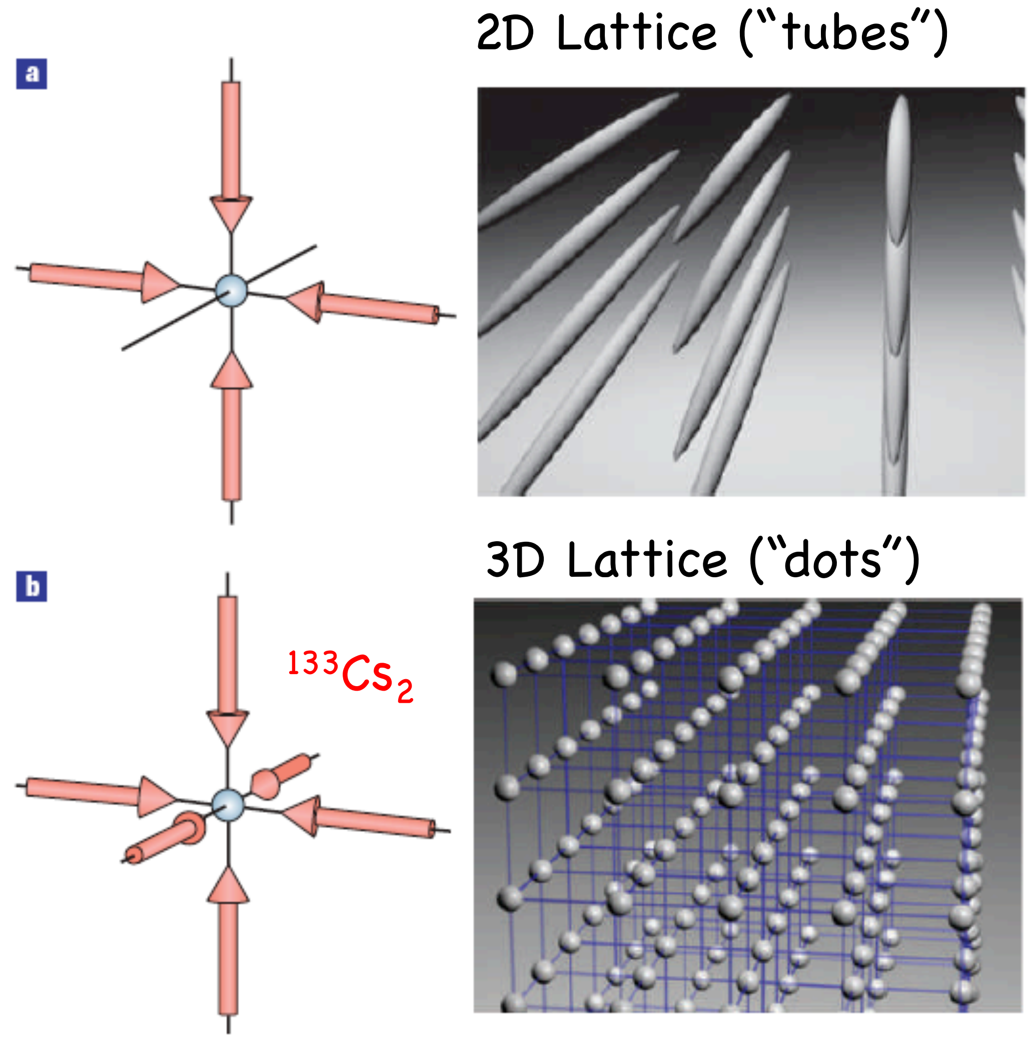


Scheme pioneered by Sage, Sainis, Bergemann and DeMille, PRL **94, 203001 (2005)**

Optical traps and lattices



From Greiner and Fölling
Nature 435, 736 (2008)



From I. Bloch, Nature Physics 1, 23 (2005)

Two kinds of collisions

Elastic: bounce off each other

Loss: go to different untrapped products

Elastic cross section: $\sigma^{\mathrm{el}}_{\alpha\alpha}(k) = \frac{\pi}{k^2}\sum_{\ell}^{\infty}(2\ell+1)|1-S_{\alpha\alpha}(k,\ell)|^2$

$S_{\alpha\alpha}(k,\ell)$ = S-matrix element for the entrance channel

Loss cross section: $\sigma^{\mathrm{loss}}_{\alpha\alpha'}(k) = \frac{\pi}{k^2}\sum_{\ell}^{\infty}(2\ell+1)|S_{\alpha\alpha'}(k,\ell)|^2$

↑ = 1 if no barrier (Langevin model)

Rate constant: $K = v\sigma = \frac{\hbar k}{\mu}\sigma$

Rate: 1/t = Kn

s-wave collision summary

If only a single *s*-wave channel, $S_{\alpha\alpha} = e^{-2ik(a-ib)}$ as $k \to 0$

Phase shift → complex scattering length *a–ib*

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

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

The long-range potential

$$\frac{V(r)}{E^*} = \frac{\ell(\ell+1)}{r^2} - \frac{C_p}{r^p}$$

where $$r = \frac{R}{R^*} \qquad E^* = \frac{\hbar}{2\mu(R^*)^2}$$

$$R^* = \left(\frac{2\mu C_p}{\hbar^2}\right)^{1/(p-2)}$$

p=1 e-ion
p=2 e-dipole
p=3 dipole-dipole (molecules)
p=4 ion-atom
p=6 van der Waals (atoms, molecules)

See Chin et al, Rev. Mod. Phys. 82, 1225 (2010) for p=6 case

The long-range potential continued

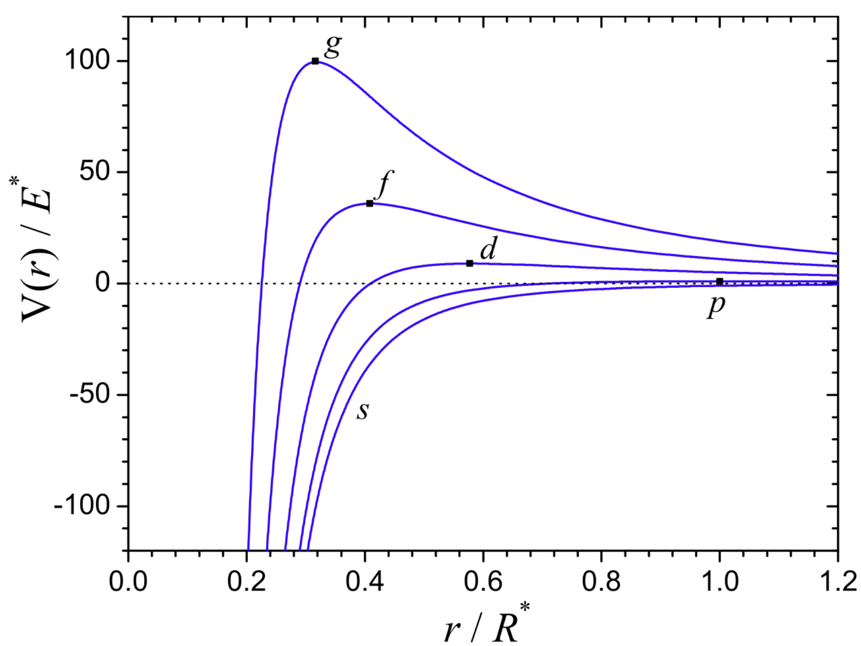
Ion-atom

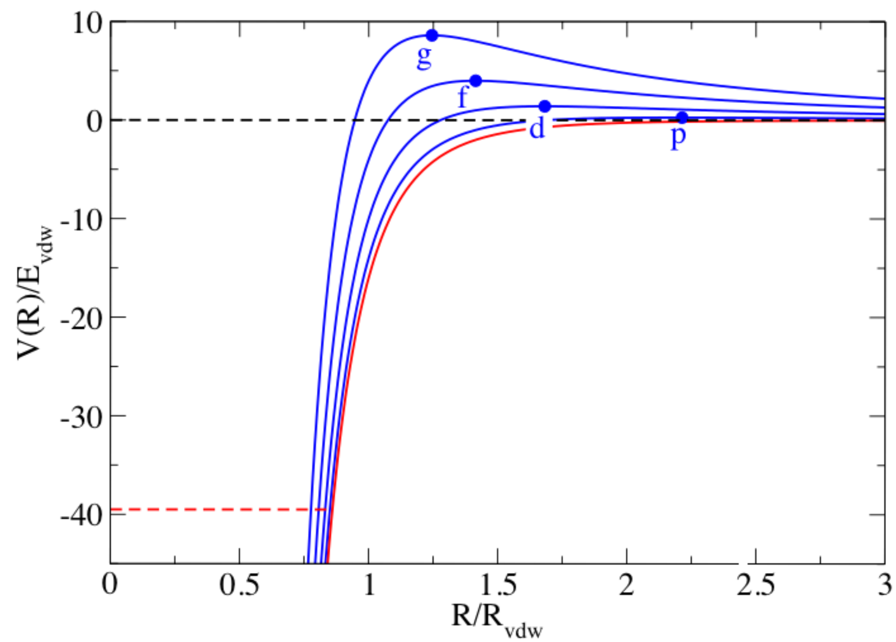
	R^* (a_0)	E^* (μK)
$^{40}Ca^+ + {}^{87}Rb$	3989	0.198
$^{138}Ba^+ + {}^{87}Rb$	5568	0.052
$^{40}Ca^+ + {}^{23}Na$	2081	1.37

Atom-atom

	R^*(a_0)	E^*(mK)
^{6}Li	31	29
^{40}K	65	1.0
^{85}Rb	83	0.35

(R* here is R_{vdW}, = | R* definition)



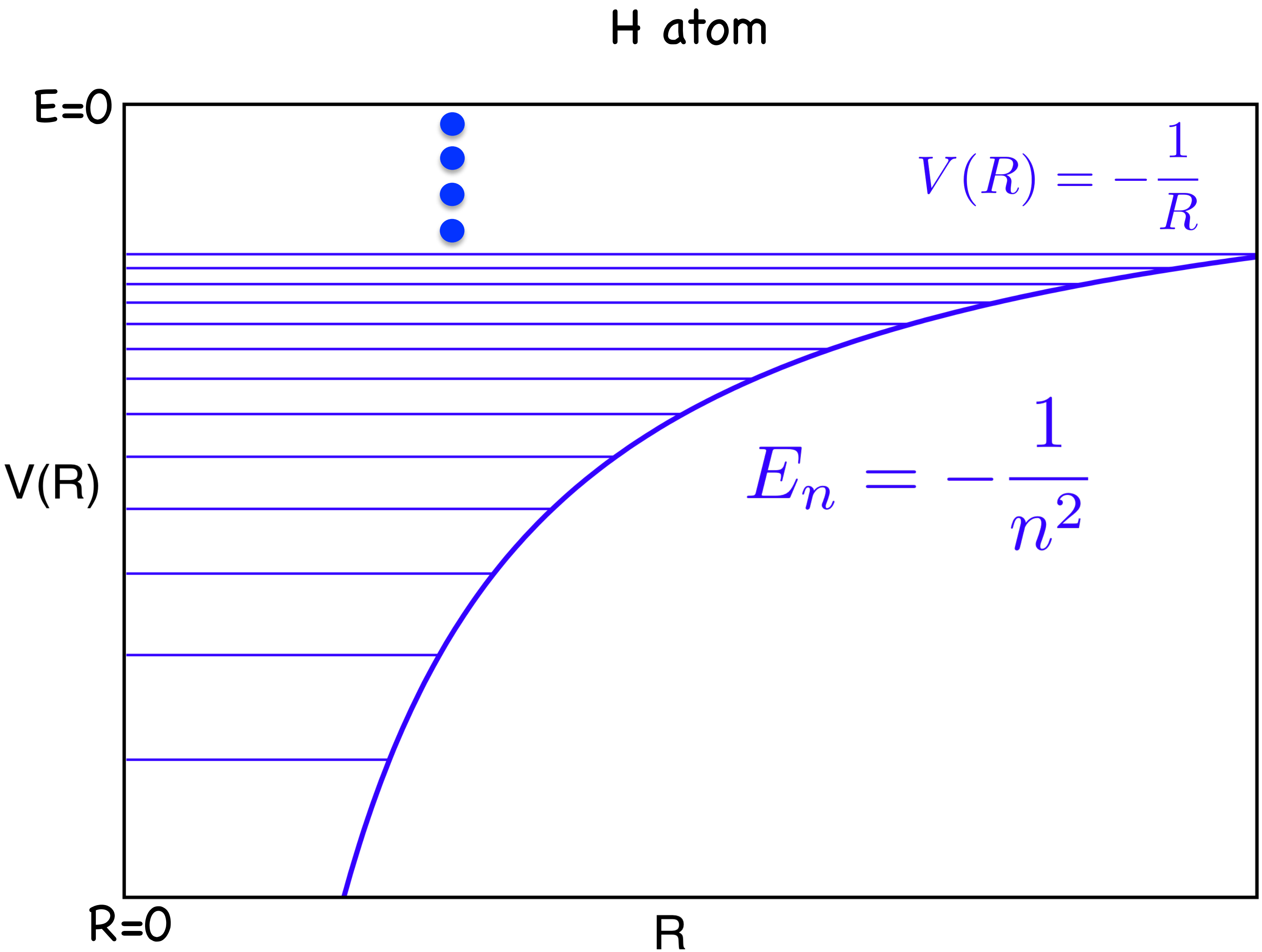


Quantum defect theory

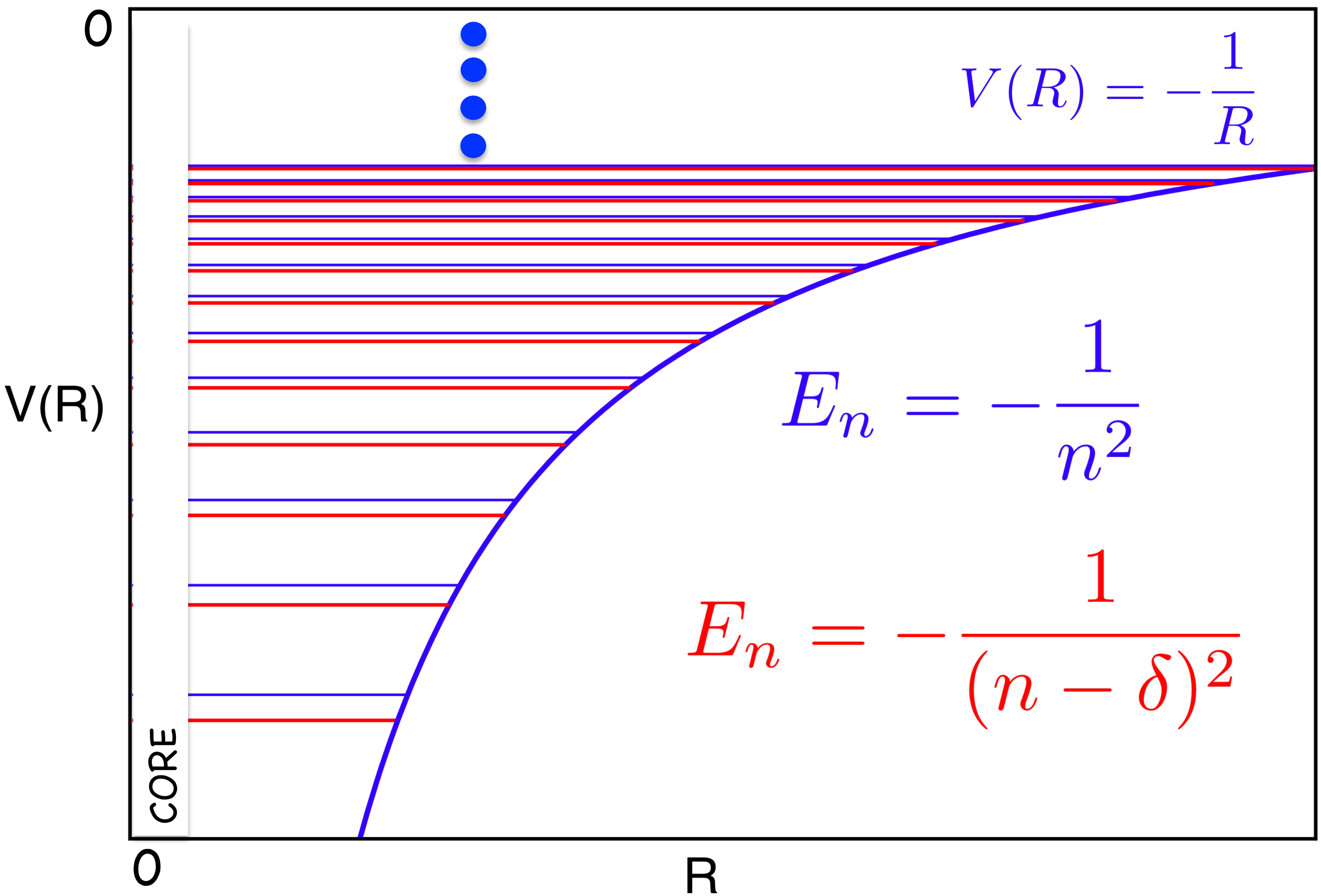
1. Pick a reference problem we can solve
   Classic example: Coulomb potential, H-like atom
   or p = 6 or p = 4 potential

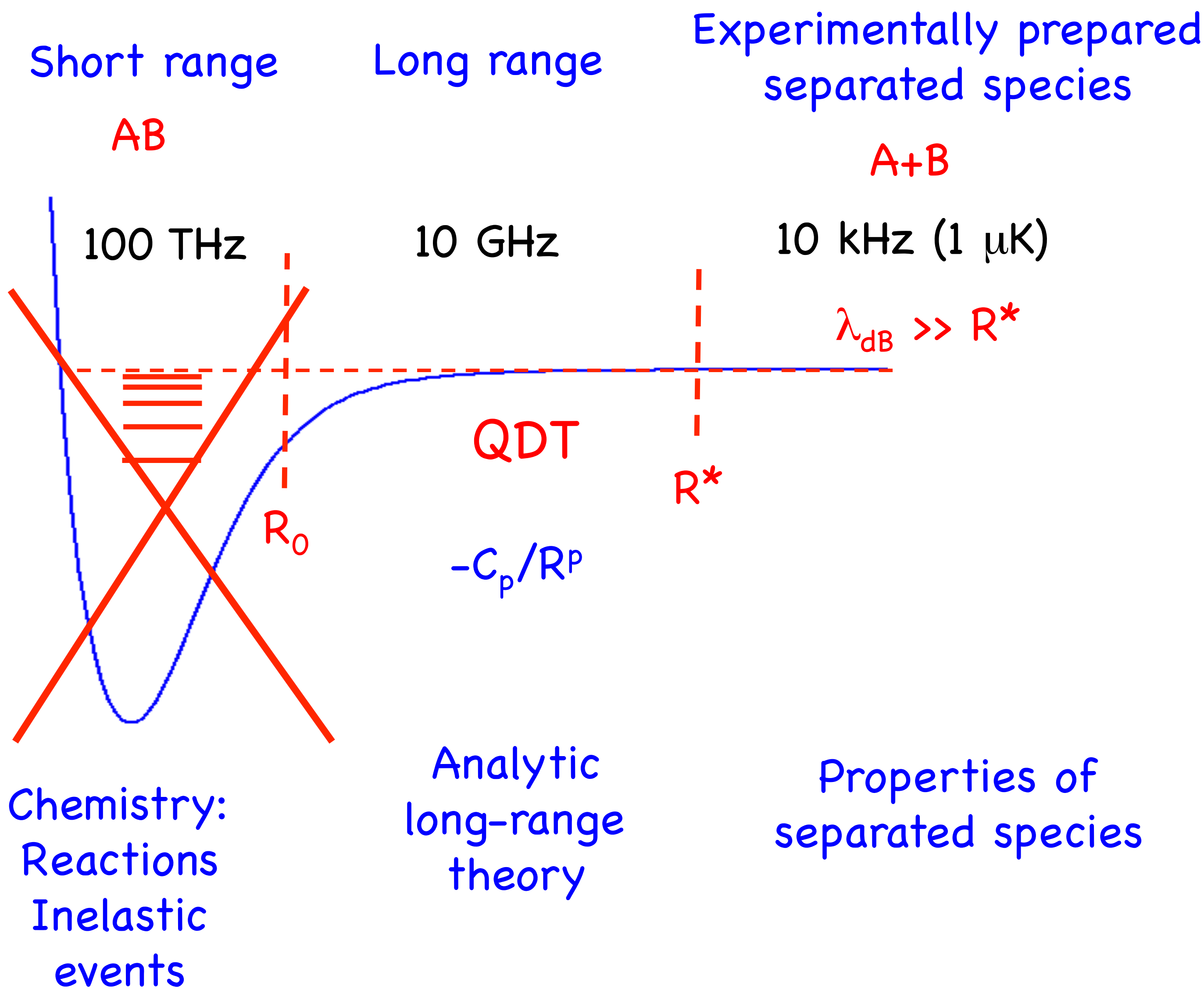
2. Parameterize dynamics by a few "physical" QDT parameters
   subject to experimental fitting
   and theoretical interpretation
   - a, phase, scattering length (singlet+triplet for alkali-like atom or ion)
   - y, probability of short range inelastic event

3. Use methods of QDT to calculate
   bound and scattering states, resonances, cross sections, etc.


H atom
E=0
$V(R) = -\frac{1}{R}$
V(R)
$E_n = -\frac{1}{n^2}$
R=0
R

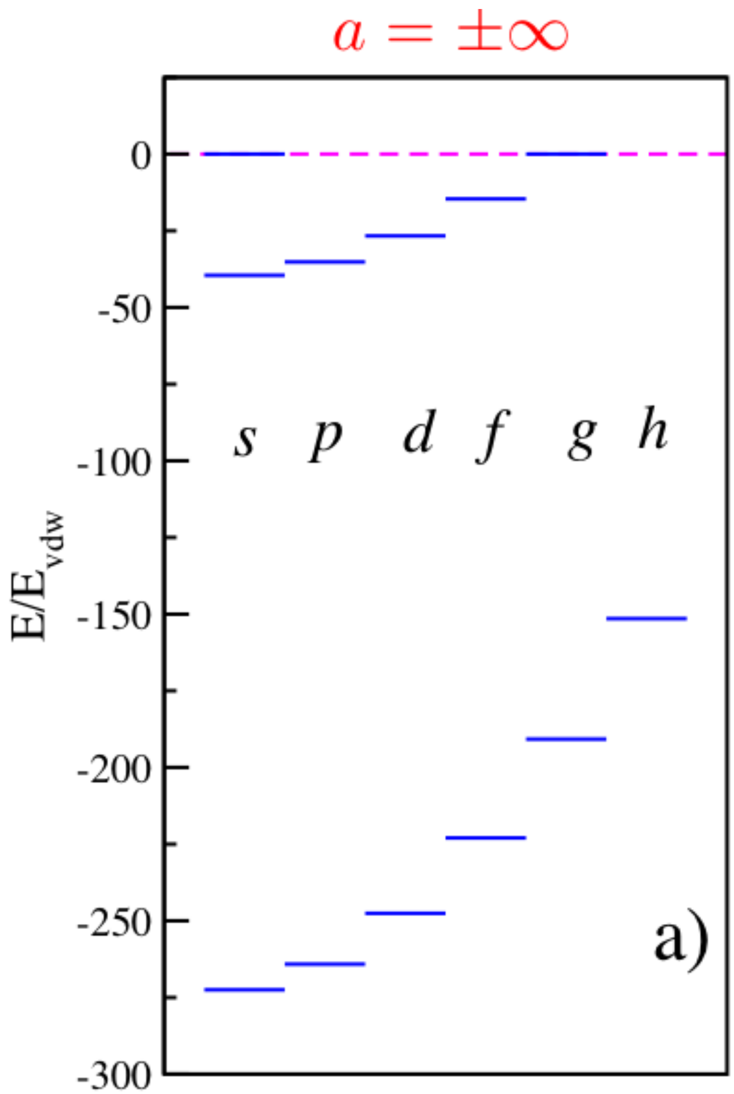
Multi-electron atom





Scattering length a (or equivalent phase) is the free QD parameter (same for all partial waves for isotropic long range V)

Bound states from van der Waals p = 6 case



a determines the pattern
(serves as QD parameter)
2 different a's needed
for H-like atoms
(singlet and triplet)

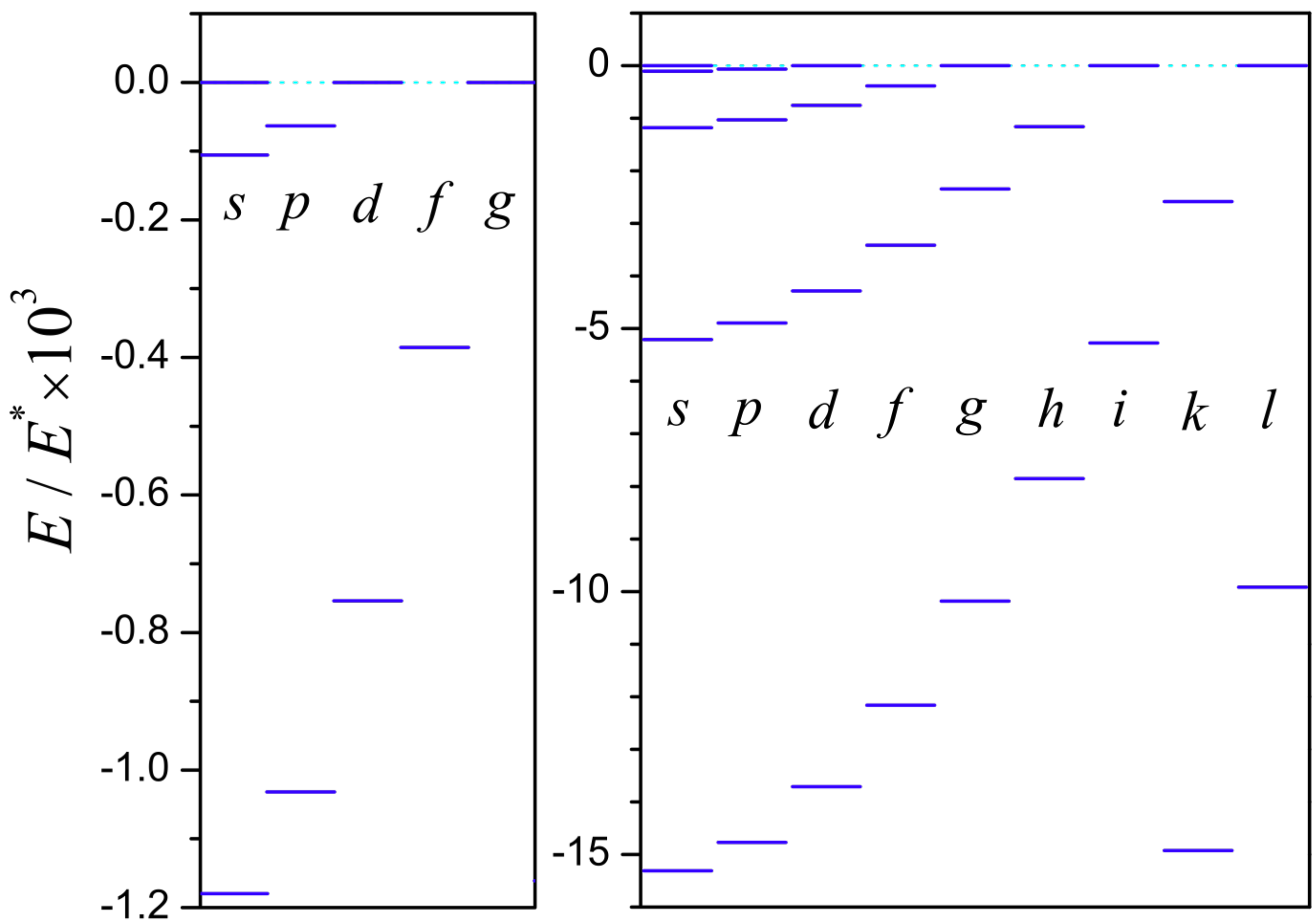
Also determines the scattering
properties and Feshbach
resonances (Hanna et al,
Phys. Rev. A 79, 040701(2009)
(multichannel version)

Found by fitting experimental data
to full Schrödinger Eq. model

Adapted from Gao, Phys. Rev. A 62, 050702 (2000); Figure from Chin et al., RMP 82, 1225(2010)

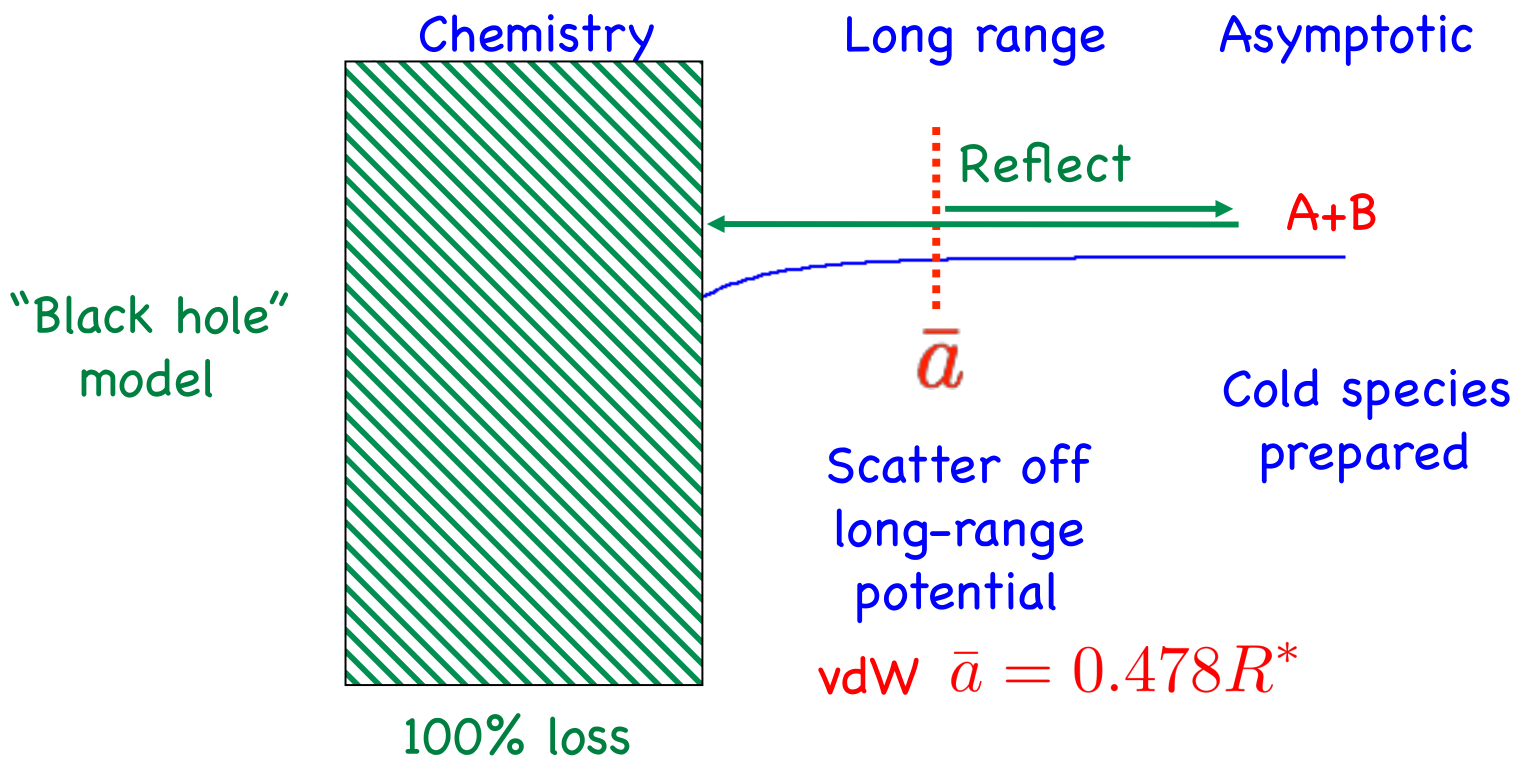
Bound states for a $-C_4/R^4$ atom-ion potential

$a = \pm\infty$



Same principle: a = R* cot(ϕ) serves as a fitting parameter for all ℓ

"Universal" loss rate constants—Quantum Threshold Langevin model



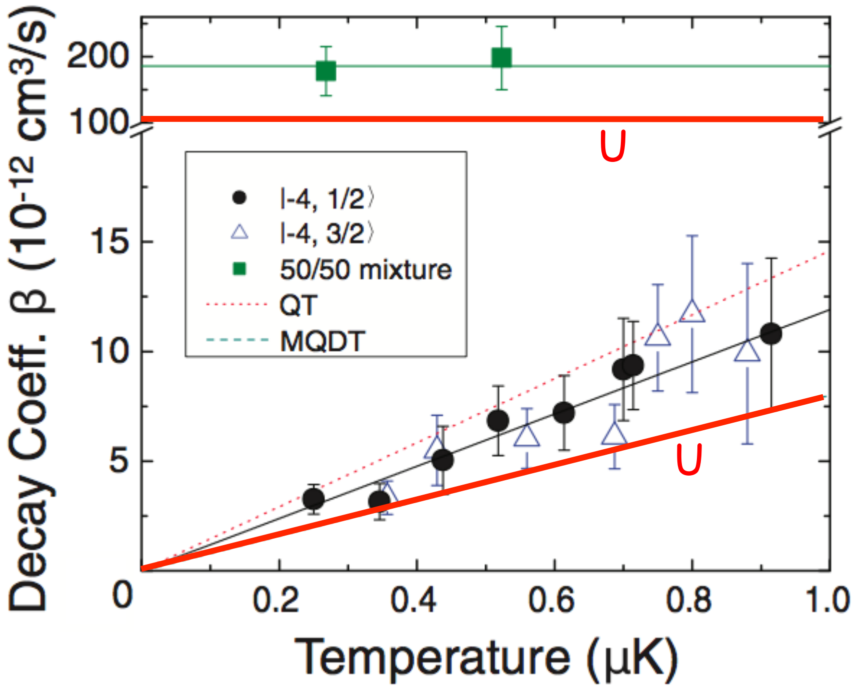
Non-identical or bosons (s-wave): $K^{\mathrm{loss}}_{\ell=0}(T) = 2\,\frac{h}{\mu}\,\bar{a}$

Identical fermions (p-wave): $K^{\mathrm{loss}}_{\ell=1}(T) = 1513\,\bar{a}^3\,\frac{k_B T}{h}$

Idziaszek & PSJ, Phys. Rev. Lett. 104, 113204 (2010)
Idziaszek, et al, Phys. Rev. A 82, 020703 (2010)

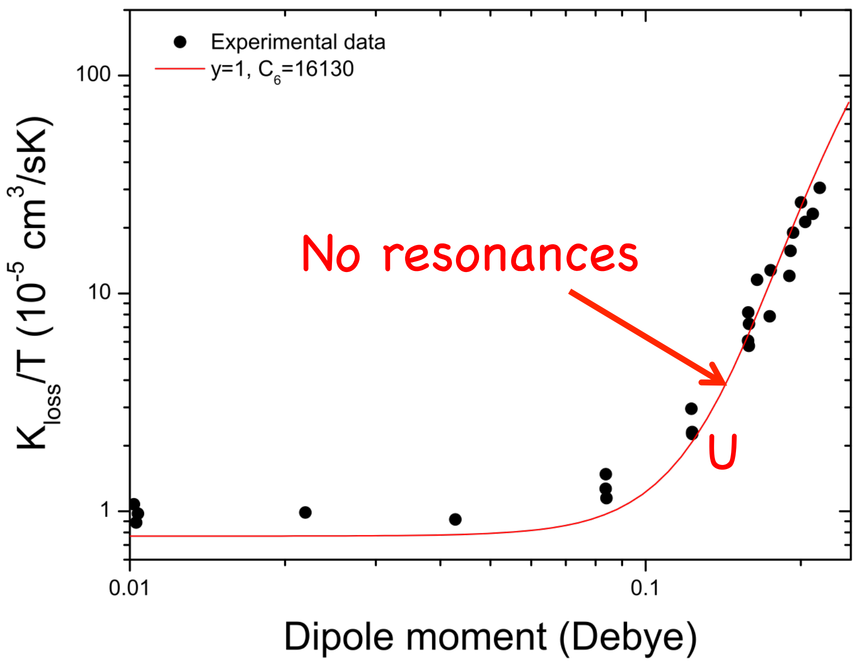
KRb + KRb → K_2 + Rb_2 JILA experiment

No E field--vdW



Ospelkaus, et al, Science 327, 853 (2010)

With E field--dipolar



Ni, et al,, Nature 464, 1324 (2010)

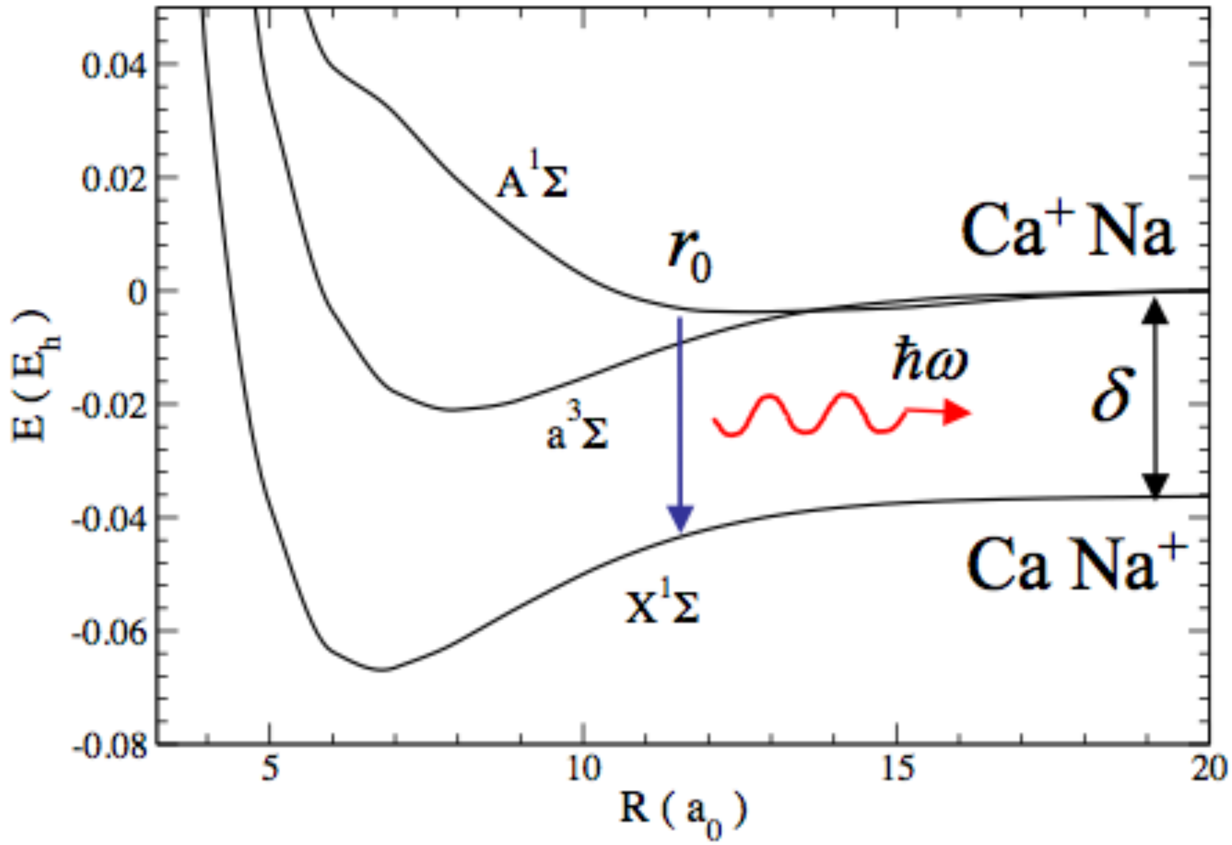
Non-reactive species (RbCs)
should have many resonances

Theory: Idziaszek & PSJ, Phys. Rev. Lett. 104, 113204 (2010)

Idziaszek, et al, Phys. Rev. A 82, 020703 (2010)

Also Quéméner and Bohn, Phys. Rev. A81, 022702(2010)

Na + Ca+ Elastic plus Charge Transfer Collisions



Full quantum scattering calculations
plus MQDT calculations and analysis
(neglect effect of ion trap—to be added later)

Z. Idziaszek, T. Calarco, PSJ, and Andrea Simoni, Phys. Rev. A 79, 010702(R) (2009).

Proposal of Makarov, Côté, Michels, and Smith, Phys. Rev. A 67, 042705 (2003)

Radiative Charge Transfer

$$K_{\mathrm{CT}}(E) = K_{\mathrm{Langevin}}(E)\, P_{\mathrm{CT}}\, Q(E)$$

Langevin capture rate

$$K_{\mathrm{Langevin}}(E) = 2\pi \sqrt{\frac{2C_4}{\mu}}$$

Long range

Emission probability

$$P_{\mathrm{CT}} = \int_{-\infty}^{\infty} A(t)dt \ll 1$$

Short range

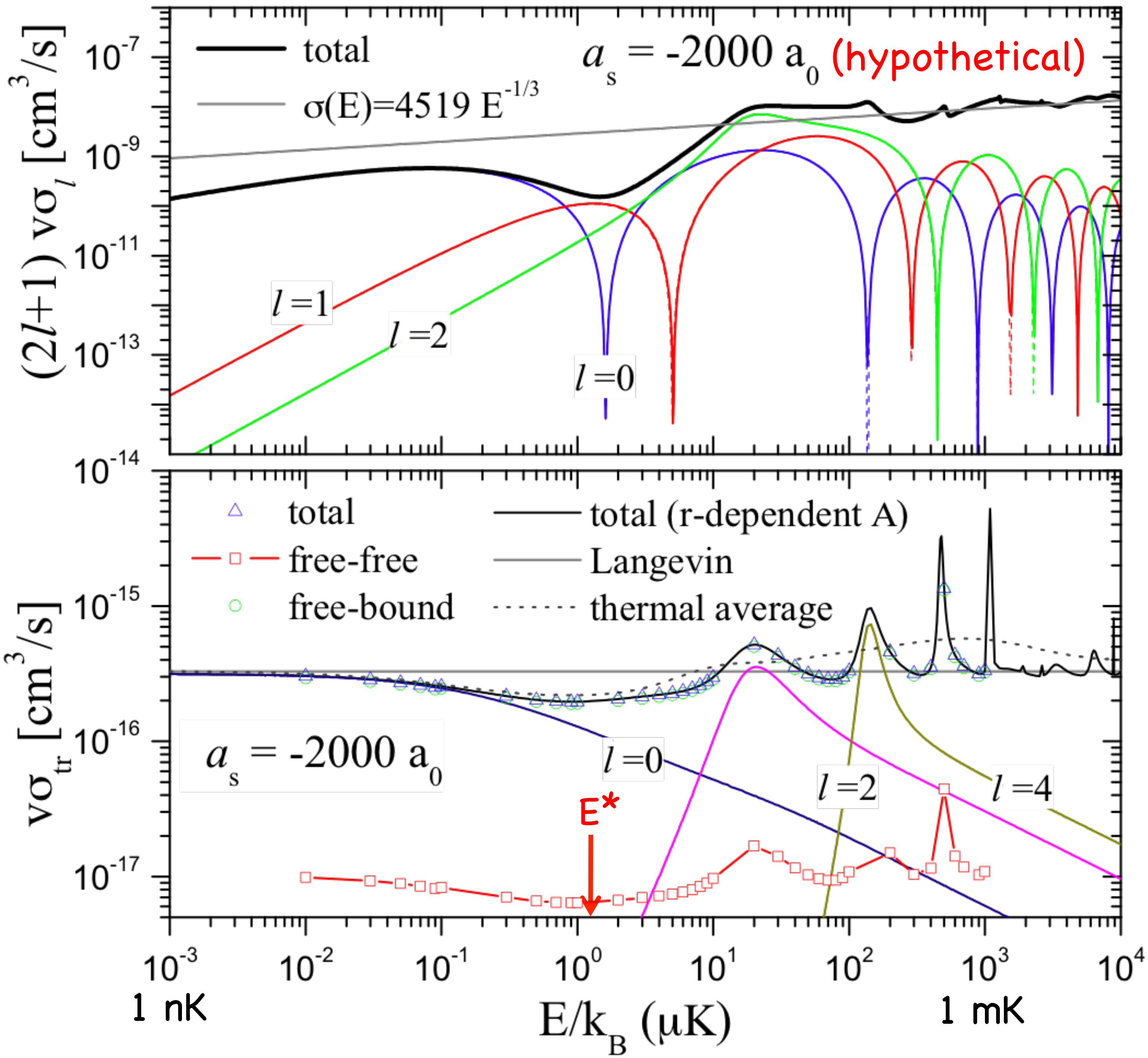
Quantum correction

$$Q(E) = \frac{1}{2kR^*} \sum_{\ell=0}^{\infty} (2\ell + 1)\, C^{-2}(E, \ell)$$

QDT function

Thermal average

$$Q(T) = \langle Q(E) \rangle_T$$



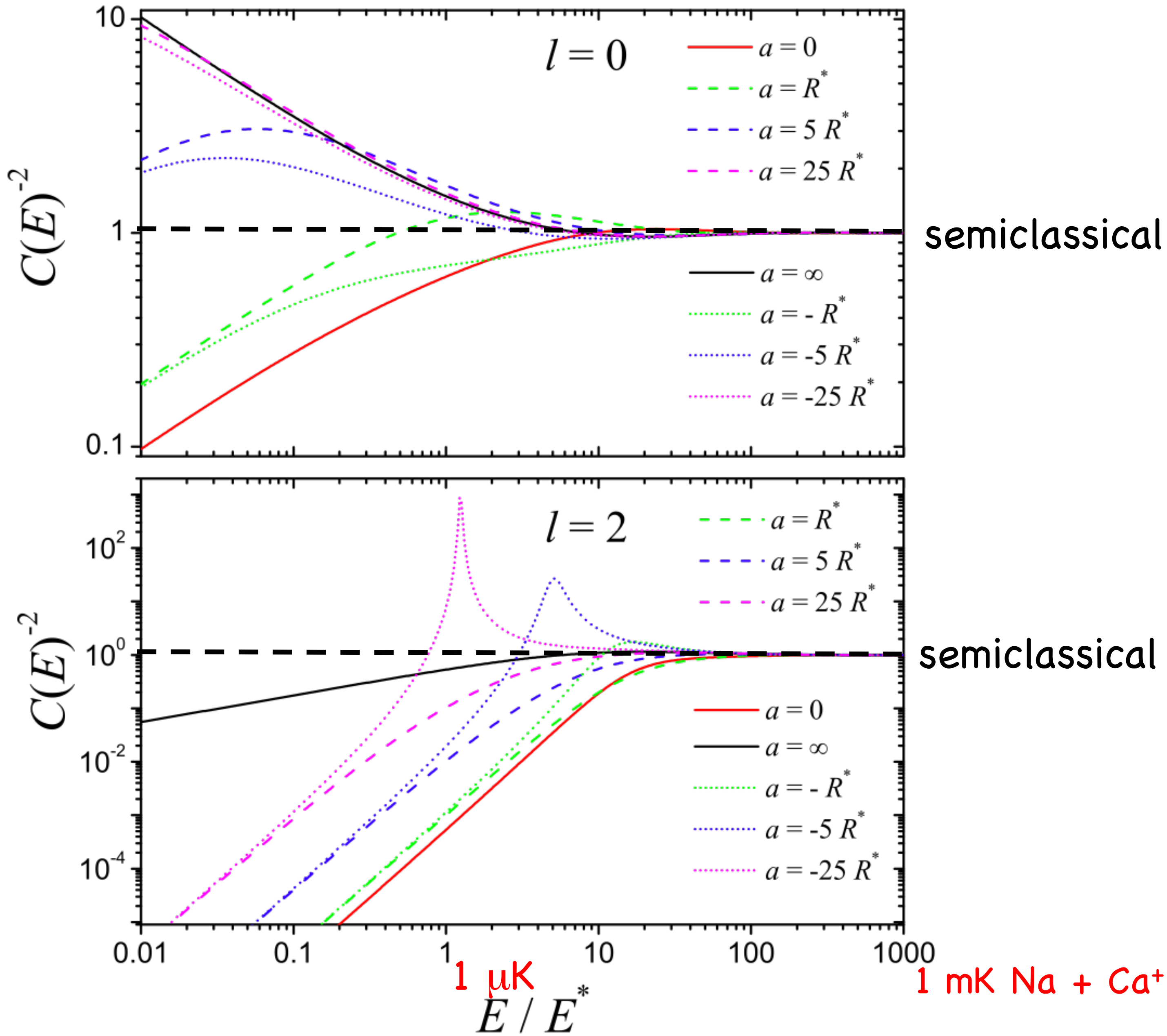
CC/QDT
Agree well

Elastic K

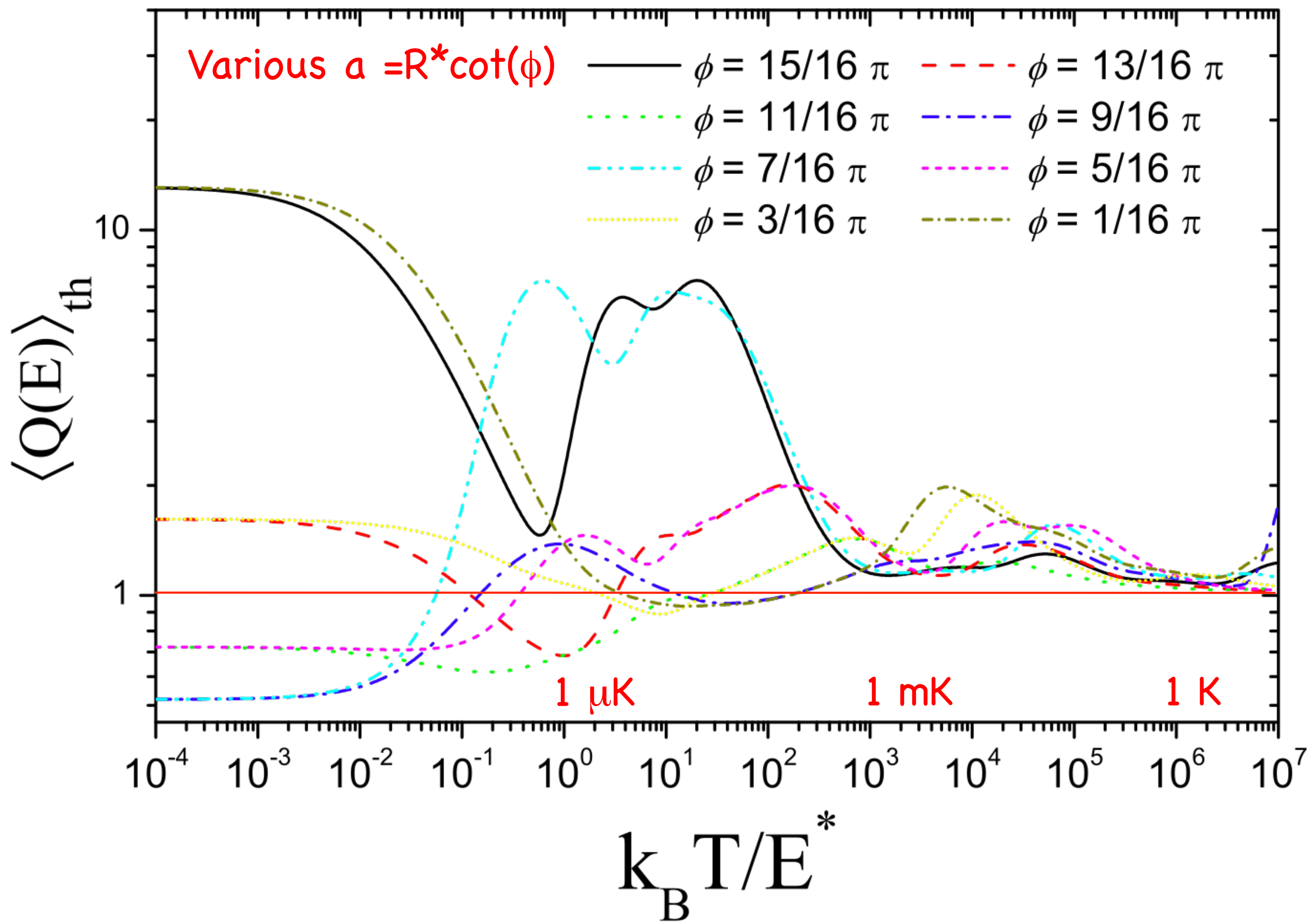
Charge
Transfer K

QDT $C^{-2}(E)$ Function

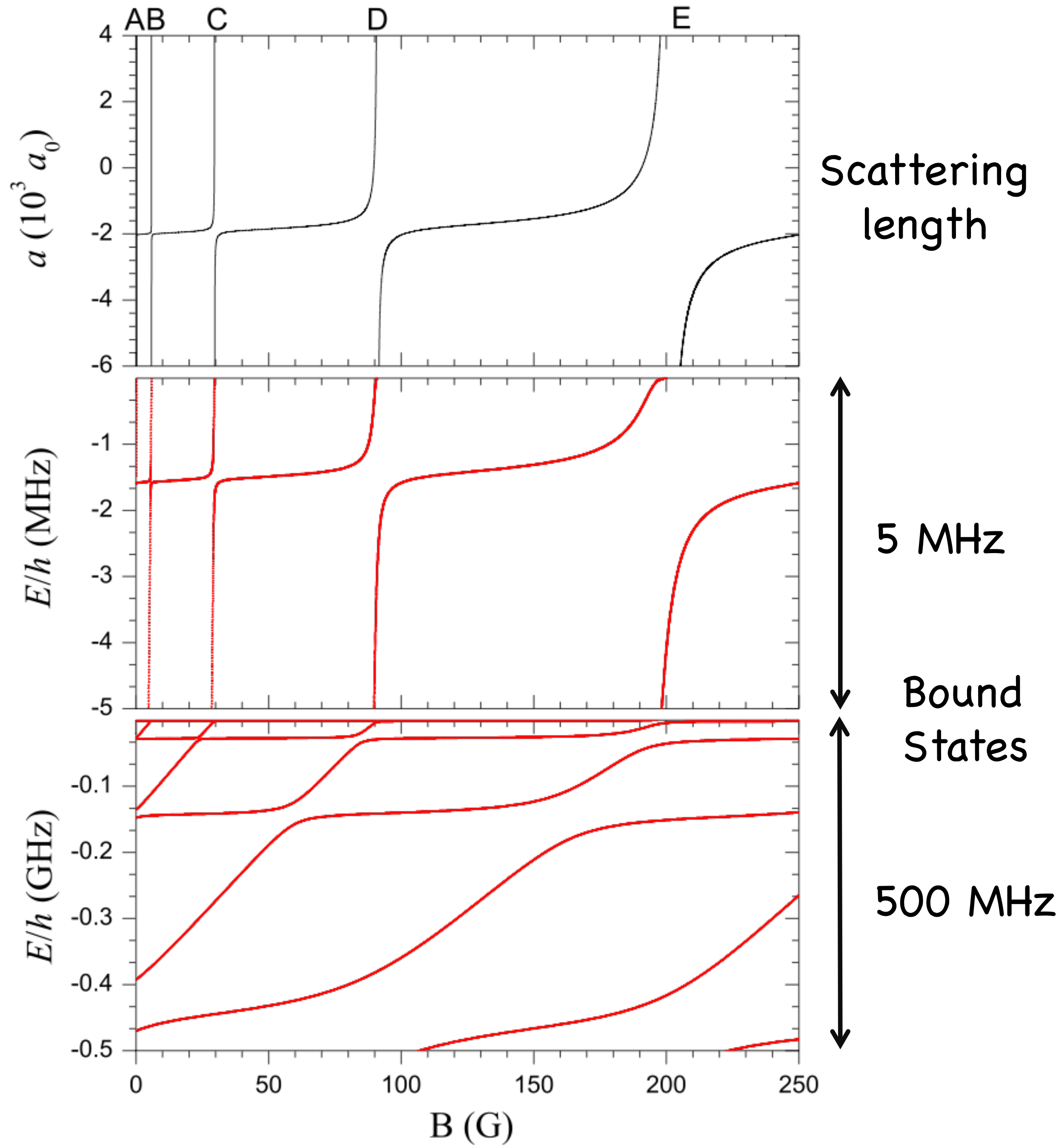
Connects quantum to semiclassical



Quantum corrections for radiative CT



Feshbach Resonance Example
a_s=+R*
a_t=-R*



Scattering length

5 MHz

Bound States

500 MHz

Some conclusions about atom-ion collisions

s-wave limit reached at very low $T \approx 1\ \mu K$. Ion typically at a higher energy scale.

Semiclassical theory useful at typical ion energy scales
But tunneling and resonances makes quantum corrections.

QDT methods agree very well with full quantum scattering calculations and are useful for analysis and calculation. QDT applies to atoms, molecules, and ions, with adaptation to the long range V.

Effect of trap potential and micromotion needs to be included in the analysis (Poster 43 S. Srinivasari)

The End