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)

Some resources

Jones et al, Rev. Mod. Phys. 78, 483 (2006)
van der Waals properties + PA review
Julienne and Mies, J. Opt. Soc. Am. B 6, 2257 (1989)
WKB/quantum connections and threshold laws

Burnett et al, Nature 416, 225 (2002)
“box”interpretation of A + simple review of cold collisions

Kohler, Goral, Julienne, cond-mat/0601429 (in press, Rev. Mod. Phys.)
Production of cold molecules via magnetically tunable
Feshbach resonances

In progress, Chin, Grimm, Tiesinga, Julienne, Rev. Mod. Phys.
Feshbach resonances in ultracold gases
(look at preprint server by end of 2006)

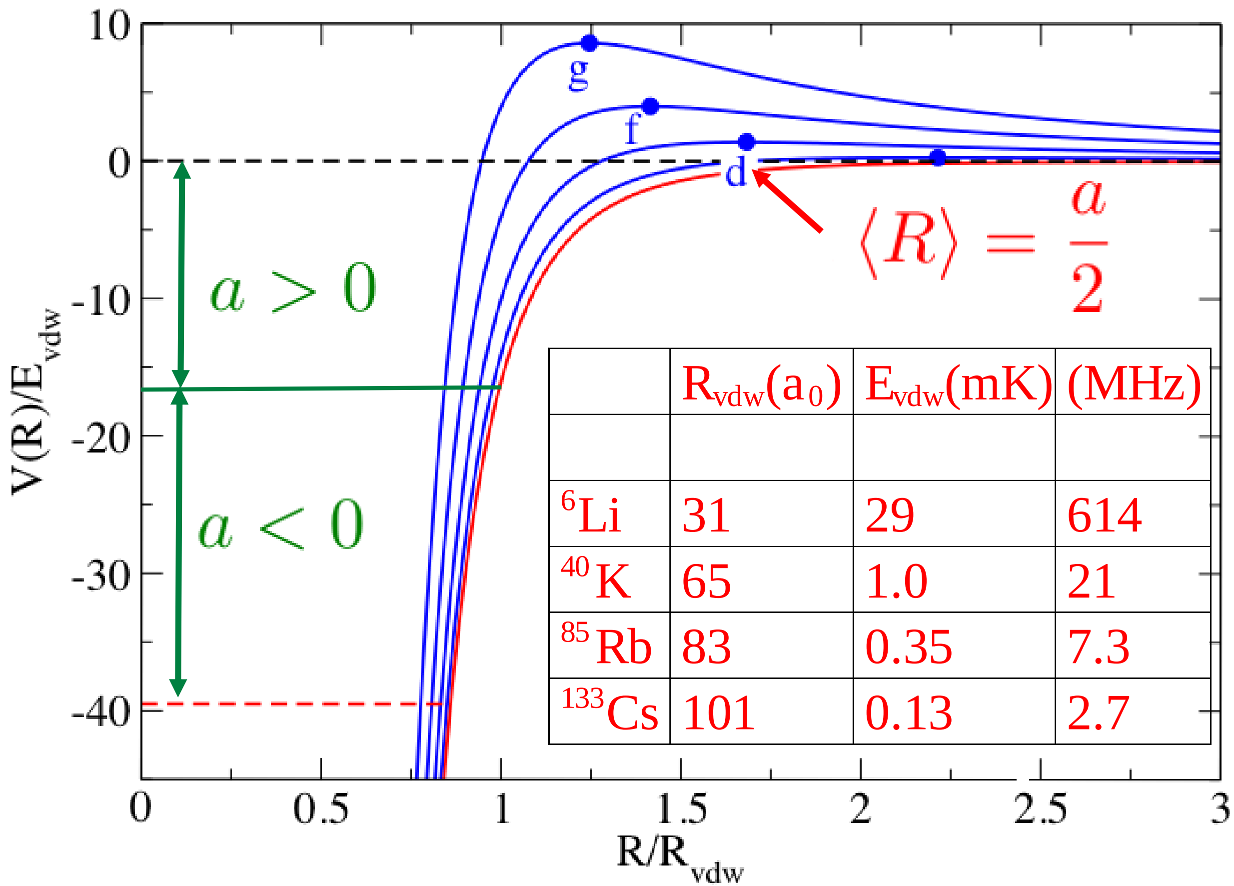
“Size” of potential V(R)

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

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

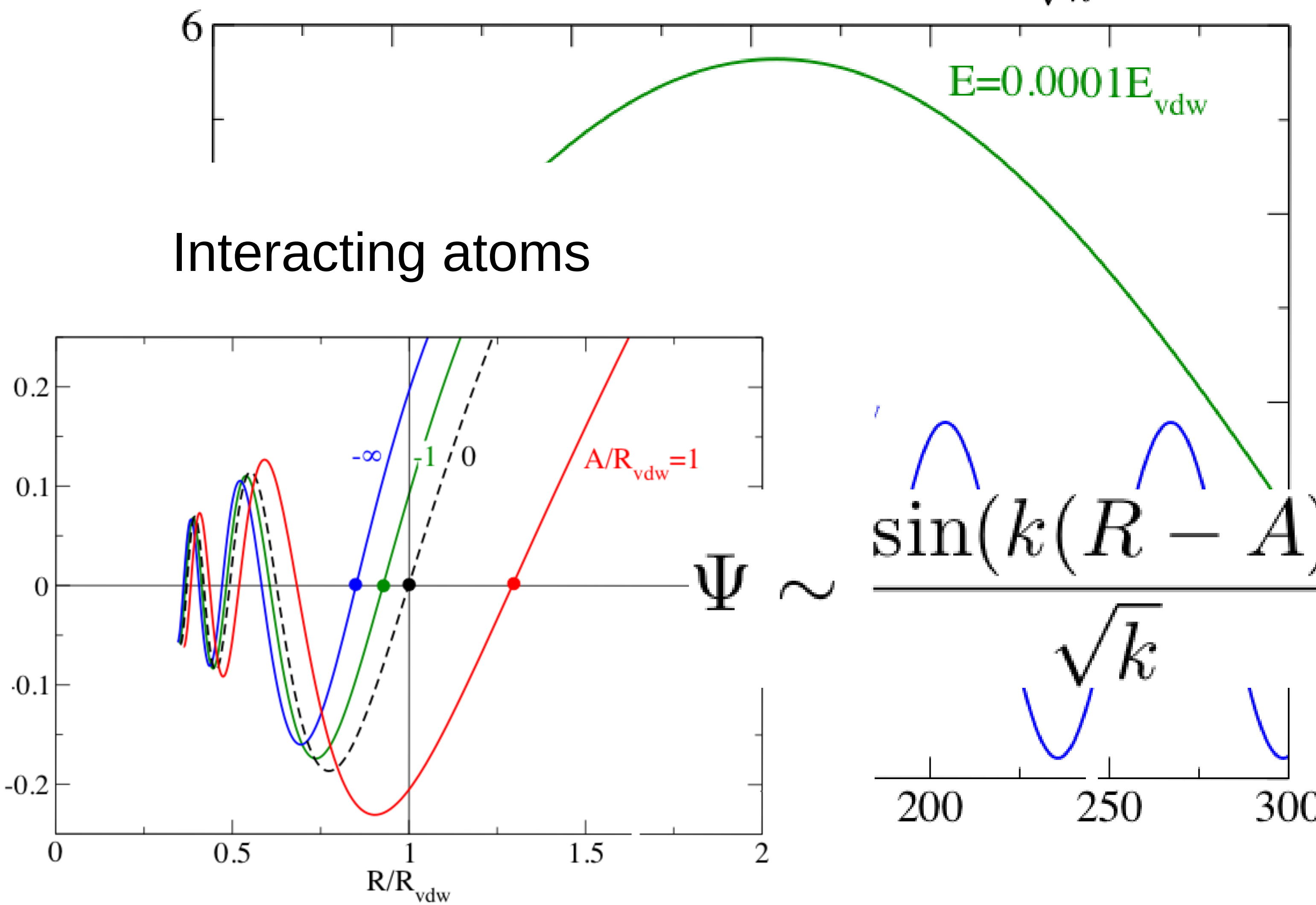
Gribakin and Flambaum, Phys. Rev. A 48, 546 (1993)

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



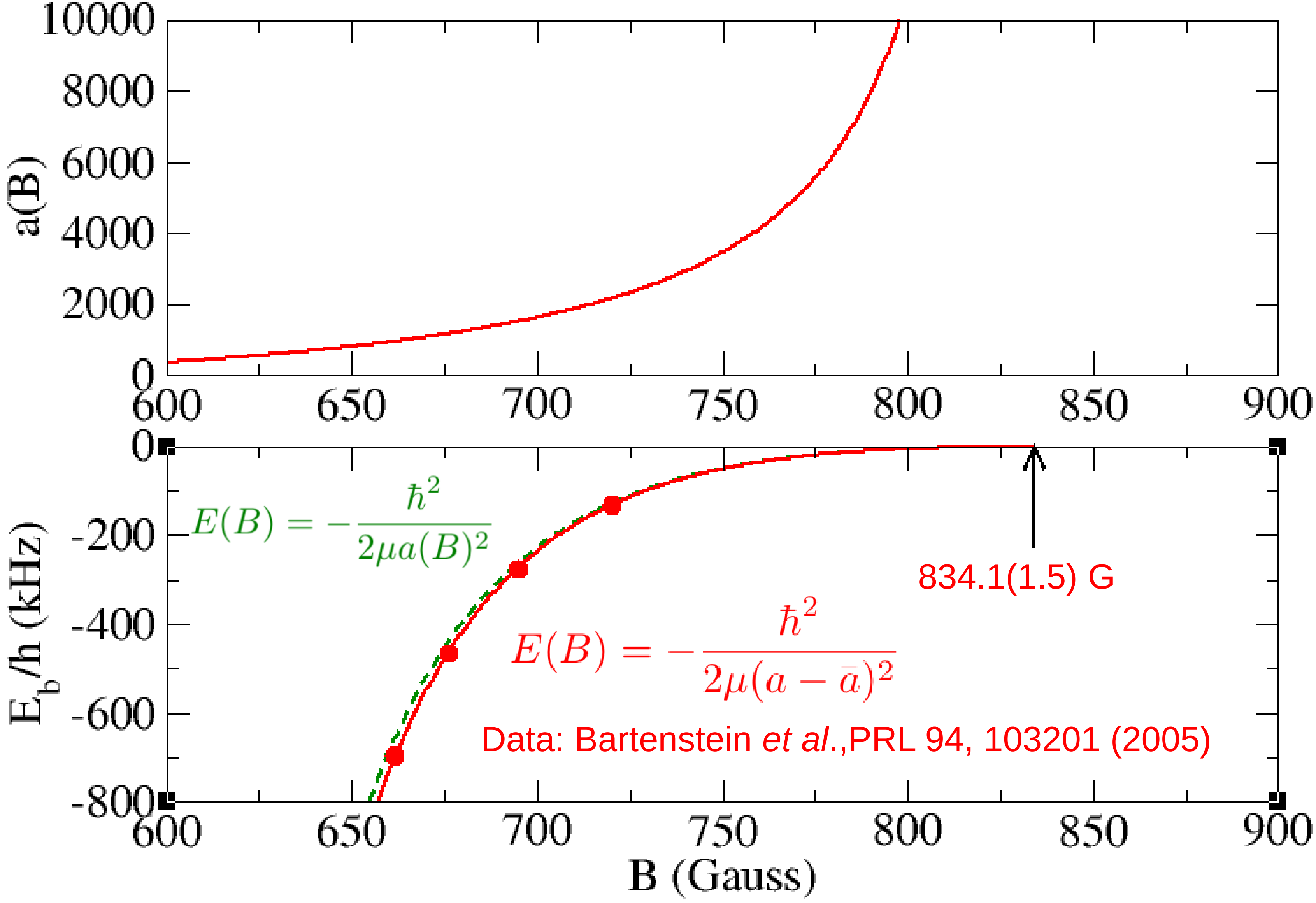
	$R_{\rm vdw}(a_0)$	$E_{\rm vdw}$(mK)	(MHz)
^{6}Li	31	29	614
^{40}K	65	1.0	21
^{85}Rb	83	0.35	7.3
^{133}Cs	101	0.13	2.7

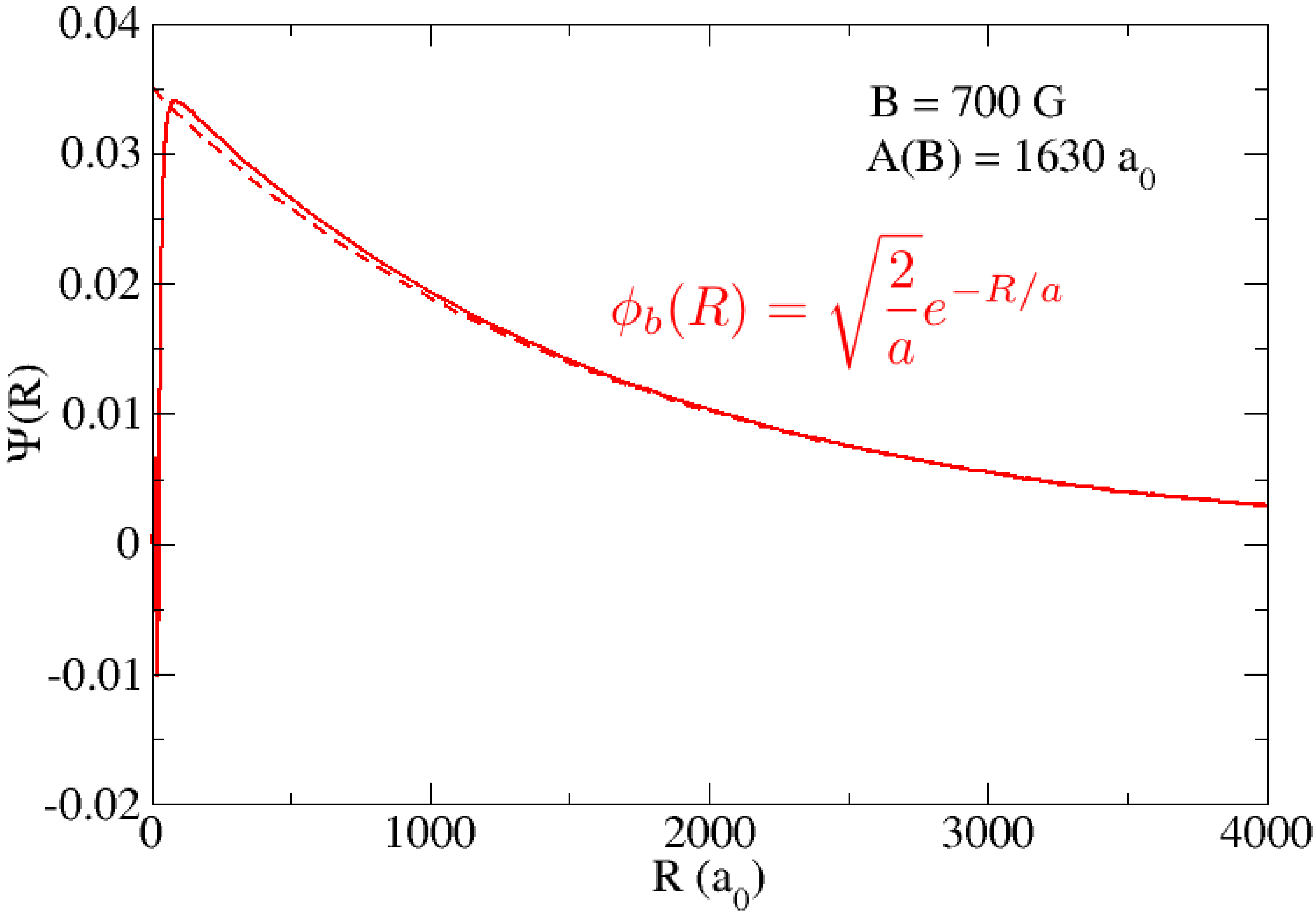
Noninteracting atoms $\Psi \sim \frac{\sin(kR)}{\sqrt{k}}$



Interacting atoms

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

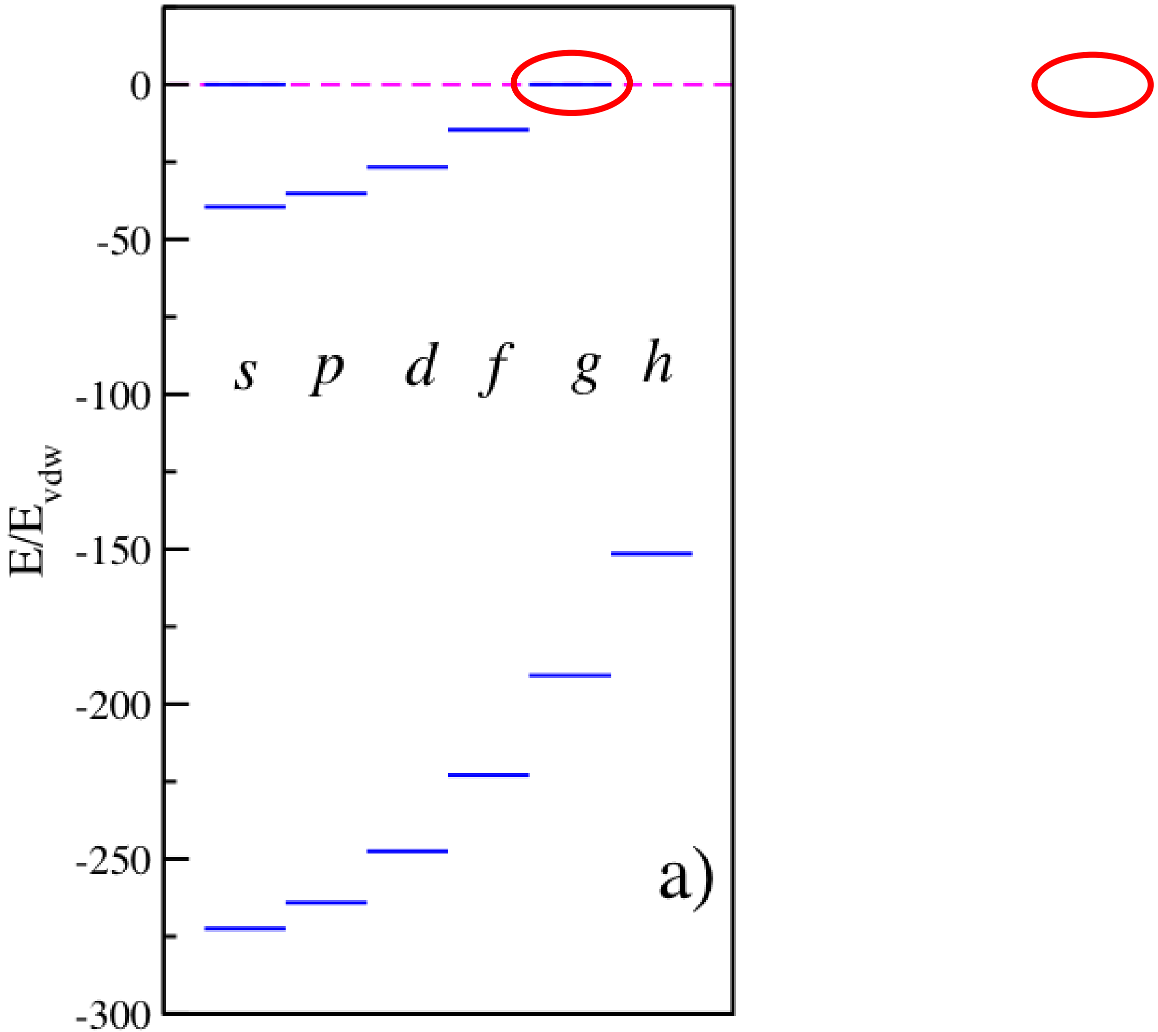

10000
8000
6000
4000
2000
0
a(B)
600
650
700
750
800
850
900
0
-200
-400
-600
-800
E_b/h (kHz)
$E(B) = -\frac{\hbar^2}{2\mu a(B)^2}$
834.1(1.5) G
$E(B) = -\frac{\hbar^2}{2\mu(a-\bar{a})^2}$
Data: Bartenstein *et al*.,PRL 94, 103201 (2005)
B (Gauss)



B = 700 G
A(B) = 1630 a0
$\phi_b(R) = \sqrt{\frac{2}{a}} e^{-R/a}$
Ψ(R)
R (a0)
0.04
0.03
0.02
0.01
0
-0.01
-0.02
0
1000
2000
3000
4000

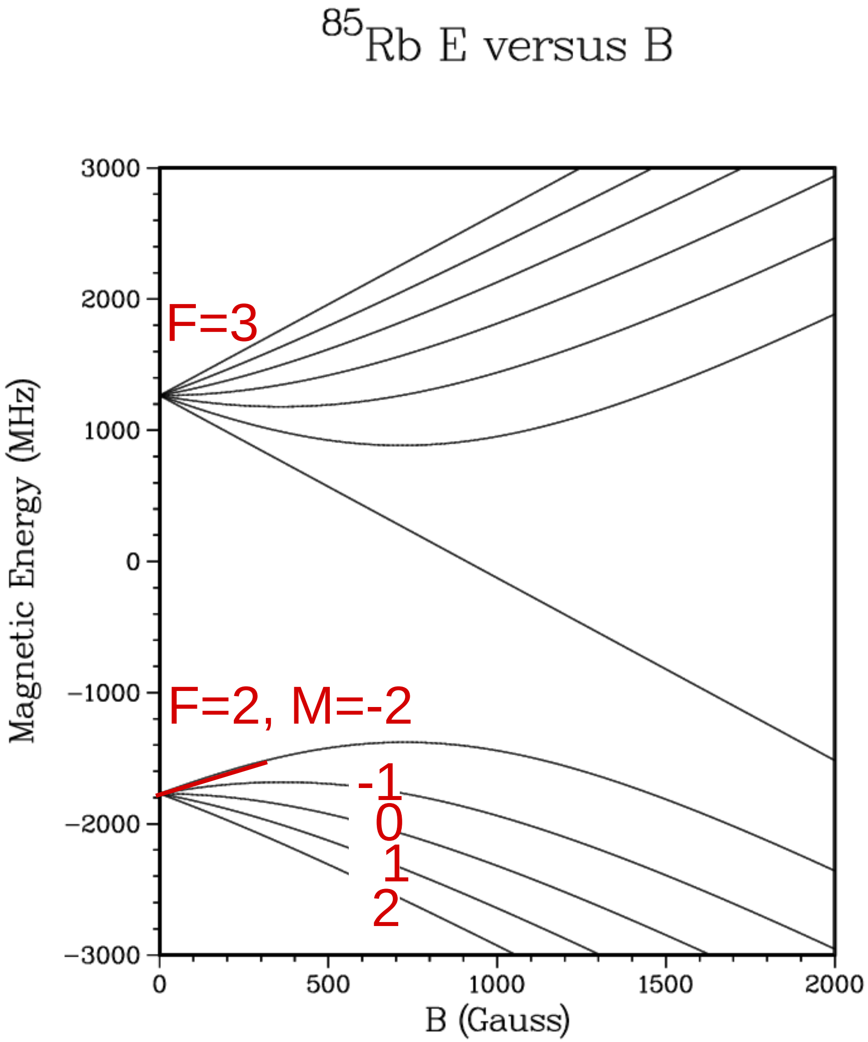
Bound states from van der Waals theory

$a = \pm\infty$ $a = \bar{a}$



Gao, Phys. Rev. A 62, 050702 (2000); Figure from E. Tiesinga

Inelastic collisions



For example:

(2,-2)+(2,-2) -->(2,-2)+(2,-1)

-->(2,-2)+(2,0)

-->(2,-1)+(2,-1)

Probability $|S_{\alpha\alpha'}|^2 \propto k^{2\ell+1}$

because

$$|\phi_\alpha(R < R_{\mathrm{vdW}})|^2 \propto k^{2\ell+1}$$

$$\text{as } k \to 0$$

For s-waves, let

$$|S_{\alpha\alpha'}|^2 = 4kb_{\alpha\alpha'}$$

Inelastic collisions

$$e^{i\vec{k}\cdot\vec{R}}|ab\rangle \; + \; \sum_{a'b'} f_{ab,a'b'}(\Omega)\frac{e^{ik'R}}{R}|a'b'\rangle$$

Scattering channels

Initial channel: $\{F_a M_a,\, F_b M_b\}\ell m_\ell = \alpha$

Final channel: $\{F_a' M_a',\, F_b' M_b'\}\ell' m_\ell' = \alpha'$

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

$$\sigma_{\alpha,\alpha'} = \frac{\pi}{k^2}|T_{\alpha,\alpha'}|^2$$

Inelastic collisions continued

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

Complex scattering length *a-ib*

$$\boxed{\begin{aligned} \sigma_{\alpha\alpha} &= 4\pi(a^2 + b^2) \\ K_{\text{loss}} &= \sum_{\alpha' \neq \alpha} K_{\alpha\alpha'} = 2\frac{h}{\mu} b \end{aligned}}$$

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

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

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

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

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

Small spin-dependent potential changes ℓ

s-wave Threshold Collisions Summary

Cross section σ cm^2

Rate coefficient $K = \langle \sigma v \rangle$ cm^3/s

Elastic collisions

$\sigma \rightarrow$ constant, $K \rightarrow v$

$\sigma = 4\pi(a^2+b^2)$

Inelastic collisions

$\sigma \rightarrow 1/v$, $K \sim$ constant

$K = (4h/m)b$

Complex scattering length $a - ib$

How fast are (inelastic s-wave) cold collisions?

$$\frac{dn}{dt} = -2Kn^2 = -\frac{1}{\tau}n \quad \text{where} \quad \frac{1}{\tau} = 2Kn$$

$$K = \frac{h}{m} 4B = (8\times 10^{-11}\,\mathrm{cm}^3/\mathrm{s})\frac{B(\mathrm{a}_0)}{m(\mathrm{amu})}$$

Typical strong event (B ~ x_0): 10^{-10} cm^3/s, MOT or BEC

$$\frac{1}{\tau} = 2Kn = n\frac{h}{m} 8B = n(1.6\times 10^{-10}\,\mathrm{cm}^3/\mathrm{s})\frac{B(\mathrm{a}_0)}{m(\mathrm{amu})}$$

In a MOT: τ ~ 0.1 to 1 s

In a BEC (use K/2): τ ~ 10 to 100 μs

How fast are inelastic cold collisions (Maxwell-Boltzmann)?

$$\frac{dn}{dt} = -2Kn^2 = -\frac{1}{\tau}n \quad \text{where} \quad \frac{1}{\tau} = 2Kn$$

$$K = \frac{1}{Q_T}\frac{k_B T}{h} \sum_{\ell}(2\ell+1)\left\langle |S(E)|^2 \right\rangle$$

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

l=0 only

Q_T = translational partition function

Λ_T = thermal de Broglie wavelength

Probability $|S|^2 < 1$

Dynamical factor

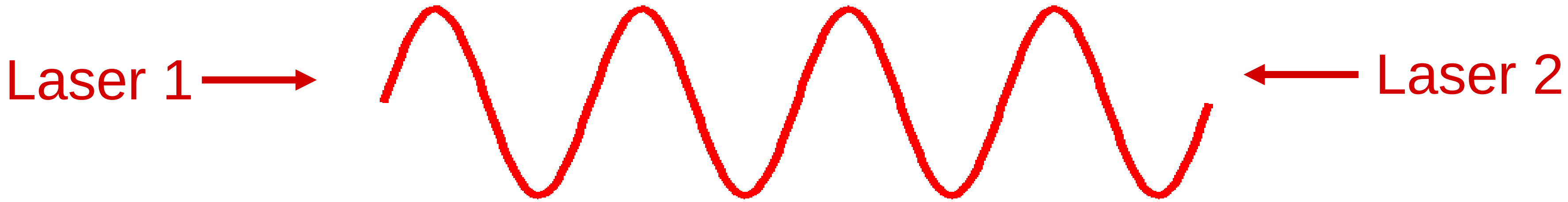
$$\frac{1}{\tau} = 2Kn = 2\,(n\Lambda_T^3)\,\frac{k_B T}{h}\,f$$

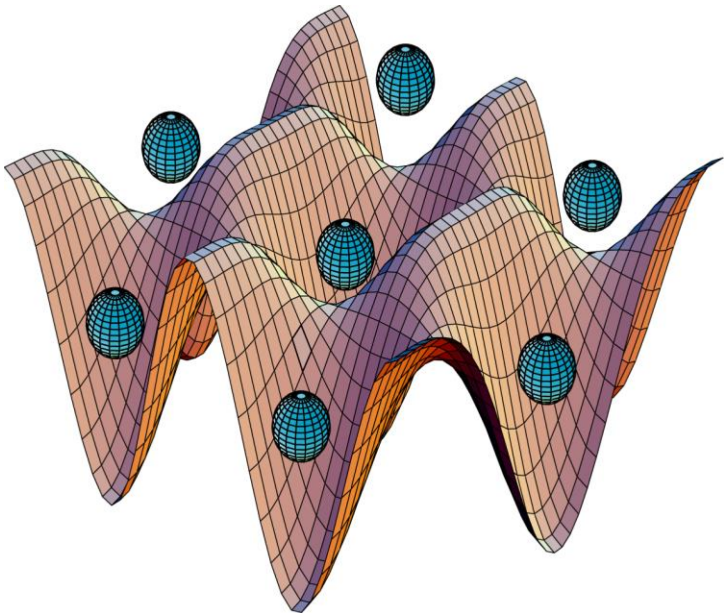
Phase Space density

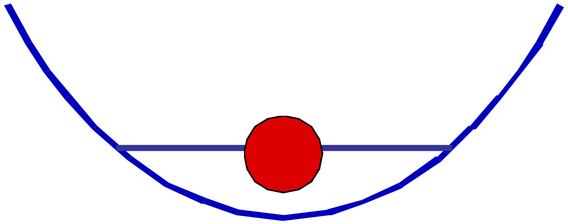
Upper bound

Dynamics

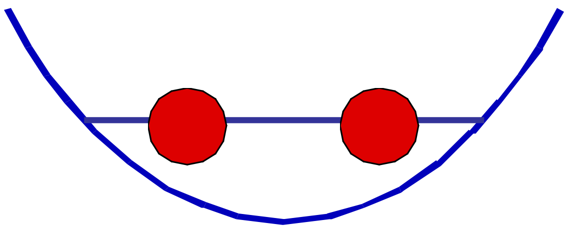
An Optical Lattice



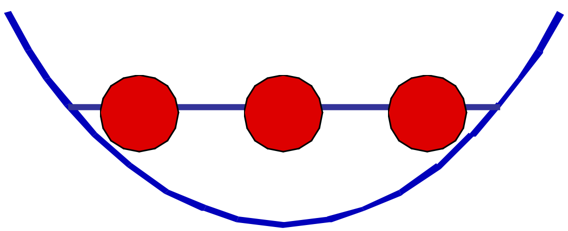




1 Atom per cell
Control



2 Atoms per cell
2-body levels, dynamics



3 Atoms per cell
3-body levels, dynamics

Two atoms in a trap

3D spherically symmetric harmonic trap: $\omega = 2\pi\nu$

2-body potential: V(r)

Separate the center of mass and relative motion

Center of mass $$\left[-\frac{\hbar^2}{2(2m)}\nabla_R^2 + \frac{1}{2}(2m)\omega^2 R^2 \right]\Psi_{cm}(R) = E_{cm}\Psi_{cm}(R)$$

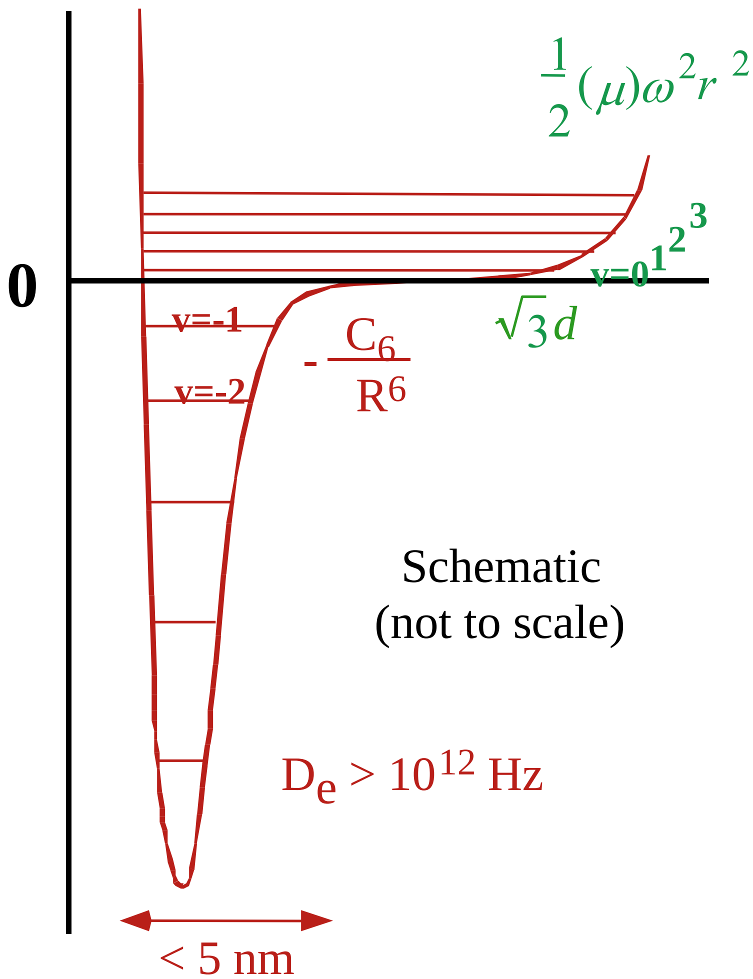
Relative $$\boxed{\left[-\frac{\hbar^2}{2(\mu)}\nabla_r^2 + \underbrace{\frac{1}{2}(\mu)\omega^2 r^2 + V(r)}_{V_{eff}(r)} \right]\Psi(r) = E\Psi(r)}$$

Scale size of trap:

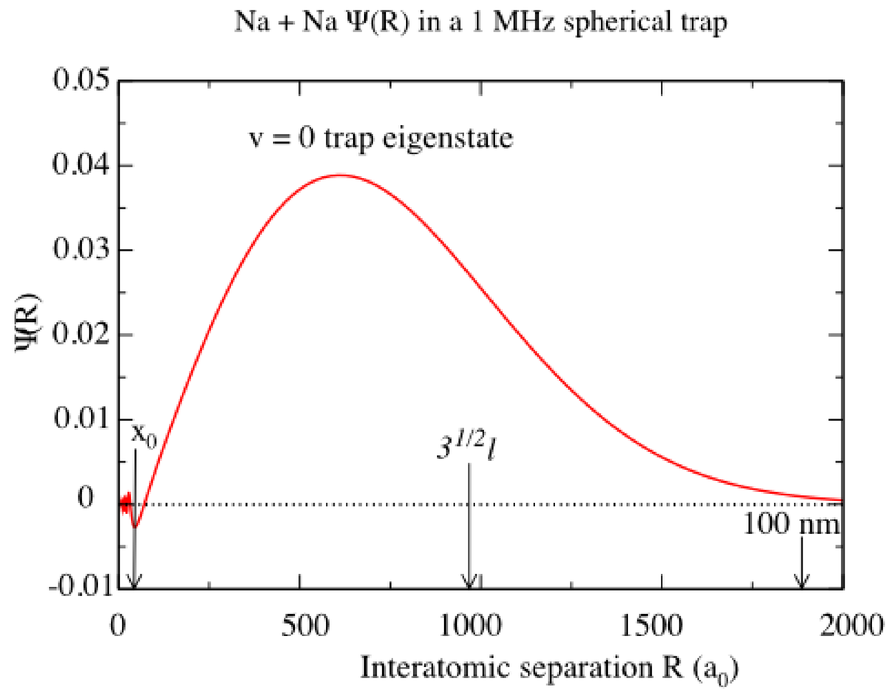
$$d = \sqrt{\frac{\hbar}{\mu\omega}}$$

Scale size of V(r)

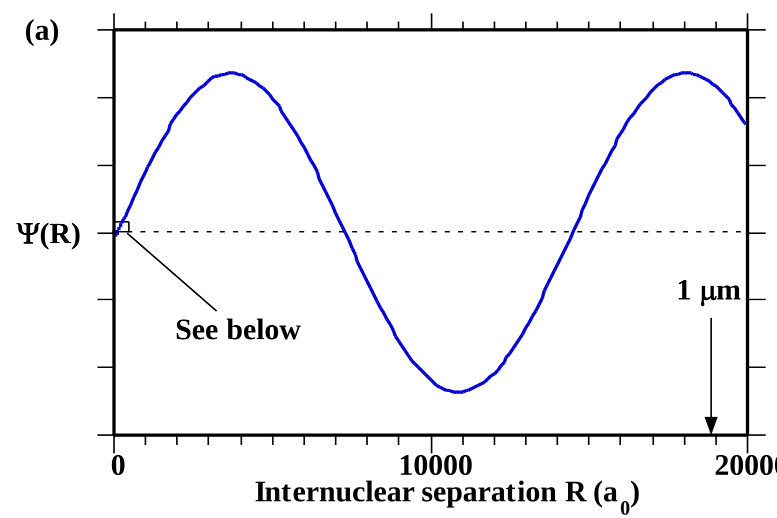
x_0



0
v=-1
v=-2
v=0
1
2
3
$\frac{1}{2}(\mu)\omega^2 r^2$
$\sqrt{3}d$
$-\frac{C_6}{R^6}$
Schematic
(not to scale)
$D_e > 10^{12}$ Hz
< 5 nm



Na + Na Ψ(R) in a 1 MHz spherical trap
v = 0 trap eigenstate
Ψ(R)
x_0
$3^{1/2} l$
100 nm
0.05
0.04
0.03
0.02
0.01
0
-0.01
0
500
1000
1500
2000
Interatomic separation R (a_0)



(a)
Ψ(R)
See below
1 μm
0
10000
20000
Internuclear separation R (a_0)

E-dependent pseudopotential

D. Blume and Chris H. Greene, Phys. Rev. A 65, 043613 (2002)
E. L. Bolda, E. Tiesinga, and P. S. Julienne, Phys. Rev. A 66, 013403 (2002)

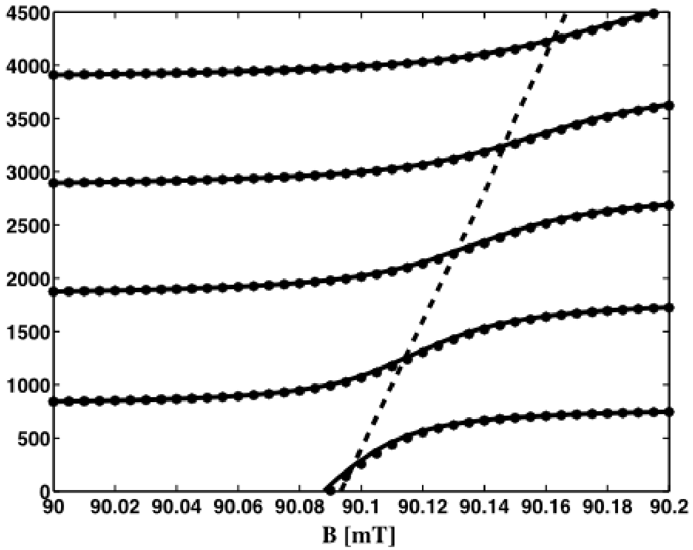
Energy-dependent pseudopotential for trap level E_n:

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

$$a(E_n) = -\frac{\tan\eta(E_n)}{k}$$

$a(E_n)$ from scatttering calculation of $\eta(E_n)$

Na F=1,M=+1
Energy levels in a
1 MHz harmonic trap
(Bolda et al., 2002)

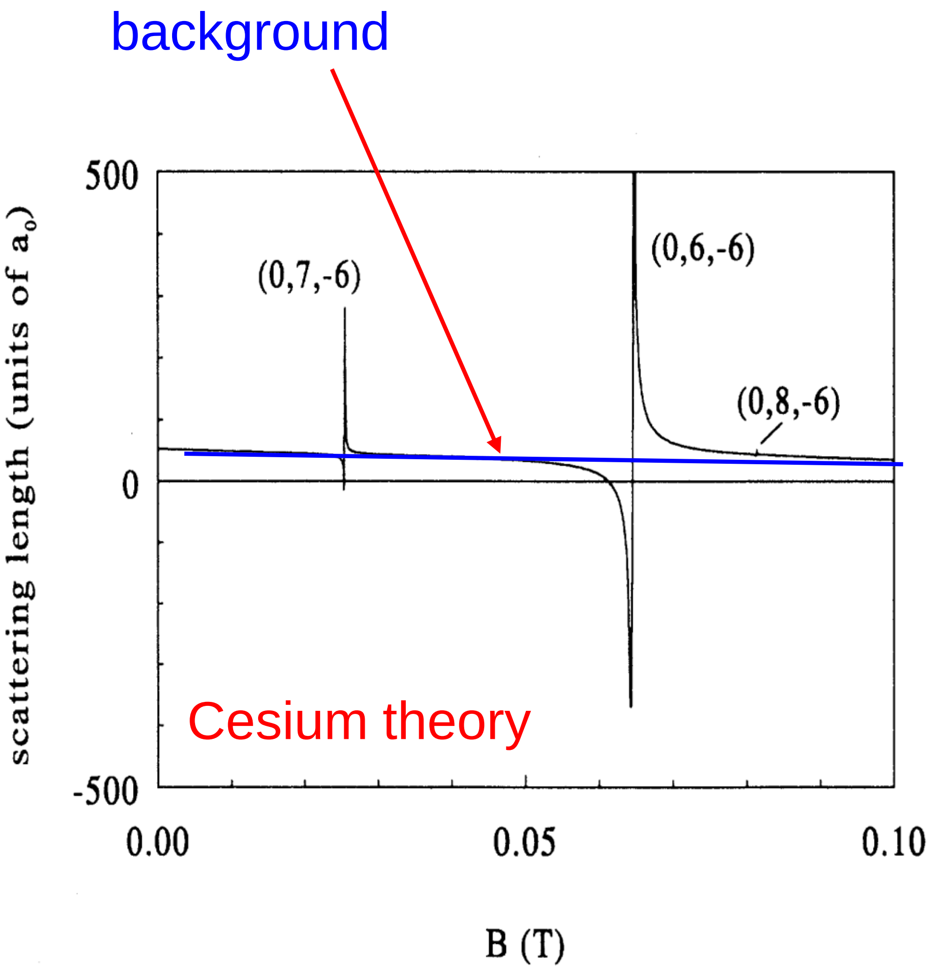


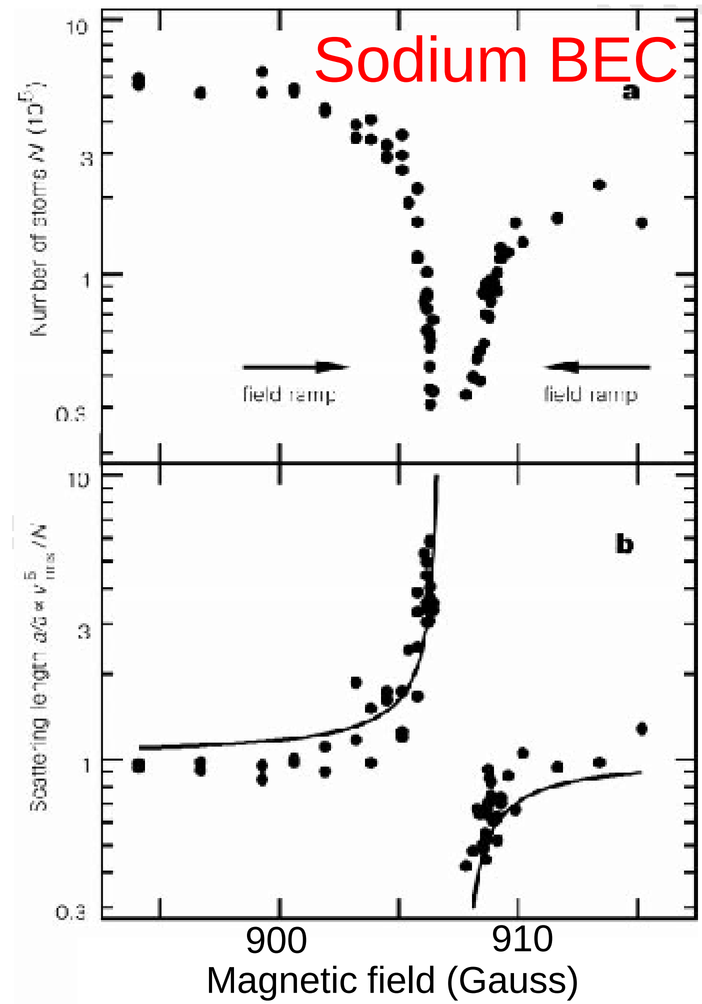
Points: numerical coupled channels
Solid Line: pseudopotential

Feshbach resonances and Feshbach molecules

- What is a scattering resonance?
- Basic properties of threshold resonance scattering and bound states
- Halo molecules
- Simple parameterization by 5 key parameters:
  - a_{bg} (background scattering length), C_6 (van der Waals coefficient), m (mass)
  - Δ (width), $\delta\mu$ (magnetic moment difference)
- Basic molecular physics of alkali atom resonances
- Illustration of typical resonances: ^{6}Li, ^{85}Rb, ^{87}Rb, ^{40}K, Cs
- Resonance dynamics—making and dissociating molecules
- Resonances in traps

Some examples of Feshbach resonances





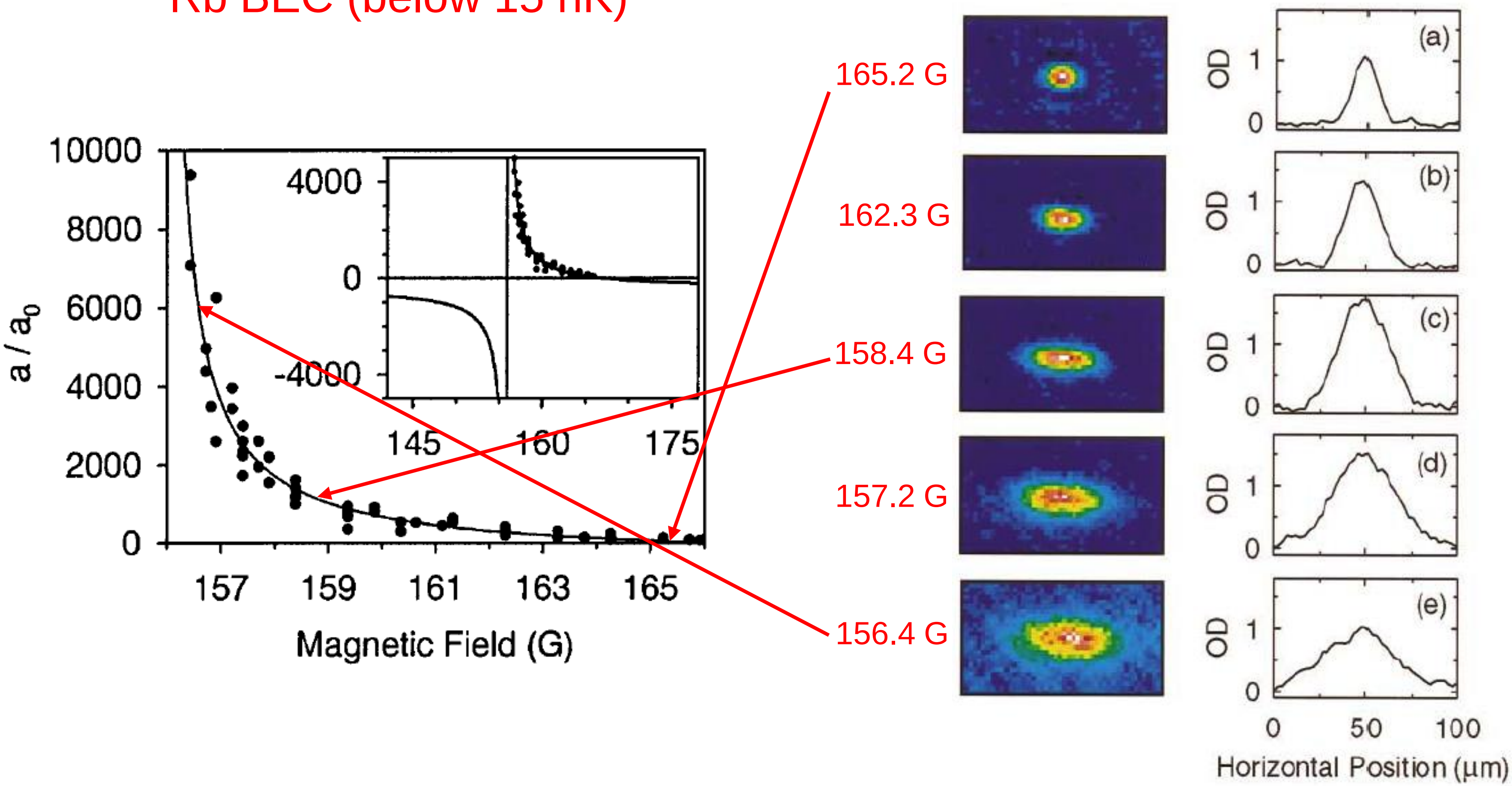
E. Tiesinga *et al*., Phys. Rev. A **47**, 4114 (1993)

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

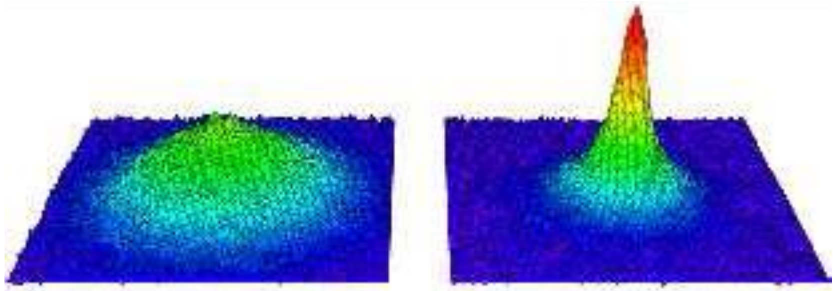
An example for E→ 0

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

^{85}Rb BEC (below 15 nK)



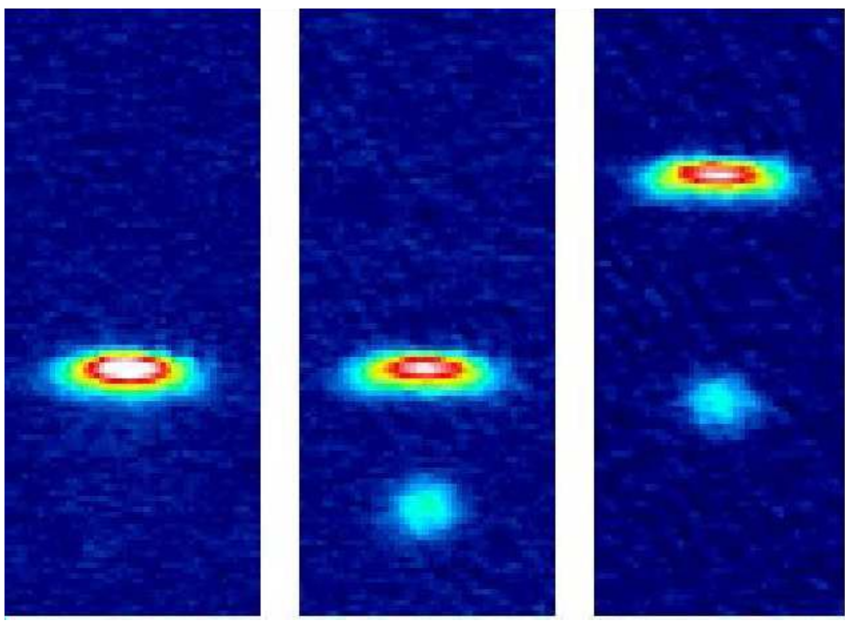
Tunable scattering resonances used for



Thermal (250 nK) BEC (79 nK)

Making $^{40}K_2$ molecules

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



Making $^{133}Cs_2$ molecules

^{133}Cs atom cloud

$^{133}Cs_2$ molecule cloud

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

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

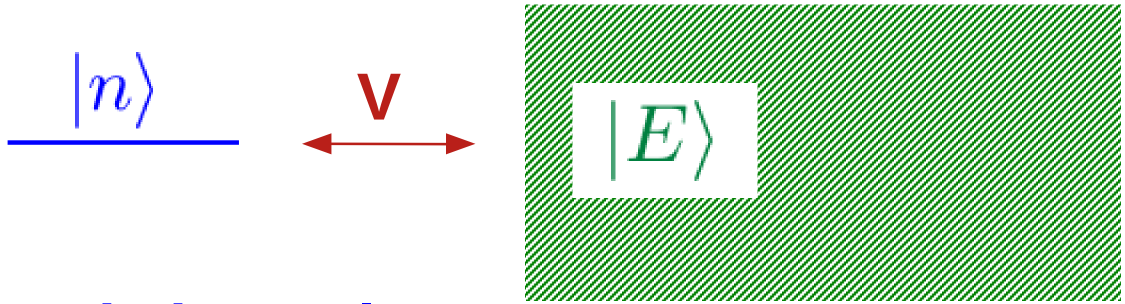
A scattering continuum

with some coupling between them

Resonant Scattering Picture

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

Bound state **Continuum**



Closed channel (Resonance) **Open channel (Background)**

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

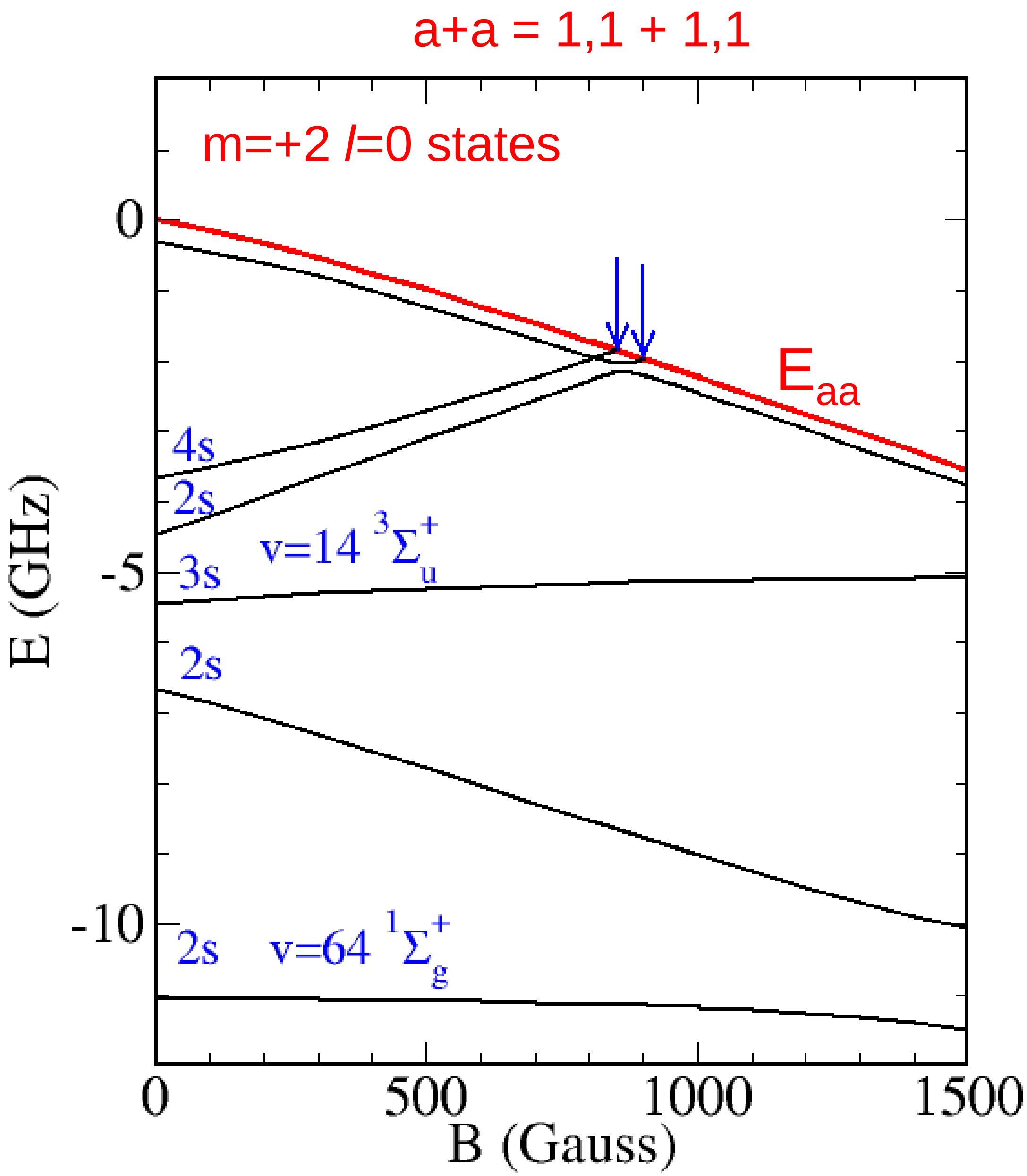
width

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

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

shift

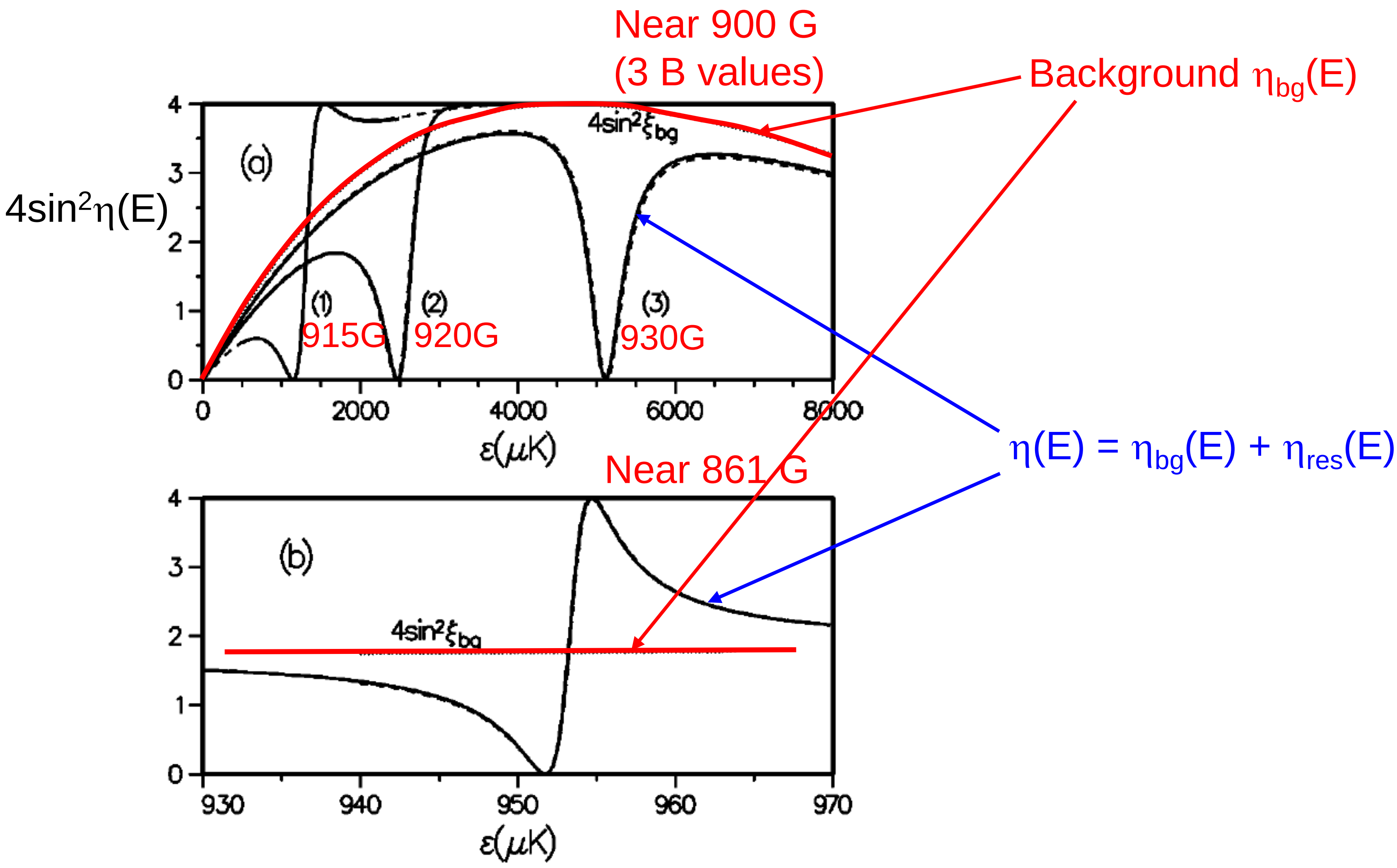
$$\delta E_n = \int \frac{|\langle n|V|E'\rangle|^2}{E_n - E'} dE'$$



Energy levels of the Na_2 dimer just below the a+a threshold

A Na example

From Mies, Tiesinga, Julienne, Phys. Rev. A 61, 022721 (2000)



Threshold Resonant Scattering

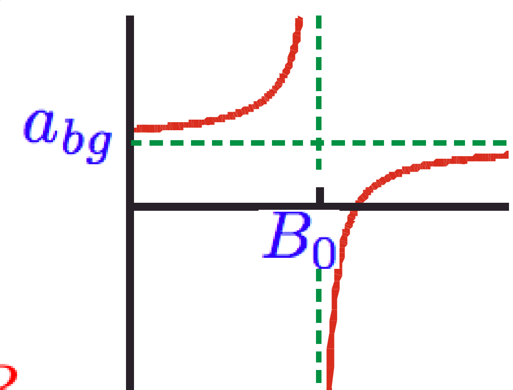
$$E_n = \delta\mu(B - B_n)$$

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

As E → 0 $\quad \eta_{\mathrm{bg}} = -ka_{\mathrm{bg}} \qquad \frac{1}{2}\Gamma_n(E) = (ka_{\mathrm{bg}})\,\delta\mu\,\Delta_n$

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

Shifted $\quad B_0 = B_n + \delta B_n$



Basic resonance parameters

For E --> 0 limit

a_{bg} *"background" scattering length*
B_0 *singularity in a(B)*
Δ *resonance width*
$\delta\mu$ *magnetic moment difference*

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

For finite E and bound states

Effect of interatomic potential
especially van der Waals $-C_6/R^6$

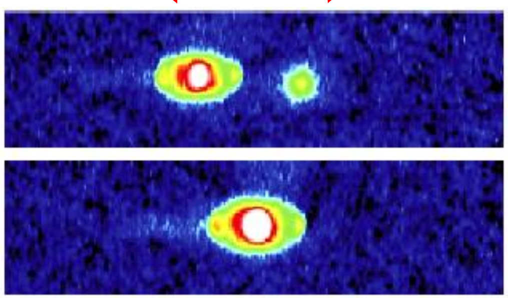
a_{bg} relative to $\bar{a}$
E relative to E_{vdw}

Example ^{87}Rb f=1, m=+1

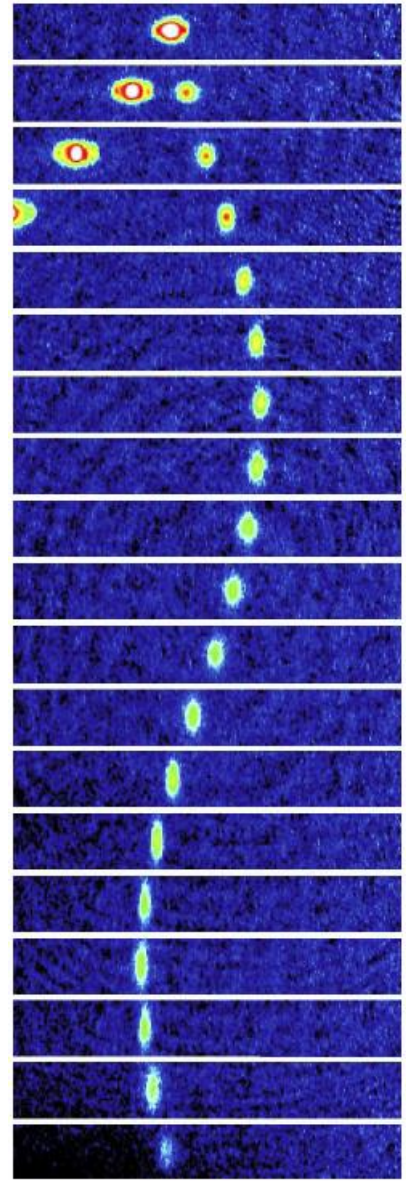
Durr, Voltz, Marte, Rempe, Phys. Rev. Lett. 92, 020406 (2004)

Stern-Gerlach separation of

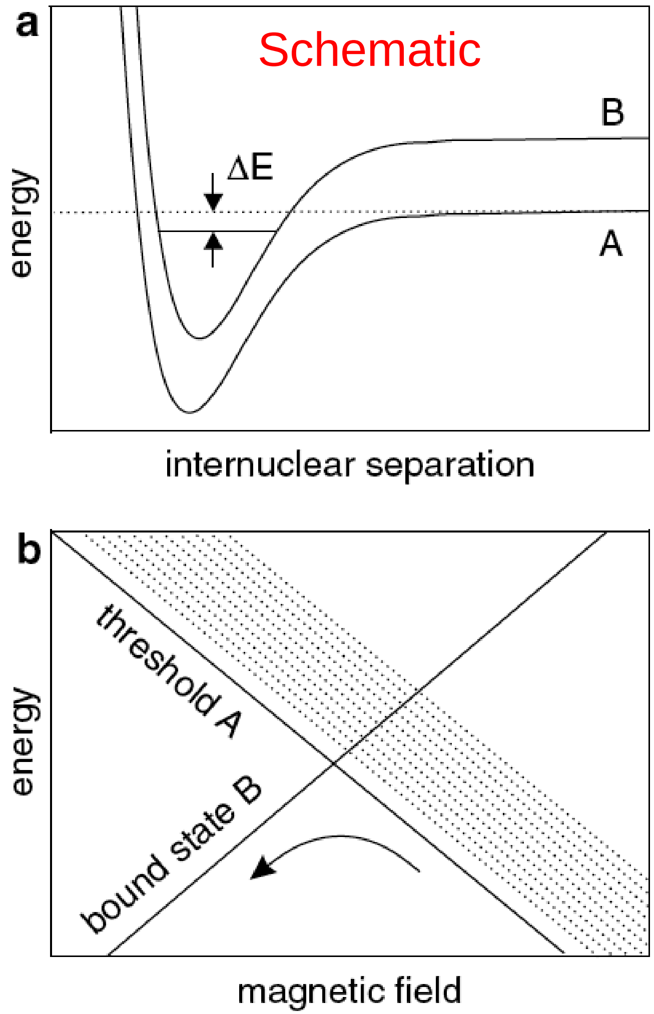
Atoms Molecules

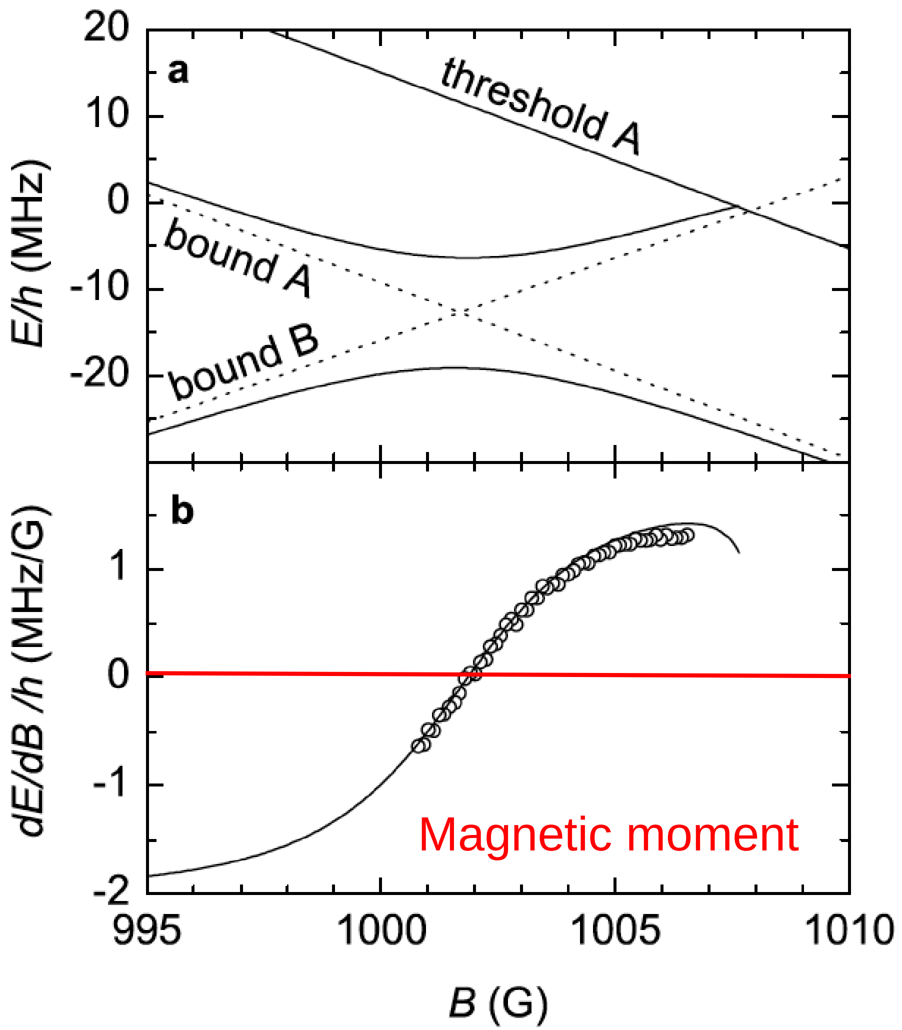


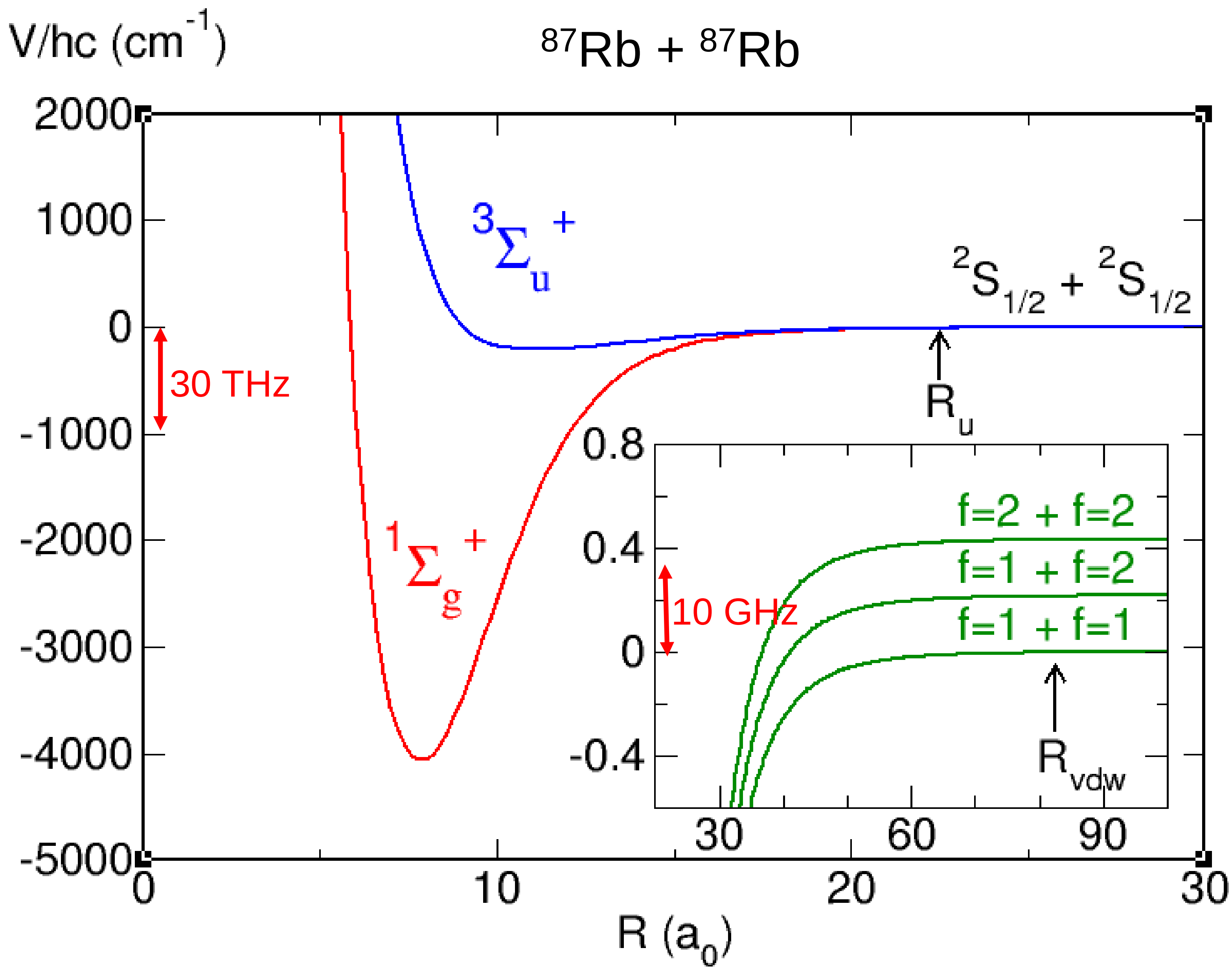
Atom cloud
in trap



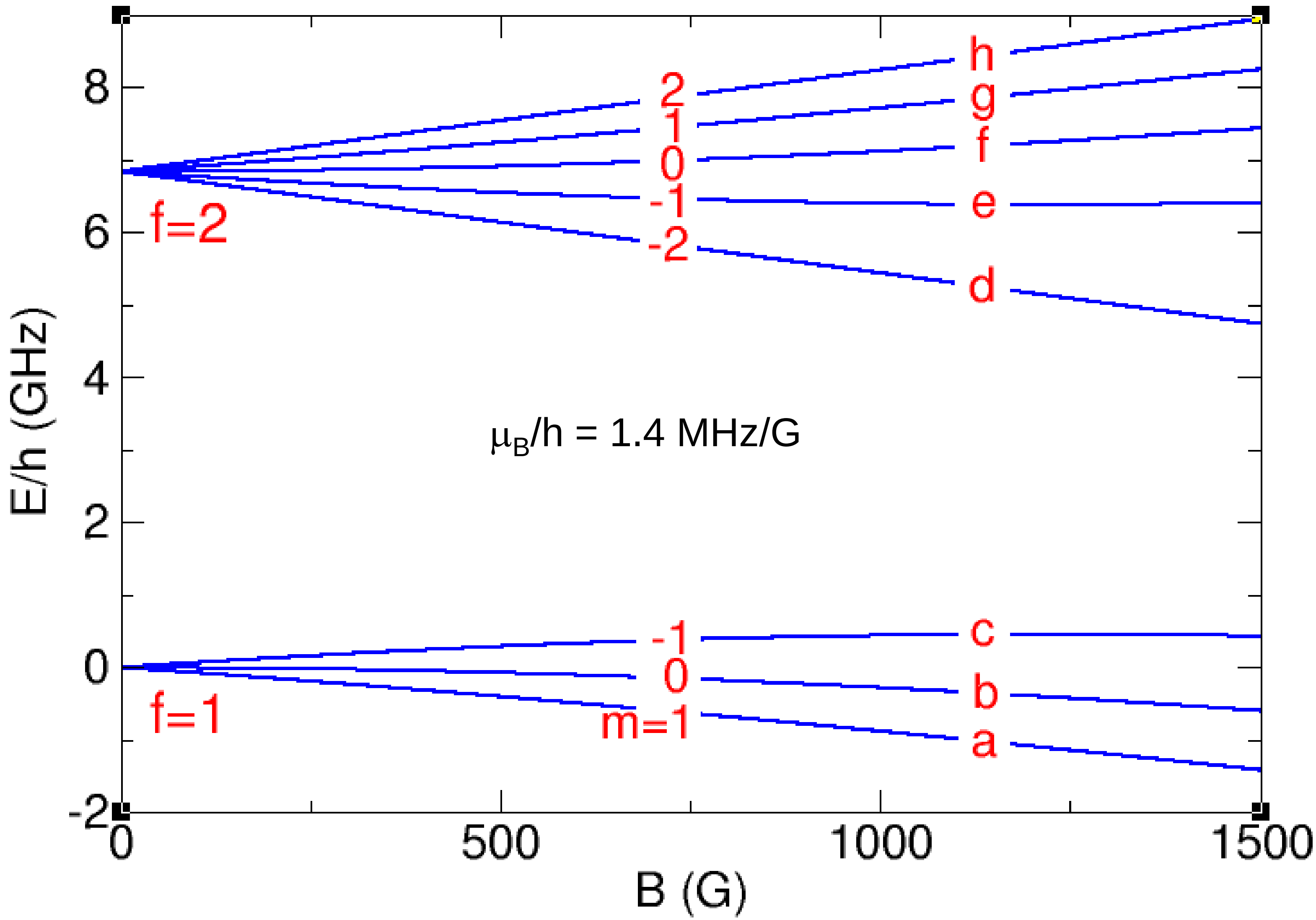
From Durr, Voltz, Marte, Rempe, Phys. Rev. Lett. 92, 020406 (2004)



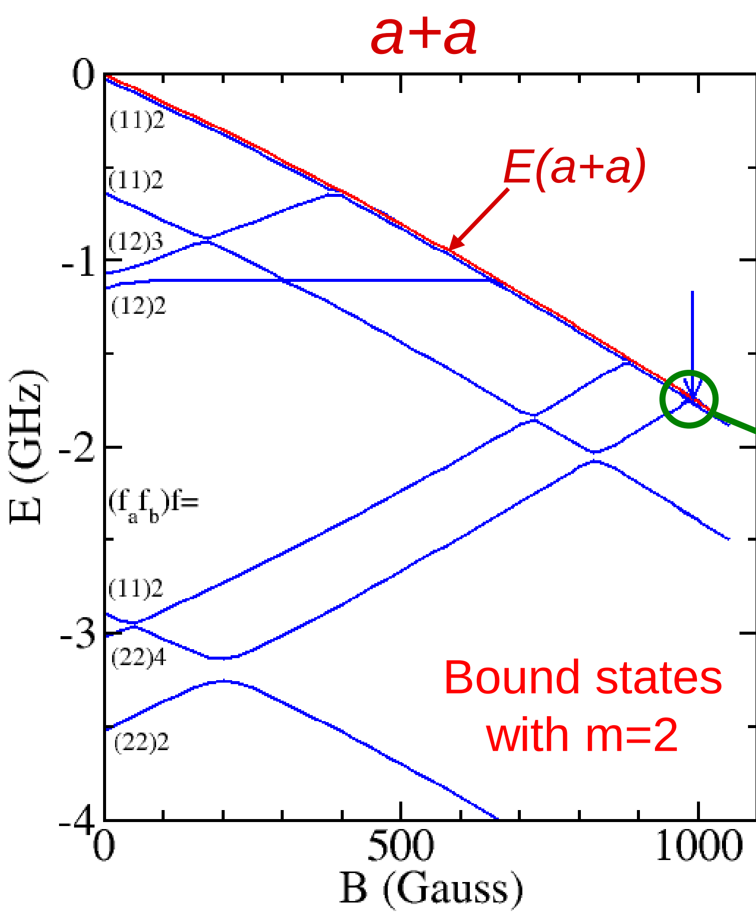


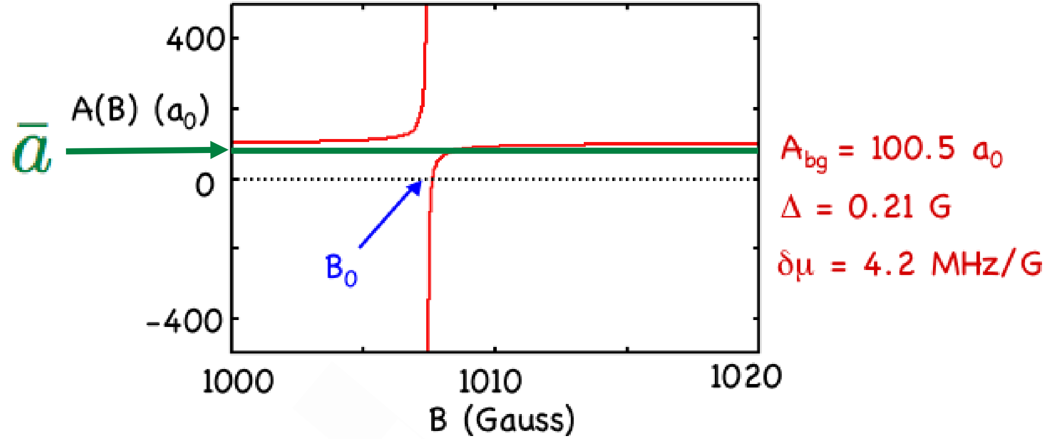

V/hc (cm^{-1})
^{87}Rb + ^{87}Rb
2000
1000
0
-1000
-2000
-3000
-4000
-5000
0
10
20
30
R (a_0)
$^3\Sigma_u^+$
$^1\Sigma_g^+$
$^2S_{1/2}$ + $^2S_{1/2}$
30 THz
R_u
0.8
0.4
0
-0.4
30
60
90
f=2 + f=2
f=1 + f=2
f=1 + f=1
10 GHz
R_{vdw}

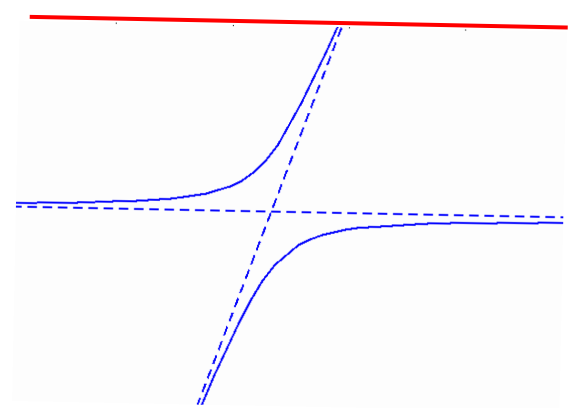
^{87}Rb Zeeman substructure

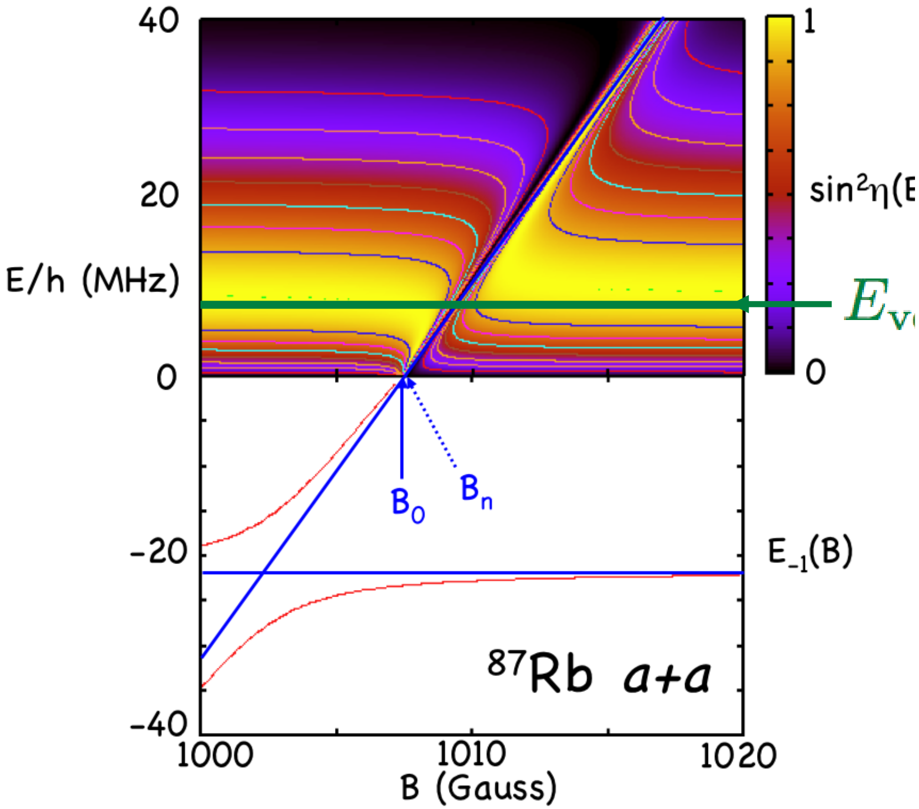


$^{87}Rb + ^{87}Rb$

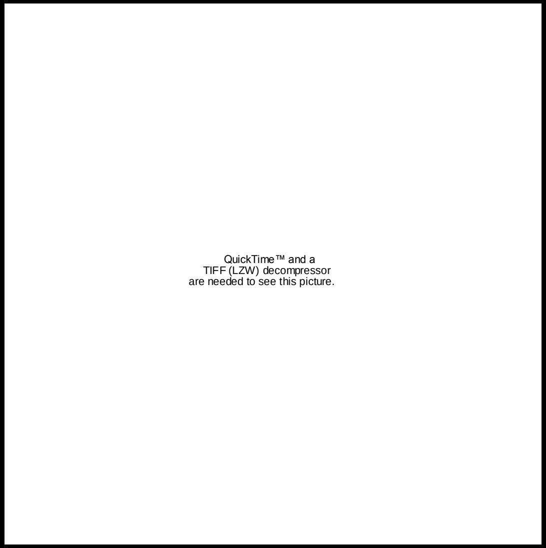

a+a
E(a+a)
Bound states
with m=2
(11)2
(11)2
(12)3
(12)2
(f a f b)f=
(11)2
(22)4
(22)2
E (GHz)
B (Gauss)
0
-1
-2
-3
-4
0
500
1000


A(B) (a_0)
$\bar{a}$
400
0
-400
1000
1010
1020
B (Gauss)
B_0
A_{bg} = 100.5 a_0
Δ = 0.21 G
$\delta\mu$ = 4.2 MHz/G





QuickTime™ and a
TIFF (LZW) decompressor
are needed to see this picture.



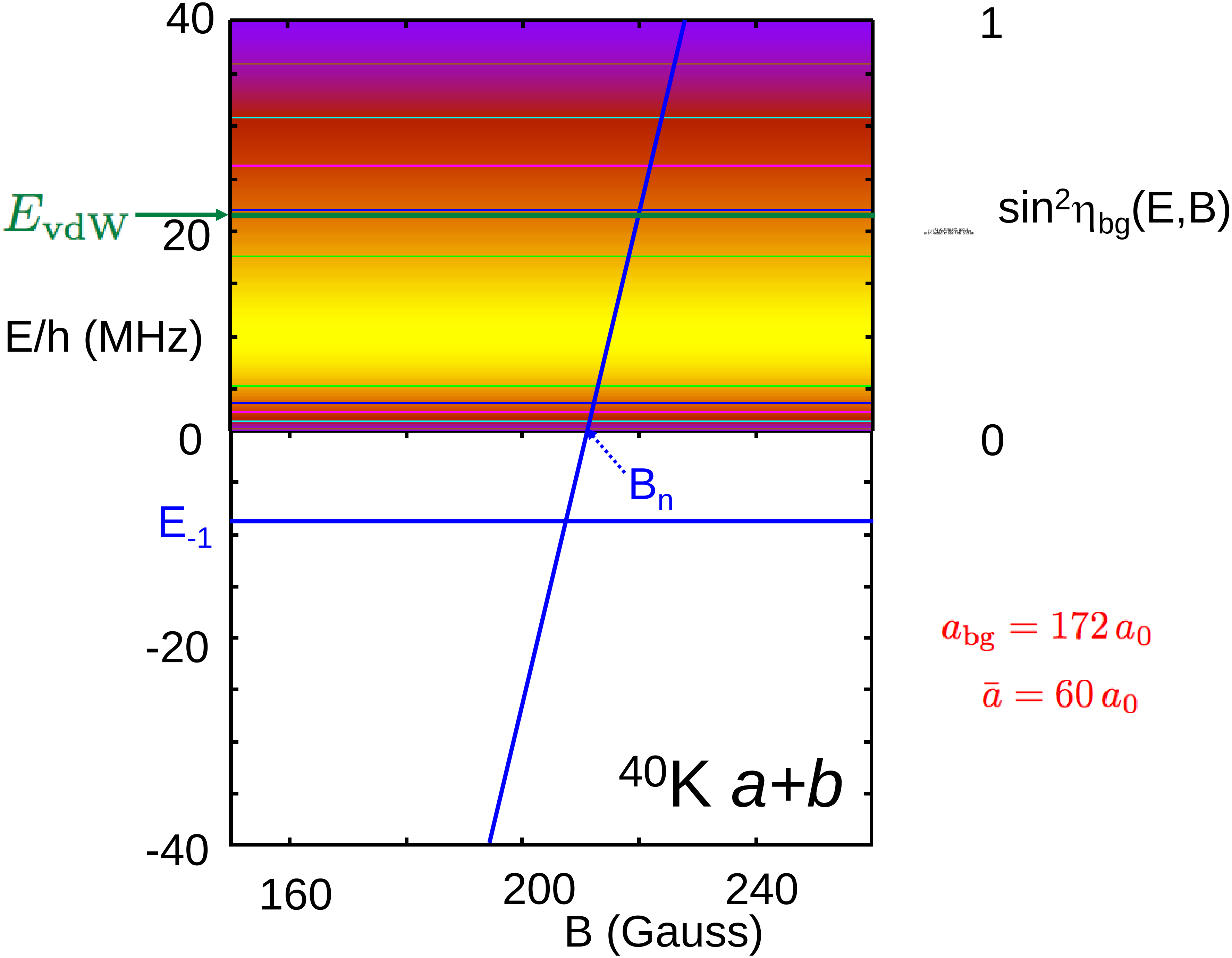
Cindy Regal, Marcus Greiner, Deborah Jin
NIST Boulder

Ultracold ^{40}K atoms, F=9/2,M=-9/2 and F=9/2,M=-7/2

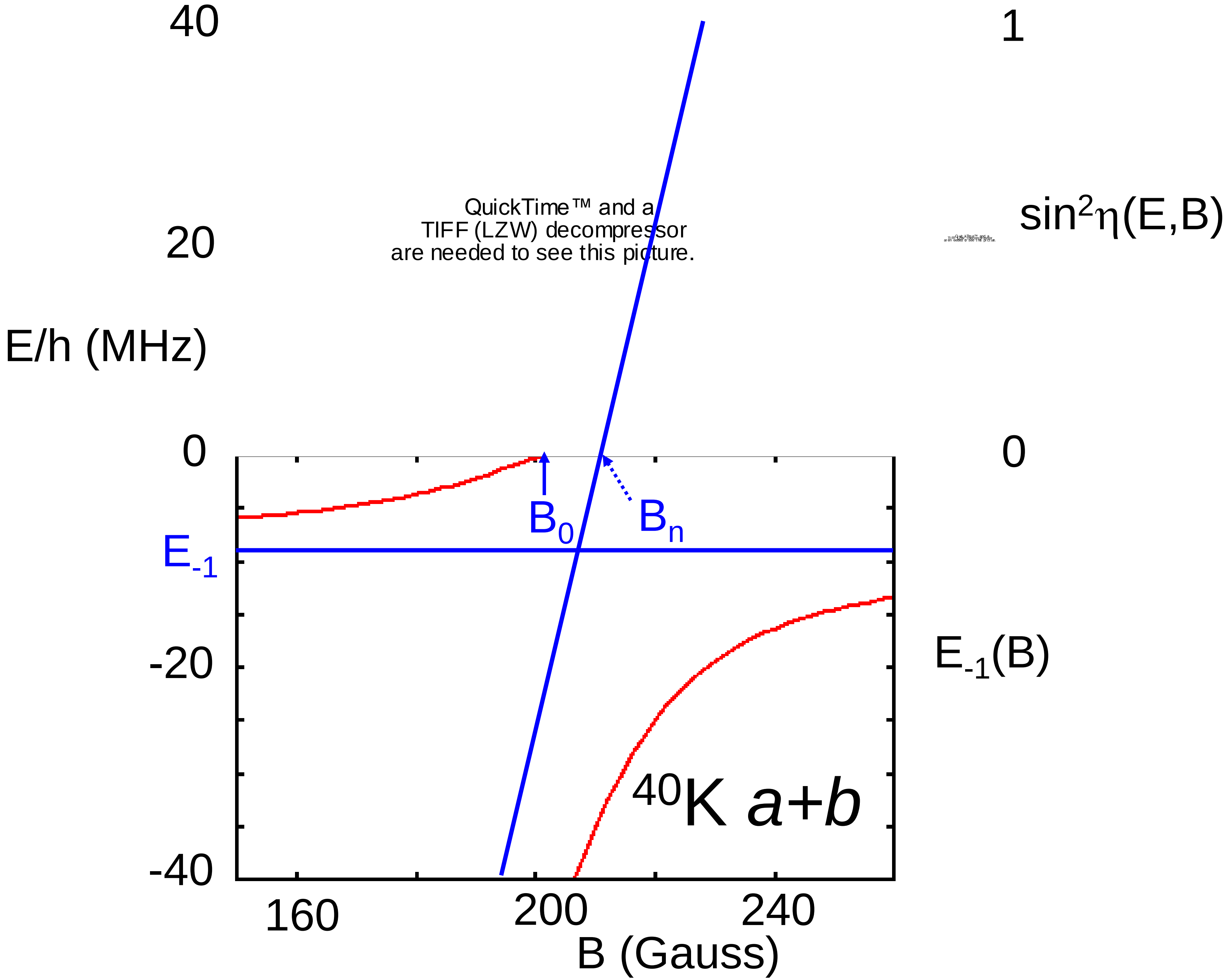
BEC of molecules
Nature 426, 537 (2003)

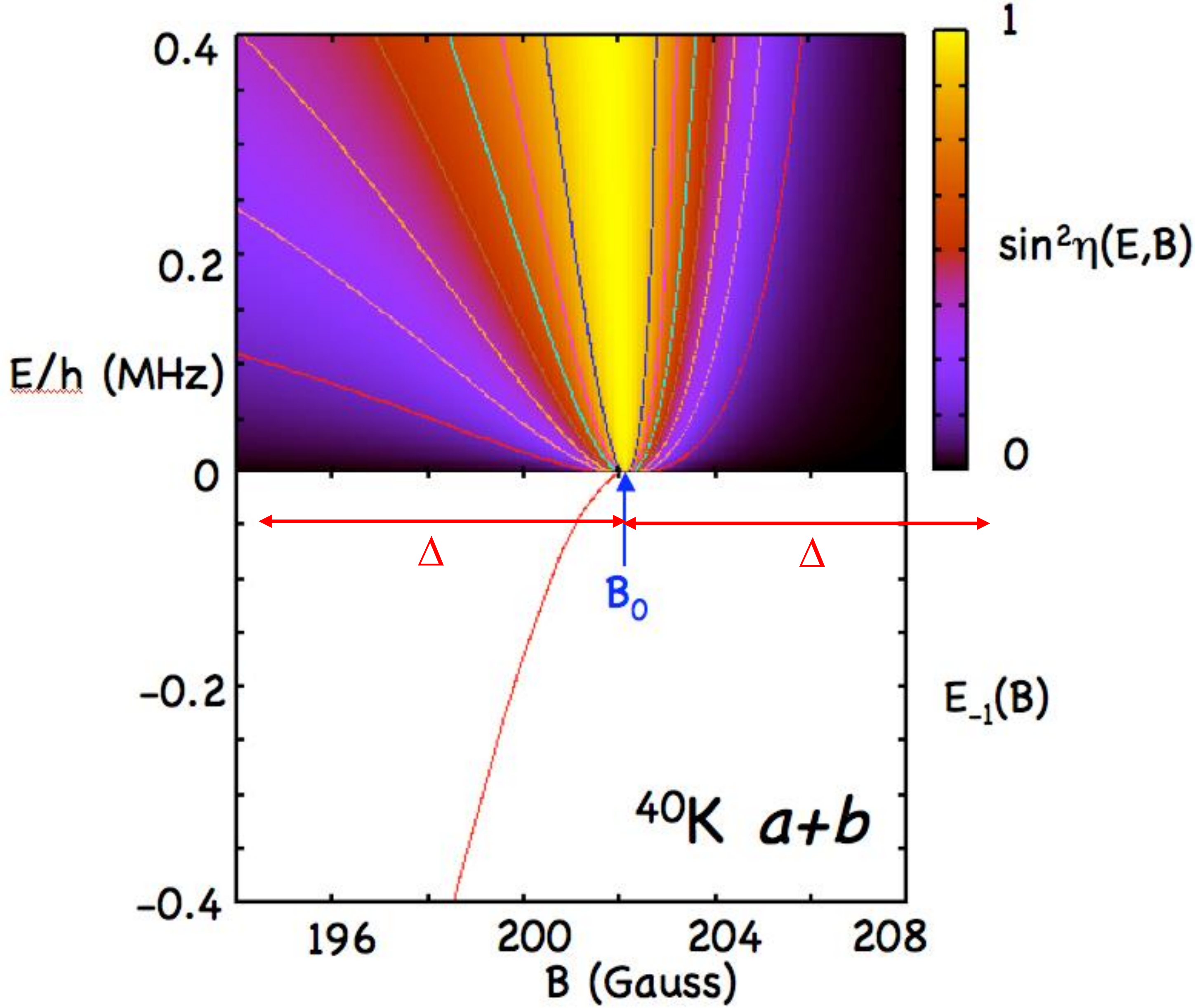
"Fermionic condensate" of paired atoms
Phys. Rev. Lett. 92, 040403 (2004)

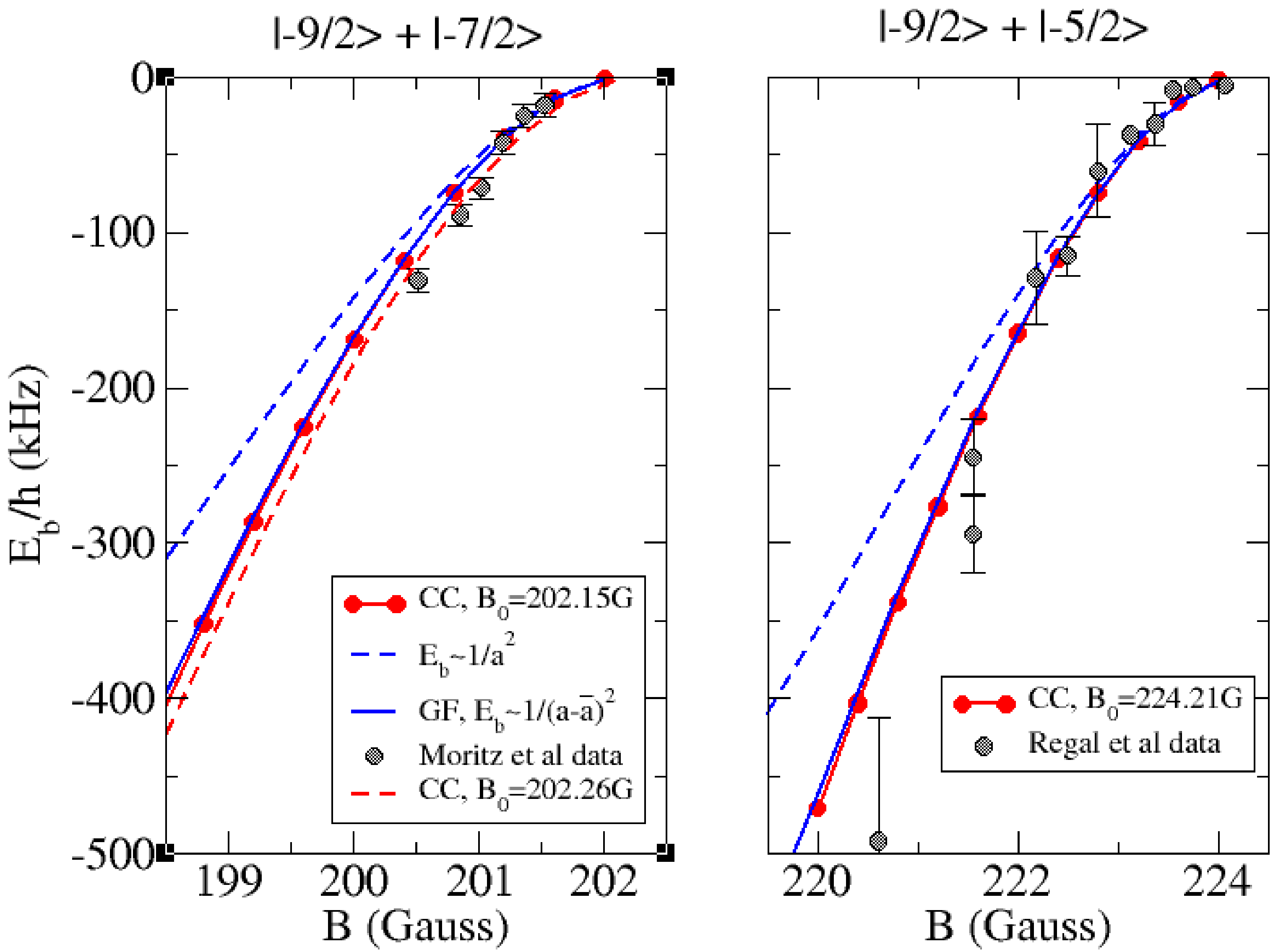
http://jilawww.colorado.edu/~jin/pictures.html



40
E_{vdW}
20
E/h (MHz)
0
-20
-40
1
$\sin^2\eta_{bg}(E,B)$
0
B_n
E_{-1}
$a_{\mathrm{bg}} = 172\, a_0$
$\bar{a} = 60\, a_0$
^{40}K a+b
160
200
240
B (Gauss)


40
20
0
-20
-40
E/h (MHz)
1
0
sin²η(E,B)
QuickTime™ and a
TIFF (LZW) decompressor
are needed to see this picture.
B0
Bn
E-1
E-1(B)
40K a+b
160
200
240
B (Gauss)


0.4
0.2
E/h (MHz)
0
-0.2
-0.4
196
200
204
208
B (Gauss)
1
0
sin²η(E,B)
Δ
Δ
B₀
E₋₁(B)
⁴⁰K a+b



|-9/2> + |-7/2>
|-9/2> + |-5/2>
E_b/h (kHz)
0
-100
-200
-300
-400
-500
199
200
201
202
B (Gauss)
220
222
224
B (Gauss)
CC, B_0=202.15G
E_b~$1/a^2$
GF, E_b~$1/(a-\bar{a})^2$
Moritz et al data
CC, B_0=202.26G
CC, B_0=224.21G
Regal et al data