YbRb
A Candidate for an Ultracold Paramagnetic Molecule

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Outline

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1. Introduction: The Yb-Rb system
2. Yb + Rb: Interactions in a conservative trap
3. YbRb*: Photoassociation spectroscopy
4. Towards YbRb in the ground state: Feshbach resonances and/or Photoassociation

1. Introduction:
The Yb-Rb system

Why Ytterbium and Rubidium?

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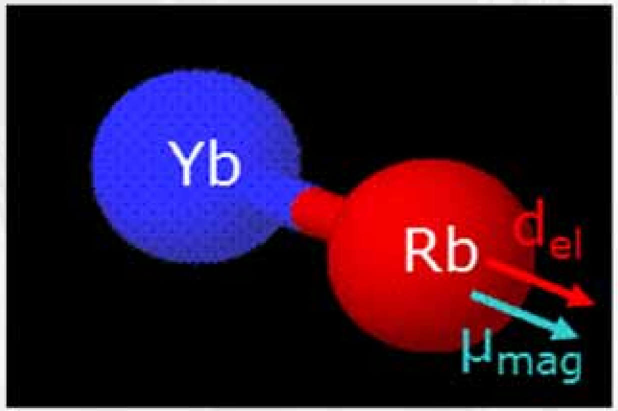
Yb + Rb as a mixture

paramagnetic diamagnetic

- unexplored interactions
- independent manipulation
- optical and (possibly) magnetic Feshbach resonances
- 5 stable bosonic and 2 stable fermionic Yb isotopes

YbRb as a molecule



- heteronuclear
- $^2\Sigma_{1/2}$ ground state
- electric and magnetic dipole
- „toolbox" for spin lattice models[1]

1) Micheli et al., Nature Physics 2, 341 (2006)

Properties of Yb-Rb mixtures

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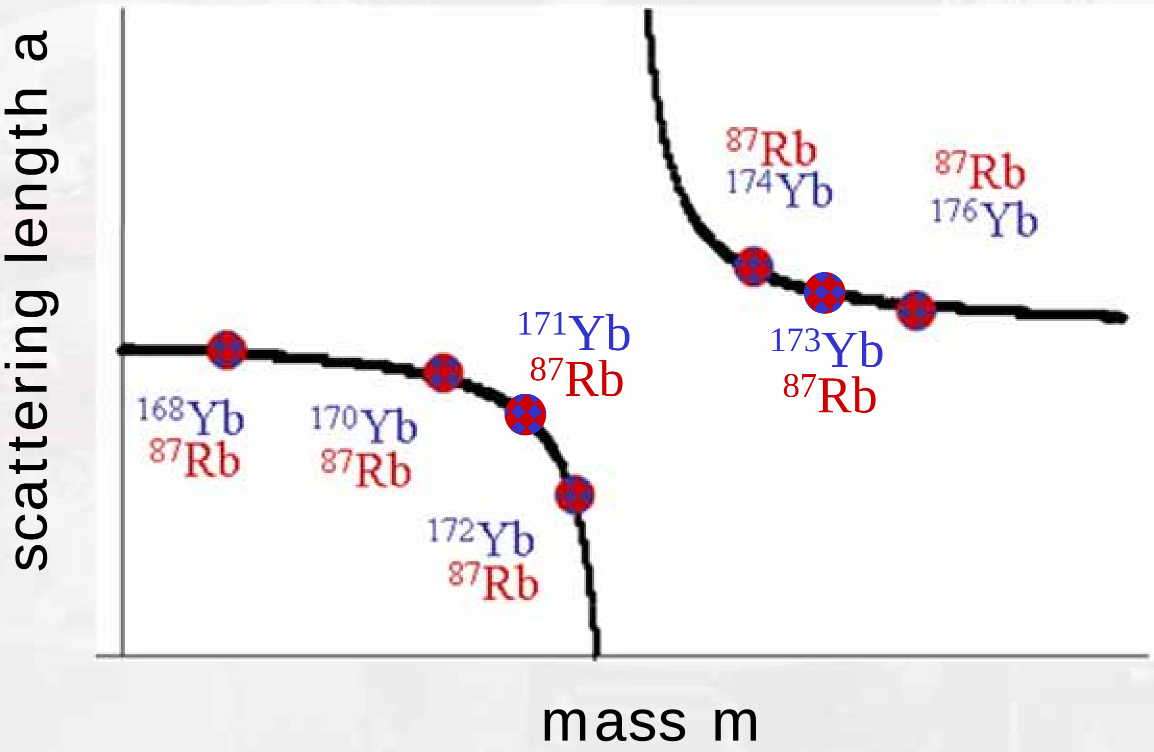
^{87}Rb

+

Bosons: ^{168}Yb, ^{170}Yb, ^{172}Yb, ^{174}Yb, ^{176}Yb

Fermions: ^{171}Yb, ^{173}Yb

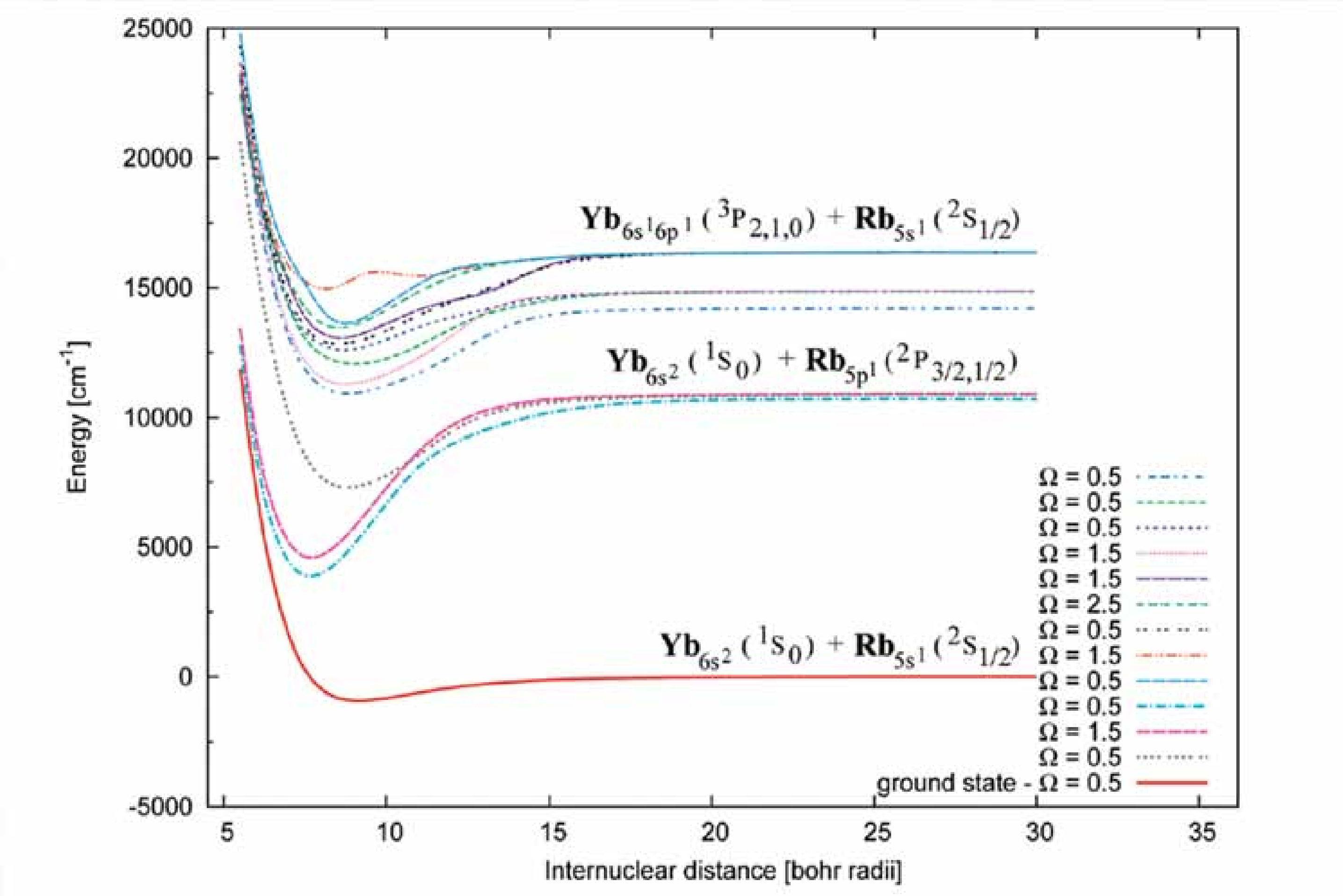
Heteronuclear scattering length (fictitious values)



⇒ **Wide range of interaction properties expected**

YbRb-Molecules

Ab-initio potentials:



Sorensen et al., *J. Phys. Chem. A* ***113, 12607 (2009)***

$D_e \sim 865\ cm^{-1}$

$R_e \sim 8.85\ a_0$

electric dipole moment:

~ 1 Debye

The Machine

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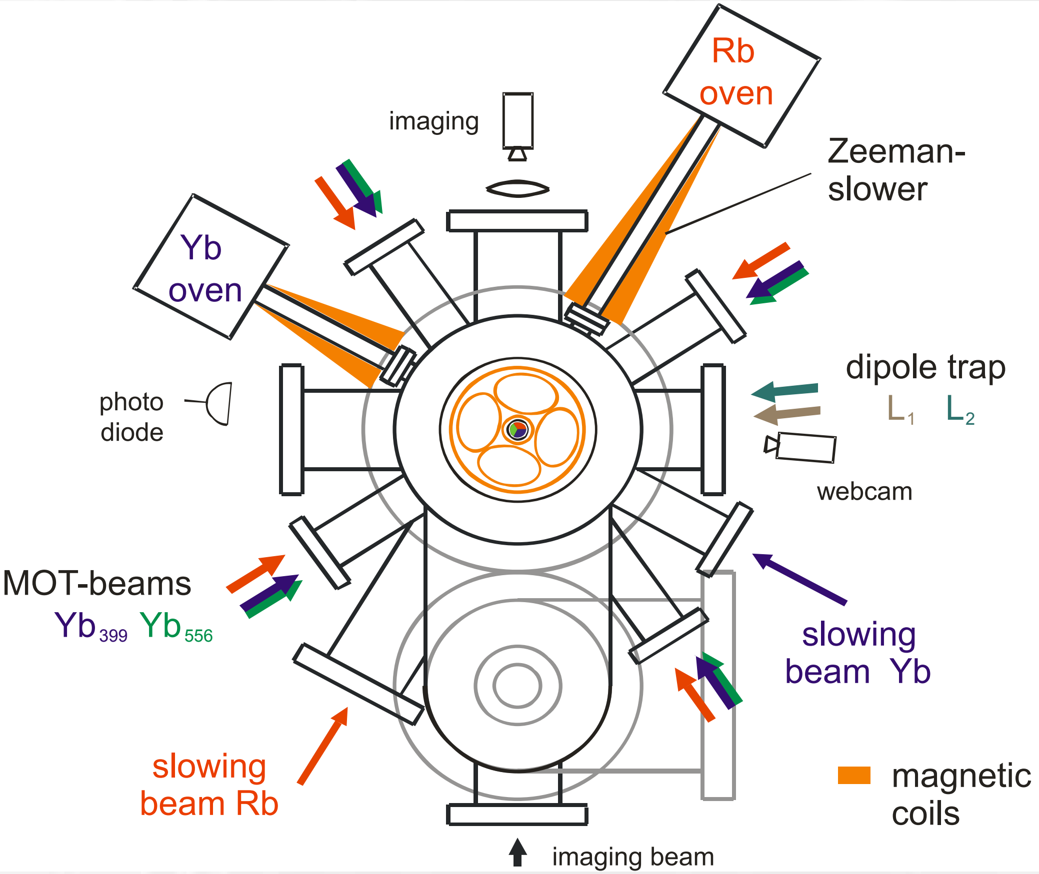
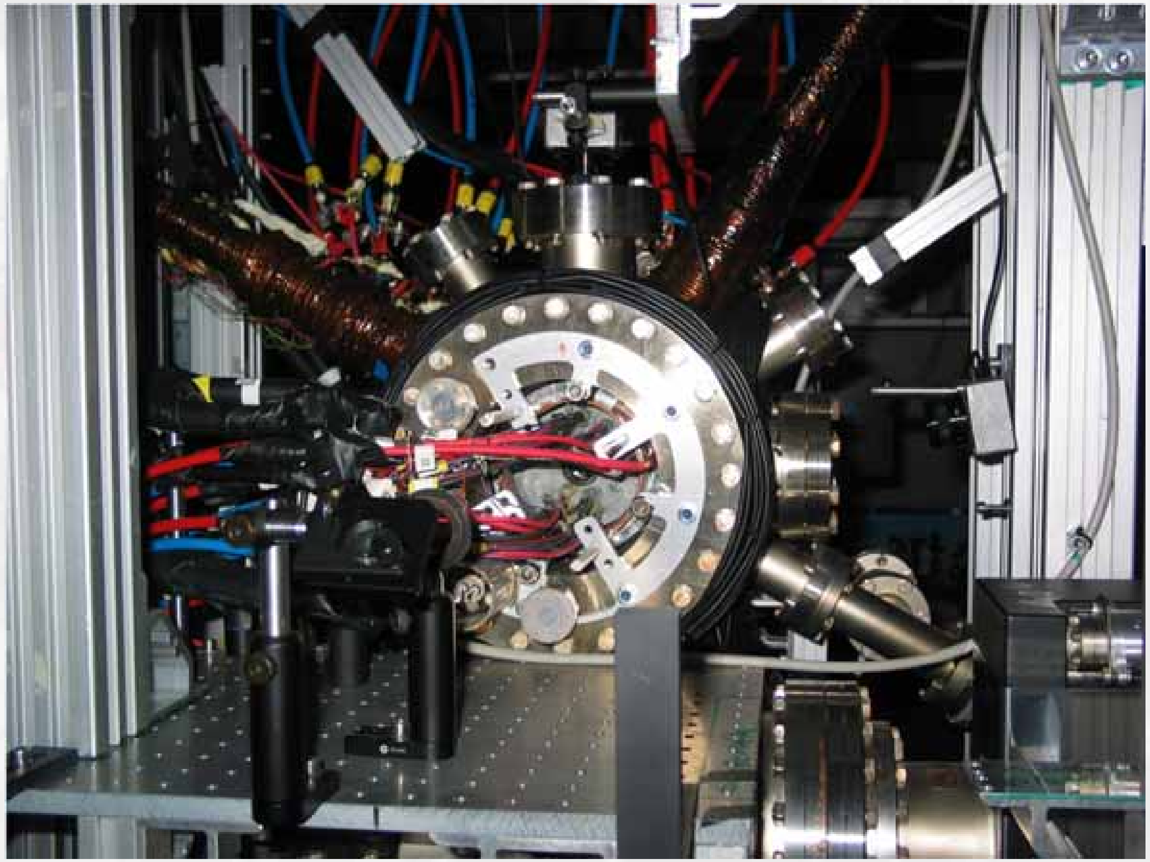
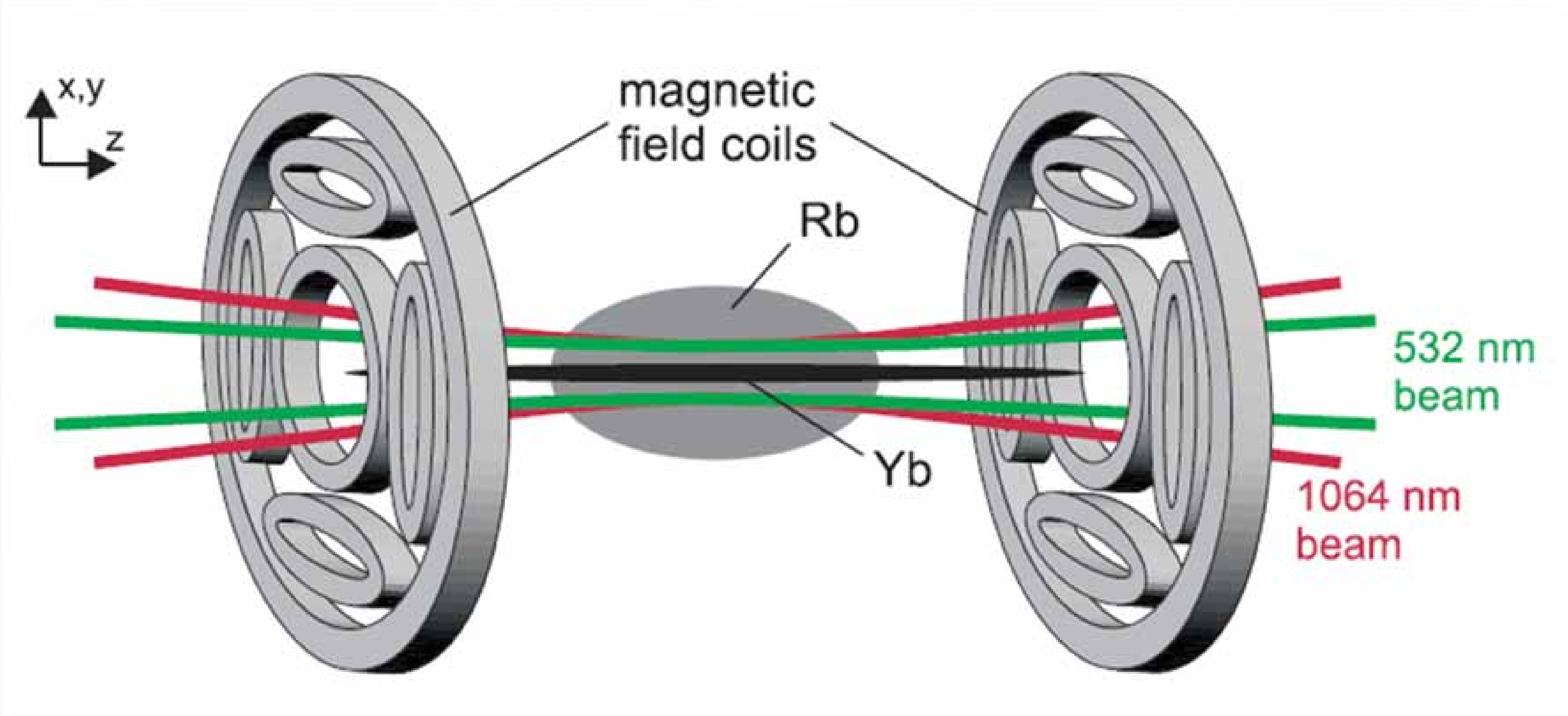


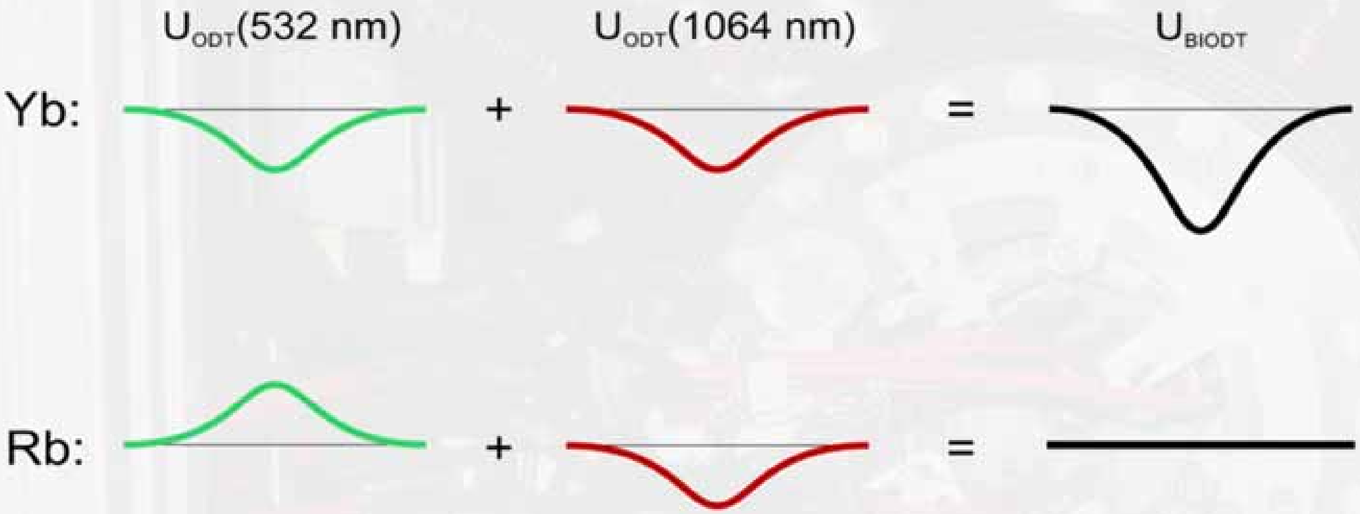


2. Yb + Rb: Interactions in a conservative trap

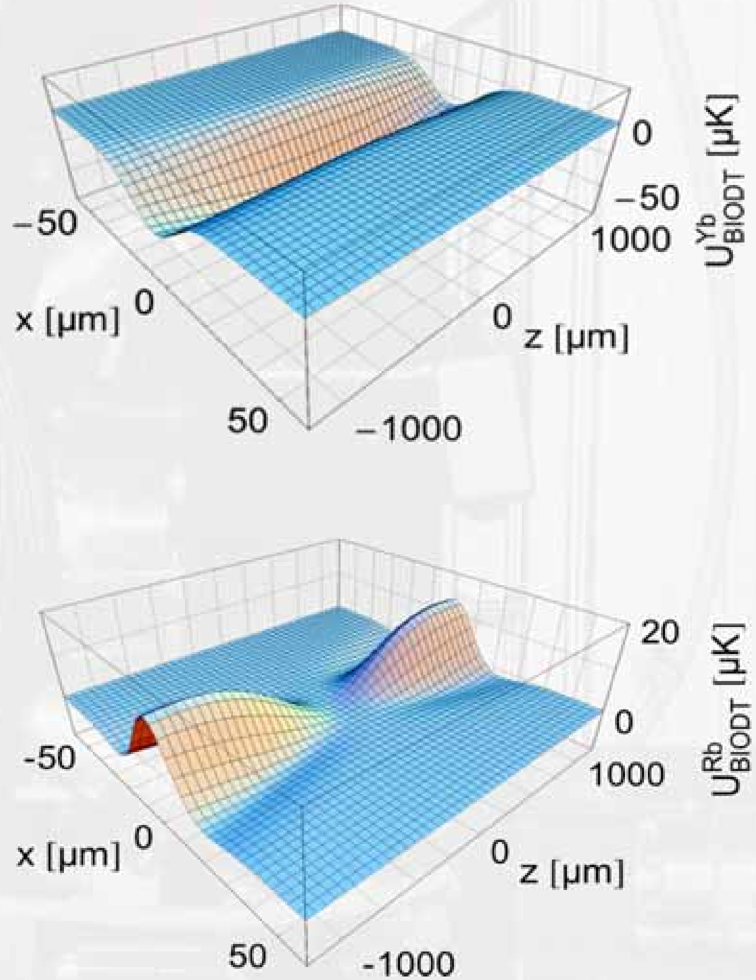
The hybrid trap



Bichromatic optical dipole trap



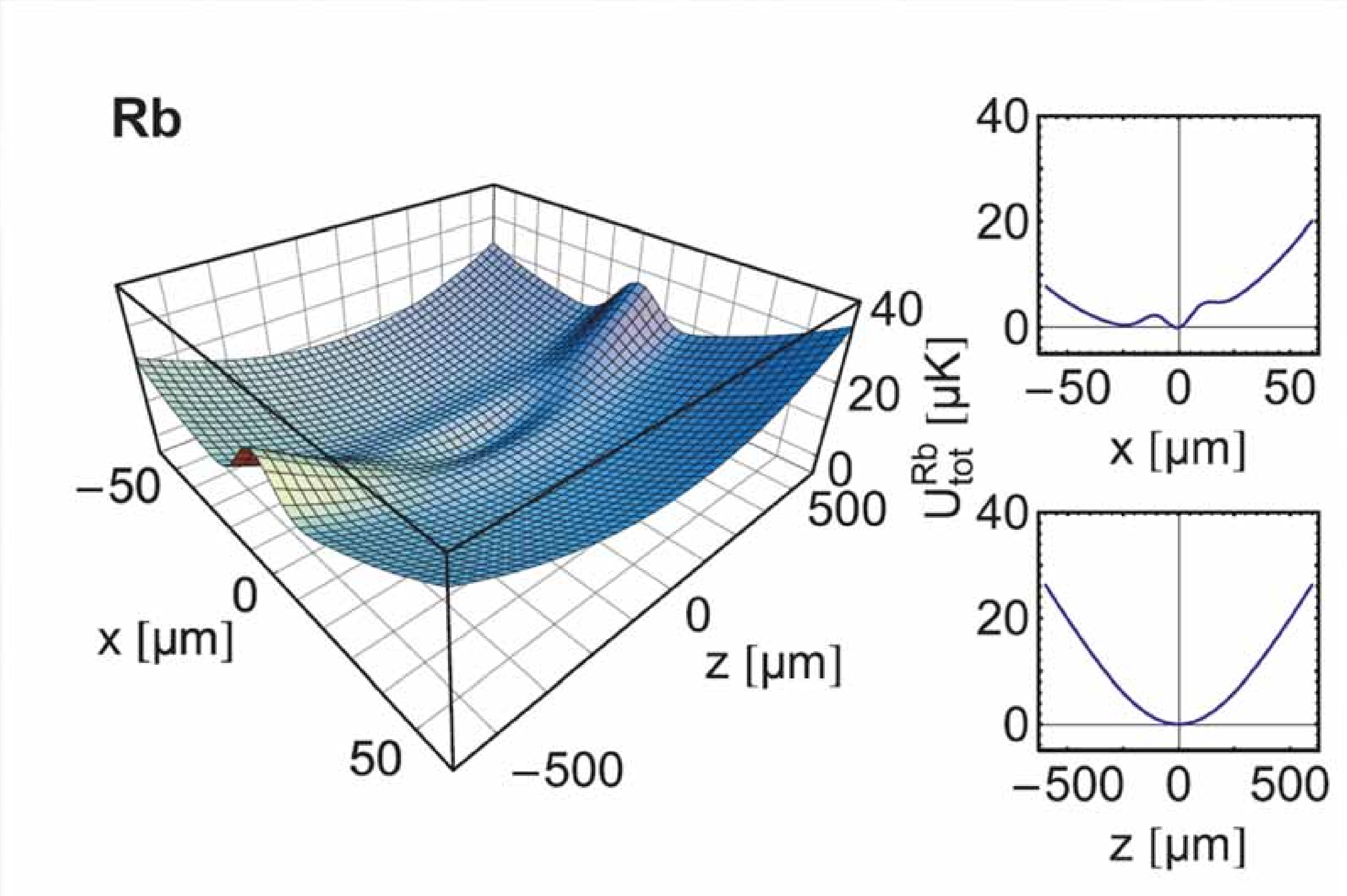
$\lambda\omega_{Yb}$	<	$\lambda_{ODT\,1}$	<	λ_{Rb}	<	$\lambda_{ODT\,2}$
399 nm	<	532 nm	<	780 nm 795 nm	<	1064 nm



$$U_{532}\,(r = 0) = U_{1064}\,(r = 0)$$

Bichromatic optical dipole trap

„Real“ potential:



Collisions at μK-temperatures

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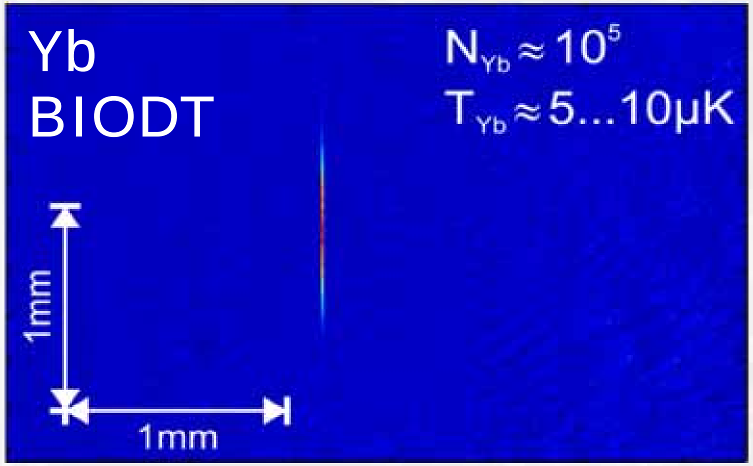
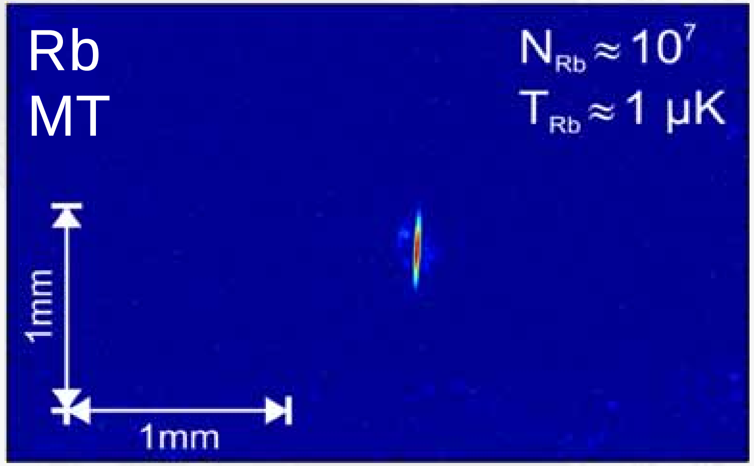
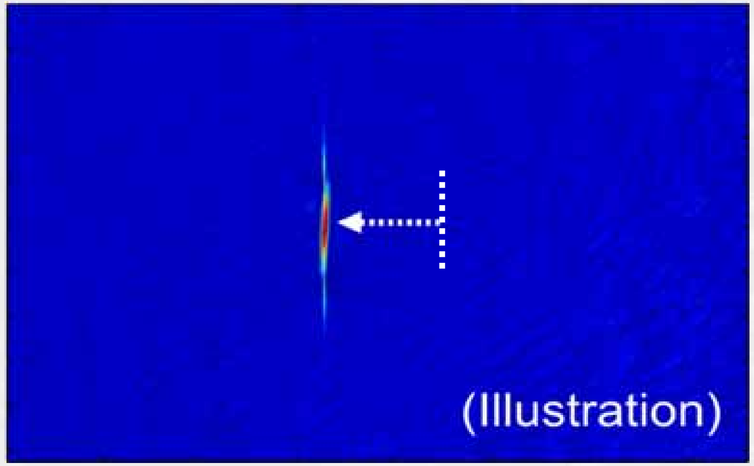
Pure s-wave collisions (p-wave threshold ~ 60 μK)





defined spatial overlap
between Yb and Rb cloud

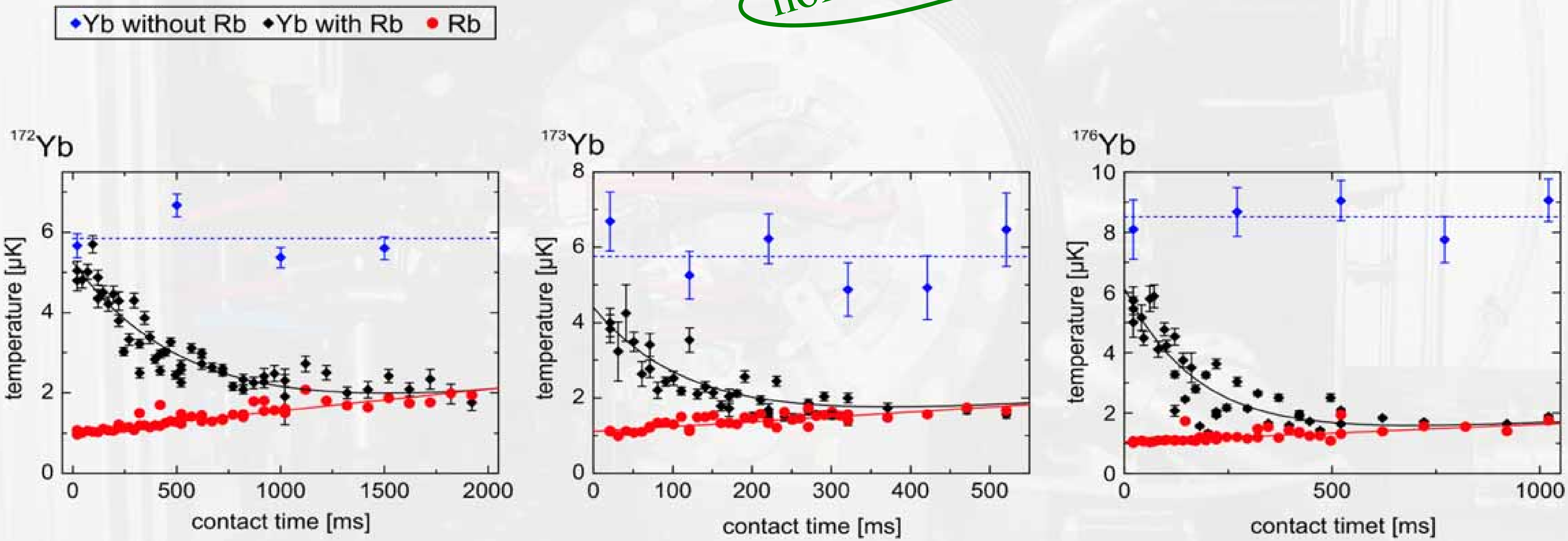


Thermalization

... between ^{170}Yb, ^{172}Yb, ^{173}Yb, ^{174}Yb, ^{176}Yb and ^{87}Rb

⇒ strong istotope dependence

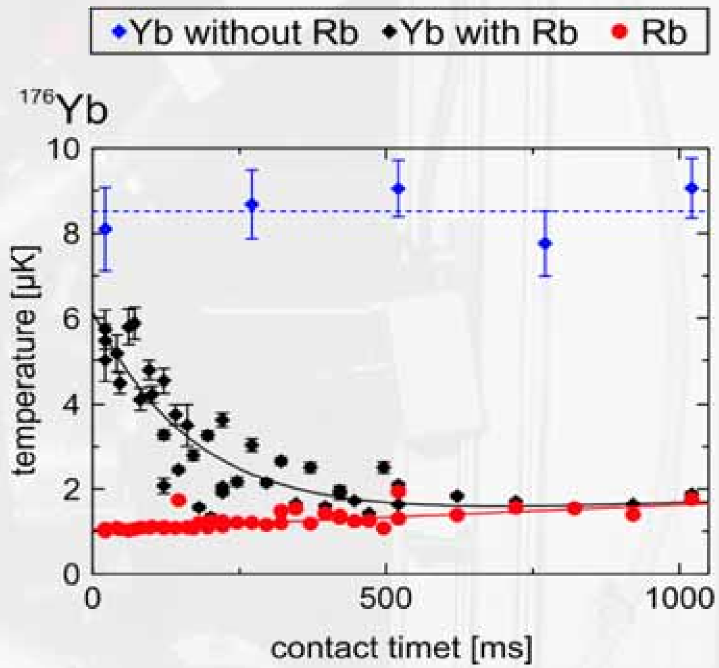
normal behavior



Thermalization

... between ^{170}Yb, ^{172}Yb, ^{173}Yb, ^{174}Yb, ^{176}Yb and ^{87}Rb

quantitative analysis:

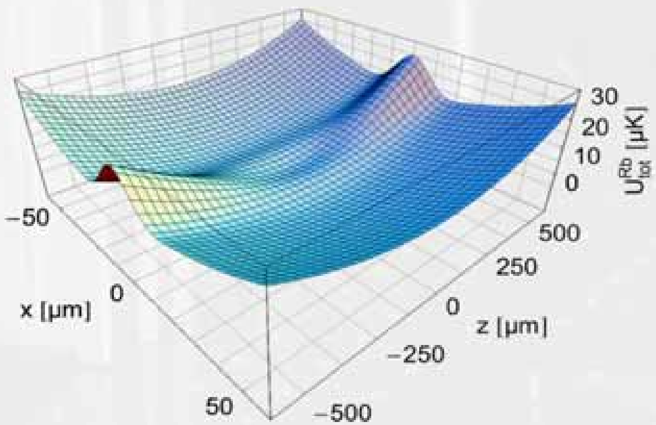


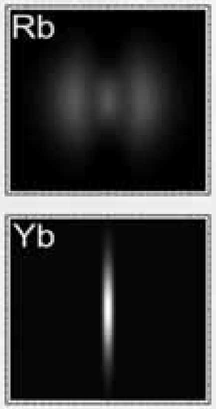
thermalization rate

Yb-Rb scattering cross section

overlap integral

$$\gamma_{\mathrm{Th}} \propto n_{\mathrm{YbRb}} \cdot \sigma_{\mathrm{YbRb}}$$





in this trap geometry:

n_{YbRb} hard to control

$\Rightarrow$ only relative values for σ_{YbRb} can be reliably deduced

Thermalization

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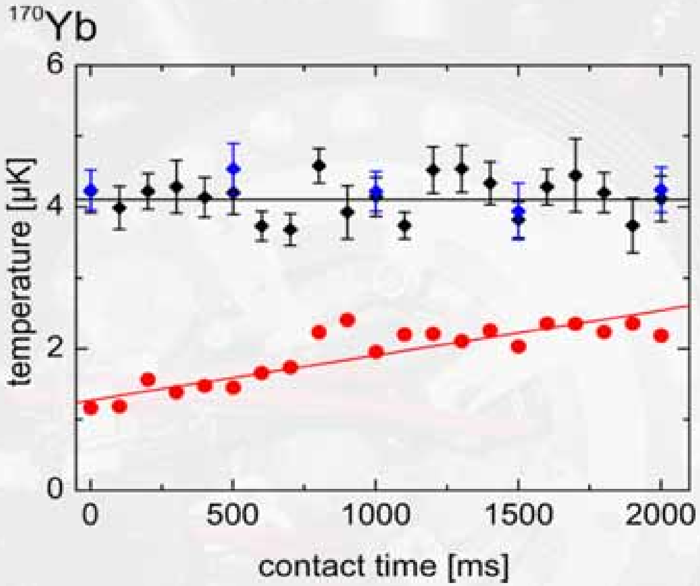
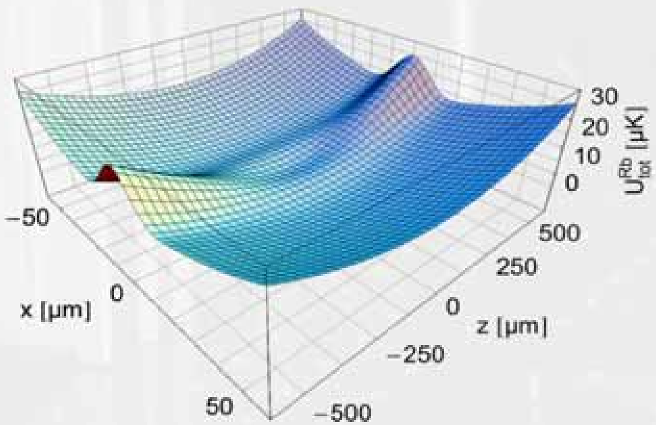
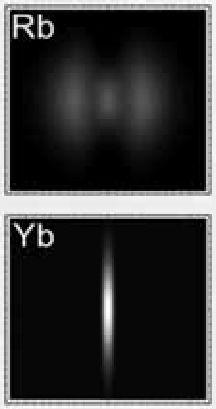
... between ^{170}Yb, ^{172}Yb, ^{173}Yb, ^{174}Yb, ^{176}Yb and ^{87}Rb

extraordinary behavior







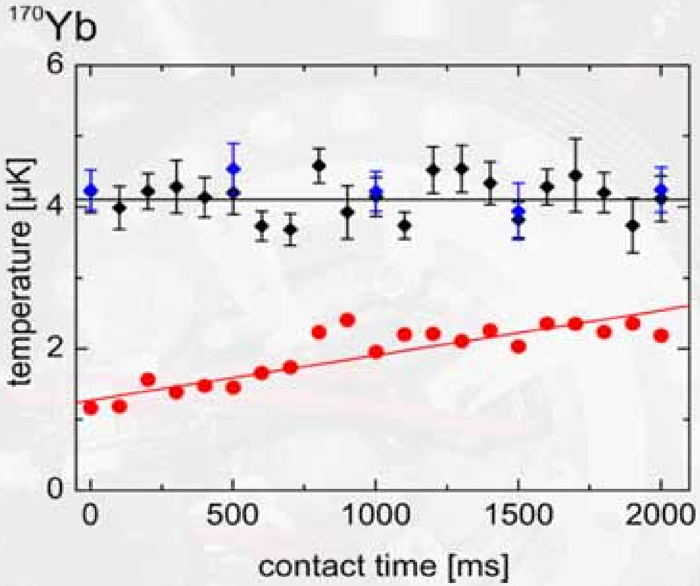
^{170}Yb does not thermalize at all

⇒ **(extremely) small elastic scattering cross section for this isotope**

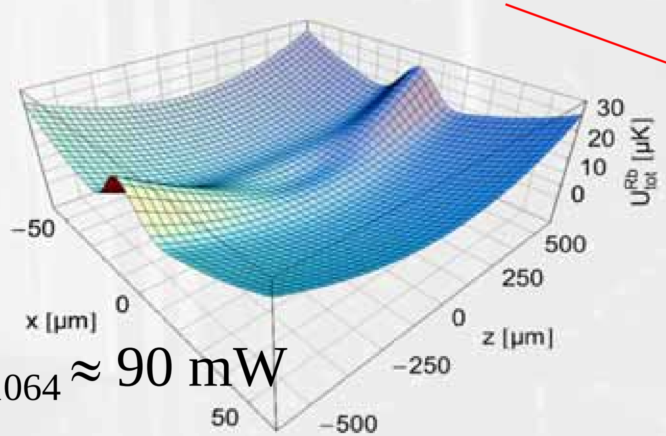
Thermalization

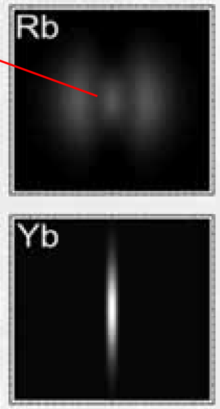
... between ^{170}Yb, ^{172}Yb, ^{173}Yb, ^{174}Yb, ^{176}Yb and ^{87}Rb

extraordinary behavior



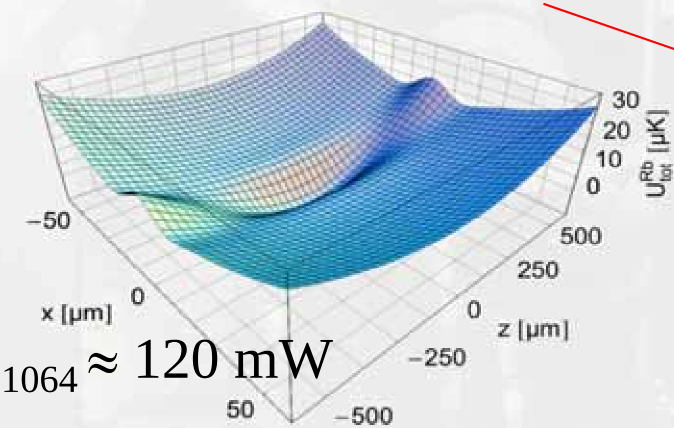
$n_{Rb} \approx 10^{10} \ldots 10^{11}$ cm^{-3}

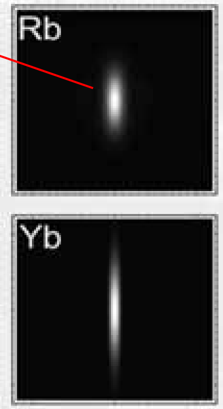




$P_{1064} \approx 90$ mW

$n_{Rb} \approx 10^{13} \ldots 10^{14}$ cm^{-3}



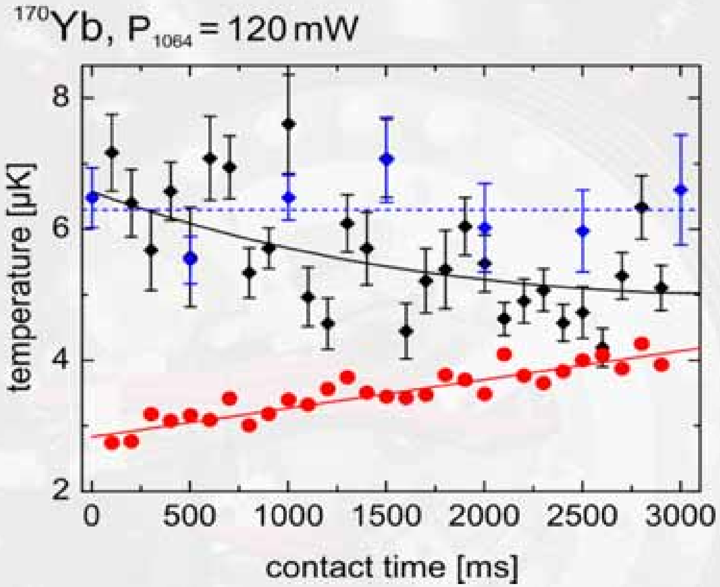


$P_{1064} \approx 120$ mW

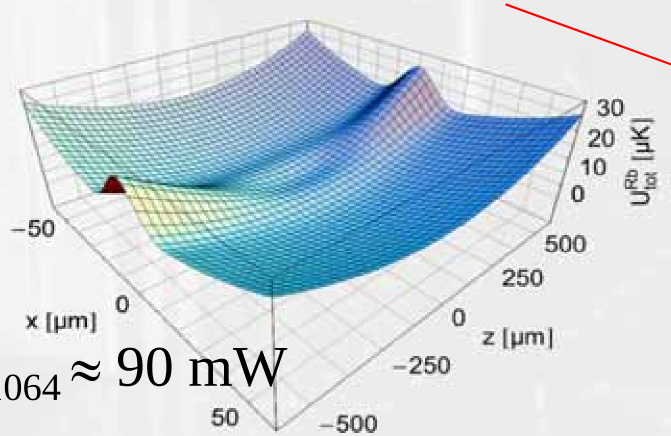
Thermalization

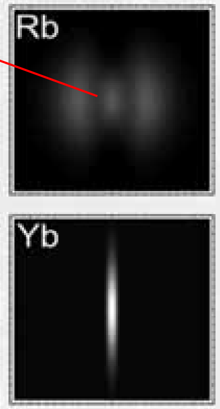
… between ^{170}Yb, ^{172}Yb, ^{173}Yb, ^{174}Yb, ^{176}Yb and ^{87}Rb

extraordinary behavior



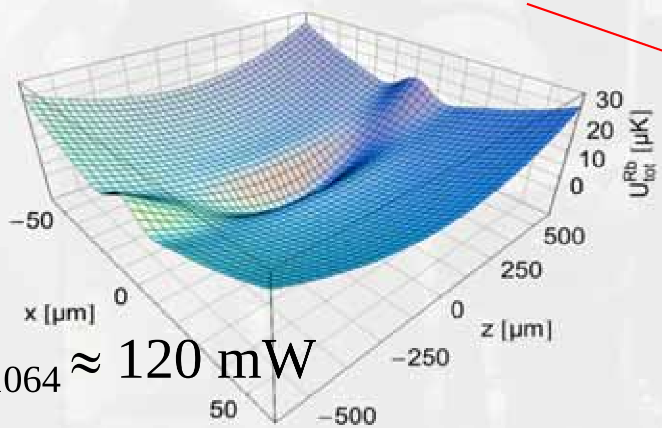
$n_{Rb} \approx 10^{10} \ldots 10^{11}\ cm^{-3}$

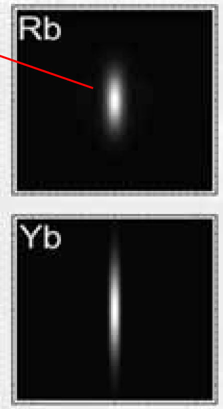




$P_{1064} \approx 90\ mW$

$n_{Rb} \approx 10^{13} \ldots 10^{14}\ cm^{-3}$





$P_{1064} \approx 120\ mW$

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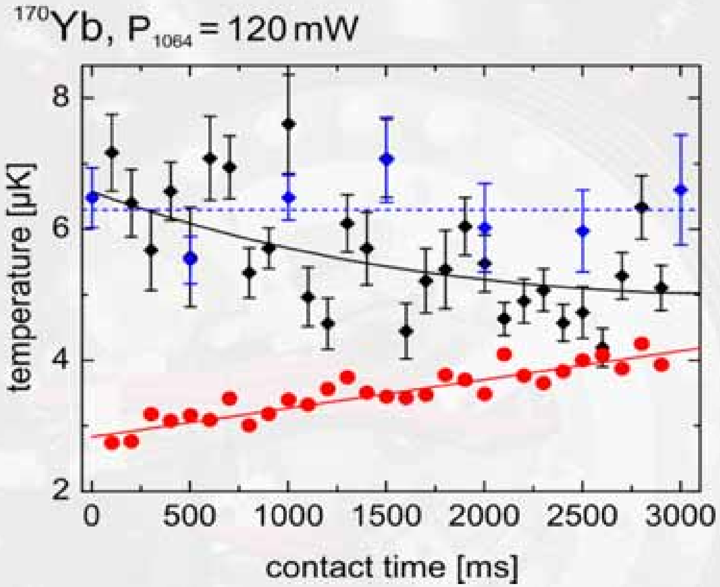
Thermalization

... between ^{170}Yb, ^{172}Yb, ^{173}Yb, ^{174}Yb, ^{176}Yb and ^{87}Rb

extraordinary behavior



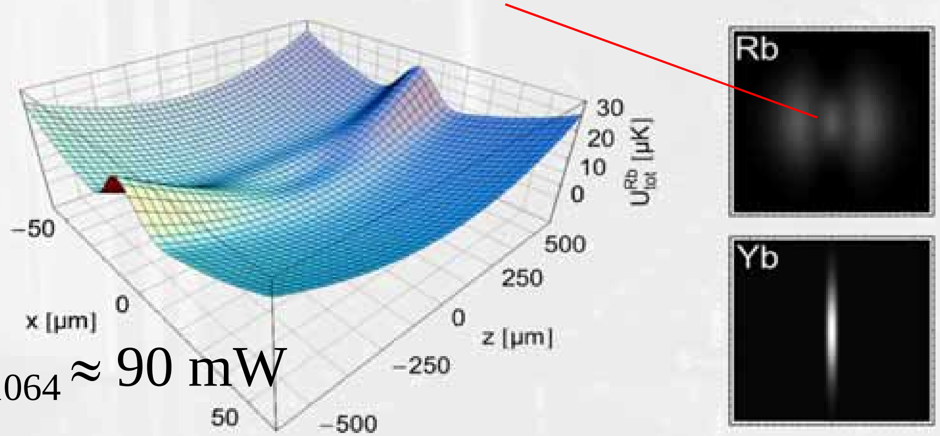
better control of n_{YbRb}

$\Rightarrow$ $\sigma_{YbRb} = 4\,\pi\,a^2$

$\Rightarrow$ scattering length:

$|a_{170\text{-}87}| \sim 10\ a_0$

$n_{Rb} \approx 10^{10} \ldots 10^{11}\ \text{cm}^{-3}$



$P_{1064} \approx 90$ mW

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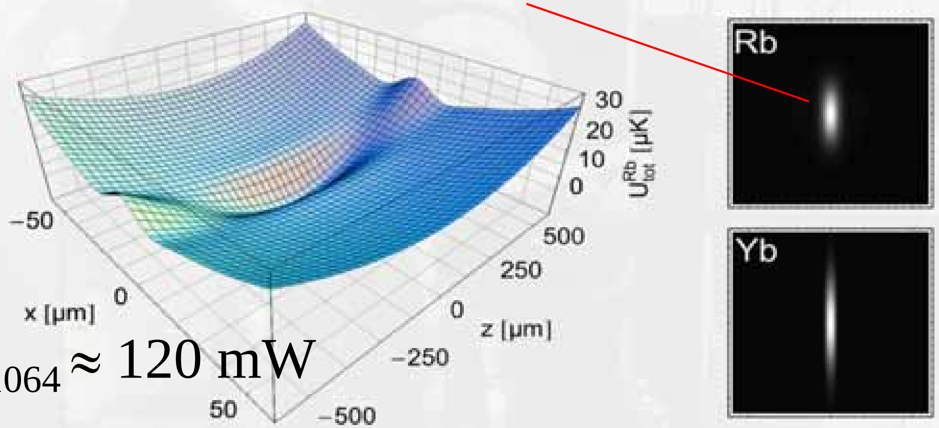

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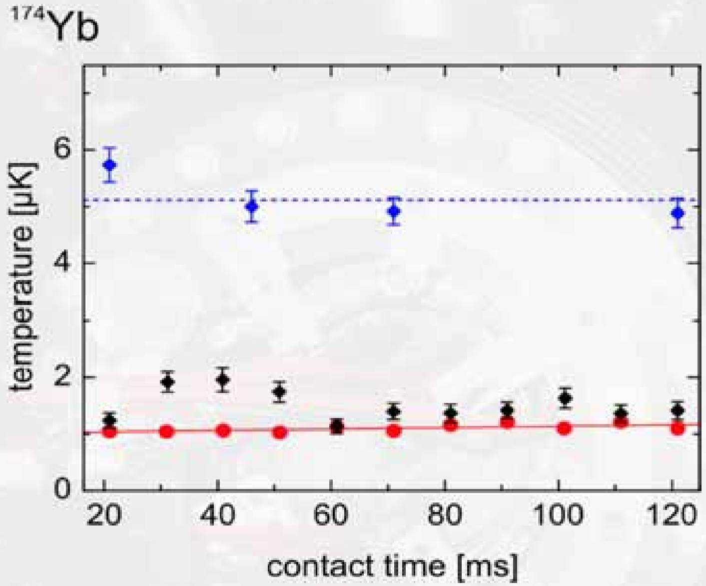

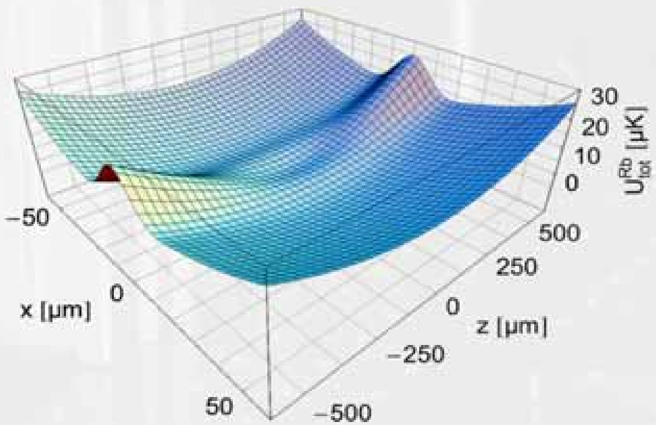

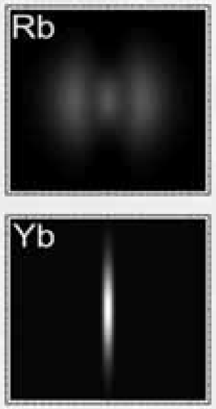

^{174}Yb thermalizes instantaneously

⇒ **(extremly) large elastic scattering cross section for this isotope**

^{174}Yb – ^{87}Rb mixture at large n_{Rb}

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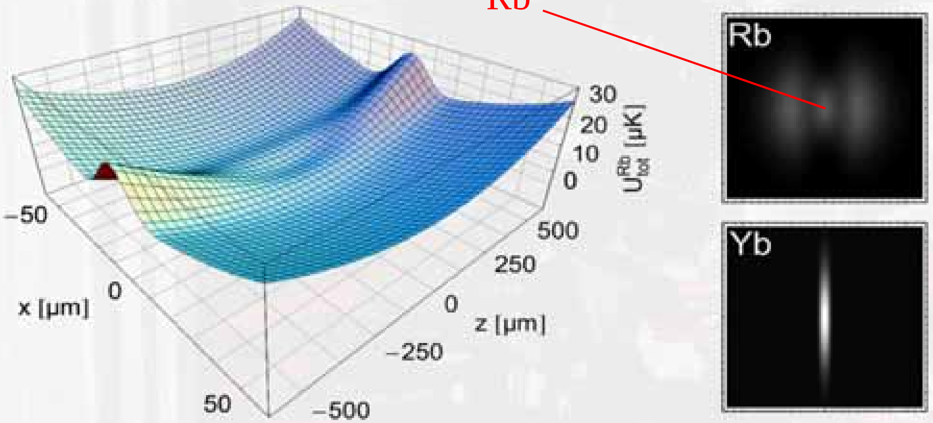
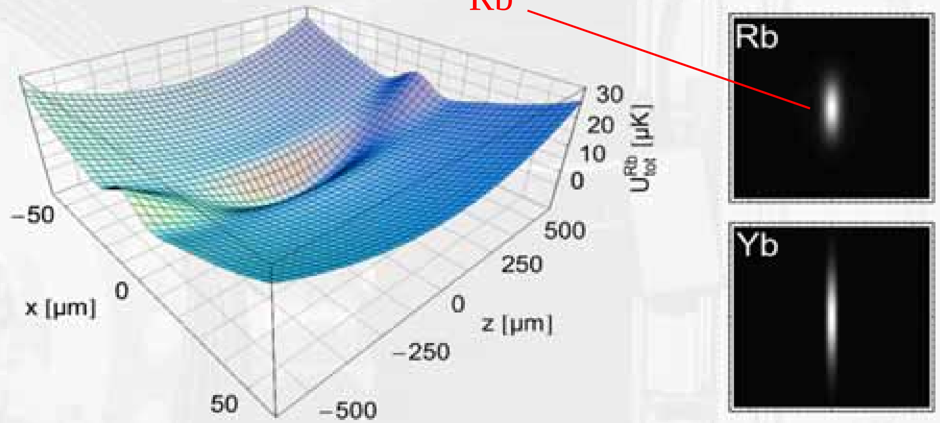
$n_{Rb} \approx 10^{10} \ldots 10^{11}$ cm^{-3}



$n_{Rb} \approx 10^{13} \ldots 10^{14}$ cm^{-3}



^{174}Yb thermalized with ^{87}Rb → ?

trap frequencies:

ω_r ~ 1 kHz, ω_z ~ 10 Hz

^{174}Yb – ^{87}Rb mixture at large n_{Rb}

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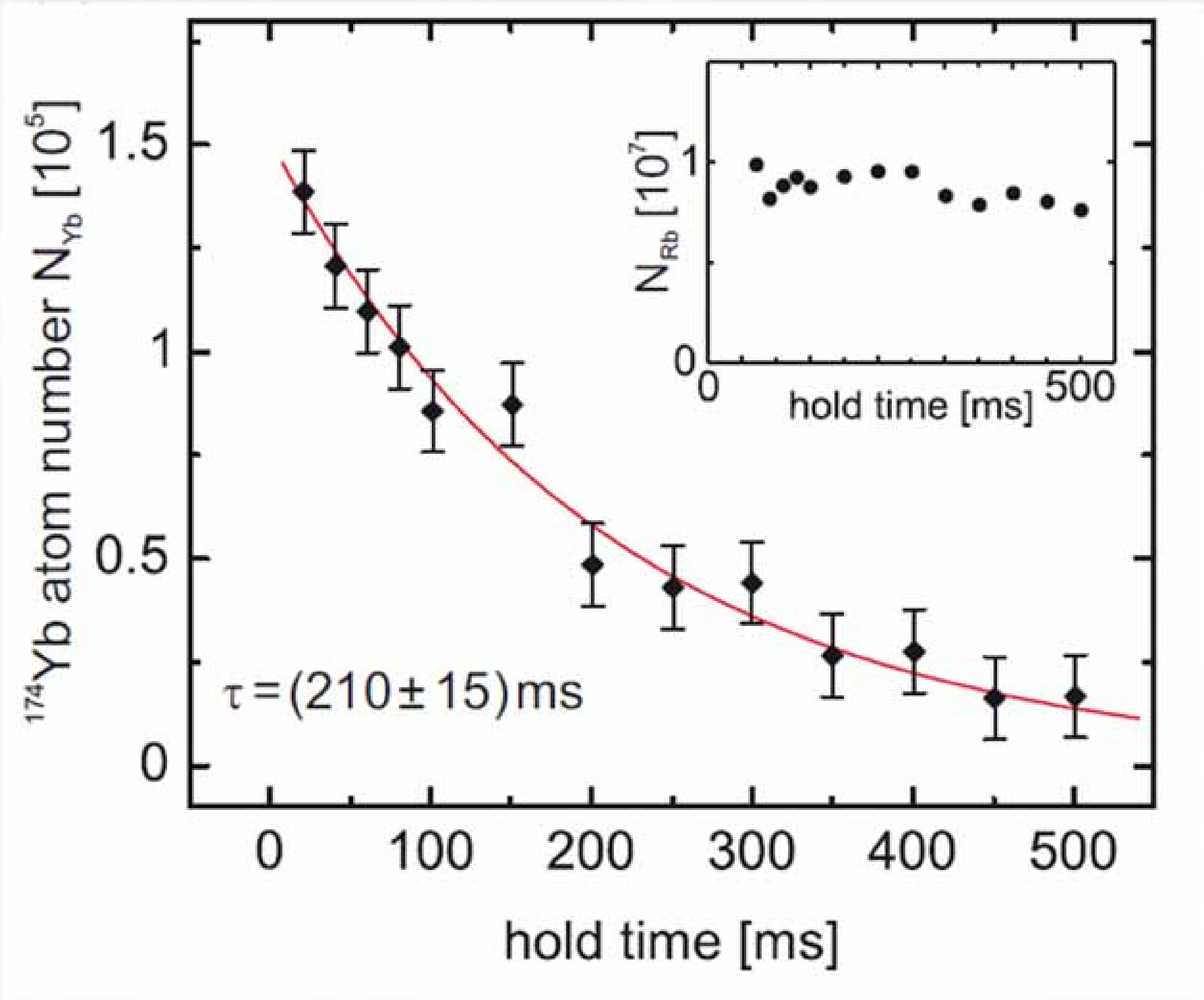


⇒ **fast loss of ^{174}Yb attributed to large 3-body loss**

Spatial separation of ^{174}Yb and ^{87}Rb

$T \approx 3\ \mu K$

$N_{Yb} \approx 10^5$

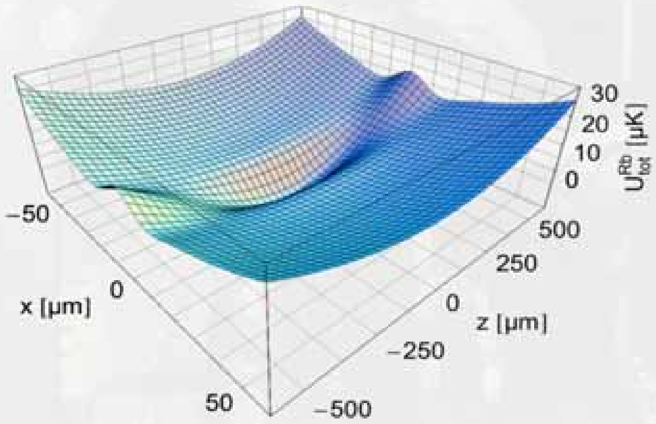
$N_{Rb} \approx$

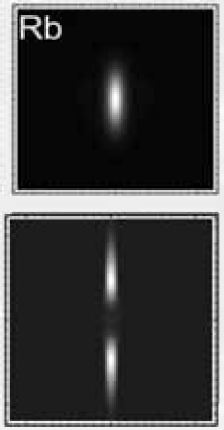
(a) 7×10^5

(b) 3×10^6

(c) 7×10^6

increasing Rb density





F. Baumer et al., PRA 83, 040702(R) (2011)

Spatial separation of ^{174}Yb and ^{87}Rb

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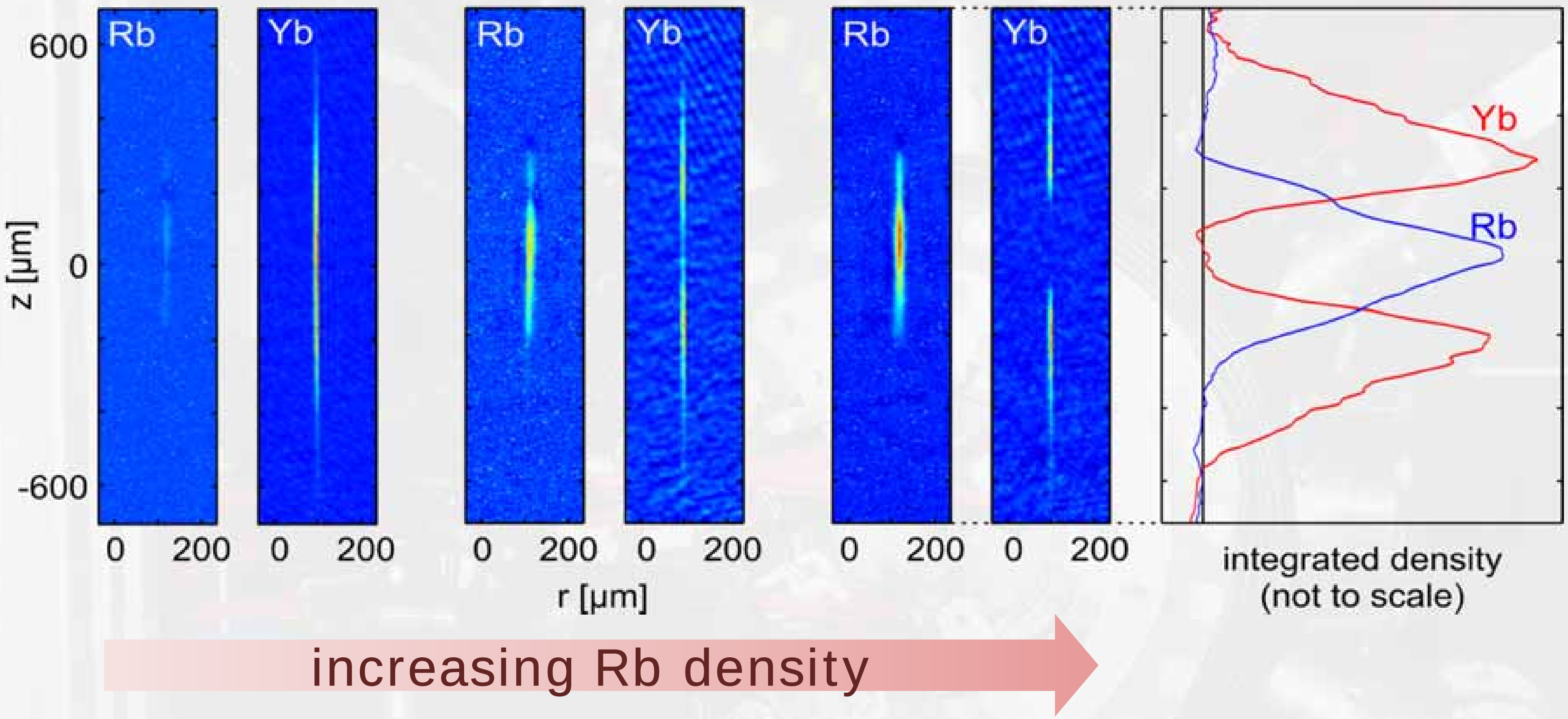


$T \approx 3$ µK

$N_{Yb} \approx 10^5$

$N_{Rb} \approx$

(a) 7×10^5

(b) 3×10^6

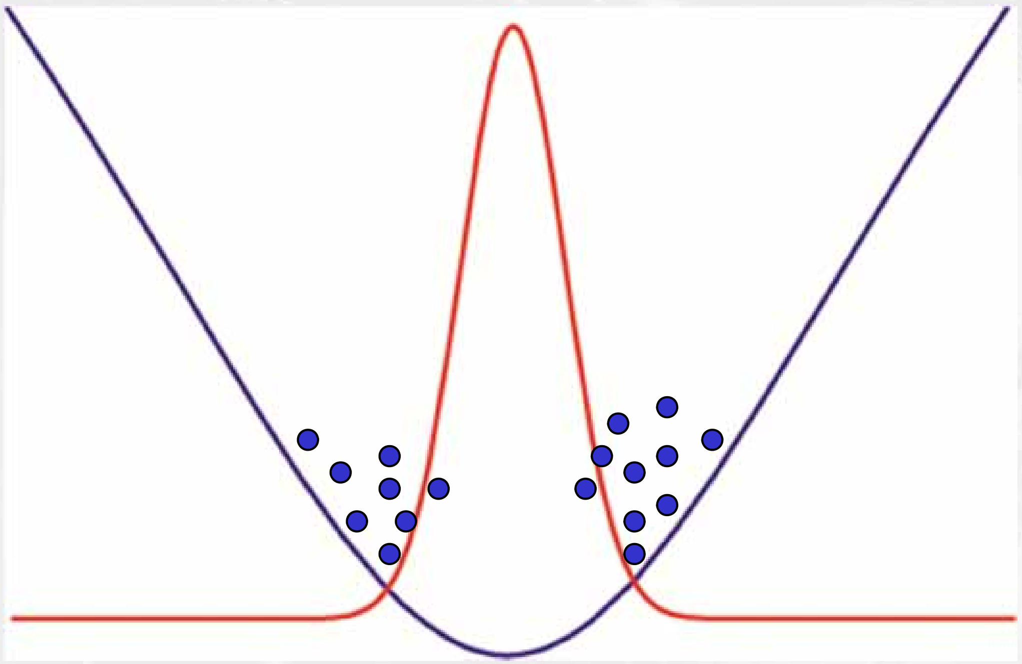
(c) 7×10^6

- separation of the ^{174}Yb-cloud and the (smaller) ^{87}Rb-cloud located in the trap center observed at temperatures 1.5 ... 7 µK
- due to $N_{Yb} \ll N_{Rb}$, no detectable effect on ^{87}Rb

⇒ unusually strong interactions between ^{87}Rb and ^{174}Yb

F. Baumer et al., PRA 83, 040702(R) (2011)

Diffusion model



- large σ_{YbRb}

$\Rightarrow$ motion of Yb is slowed

- large K_3

$\Rightarrow$ loss of Yb due to Rb+Rb+Yb collisions primarily in trap center

- Slowed, spatially dependent Yb loss

$\Rightarrow$ „hole“ in Yb distribution

Diffusion model

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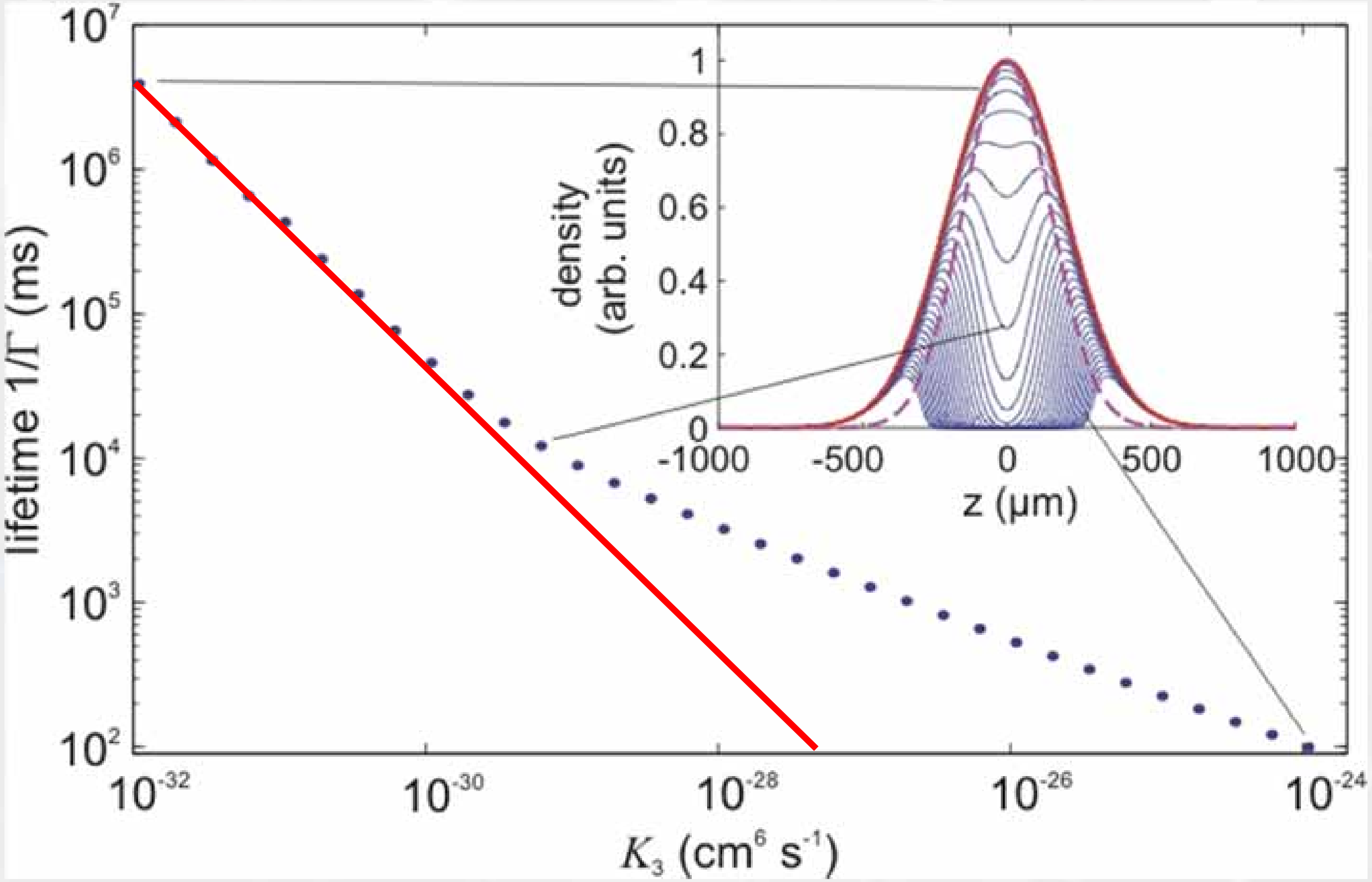
Calculated axial density distribution for 1D diffusion model



Assumption: unitarity-limited σ_{YbRb}, $n_{Rb} = 3 \times 10^{14}$ cm^{-3}

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3. YbRb: Photoassociation Spectroscopy

Photoassociative production of YbRb*

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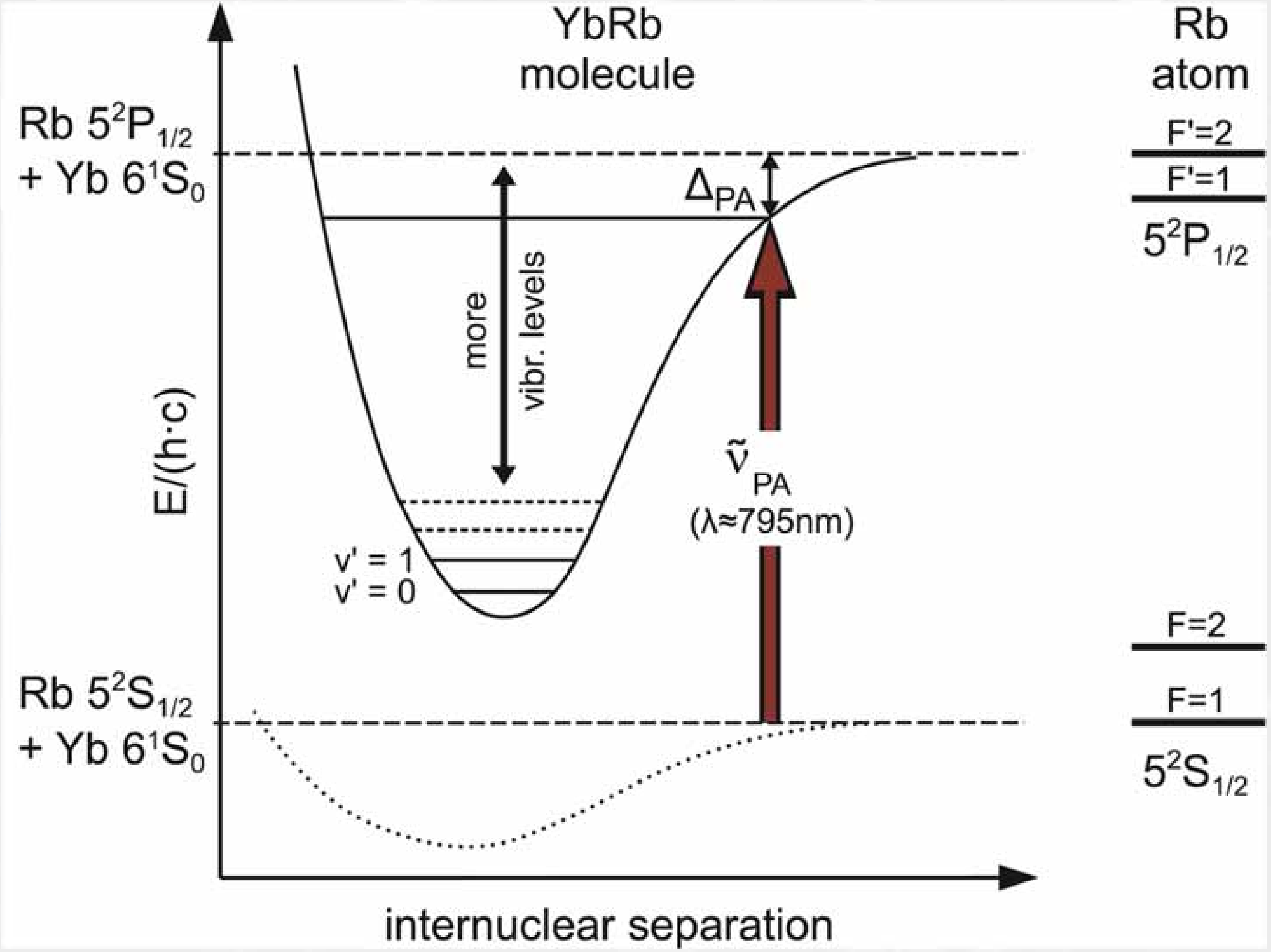
1-Photon photoassociation



Experimental scheme

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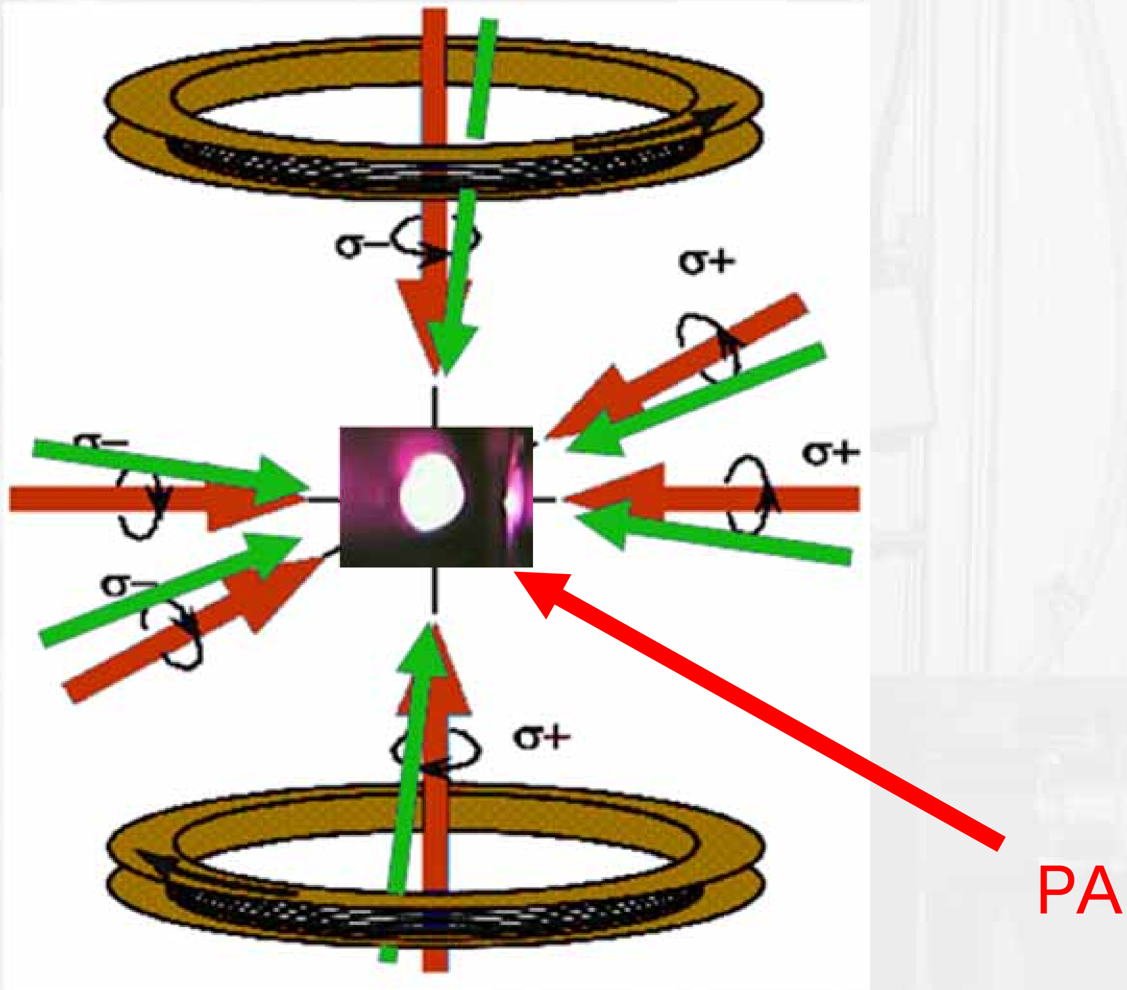
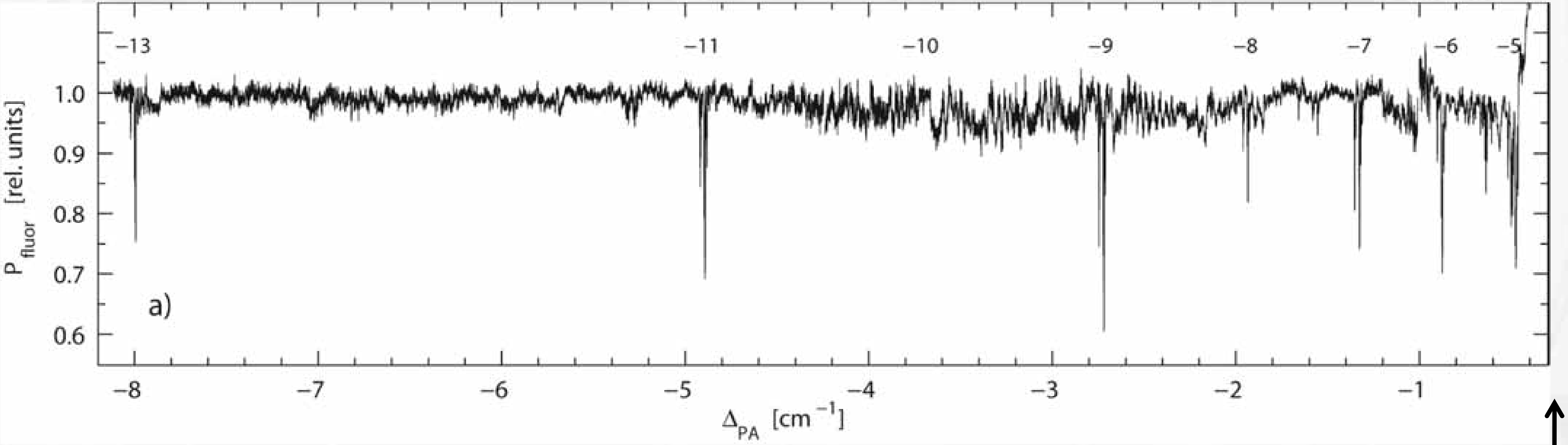
Continuously loaded simultaneous MOTs:

- Yb – „green“ MOT:
  ~ 10^6 atoms (loaded directly from slower)
- Rb - Dark Spot MOT:
  ~ 10^9 atoms; n ~ 10^{10}-10^{11} cm^{-3}
- PA-laser induces loss
- Rb-loss ⇒ Rb_2 formation
- Yb-loss ⇒ YbRb* formation



Photoassociative production of YbRb*

$^{176}Yb^{87}Rb$



Rb D1-line
@ 795 nm

YbRb* photoassociation

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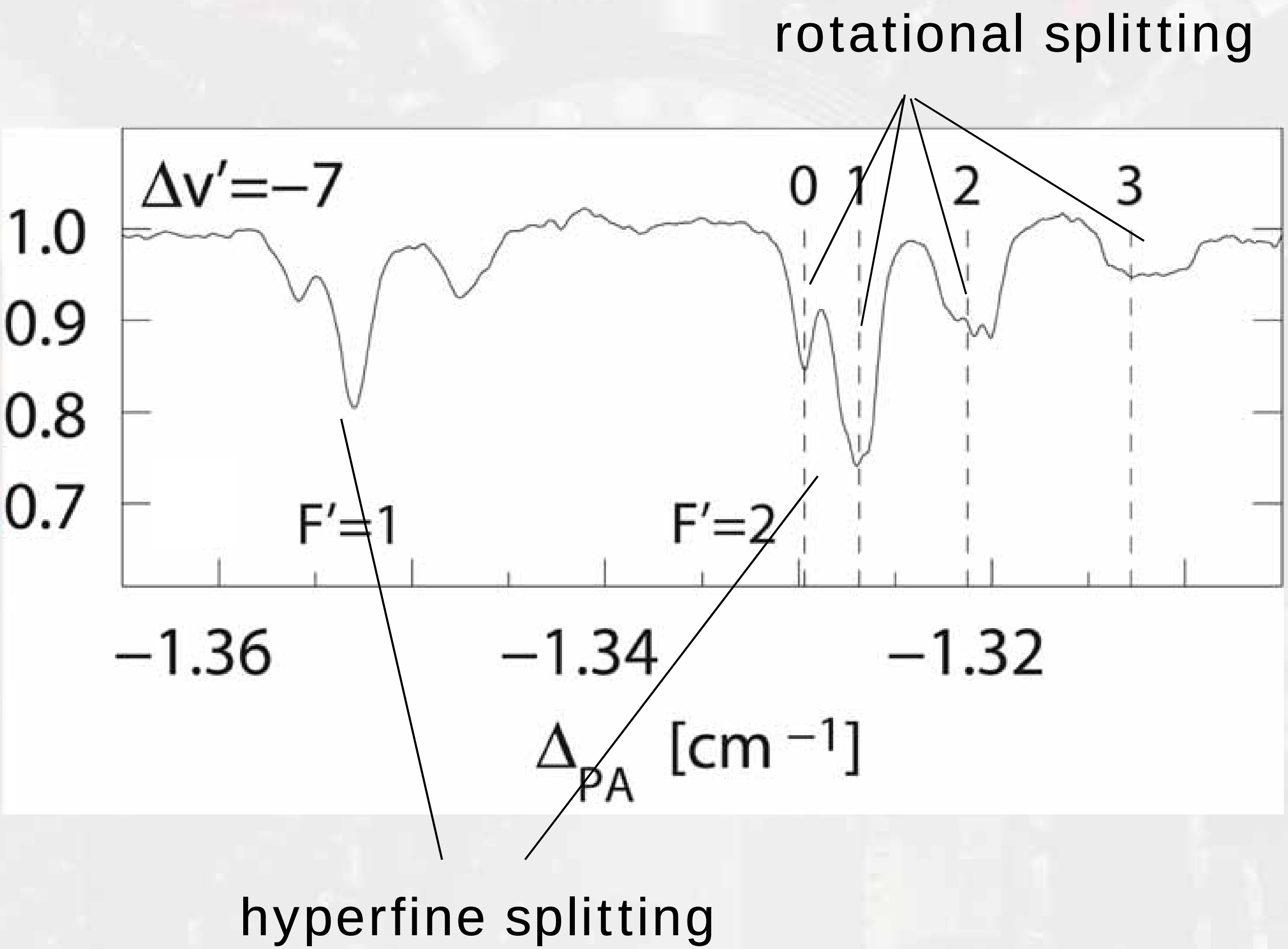
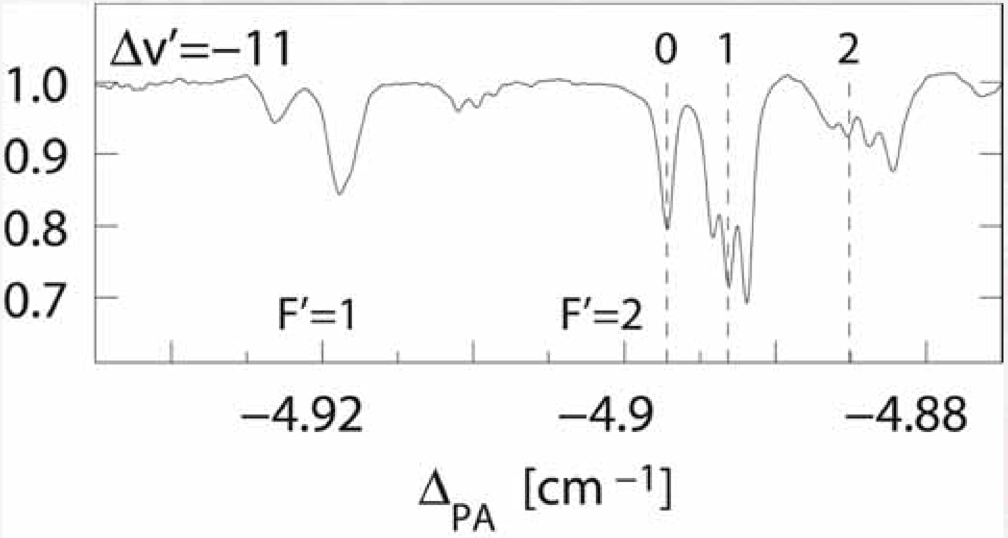
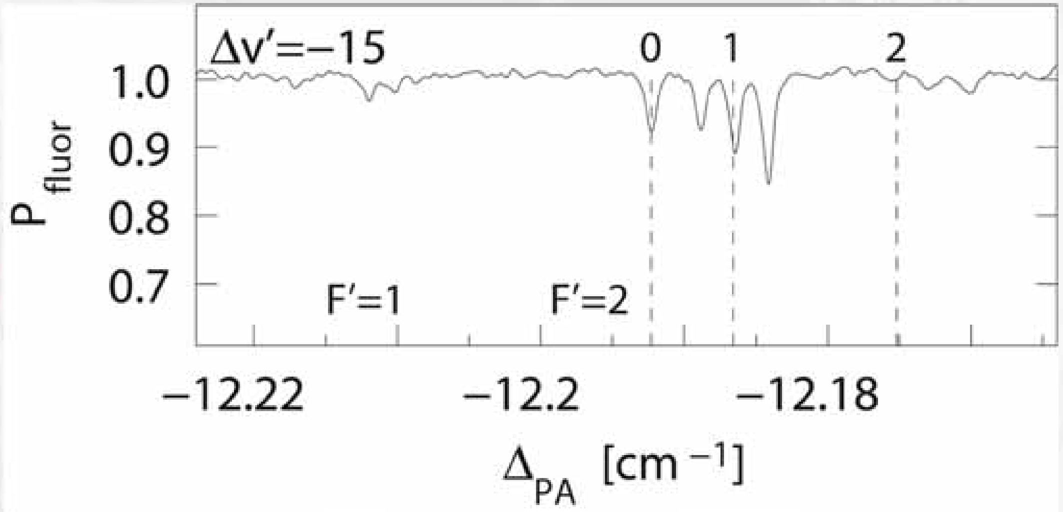
Resolved structure of vibrational level:



YbRb* photoassociation

Splitting of rotational levels:



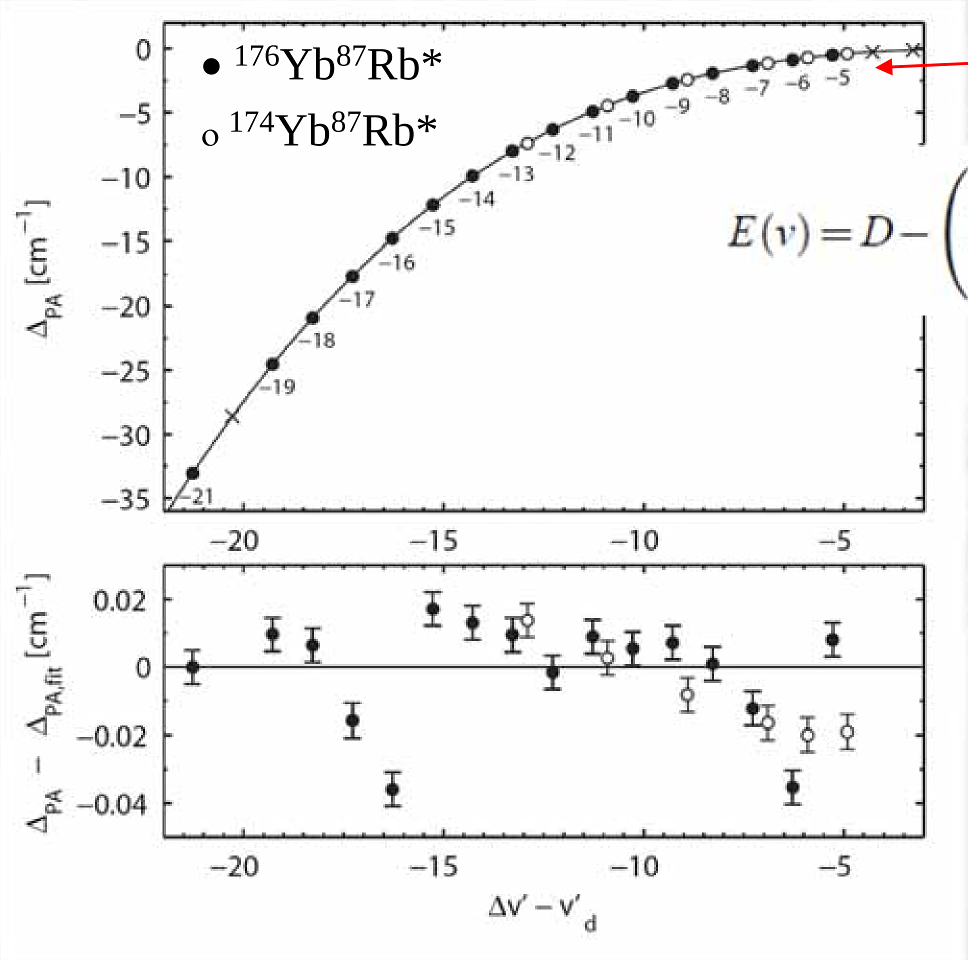


explanation: coupling of F‘ to R‘ (Hund‘s case (e))

F‘: Rb total angular momentum

R‘: nuclear rotation

Interpretation of results: Leroy-Bernstein Fit



Fit to Leroy-Bernstein formula[1]

$$E(v) = D - \left(\hbar \left(\frac{2\pi}{\mu} \right)^{1/2} \frac{\Gamma(1+1/n)}{\Gamma(\frac{1}{2}+1/n)} \frac{n}{C_n^{1/n}} (v_D - v) \frac{n-2}{2n} \right)^{\frac{2n}{n-2}}$$

assuming potential:

$V(r) = - C_6/R^6$

$\Rightarrow$ C_6-coefficient for YbRb*:

C_6 = 5684 a.u.

Nemitz et al., PRA 79, 061403 (2009)

1) R. J. LeRoy and R. B. Bernstein, J. Chem. Phys. 52, 3869 (1970).

2-Photon PA-spectroscopy

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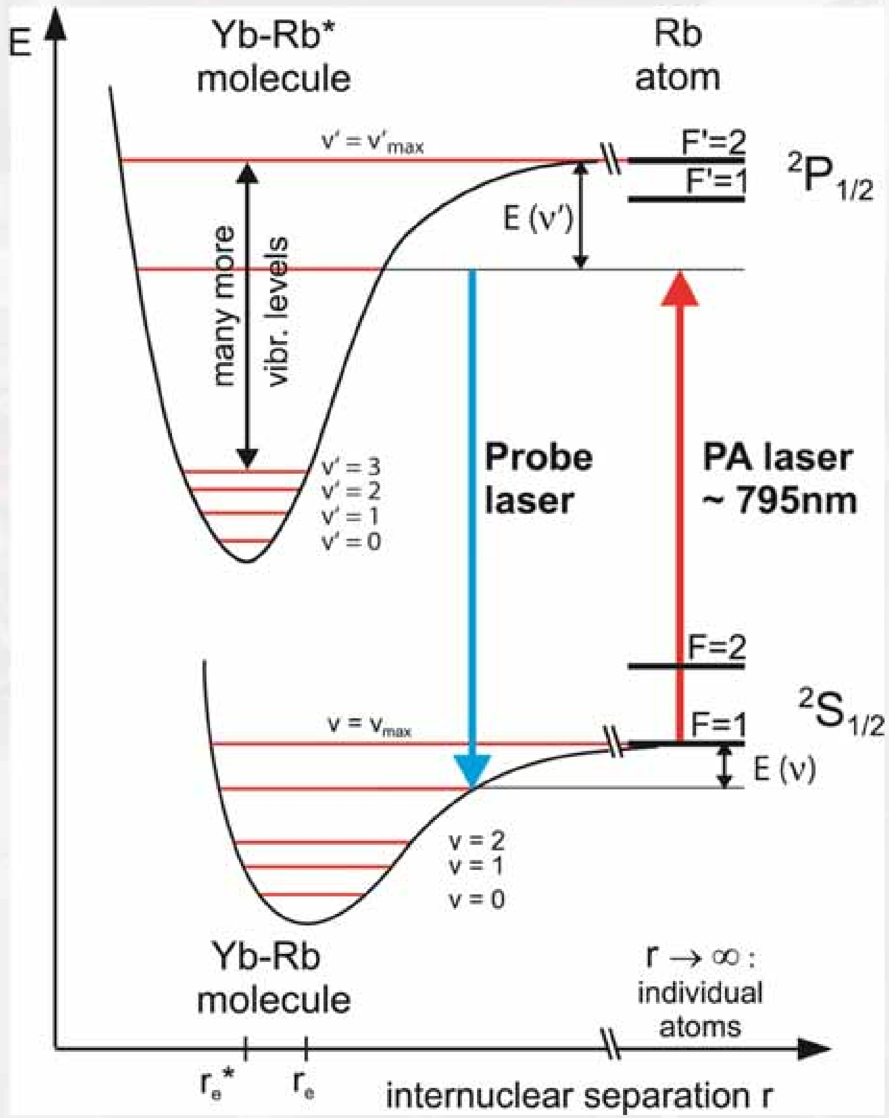
binding energy
of ground state level

$$\nu_{PA} - \nu_{Probe} = E(\nu)/h \quad (+\ \nu_{Hyperfine})$$

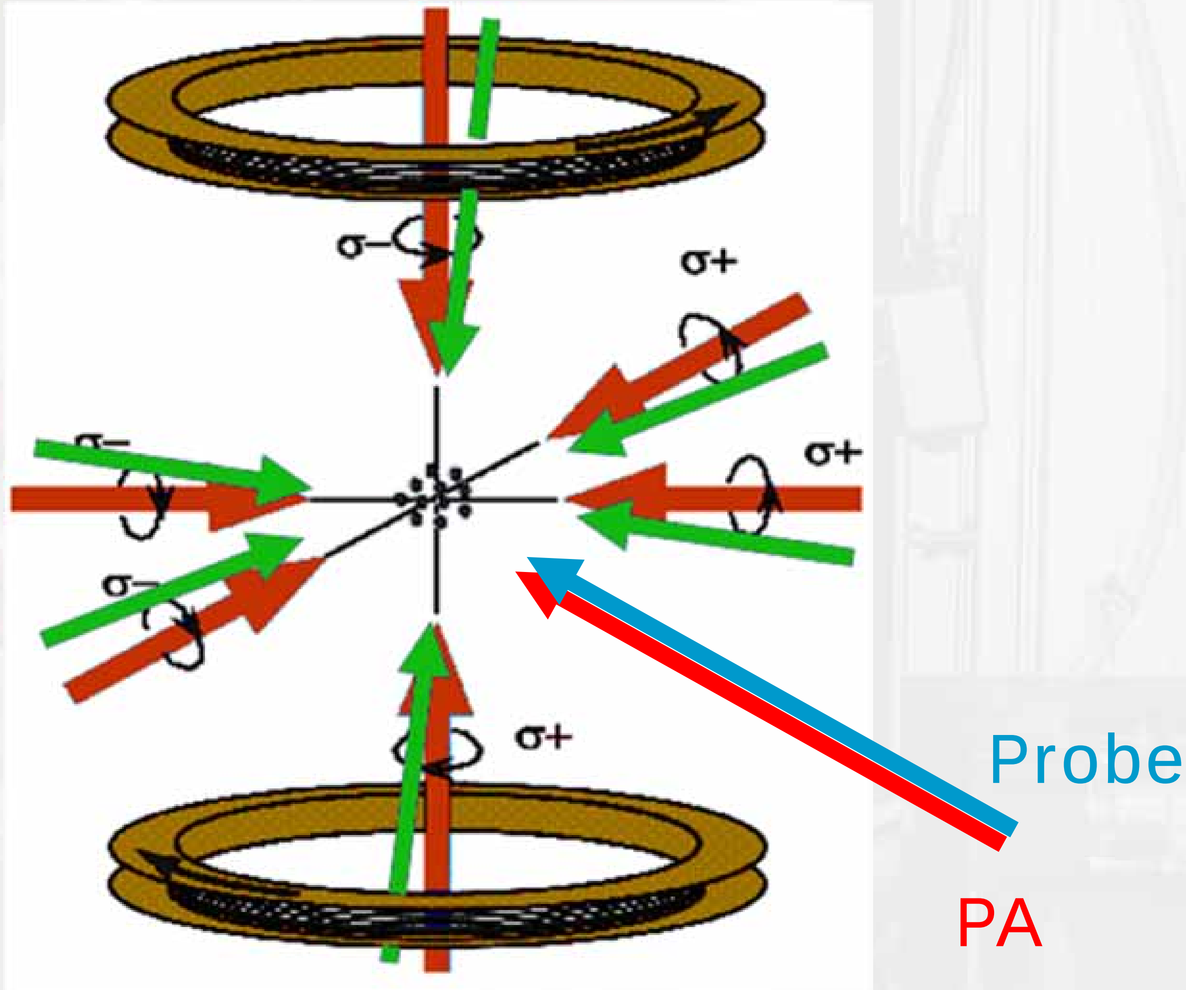
Probe laser only couples to transitions with $\Delta R = R\text{-}R' = 0$



Experimental scheme

- PA laser frequency set to single photon resonance $[\nu_{PA} = \nu_{D1} - E(\nu')/h]$
  $\Rightarrow$ continuous trap loss

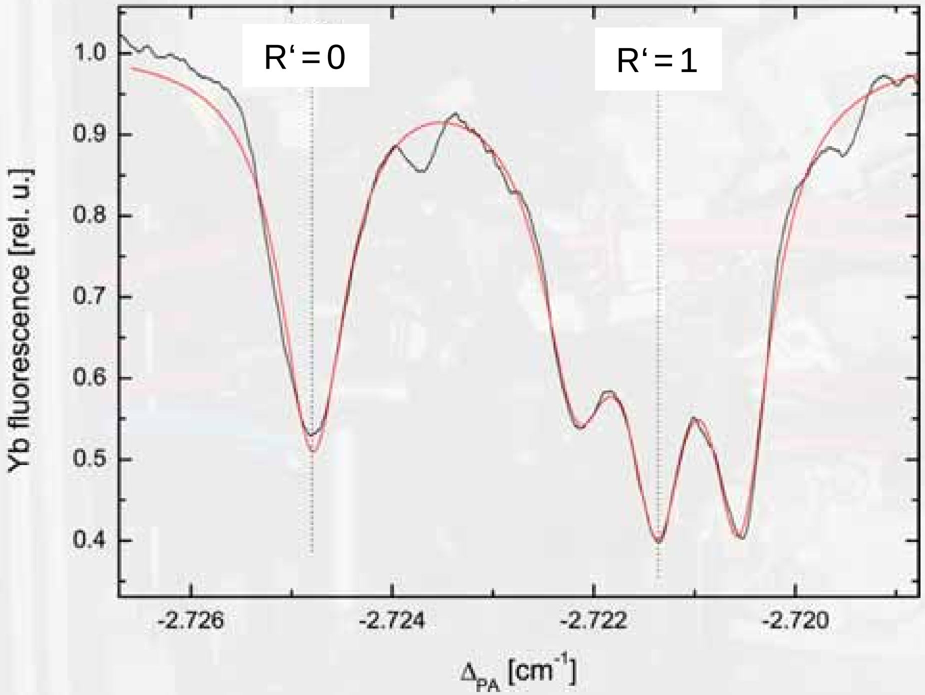
- if $\nu_{probe} = \nu_{PA} - E(\nu)/h$
  $\Rightarrow$ reduced trap loss due to light shift of probe beam on molecular transition $\nu \rightarrow \nu'$



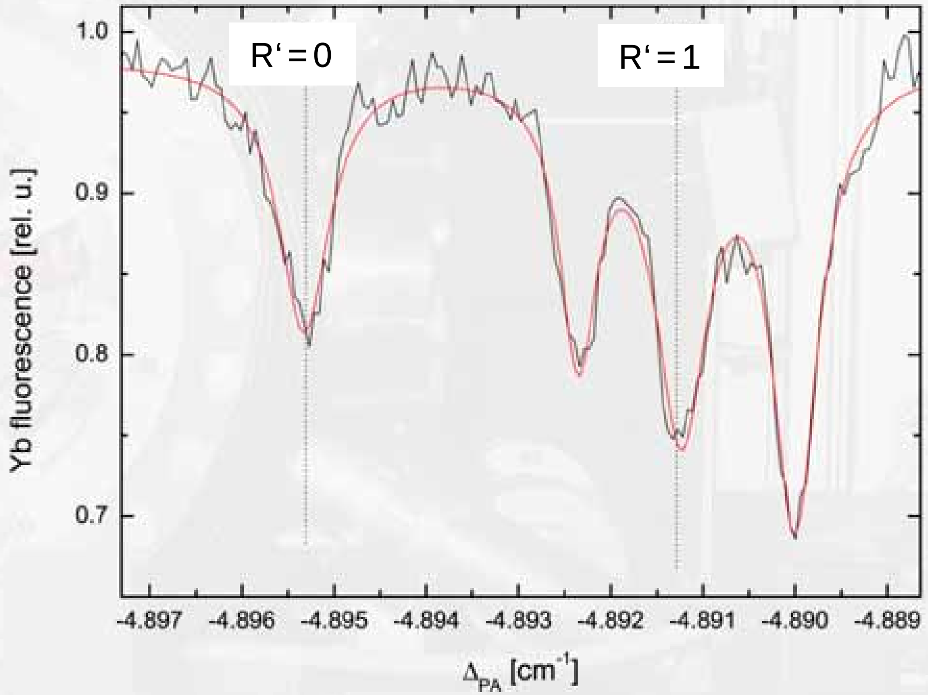
2-Photon PA-spectroscopy

Single-photon PA resonances used:

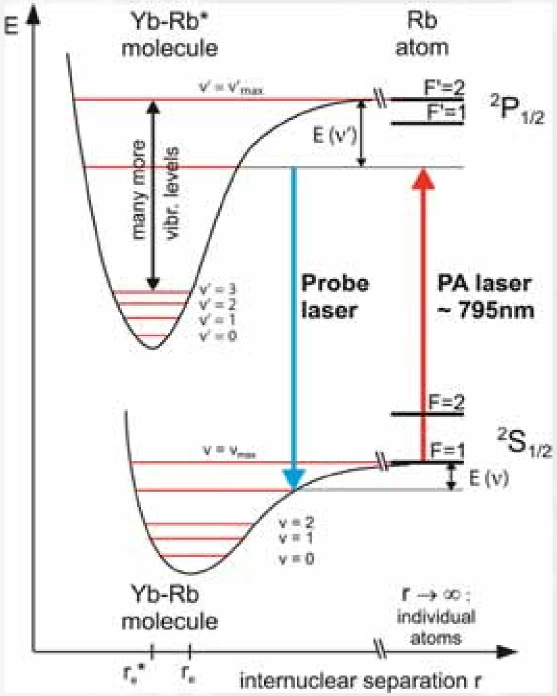
$\Delta v' = -9$

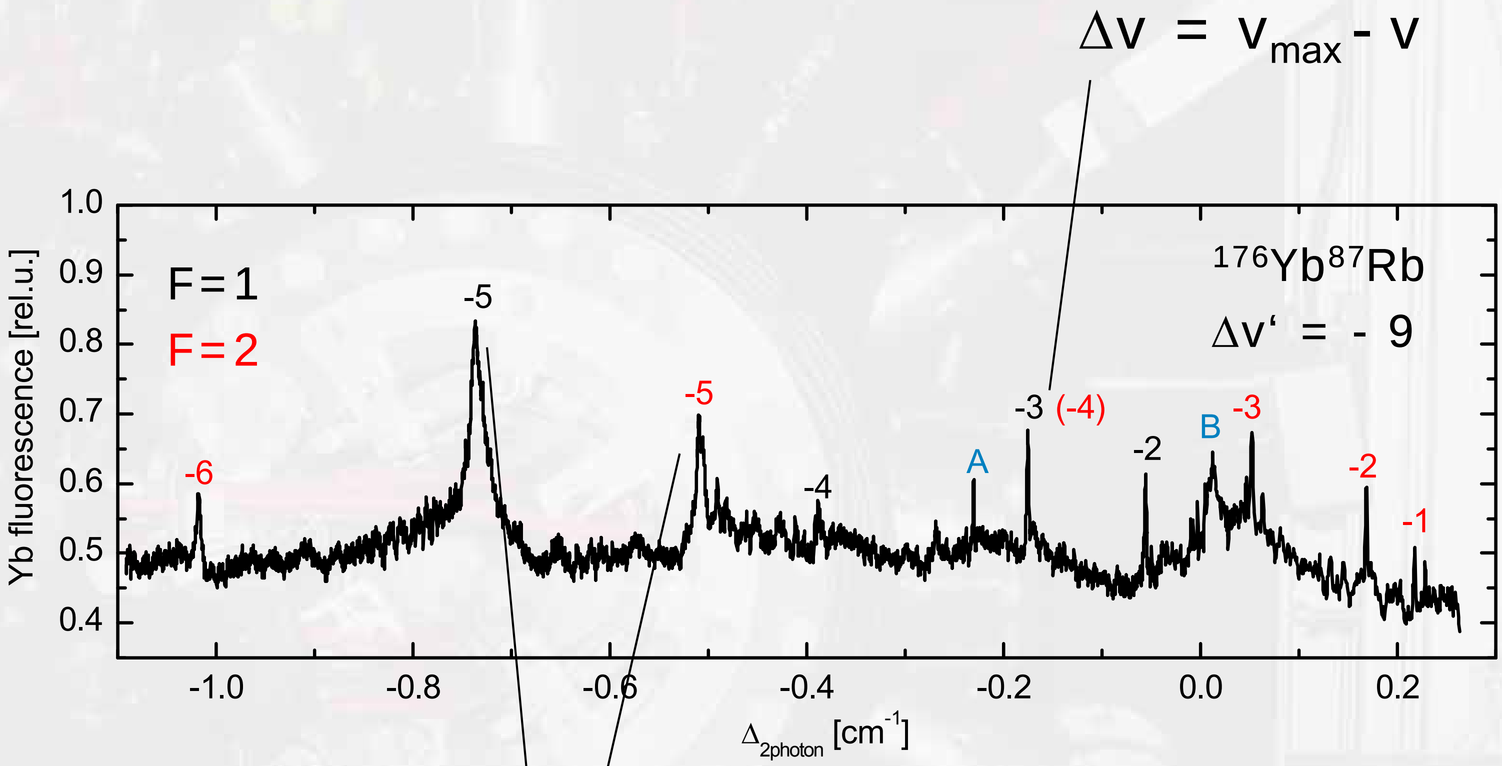


$\Delta v' = -11$



2-Photon PA-spectroscopy





- PA laser is fixed
- probe laser is scanned

Münchow et al., Phys.Chem.Chem.Phys. 13,18734 (2011)

Binding energies: LeRoy-Bernstein Fit

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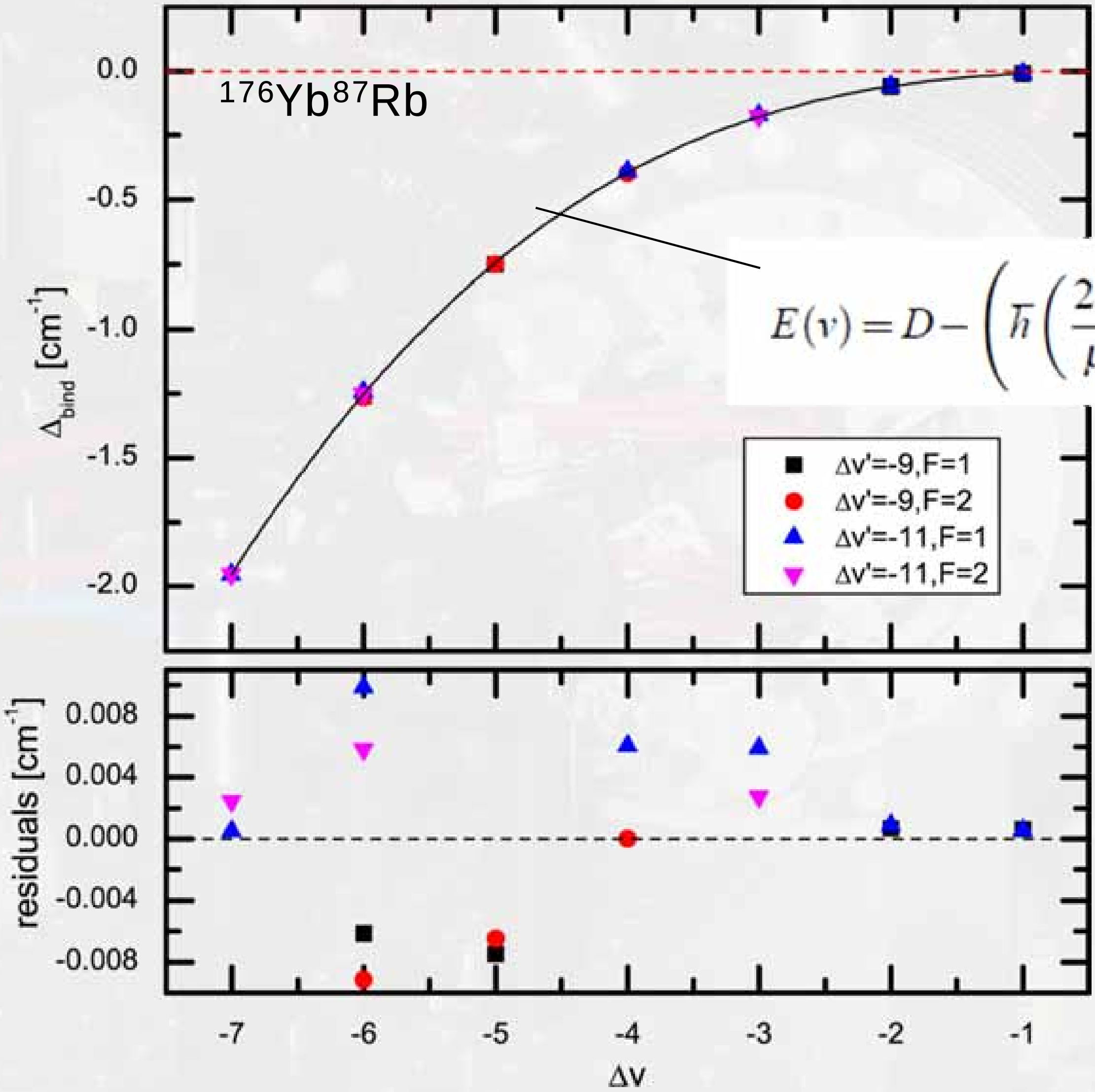


Assuming

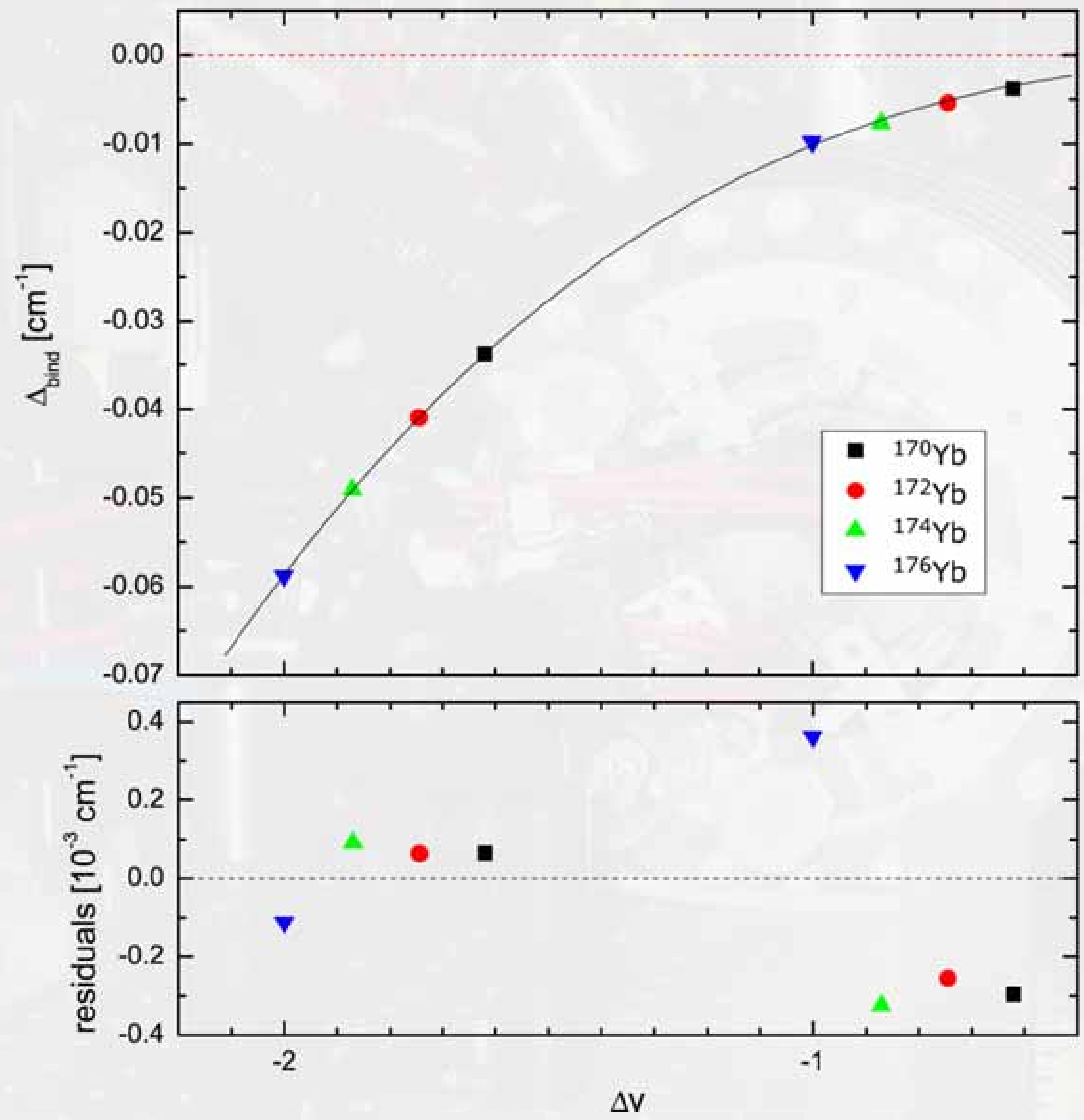
Long-range potential:

$V(R) = -C_6/R^6$

$$E(v) = D - \left(\hbar \left(\frac{2\pi}{\mu} \right)^{1/2} \frac{\Gamma(1+1/n)}{\Gamma(\frac{1}{2}+1/n)} \frac{n}{C_n^{1/n}} (v_D - v) \frac{n-2}{2n} \right)^{\frac{2n}{n-2}}$$

$\Rightarrow C_6 \sim 2600$ a.u.

Binding energies of $^{x}Yb^{87}Rb$



- binding energy of high-lying levels detected with ±10 MHz inaccuracy
- v_D adjusted for each Yb isotope (corresponding to mass scaling)

Scattering lengths

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Theoretical modelling by M. Borkowski, P. Zuchowski, R. Ciurylo, P. Julienne*

Binding energies are fit by:

scaling parameter

switching function

$$V(r) = dV_{\mathrm{sh}}(r)\,(1 - f(r)) - f(r)\left(C_6 R^{-6} + C_8 R^{-8}\right)$$

ab-initio potential

Fit parameters: C_6, C_8, d (corresponding to D_e)

*M. Borkowski et al., (in preparation)

Scattering lengths

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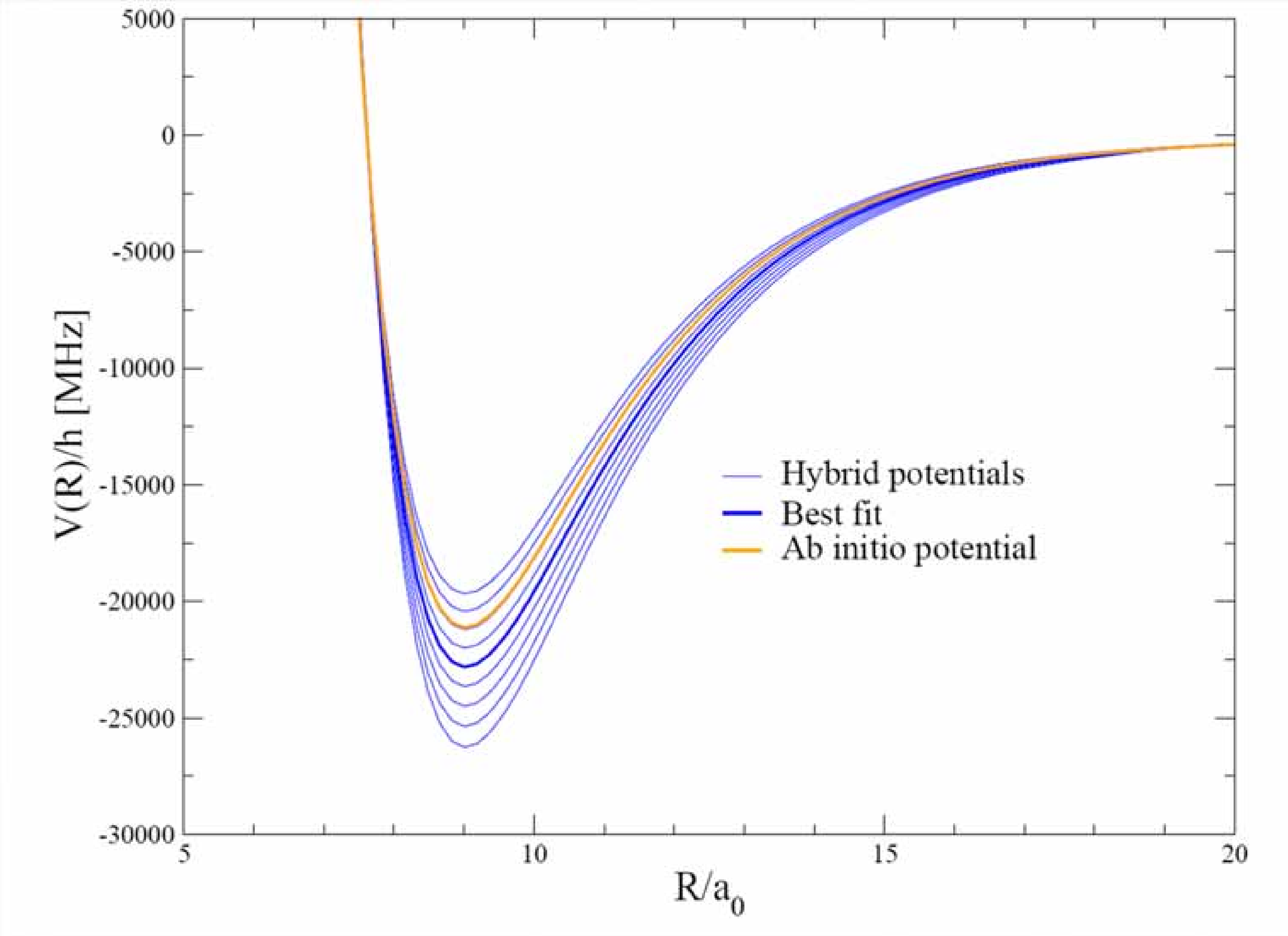

Best fit:

C_6 = 2813 a.u.

C_8 = 4.37 x 10^5 a.u.

D_e = 761 cm^{-1}

*M. Borkowski et al., (in preparation)

Scattering lengths

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$\Rightarrow$ scattering length given by*

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

with background scattering length:

$$\bar{a} \;=\; 2^{-\frac{3}{2}}\frac{\Gamma(3/4)}{\Gamma(5/4)}(2\mu C_6/\hbar^2)^{\frac{1}{4}}$$

and phase:

$$\Phi = \frac{\sqrt{2\mu}}{\hbar}\int_{R_{\mathrm{in}}}^{\infty}\sqrt{-V(r)}\mathrm{d}r.$$

*G. F. Gribakin and V. V. Flambaum, PRA 48, 546 (1993).

Scattering lengths

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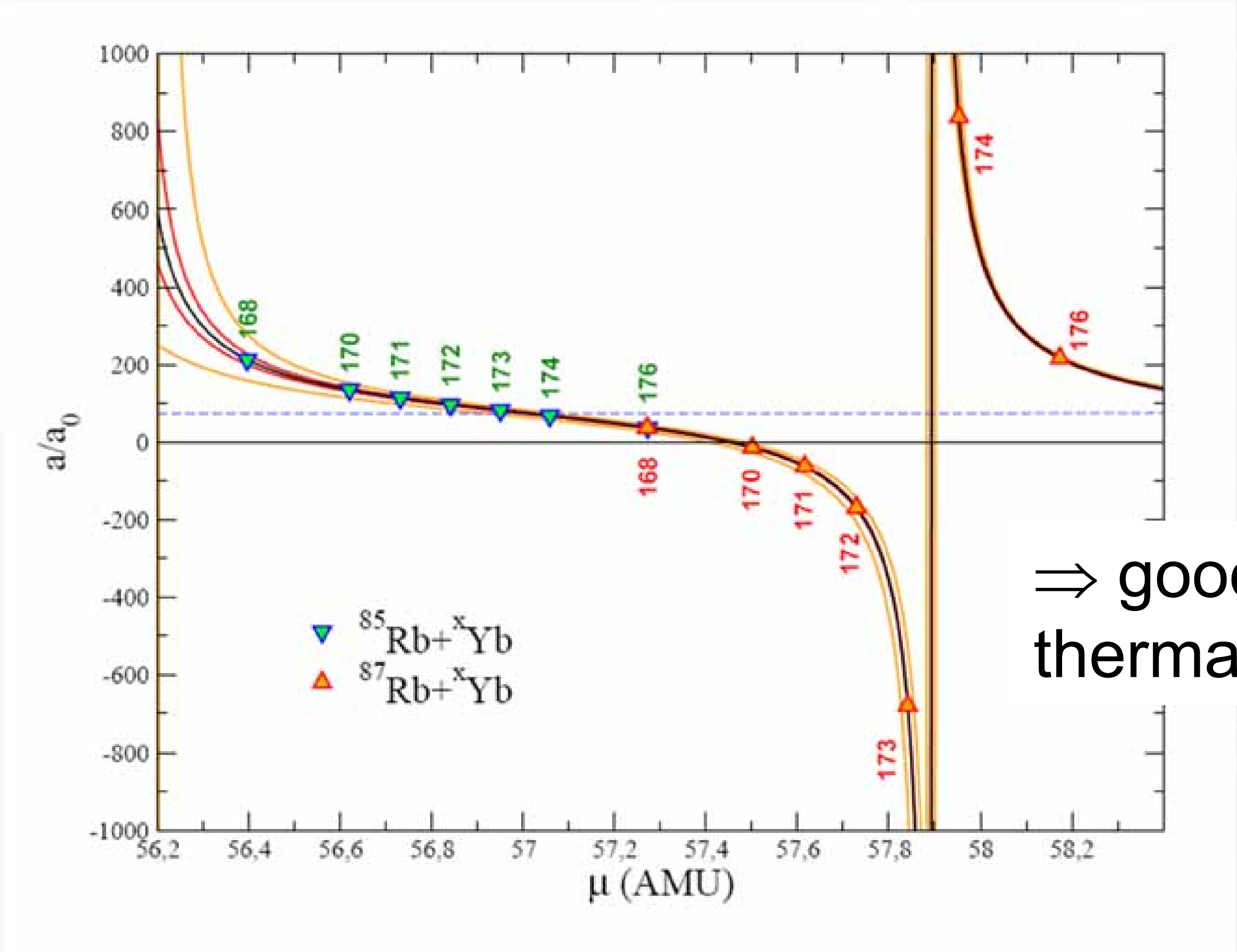
From best fit:



$\Rightarrow a_{87,170} \sim -14.5\ a_0$

$a_{87,\ 174} \sim 840\ a_0$

$\Rightarrow$ good agreement with thermalization measurements

Autler-Townes Spectroscopy

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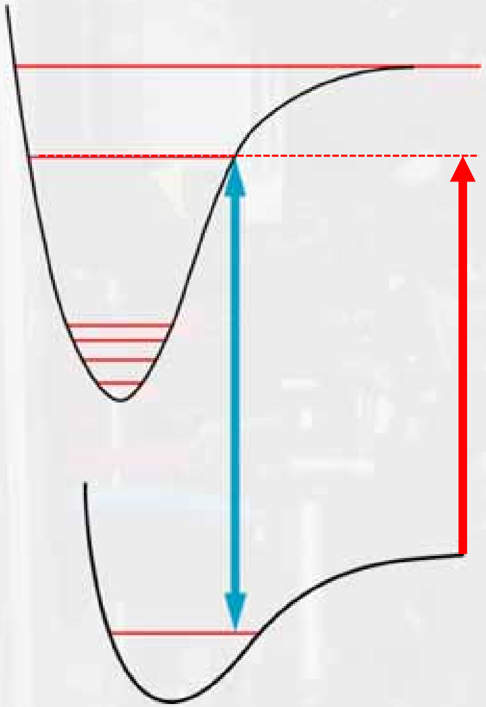
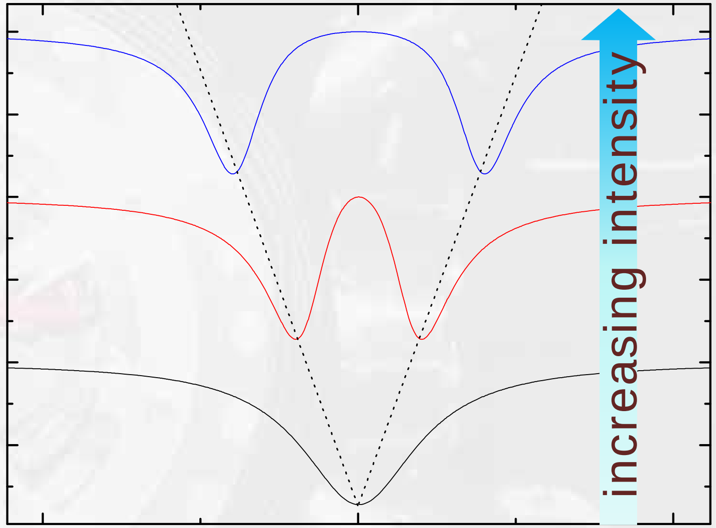
transition dressed by coupling laser

splitting of line



$\Rightarrow$



Splitting

$$\Delta = \sqrt{\delta^2 + \Omega_0^2}$$

S. H. Autler and C. H. Townes, Phys. Rev. 100, 703 (1955).

Autler-Townes Spectroscopy

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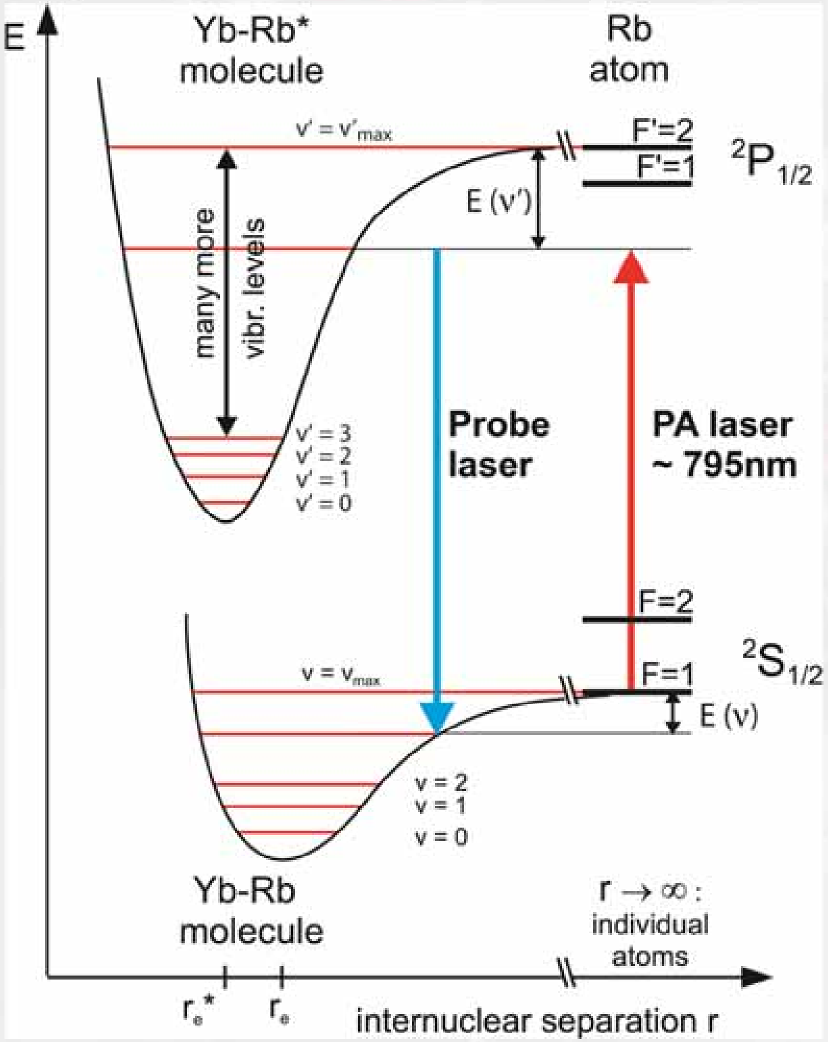
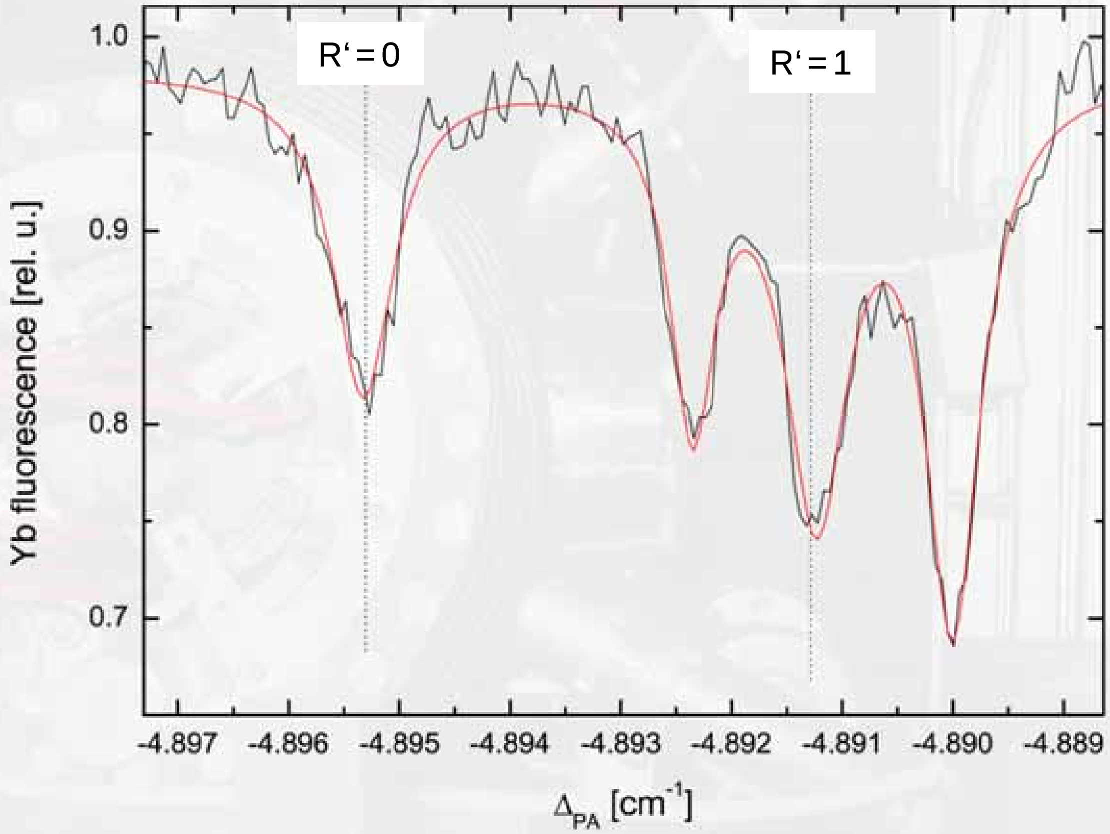


- probe laser couples to a bound-bound transition
- PA laser scanned over 1-Photon-PA resonance (free – bound)
  $\Rightarrow$ observation of splitting
  $\Rightarrow$ determination of Rabi frequency

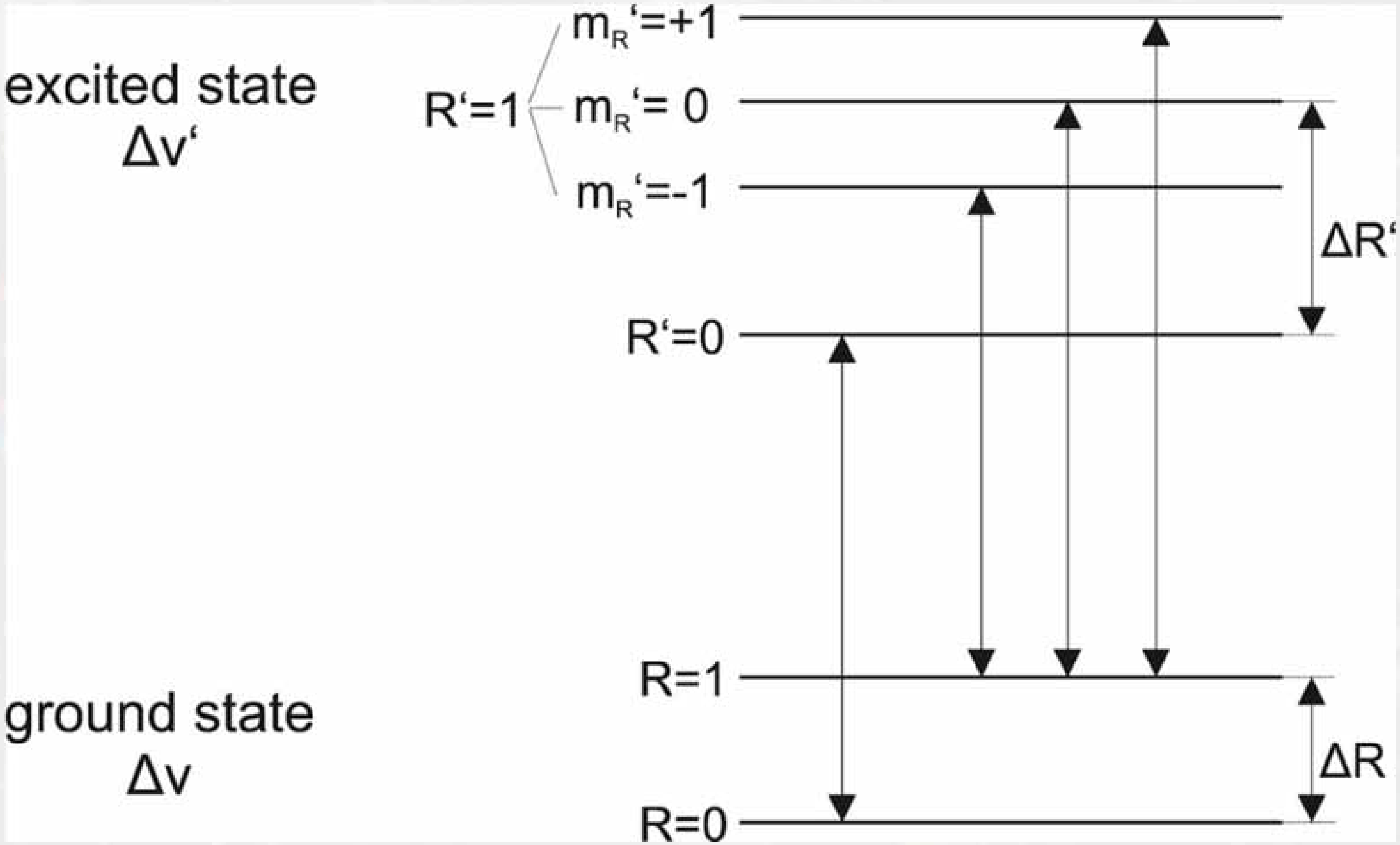
Autler-Townes Spectroscopy

1-photon PA spectrum
without coupling laser
(Δv= - 6 -> Δv' = -11)



Autler-Townes Spectroscopy

relevant levels for coupling laser



Autler-Townes Spectroscopy

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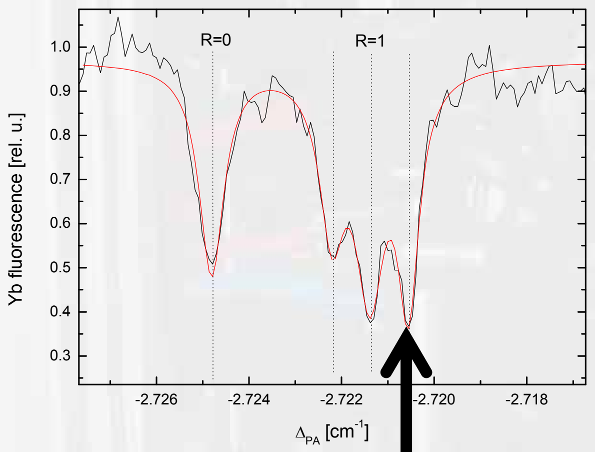
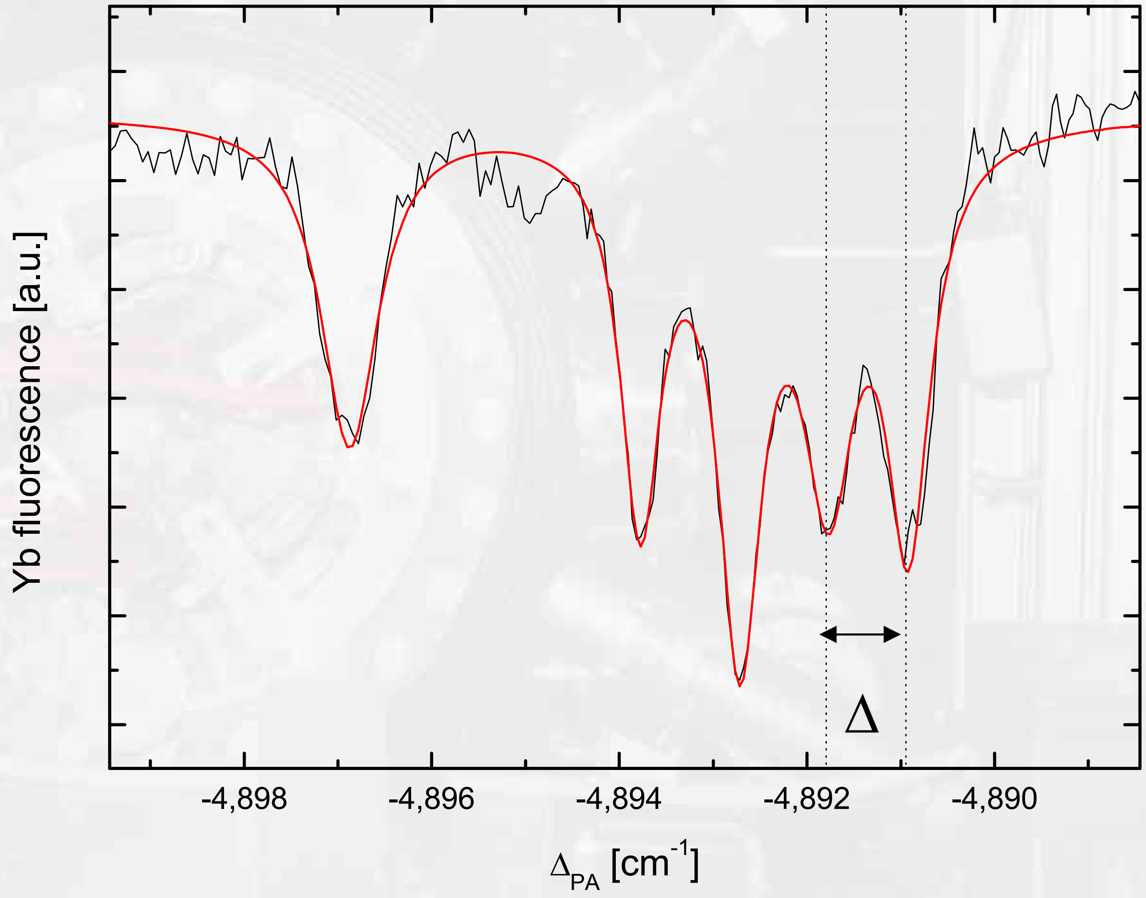
1-photon PA spectrum
with coupling laser

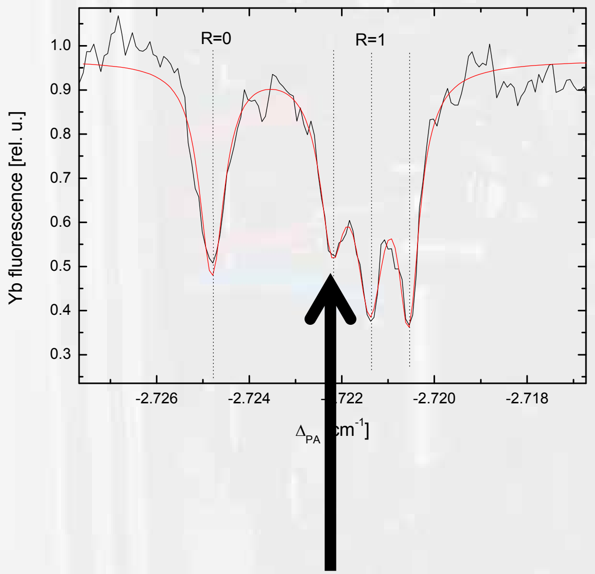


coupling laser
(Δv=-6 -> Δv‘=-11)

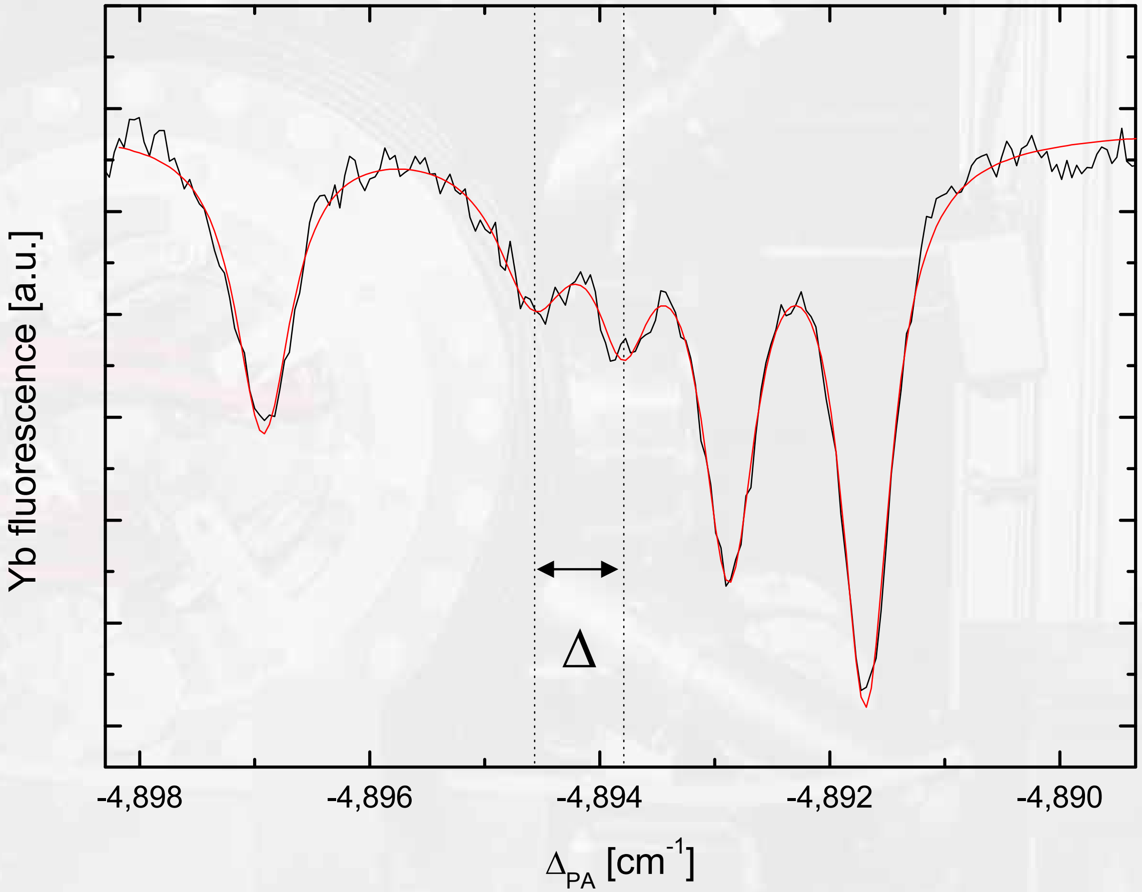


Autler-Townes Spectroscopy

1-photon PA spectrum
with coupling laser



coupling laser
(Δv=-6 -> Δv'=-11)



Autler-Townes Spectroscopy

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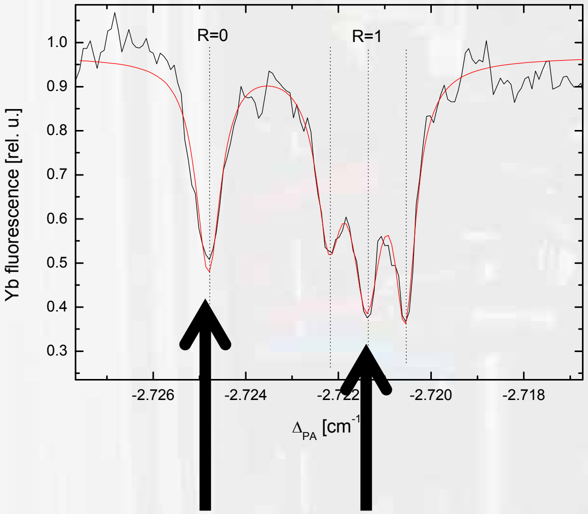
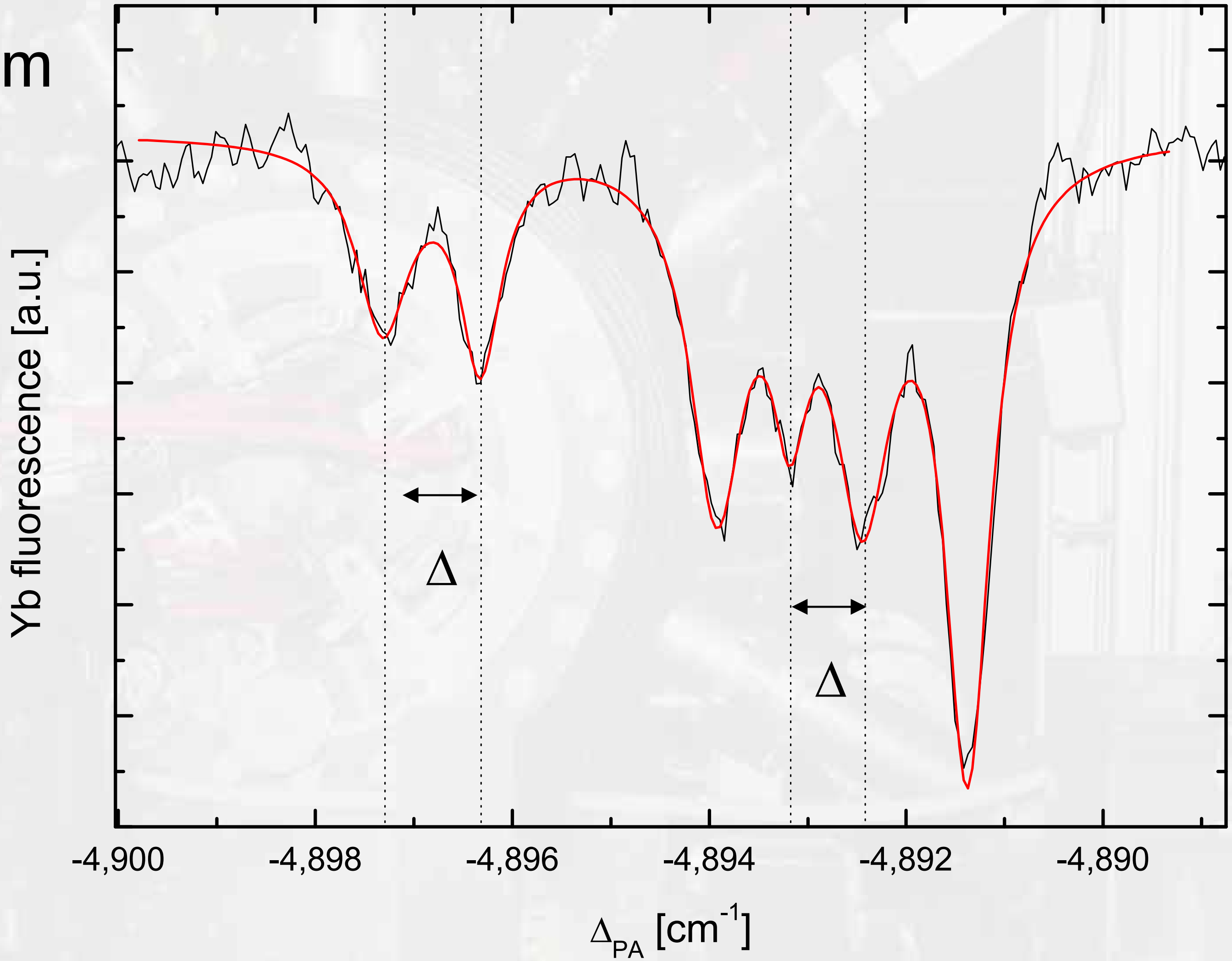
1-photon PA spectrum with coupling laser



coupling laser
(Δv=-6 -> Δv'=-11)



Autler-Townes Spectroscopy

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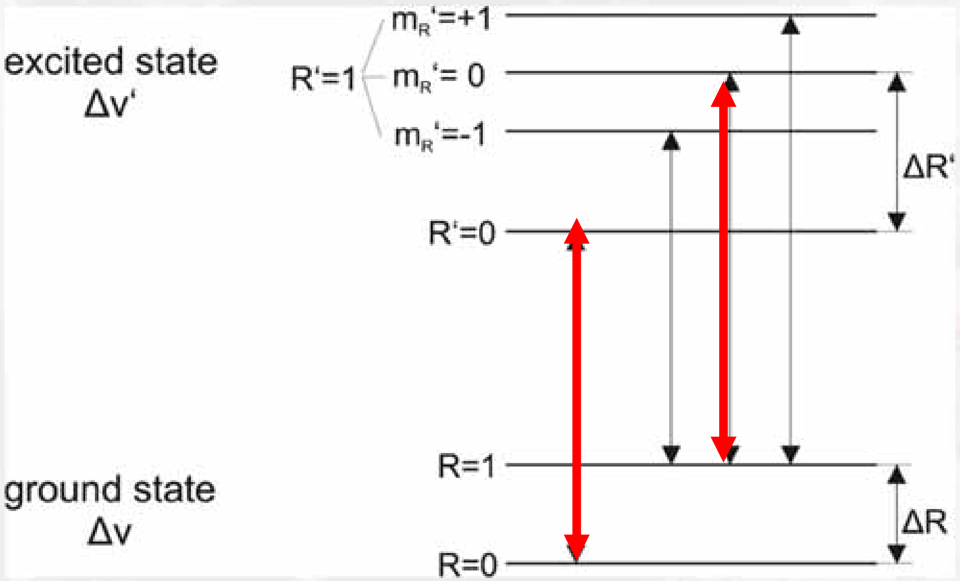
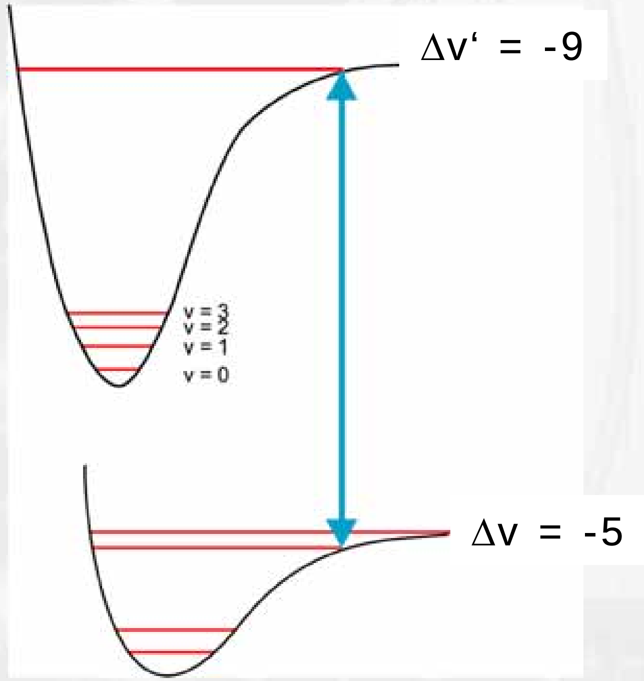
⇒ coupling laser couples R=1 and R= 0 transitions



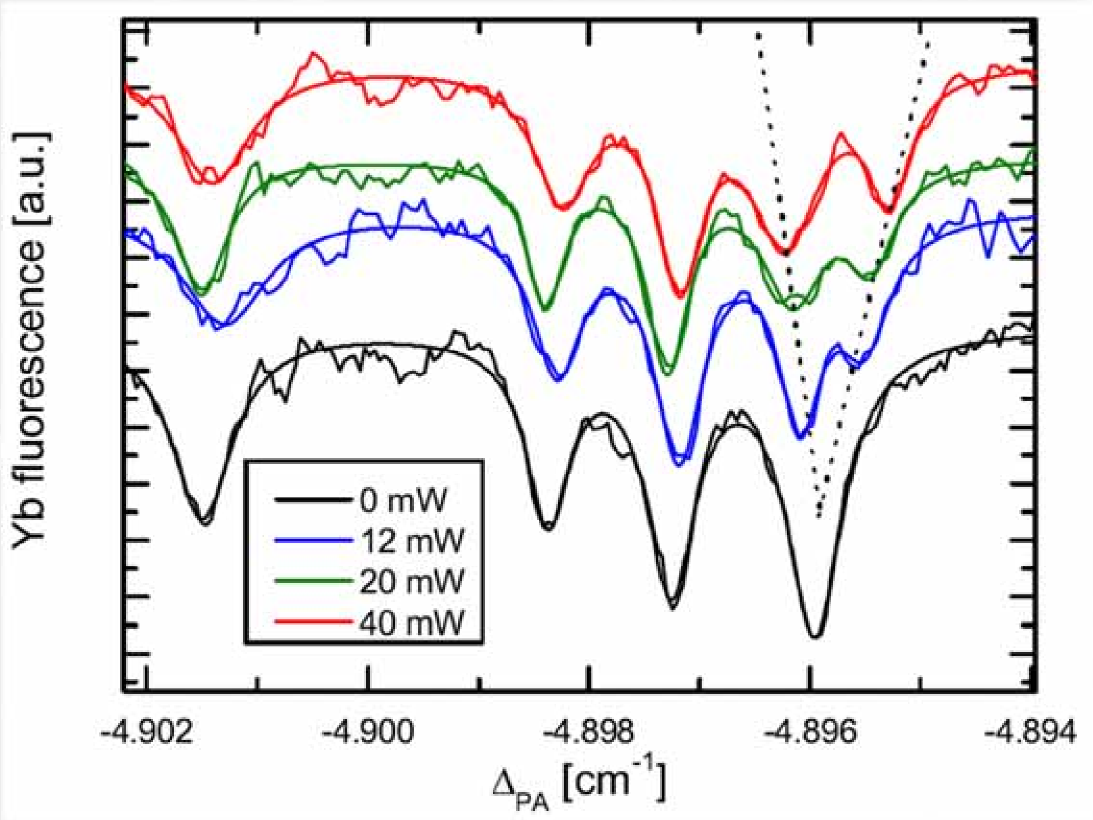


⇒ ΔR ~ ΔR'

⇒ similar classical outer turning points for ground and excited state

Autler-Townes Spectroscopy

Intensity-dependent splitting

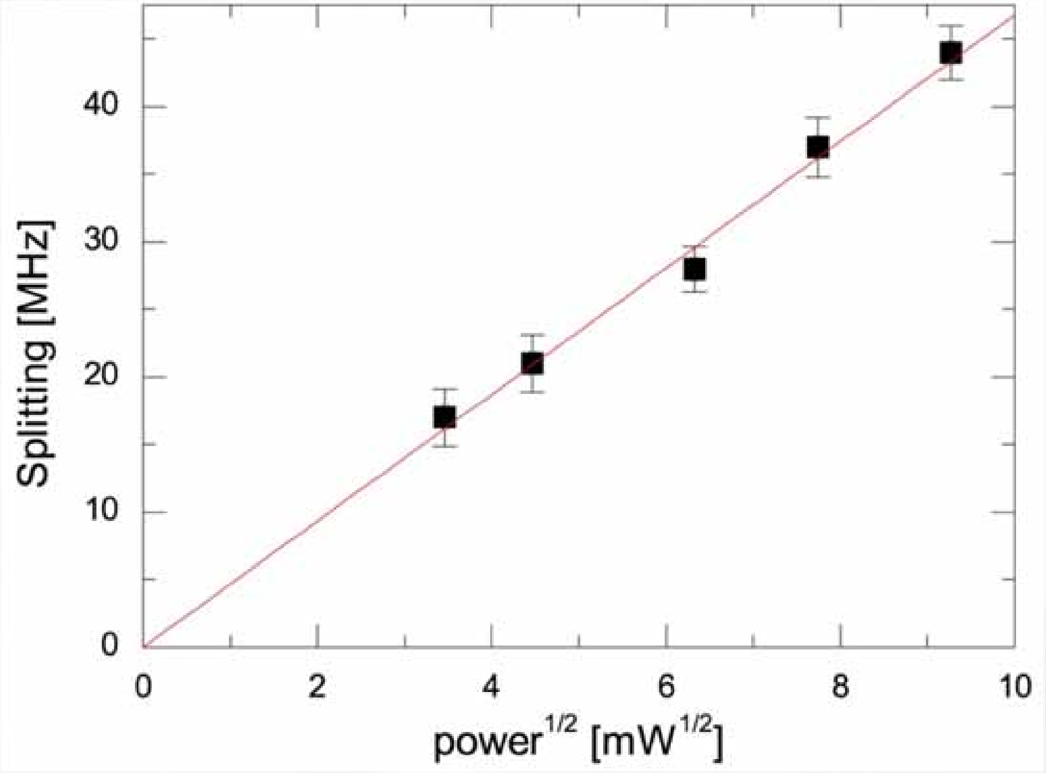


coupling laser
(Δv=-7 -> Δv'=-11)

Autler-Townes Spectroscopy

Rabi frequency:

$$\Omega_{12} = \alpha \, |\langle b_1 | b_2 \rangle| \, \gamma_1 \sqrt{\frac{I}{4 I_{\mathrm{sat}}}}$$



coupling laser
(Δv=-7 -> Δv‘=-11)

Autler-Townes Spectroscopy

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Franck-Condon factor

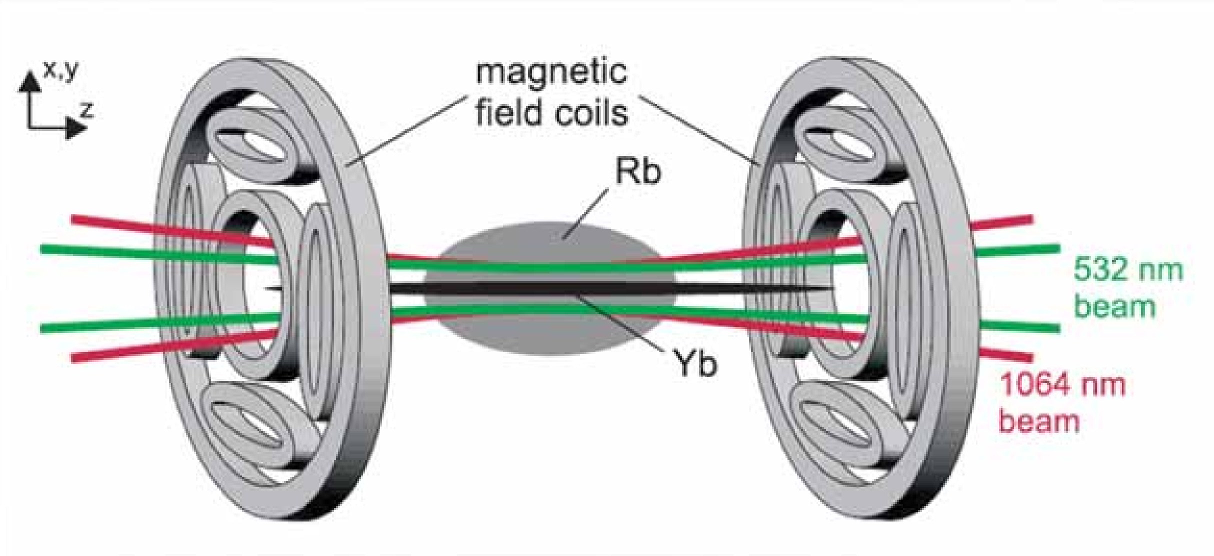
$$f_{\mathrm{FC}} = |\langle b_1 | b_2 \rangle|^2 = \frac{\Omega_{12}^2}{\alpha^2 \gamma_1^2} \frac{4 I_{\mathrm{sat}}}{I}$$

$\Delta v'$	Δv	Δ_{bind} (cm^{-1})	f_{FC} (rel.units)
-11	-4 (F=1)	-0.390	0.036 ± 0.008
	-6 (F=1)	-1.248	0.35 ± 0.10
	-6 (F=2)	-1.248	0.17 ± 0.03
	-7 (F=1)	-1.954	0.030 ± 0.002
-9	-5 (F=1)	-0.751	0.37 ± 0.04
	-5 (F=2)	-0.751	0.41 ± 0.02

4. YbRb in the ground state: Feshbach resonances and / or Photoassociation

Back to the conservative trap

Hybrid trap

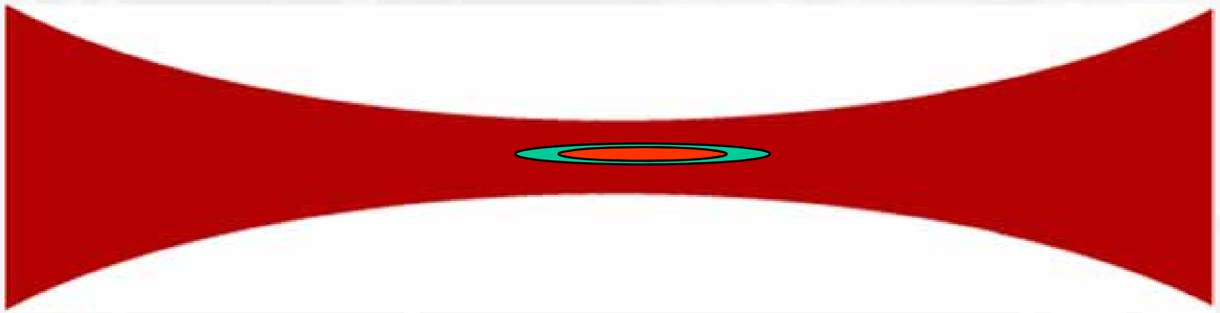


+ independent manipulation
+ similar trap dephts for Yb and Rb

- imperfect overlap
- hard to control experimentally

Back to the conservative trap

or simple optical trap?



+ experimentally simple
+ automatic overlap of atomic clouds (for tight confinement)

- 5 x deeper trap for Rb
- no independent manipulation

Back to the conservative trap

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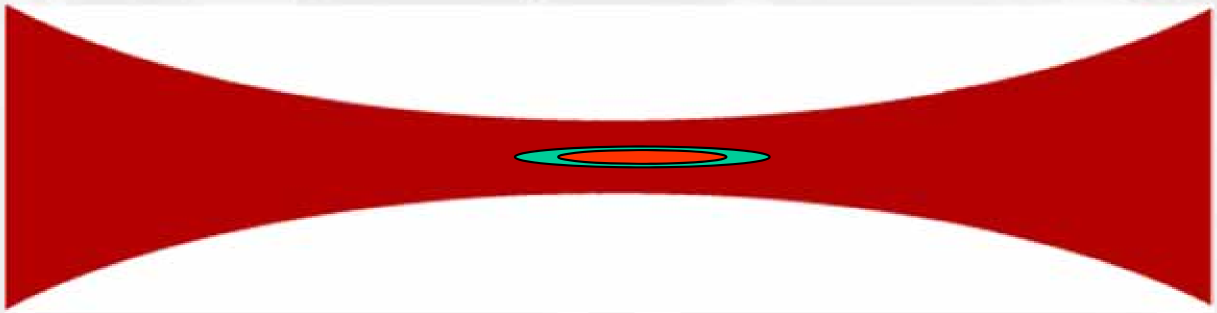
1st try: simple optical trap



1st goal: Find Route to create vibrationally excited molecules

Feshbach **Photoassociation**

Feshbach resonances in YbRb

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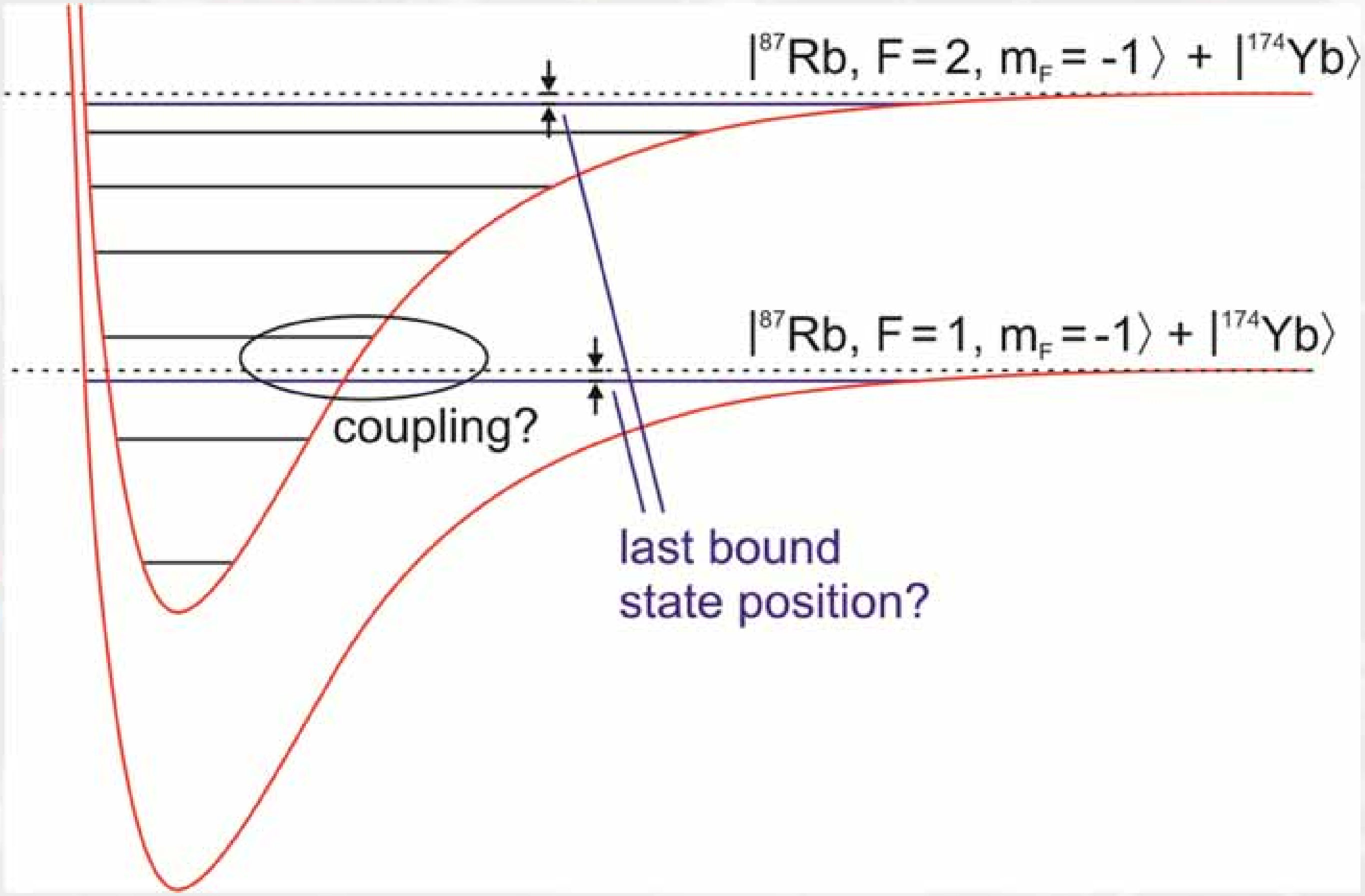

Predictions for SrRb

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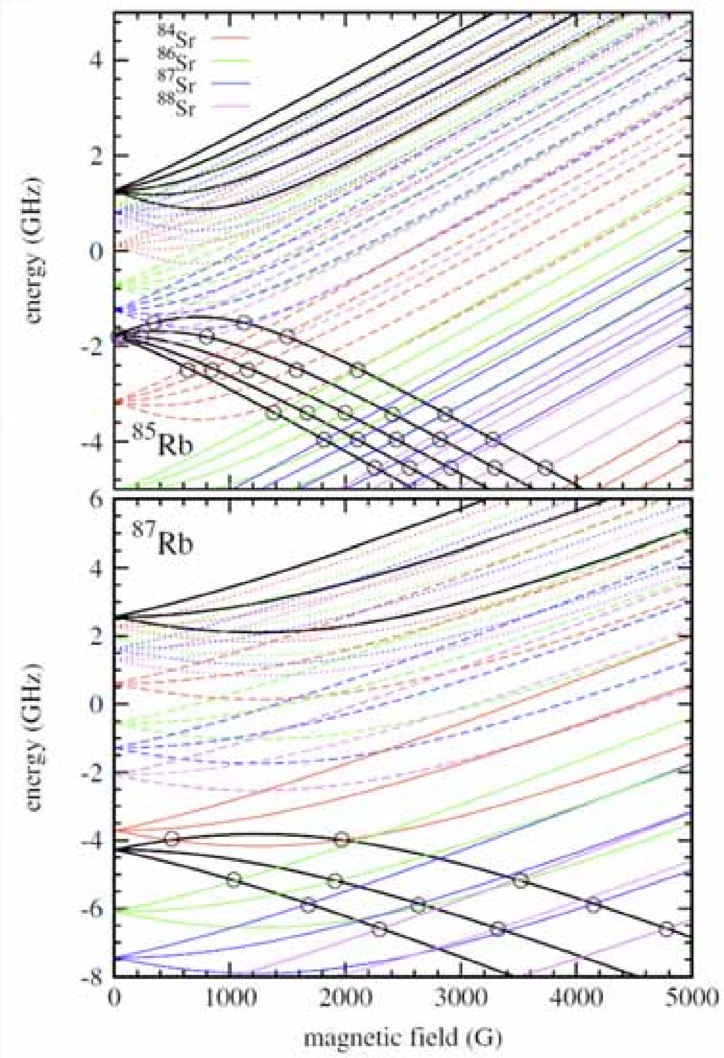
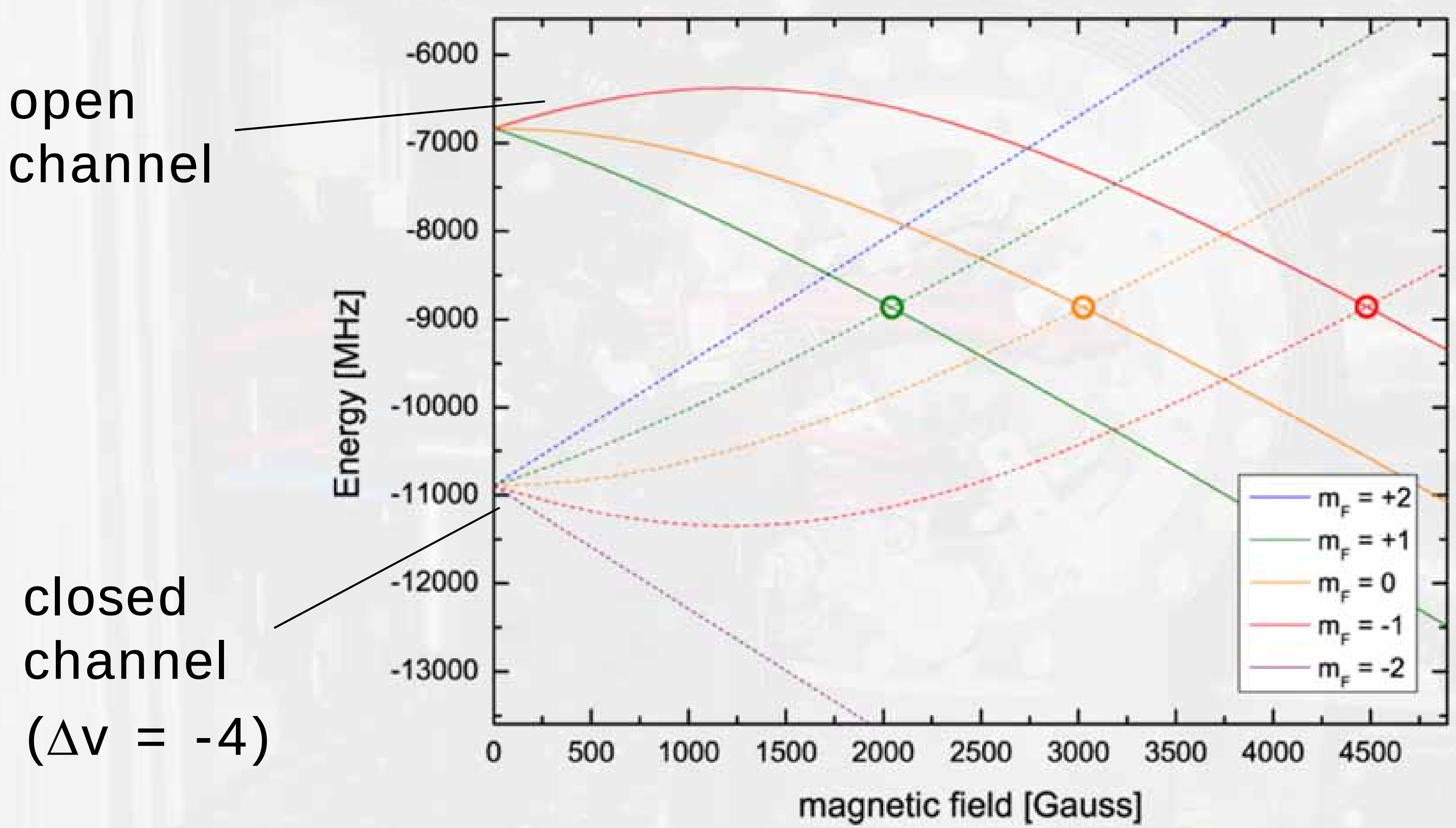


	B (G)	a_{bg}	ΔB (mG)
^{87}Rb^{84}Sr	477	1715.0	7.41
	1959	1700.3	− 122
^{87}Rb^{86}Sr	1036	55.0	− 0.209
	1896	55.0	− 1.08
	3472	55.0	− 2.29
^{87}Rb^{87}Sr	1660	31.5	− 0.636
	2608	31.5	− 2.27
	4096	31.5	− 3.79
^{87}Rb^{88}Sr	2281	1.6	− 33.6
	3280	1.6	− 101
	4716	1.5	− 153

P. Zuchowski et al., PRL 105, 153201 (2010)
for YbLi see D. Brue et al., PRL 108, 043201 (2012).

Feshbach resonances in $^{X}Yb^{87}Rb$

$^{174}Yb^{87}Rb$



bosonic Yb:

⇒ I_{Yb} = 0

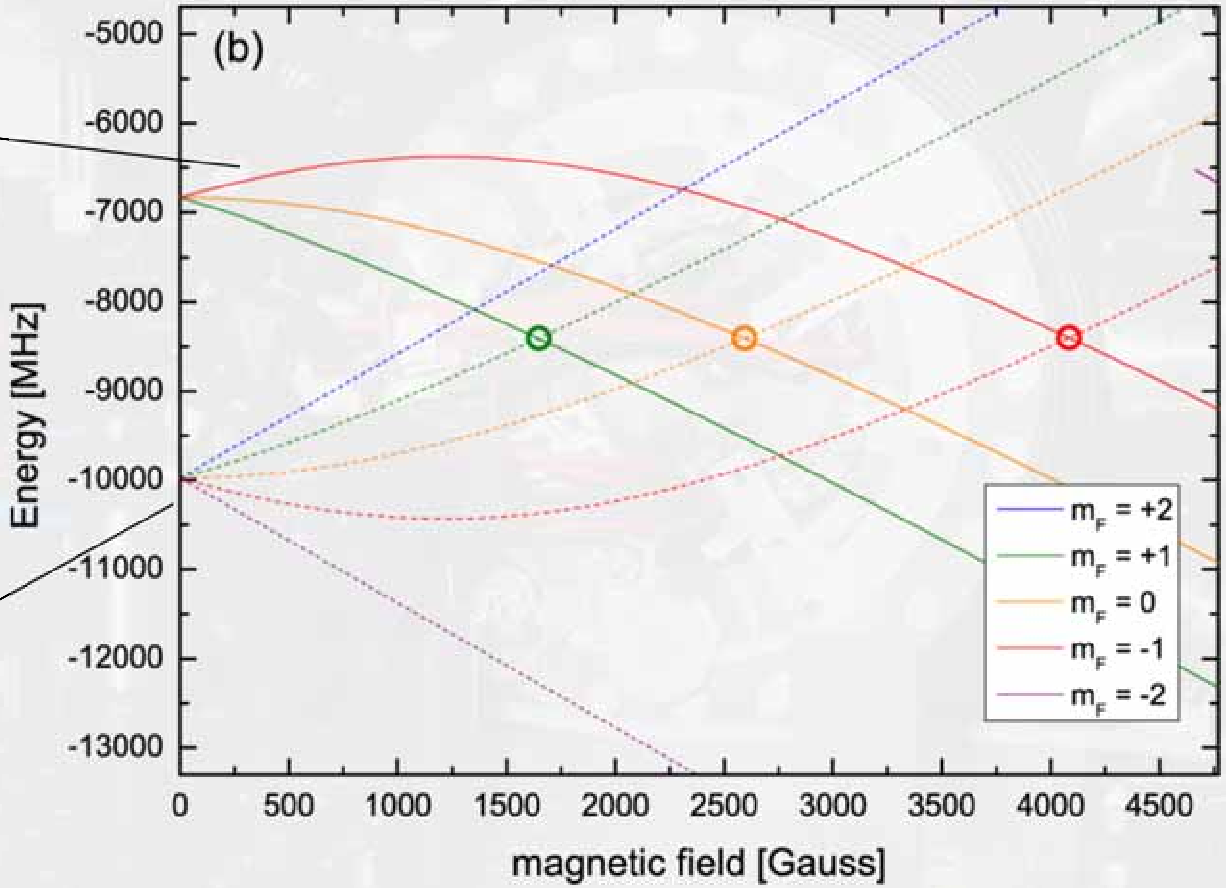
⇒ only $\Delta m_F = 0$ resonances

Feshbach resonances in $^{X}Yb^{87}Rb$

$^{172}Yb^{87}Rb$

open channel

closed channel (Δv = -4)



*lowest resonances with ^{87}Rb:

^{168}Yb ~ 850 G

^{170}Yb ~ 1250 G

^{172}Yb ~ 1650 G

^{174}Yb ~ 2000 G

^{176}Yb ~ 2500 G

^{171}Yb ~ 1150 G

^{173}Yb ~ 1550 G

* values derived from simplified model

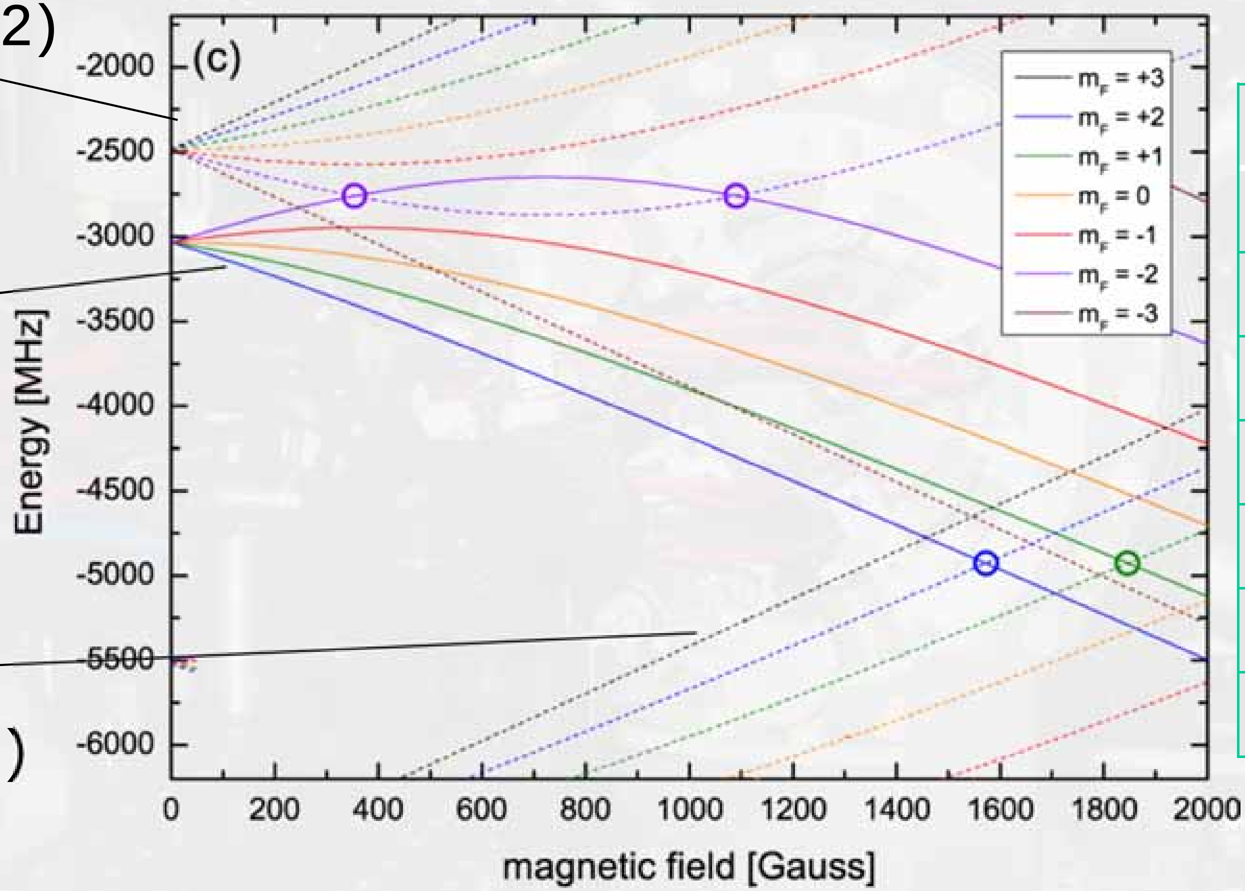
Feshbach resonances in $^{X}Yb^{85}Rb$

$^{172}Yb^{85}Rb$

closed channel (Δv = -2)

open channel

closed channel (Δv = -3)



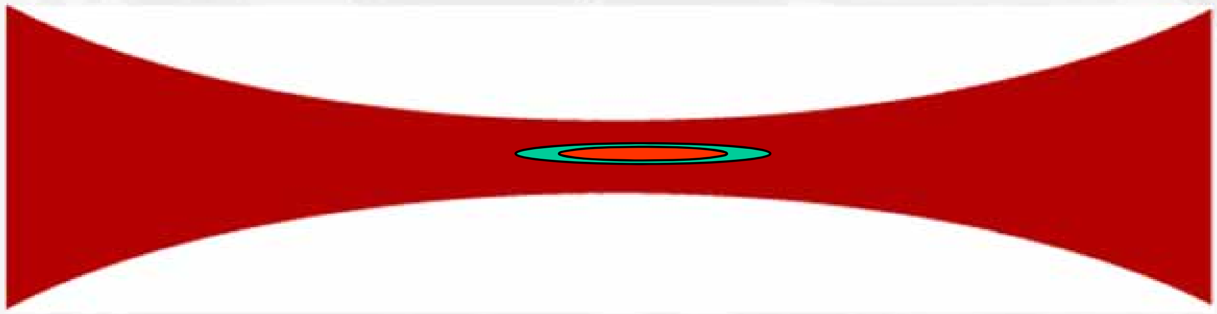
◊ lowest resonances with ^{85}Rb :

Isotope	B (G)	F, m_F
^{168}Yb	1078	2, 2 (a)
^{170}Yb	1323	2, 2 (a)
^{172}Yb	348	2, -2 (e)
^{174}Yb	98	2, -2 (e)
^{176}Yb	111	2, 2 (a)
^{171}Yb	539	2, -2 (e)
^{173}Yb	215	2, -2 (e)

◊ from model potential

Searching Feshbach resonances

^{174}Yb and ^{85}Rb in single-beam optical trap



+ tunable magnetic field

⇒ Feshbach loss spectroscopy

Searching Feshbach resonances

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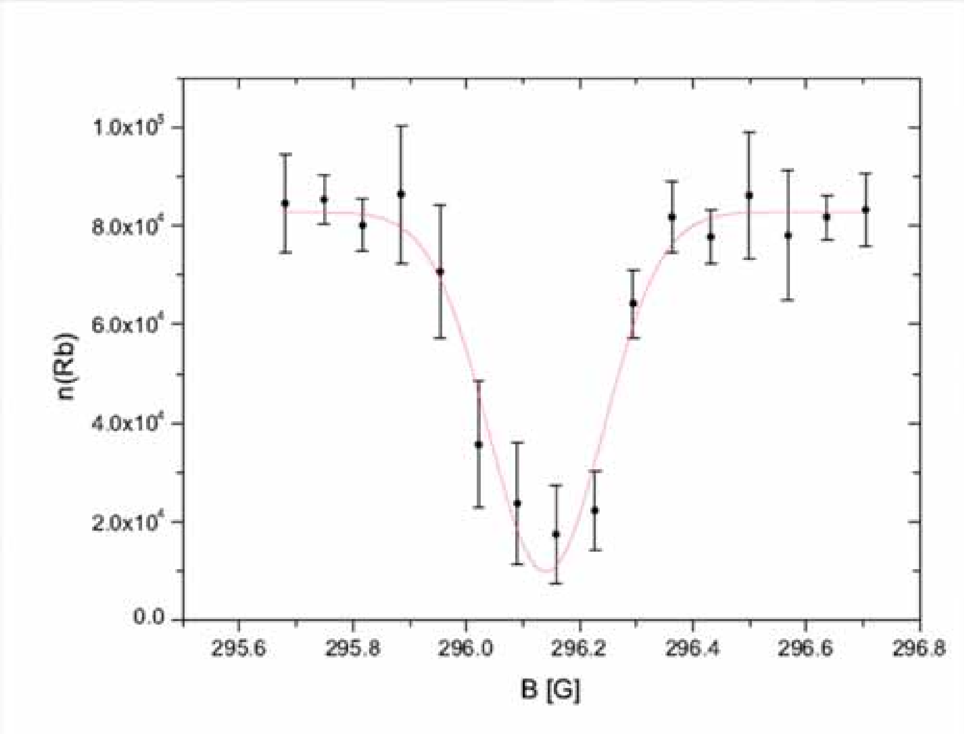
^{85}Rb + ^{85}Rb Feshbach resonance



theoretical width[1]:

Δ ~ 1.8 mG

[1] C.Blackley et al. , arXiv:1212.5446

Searching Feshbach resonances

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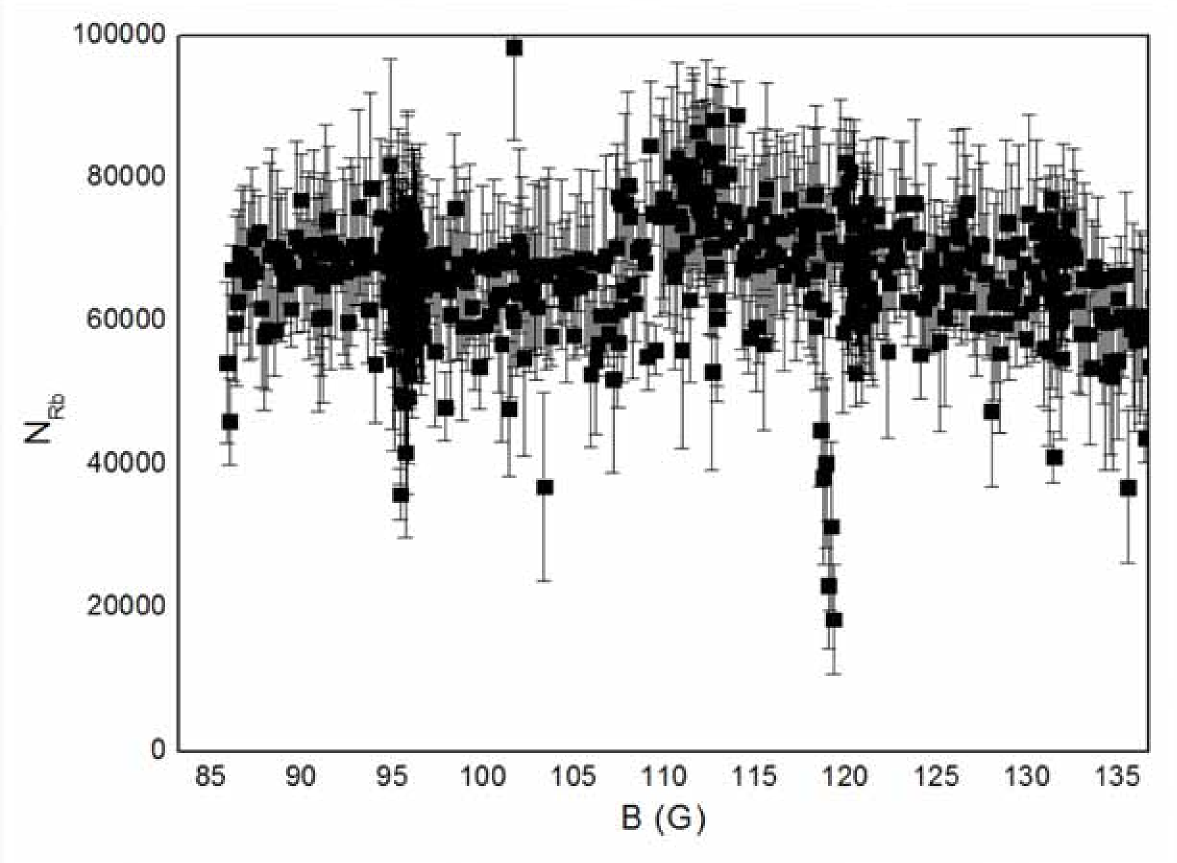
Search for ^{85}Rb + ^{174}Yb Feshbach resonance



⇒ **No Yb-Rb resonances observed so far**

Alternative Route: 1-Photon PA + spontaneous decay

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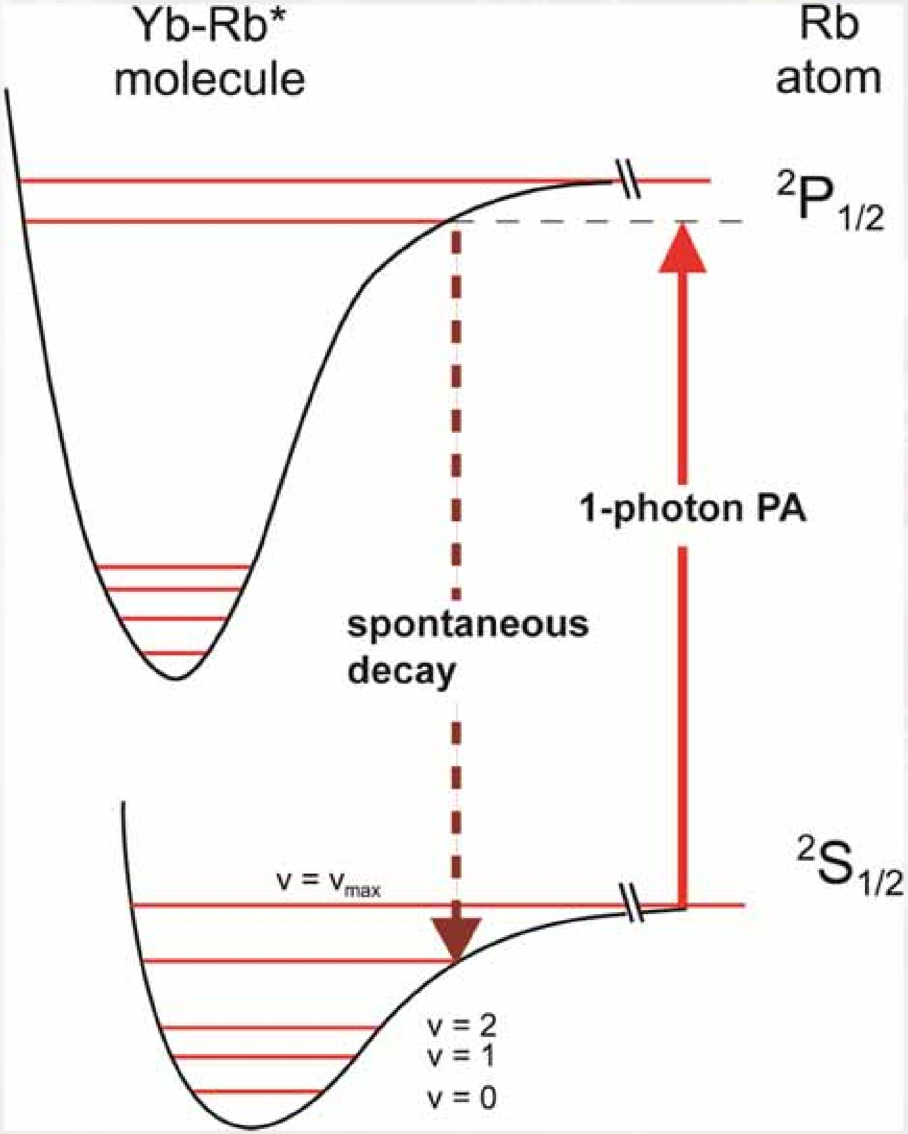

- Excitation of YbRb* (or Yb*Rb) by single-photon PA
- Make use of large FC-Factors to poulate only few vibrational levels of the ground state

Final Step: STIRAP to lowest vibrational level

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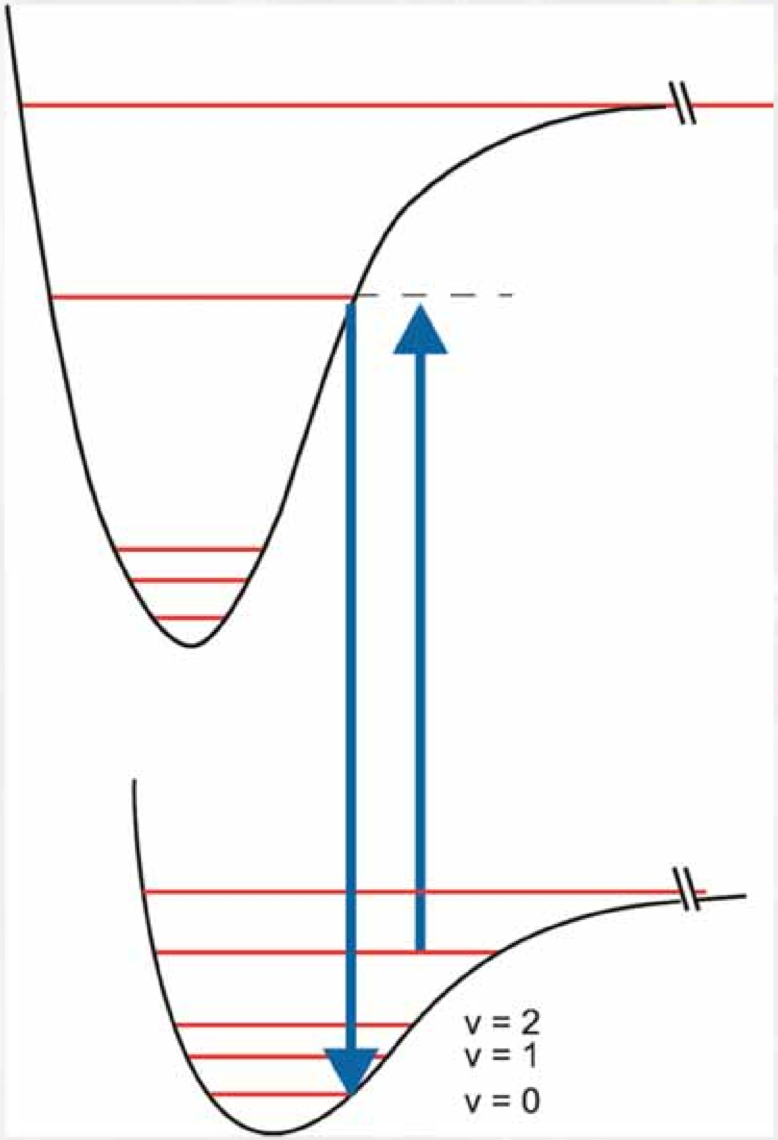


- STIRAP to v=0 by choice of appropriate intermediate level
- YbRb is not chemically stable
- Possible environment: optical lattice @ 2 µm

The Team

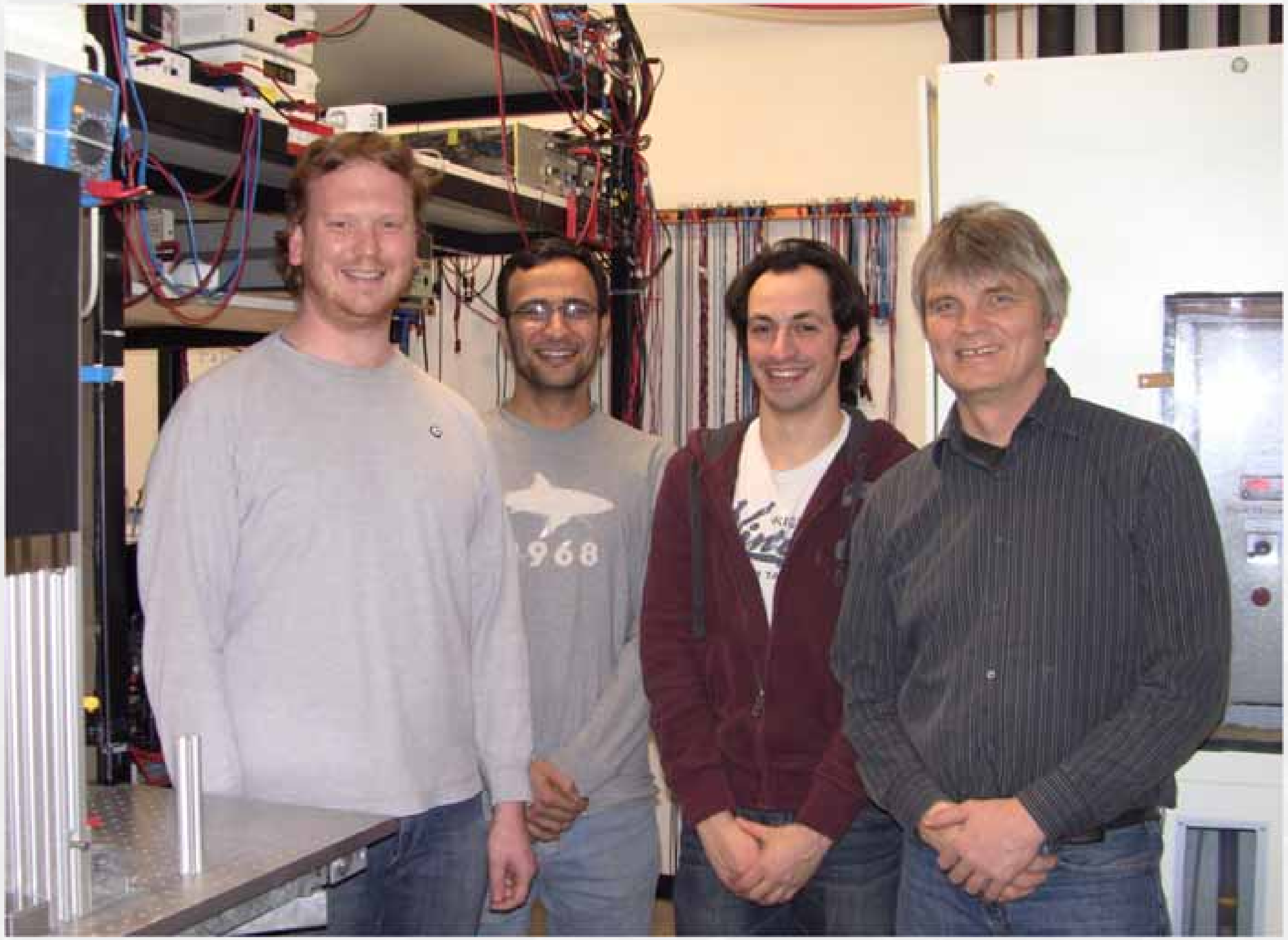
Axel Görlitz (PI)

Frank Münchow
(former PhD-student)

Cristian Bruni
(PhD-student)

Ali Al-Massoudi
(former MSc-student)

Fabian Wolf
(MSc-student, not in picture)



Former members:

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Nils Nemitz (PhD)

S.Tassy (PhD)

M. Madalinski (MSc)