Fun with triplet state molecules: Li2, LiRb, and RbH Ultra-Cold atoms and molecules at UBC Kirk Madison



February 19, 2013 - KITP

### Li+Rb mixtures

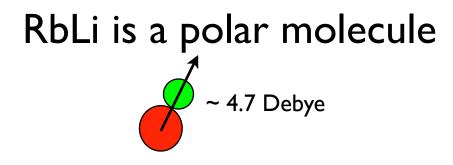


### Theory support for $\text{Li}_2$ from Xuan $\text{Li}^1$ and Nike Dattani^2

<sup>1</sup>Chemical Science Division, Lawrence Berkeley National Laboratory, Berkeley, USA <sup>2</sup>Department of Chemistry, University of Oxford, Oxford, UK

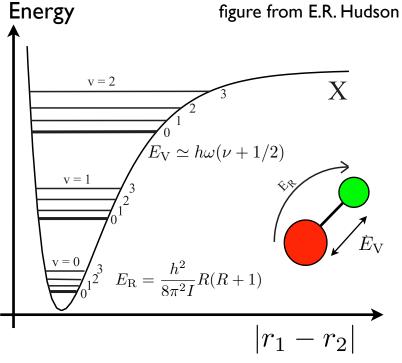


## Long term goal: production of dense, ultracold ensembles of polar molecules



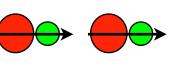


Rich internal structure: - rotational, vibrational



# Dipolar interactions: - large and long range $\sim 1/r^3$ - angular dependence (anisotropic) $U_{dd}^{electric} = \frac{1}{4\pi\epsilon_0} \frac{\mathbf{d_1} \cdot \mathbf{d_2} - 3(\mathbf{d_1} \cdot \hat{r})(\mathbf{d_2} \cdot \hat{r})}{r^3}$

repulsion



attraction

... and zero at the 'magic angle'

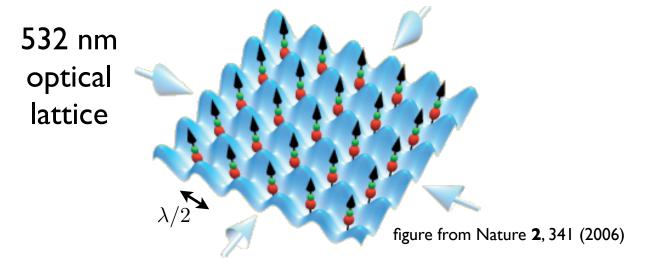
Dipolar interactions - how strong?

\* fully polarized

Inter-particle interactions between RbLi dimers (4.7 Debye)\*

- ~1000x larger than mean field interaction in a BEC
- ~10,000x larger than magnetic dipolar interactions in Cr

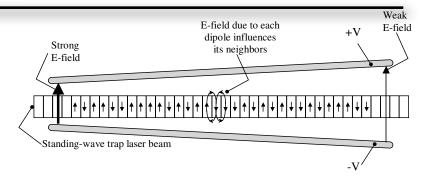
Dipolar interactions - at what range?



$$\left. U_{\rm dd} \sim \frac{(4.7 \text{ Debye})^2}{4\pi\epsilon_0 r^3} \right|_{r=0.266\mu \rm m} = k_{\rm B} \times 8.5 \ \mu \rm K = h \times 177 \ \rm kHz$$

few and many body QM

• 2002, Quantum logic gates [DeMille]





• 2004, Quo vadis, cold molecules? [Doyle, Friedrich, Krems, Masnou-Seeuws]

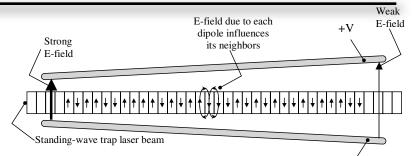


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"Inelastic collisions and chemical reactions of cold molecules in external fields"

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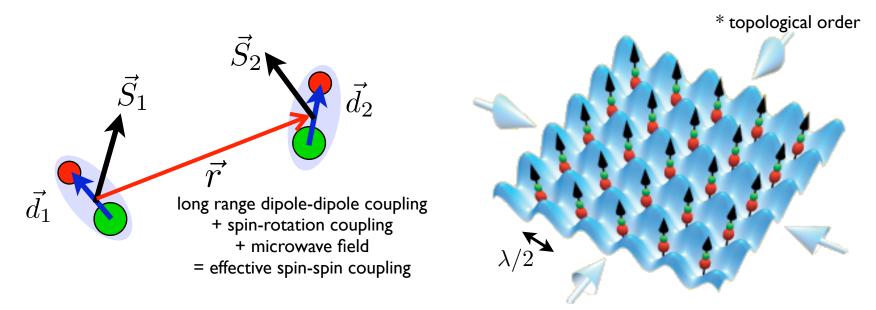


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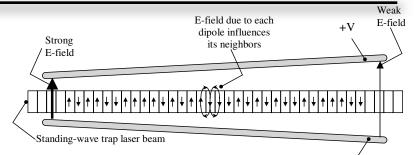
### • 2006 Exotic many body quantum mechanics [Micheli, Brennen, Zoller]

with polar molecules in an optical lattice dressed with a microwave field, you can realize just about any spin lattice model : I D xyz, 2D Ising, 3D Heisenberg, Kitaev model\*, etc...



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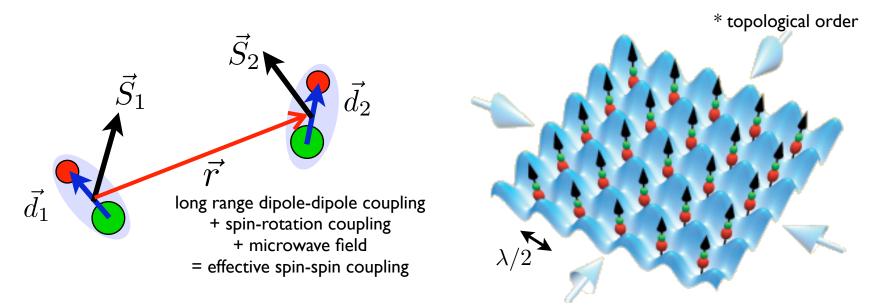


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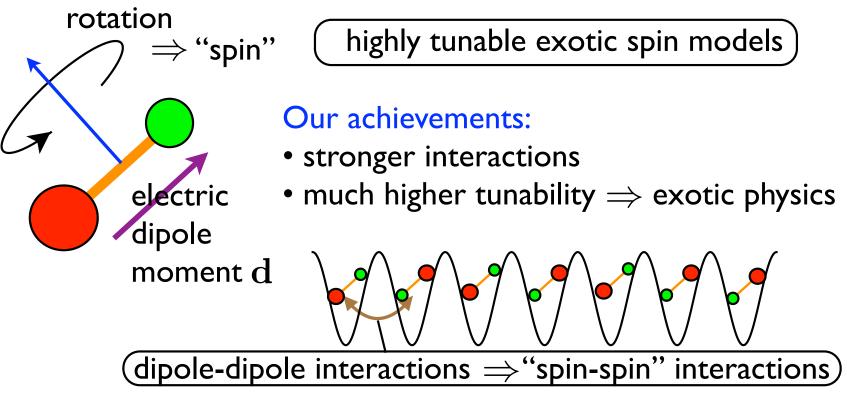
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#### for this, you need paramagnetic, polar molecules !

from Alexey V. Gorshkov's Jan. 24th talk, "Topological Phases in Polar-Molecule Quantum Magnets"



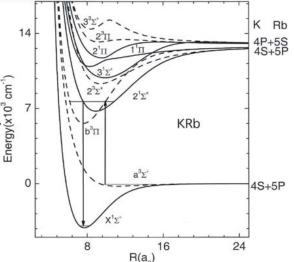
Barnett et al., PRL (2006) Micheli, Brennen, Zoller, Nat Phys (2006) Brennen, Micheli, Zoller, NJP (2007) Buchler, Micheli, Zoller, Nat Phys (2007) Watanabe, PRA (2009) Wall, Carr, NJP(2009) Pupillo et al, in *Cold Molecules* (2009) Wall, Carr, PRA (2010) Schachenmayer et al., NJP (2010) Perez-Rios, Herrera, Krems, NJP (2010) Trefzger et al., NJP (2010) Herrera, Litinskaya, Krems, PRA (2010) Kestner et al., PRB (2011), Lemeshko et al, PRL (2012), etc...

4

#### for some of these proposals, you need paramagnetic, polar molecules !

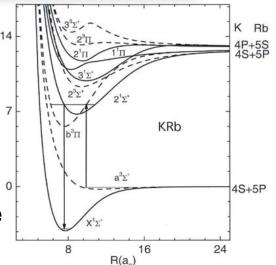
**2004 Proposal**: Efficient conversion of ultracold Feshbach-resonance-related polar molecules into ultracold ground state molecules [**Stwalley**], Eur. Phys. J. D **31**, 221–225 (2004)

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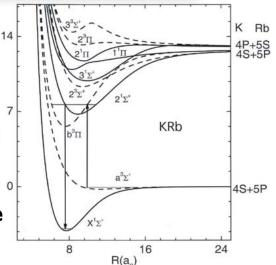
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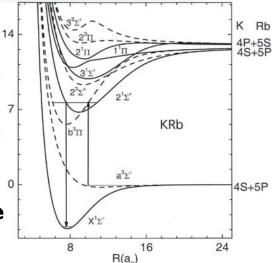
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### Limitations of KRb ?

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### **Limitations of KRb ?**

• chemically reactive  $KRb + KRb \rightarrow K_2 + Rb_2$ 

Dipole moments (Debye)

x	Na	К	Rb	Cs
Li	0.53 (0.45°)	3.50 (3.41 <sup>b</sup> )	4.13 (4.01°)	5.48
Na	(0.45)	2.75	3.33	4.60
к		(2.73 <sup>d</sup> )	(3.05°) 0.64	(4.57°) 1.92
Rb				1.26

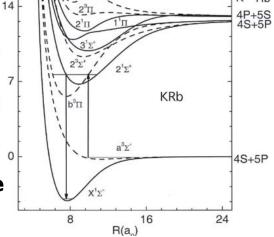
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chemically reactive KRb + KRb -> K<sub>2</sub> + Rb<sub>2</sub>
 solution: other alkali mixtures are chemically stable

NaK, NaRb, NaCs, KCs, RbCs (endoergic - stable) LiNa, LiK, LiRb, LiCs and KRb (exoergic - unstable)



K Rb

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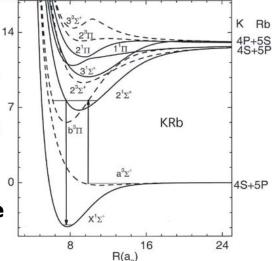
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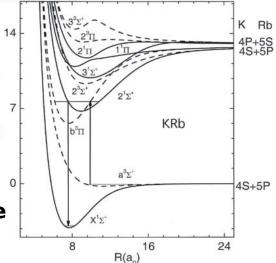
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solution : ultra-cold paramagnetic polar molecules made from alkaline-earth or rare earth + alkali atoms : SrLi, YbLi



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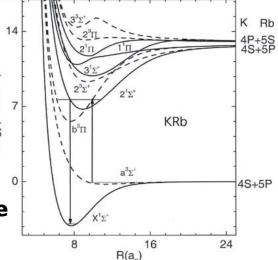
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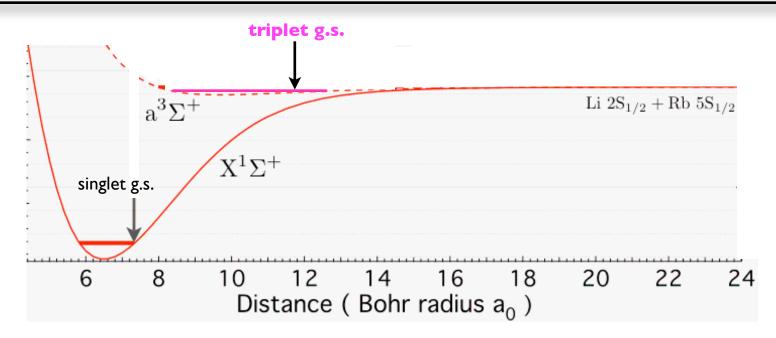
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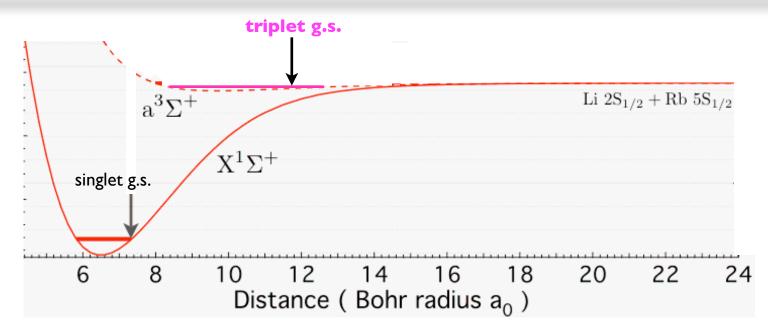
what about the triplet state of a bi-alkali molecule?



Dipole moments (Debye)						
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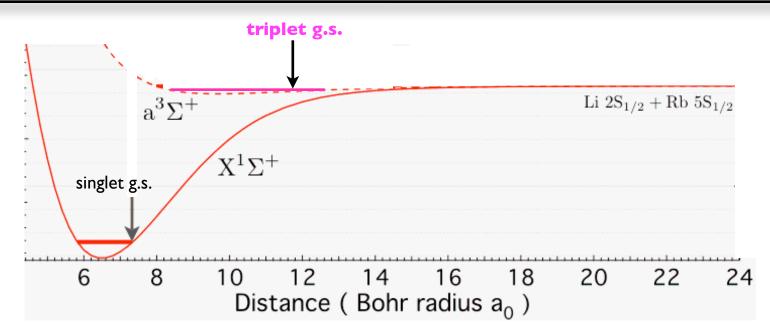
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#### $\sqrt{\mathbf{paramagnetic}}$

magnetically tunable collisions (FRs)



### √ paramagnetic

magnetically tunable collisions (FRs)

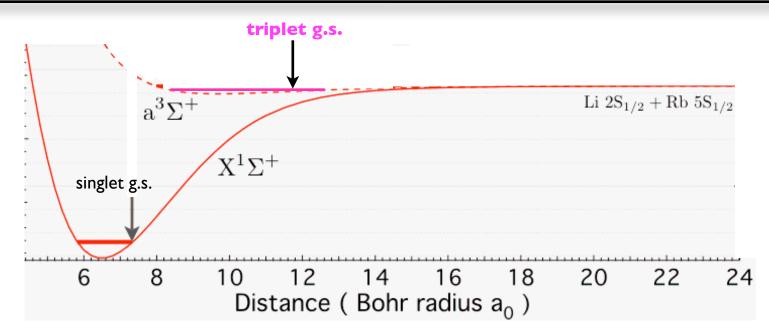
### $\sqrt{}$ somewhat polar (triplet DM ~1/10 that of singlet)

#### DM of triplet state LiRb is about 0.4 Debye

(DM of singlet state KRb is about 0.5 Debye)

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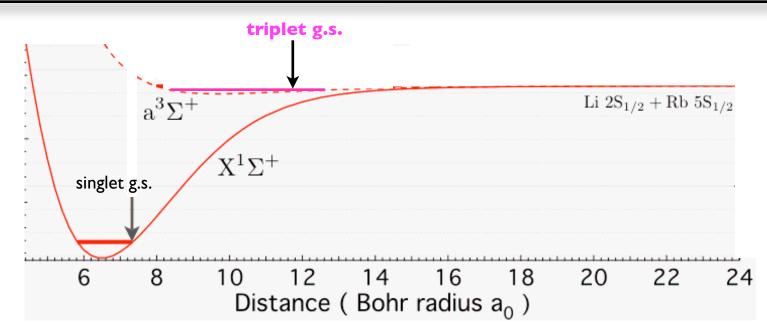
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magnetically tunable collisions (FRs)

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#### ??? Is it stable ???

- spin relaxation collisions (triplet to singlet coupling) ?
- chemical reactivity ?
- spontaneous emission ?

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• spin relaxation collisions (triplet to singlet coupling) ?

• chemical reactivity ?

### by some magic<sup>\*</sup>, is the triplet state stable?

\* or suitably physical reasons

#### • spin relaxation collisions (triplet to singlet coupling)?

"Spin-orbit couplings are small in light systems. For Li<sub>2</sub>, one wouldn't expect fast relaxation. ... but will be more important in heavy systems (like LiRb), but how important?"

#### • chemical reactivity ?

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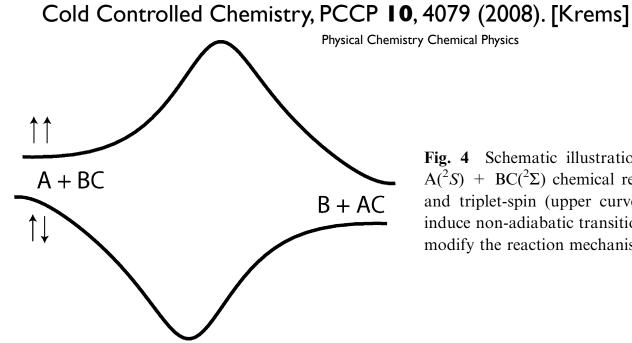


Fig. 4 Schematic illustration of minimum energy profiles for an  $A(^2S) + BC(^2\Sigma)$  chemical reaction in the singlet-spin (lower curve) and triplet-spin (upper curve) electronic states. Electric fields may induce non-adiabatic transitions between the different spin states and modify the reaction mechanism.

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"The interactions between 2S atoms and 2S molecules in the triplet spin state are typically characterized by strongly repulsive exchange forces, leading to significant reaction barriers."

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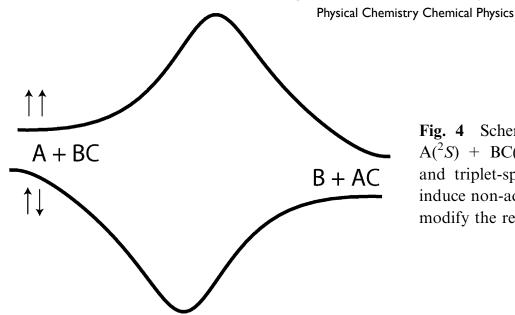


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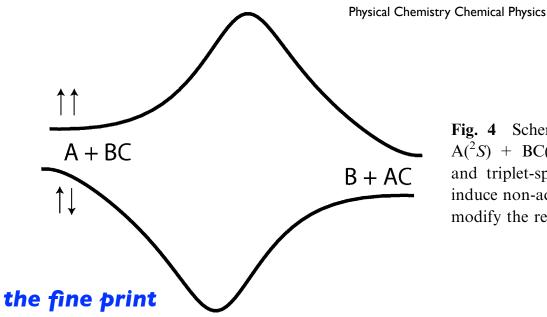
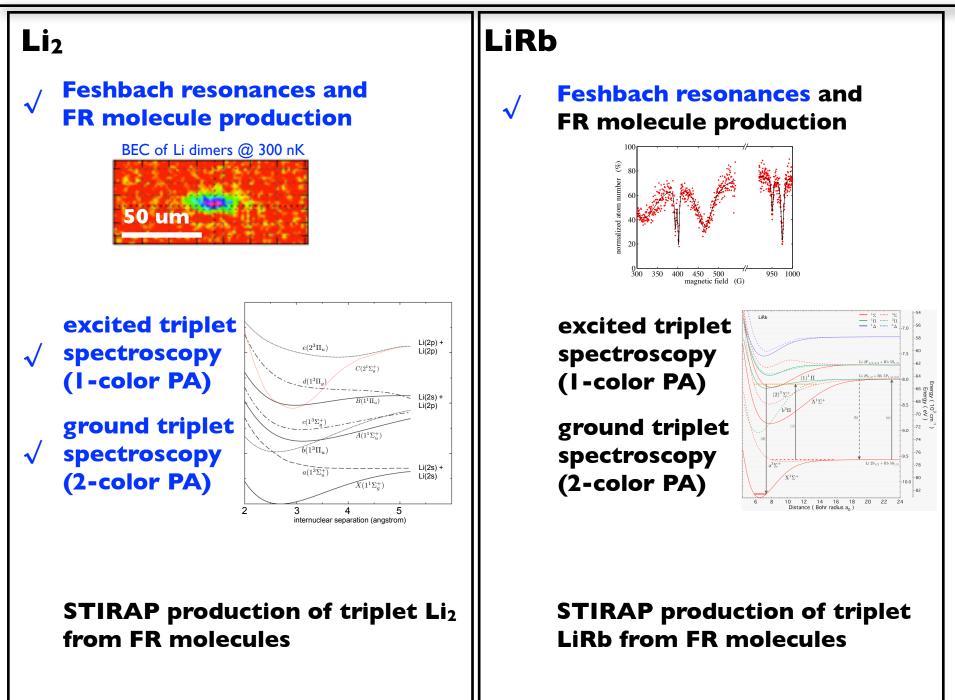


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"... non-adiabatic coupling ... may be induced by the spin-rotation interaction and the magnetic dipole-dipole interaction. The latter is negligibly small and ... transitions are determined by the spin-rotation interaction in the open-shell molecule. The spin-rotation interaction can be effectively manipulated with an external electric field."

### **Experimental goals and results**



## **Experimental goals and results**

table from Eberhard Tiemann's Jan. 25th talk, "Molecular Properties and Potentials"

### Overview of results

FR: Feshbach resonances observed

a: potential for  $a^3\Sigma^+$  determined

	Li	Na	К	Rb	Cs
Li	FR				
Na	FR	FR (a)			
К	FR a	FR a	FR a		
Rb	FR (a)	FR a	FR a	FR a	
Cs	FR (a)	а	а	FR a	FR (a)



## **Experimental goals and results**

table from Eberhard Tiemann's Jan. 25th talk, "Molecular Properties and Potentials"

Κ

### Overview of results

Li

Na

FR: Feshbach resonances observed

Li

FR

FR a

a: potential for  $a^3\Sigma^+$  determined

Rb

Cs

FR (a)

К	FR a	FR a	FR a			
Rb	FR (a) a	FR a	FR a	FR a		
Cs	FR (a)	а	а	FR a		
our contributions in blue pending contributions in red						

Na

FR (a)



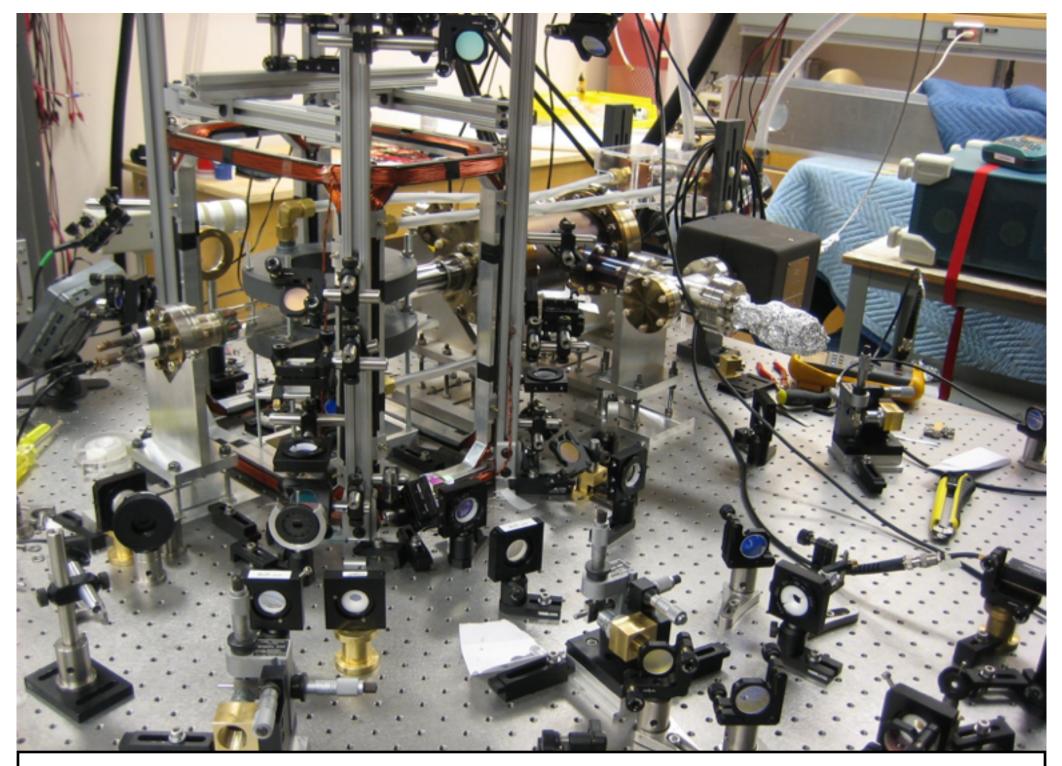


ultra-cold Li+Rb mixtures

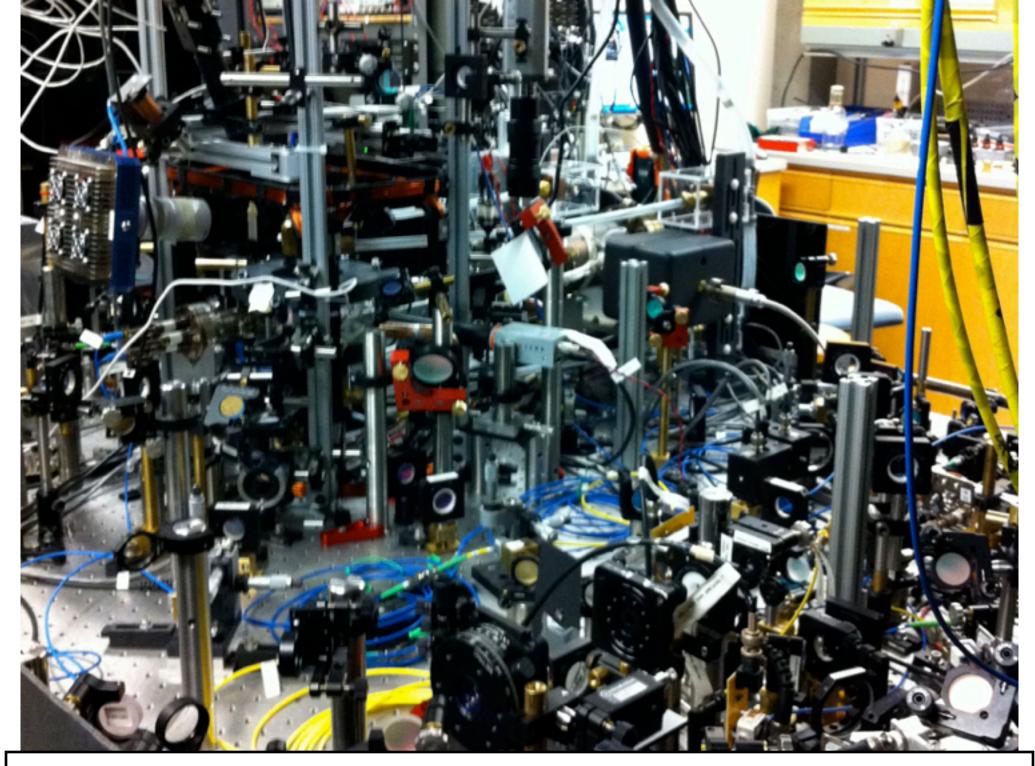


MOT cell

### ultra-cold Li+Rb mixtures



### ultra-cold Li+Rb mixtures



ultra-cold Li+Rb mixtures

Feshbach coil

MOT cell<sup>-</sup>

Feshbach coil

oven

ultra-cold Li+Rb mixtures

#### Feshbach coil

#### **Electric Field Plate**

#### **Electric Field Plate**

#### Feshbach coil

#### ultra-cold Li+Rb mixtures

**MOT Cell** 



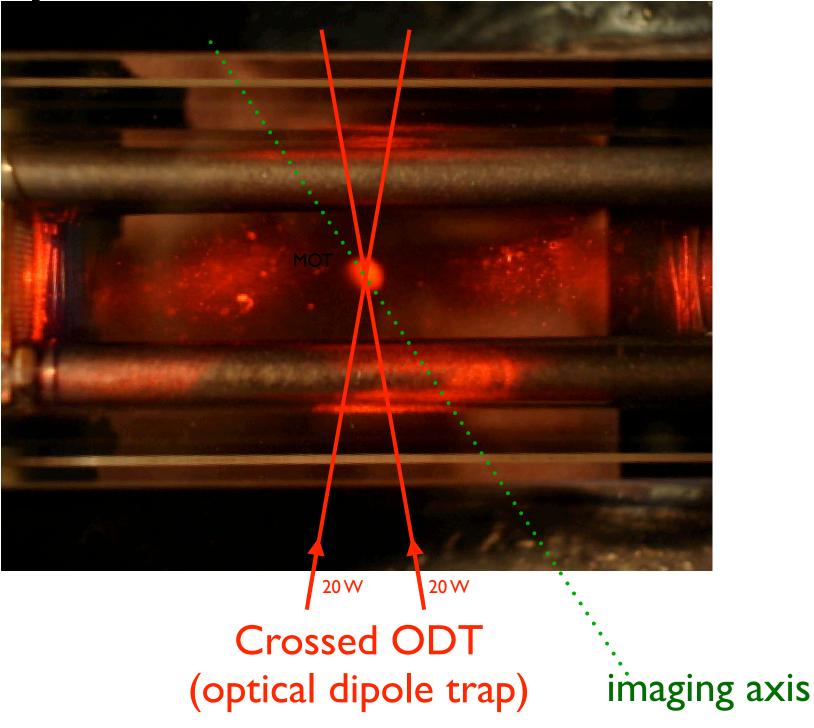


#### ultra-cold Li+Rb mixtures

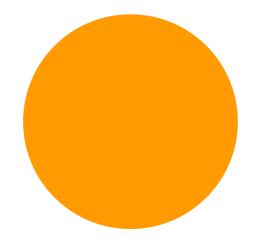
# observing Rb+Li Feshbach resonances



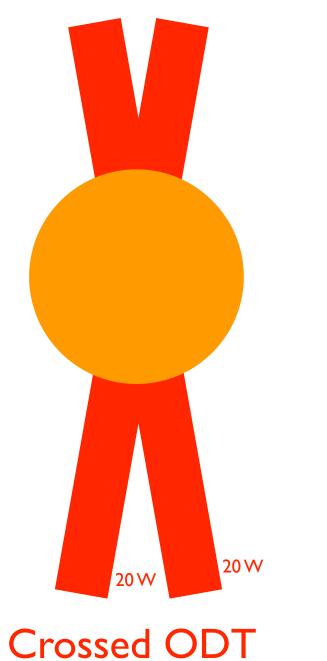
# **Trap Schematic**



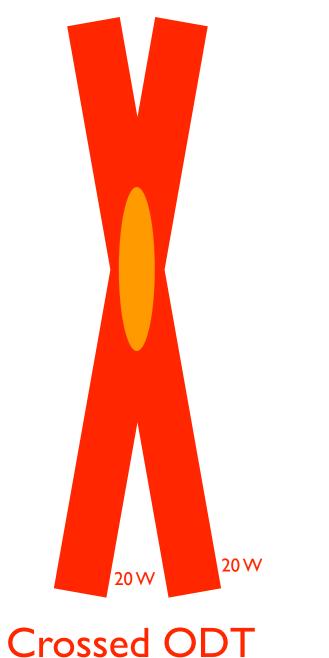
# Load Lithium MOT



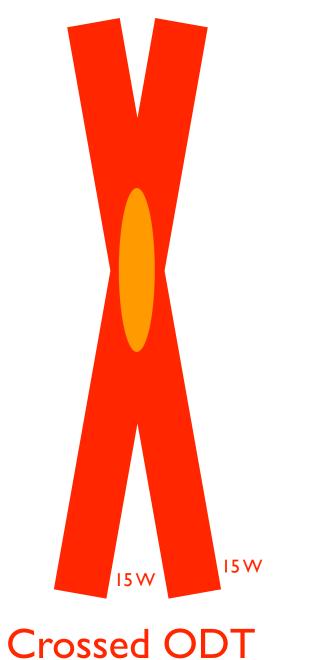
### Transfer Li from MOT to crossed trap



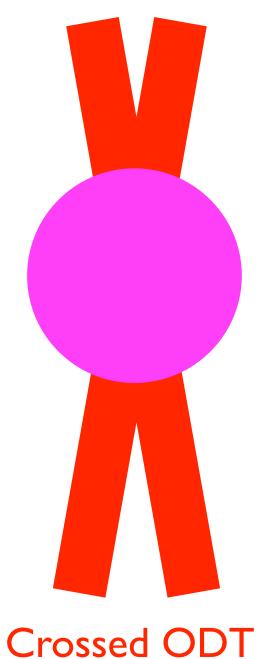
# Transfer Li from MOT to crossed trap



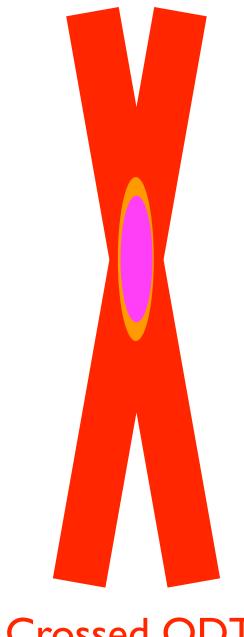
# **Evaporate Li from crossed trap**



# Load Rb MOT while holding Li



### **Transfer Rb to crossed trap**

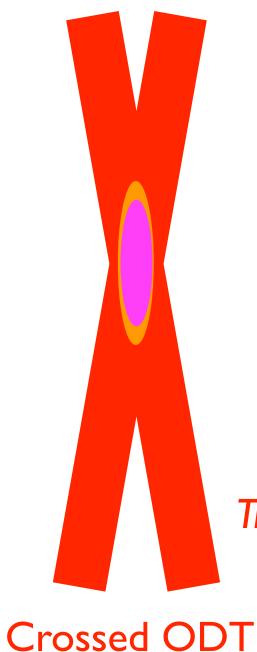


Rb MOT turned off:

In trap: Rubidium and Lithium



# Both Rb and Li in trap: trap depths different



Trap for Li half as deep for Rb

# Simultaneous evaporation of Li and Rb

Trap power lowered to force evaporation losses

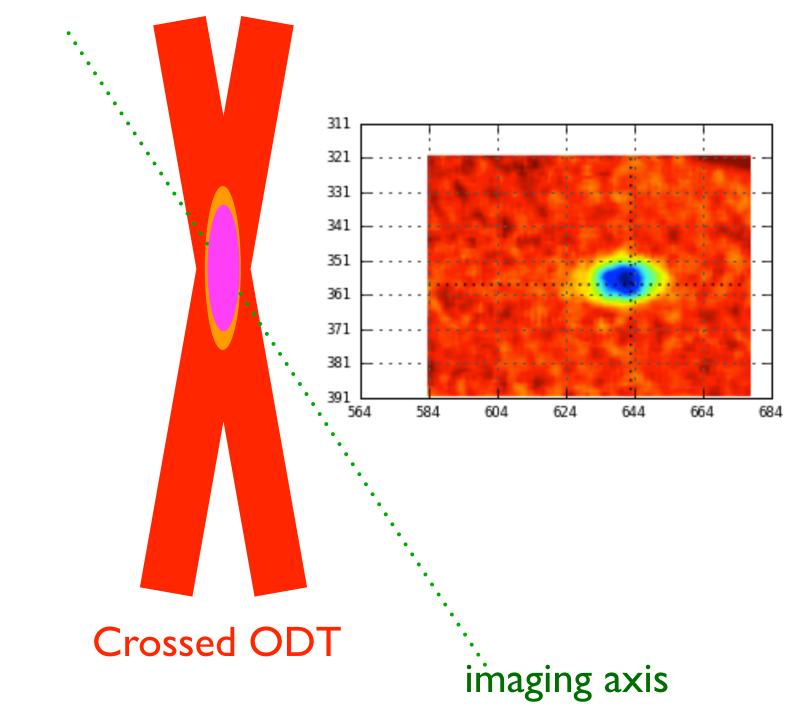
A) If Li+Rb reach thermal equilibrium, Li leaves trap quickly

B) If Li+Rb decoupled, Li evaporatively cools and leaves trap slowly

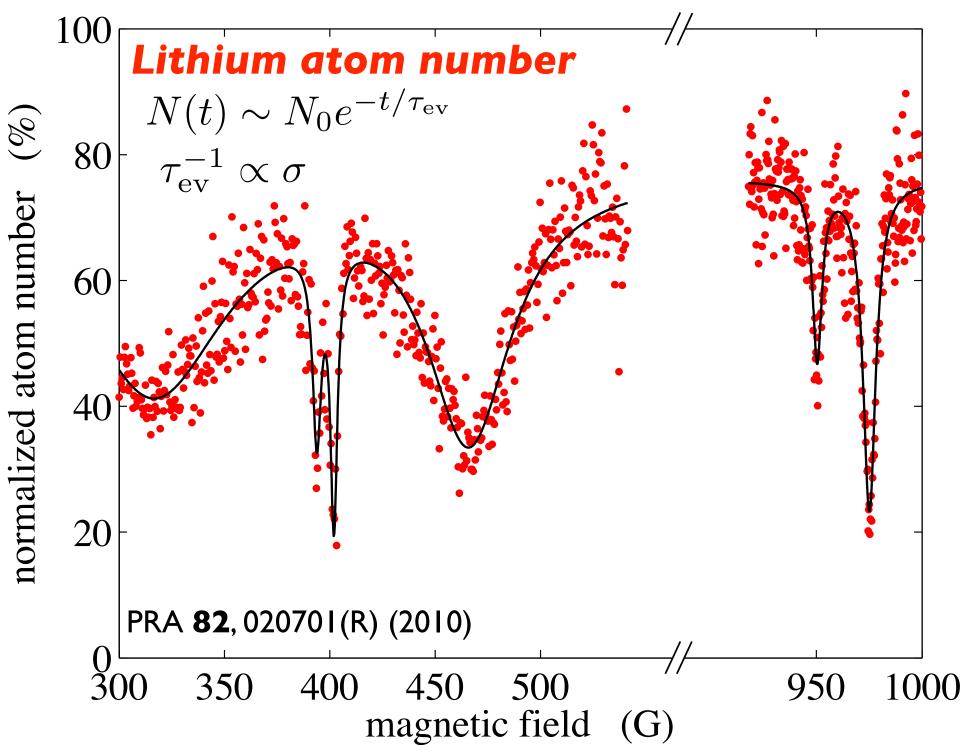
Trap for Li half as deep for Rb

**Crossed ODT** 

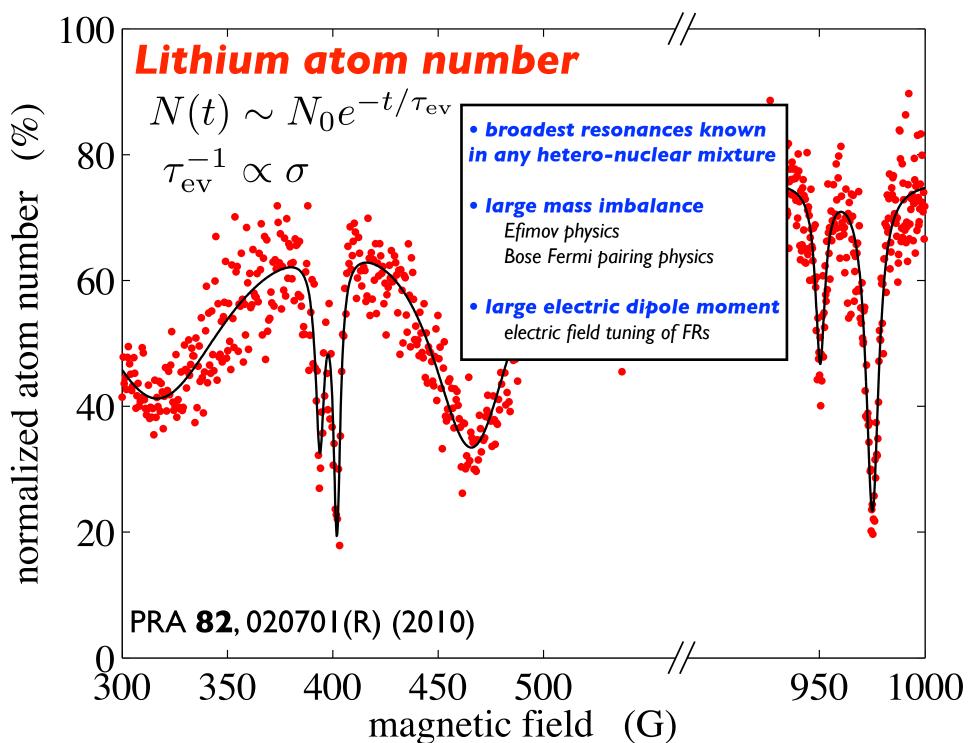
# Image Li or Rb

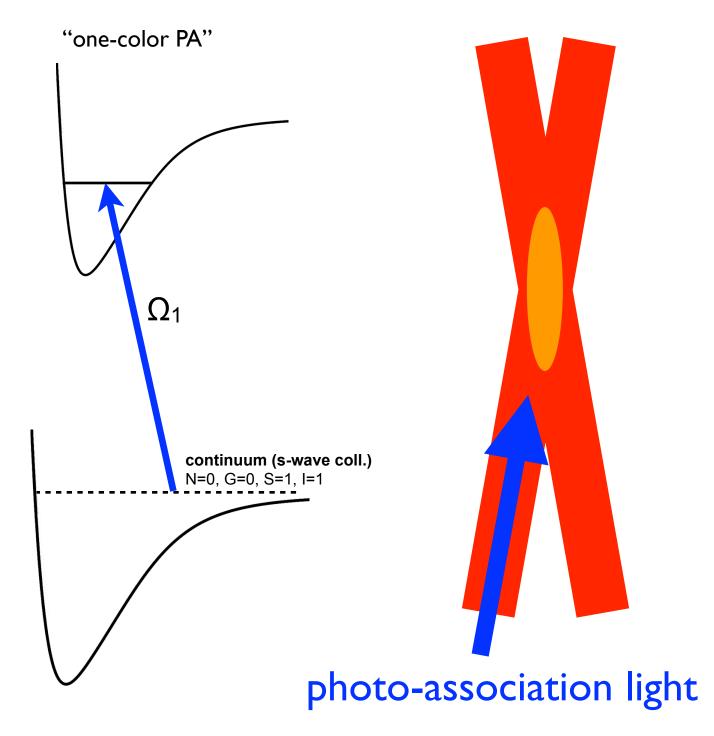


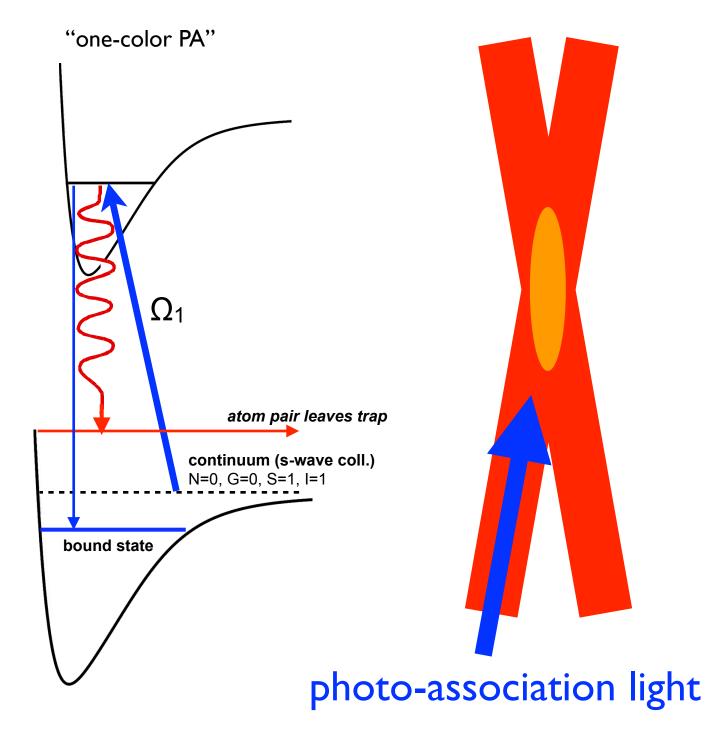
### Feshbach resonances in <sup>6</sup>Li+<sup>85</sup>Rb mixtures

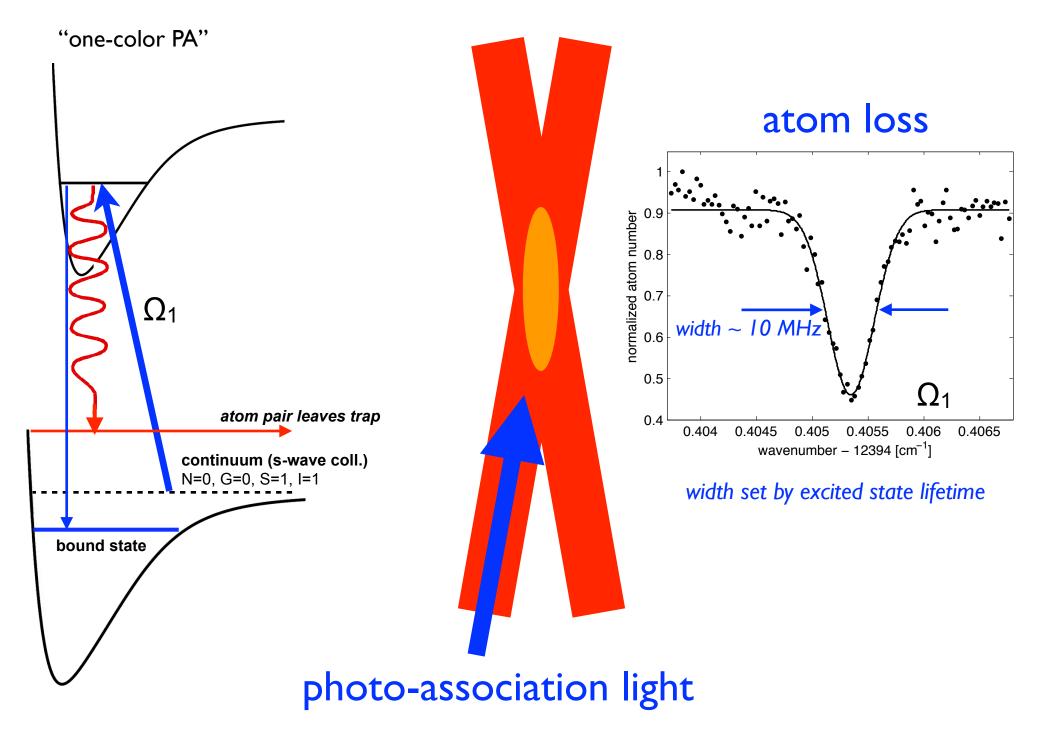


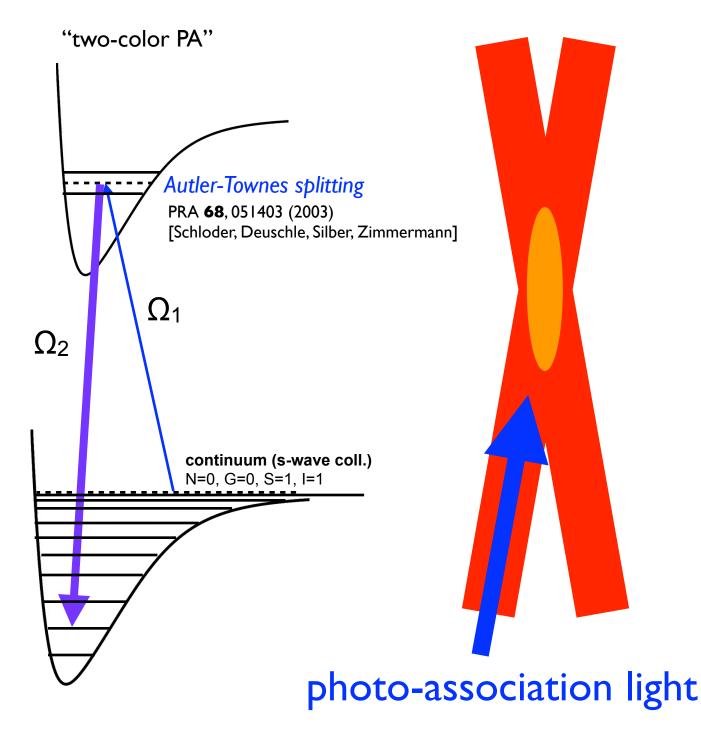
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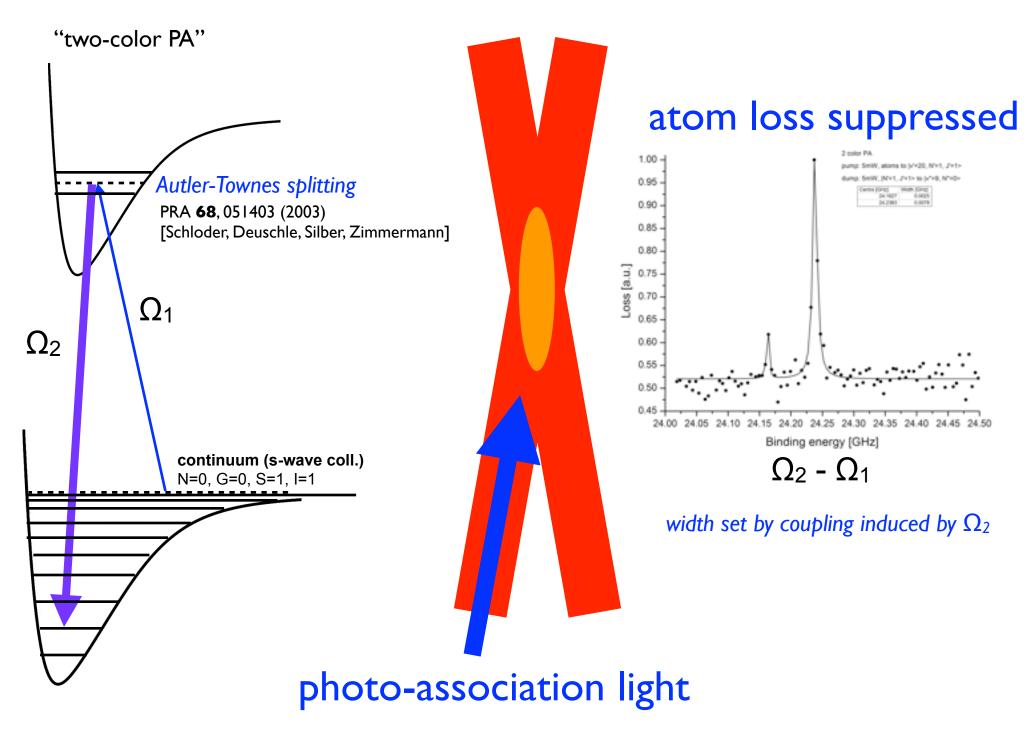


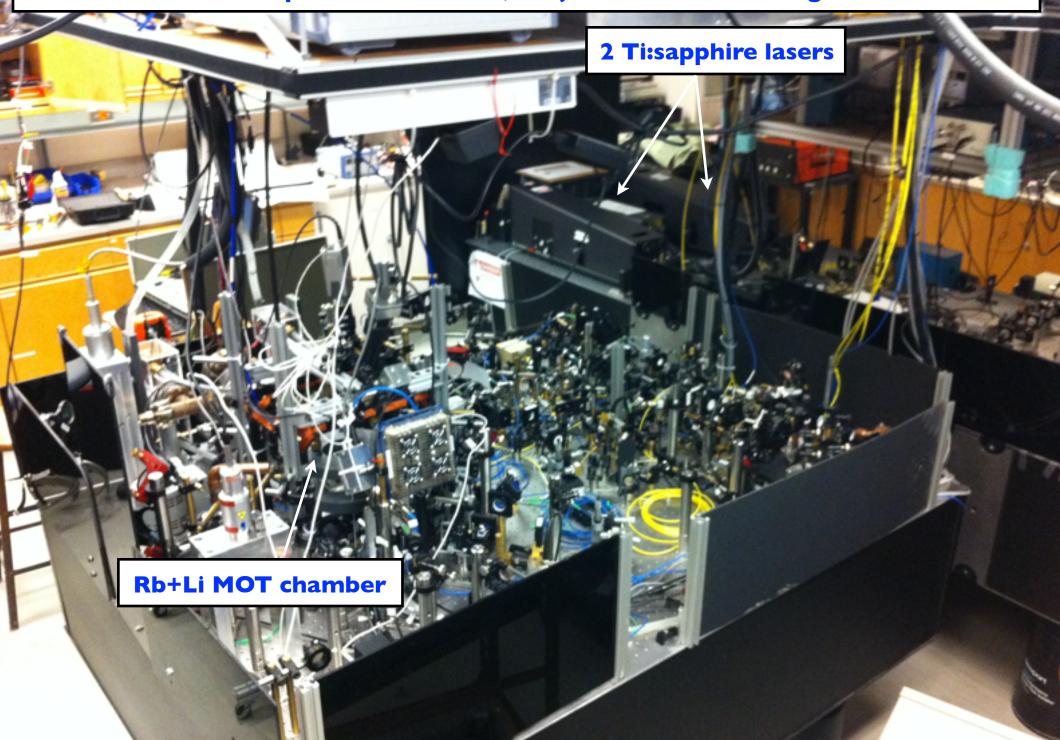


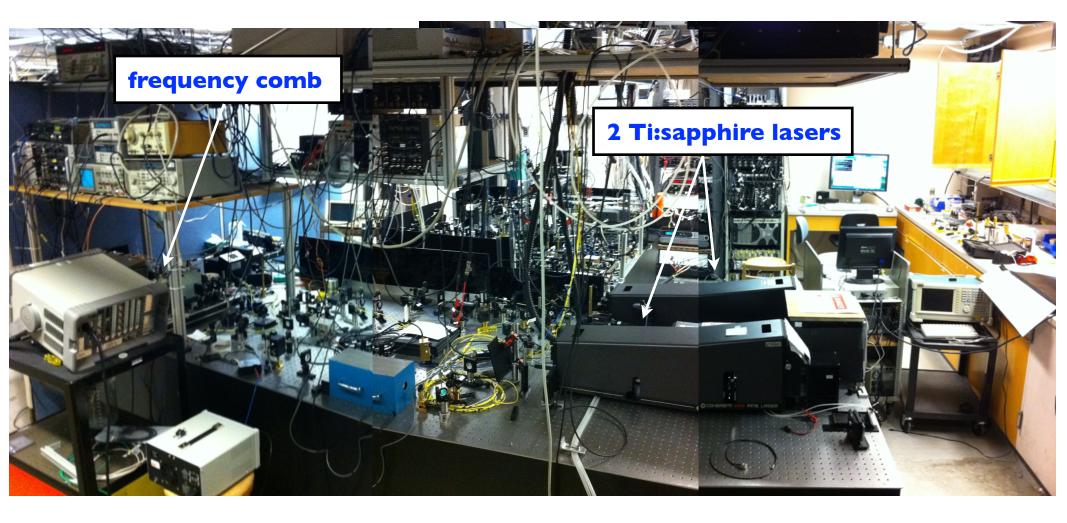






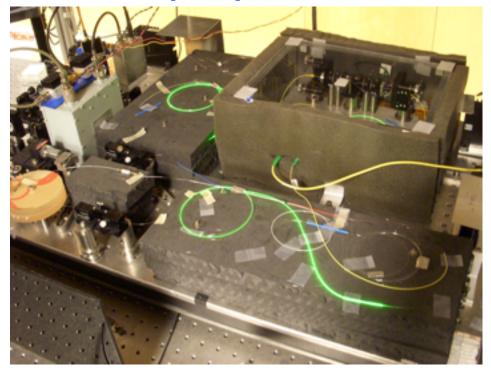


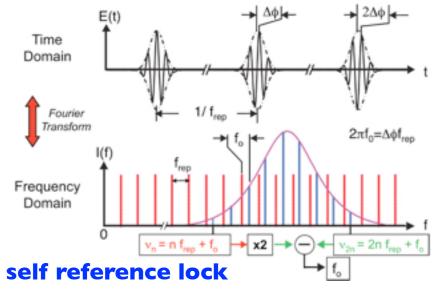




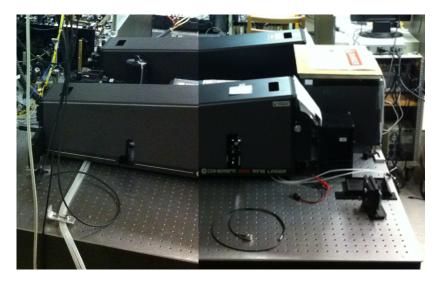
### **Photo-association (PA) laser system**

#### frequency comb

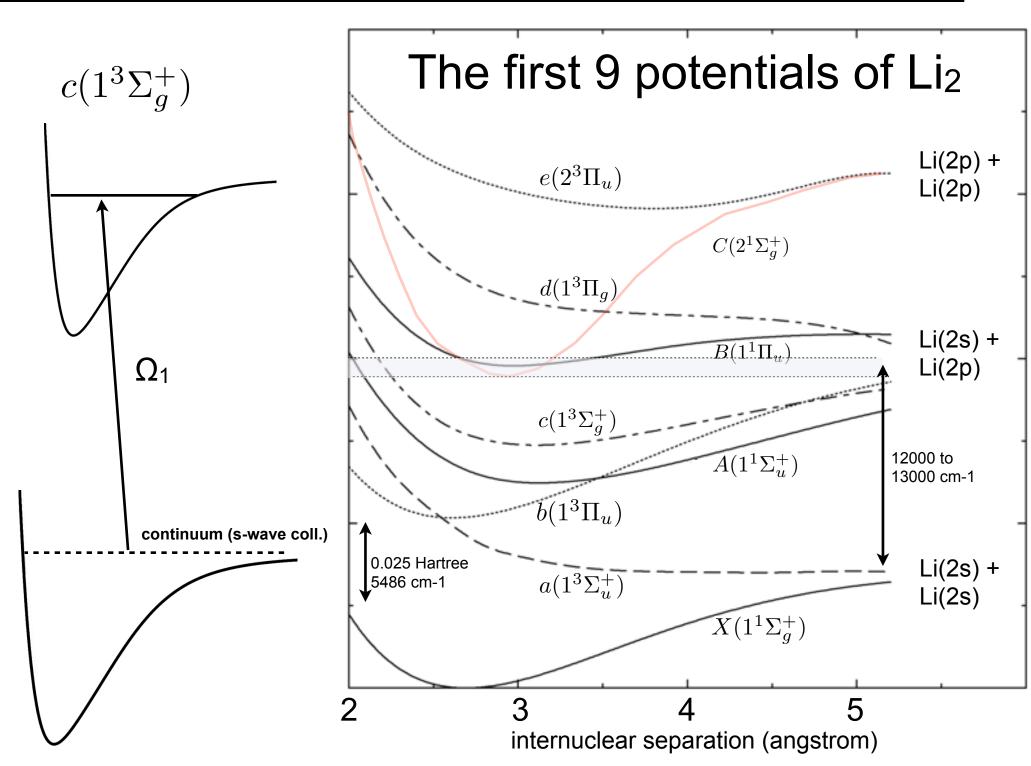


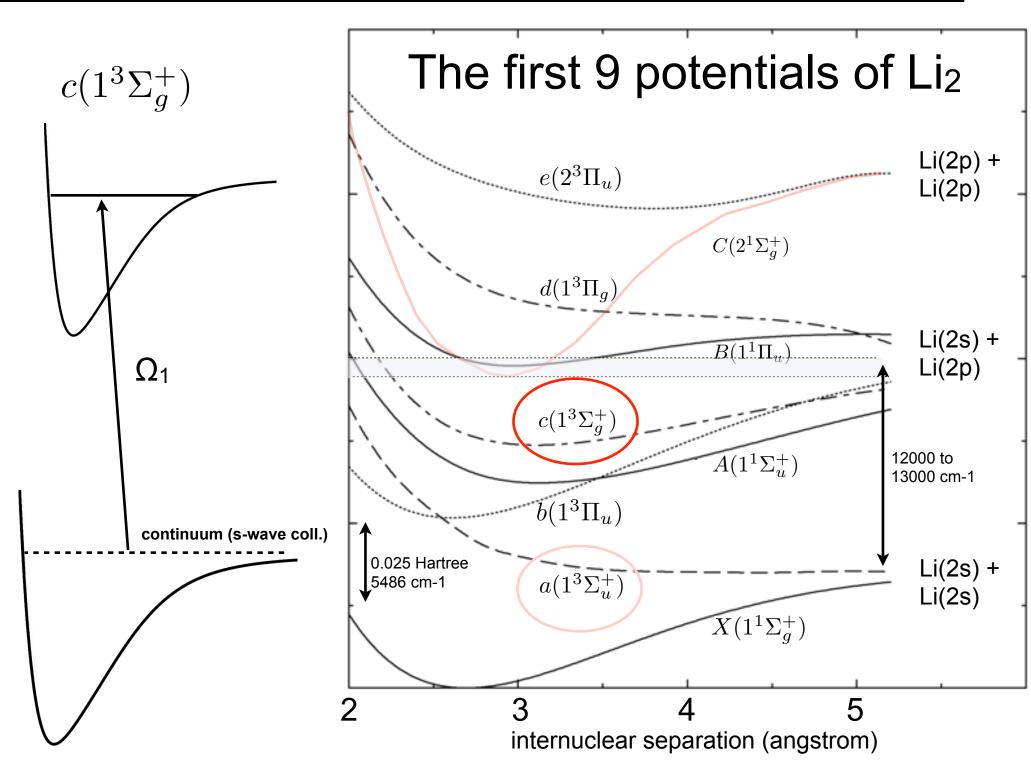


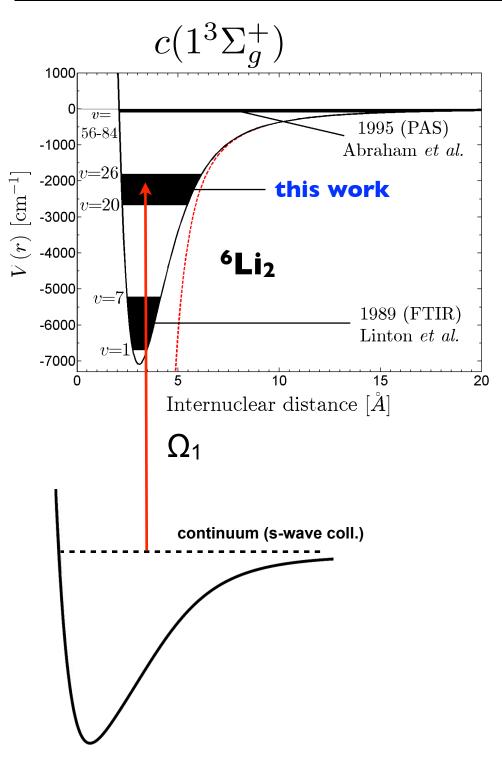
#### 2 Ti:sapphire lasers

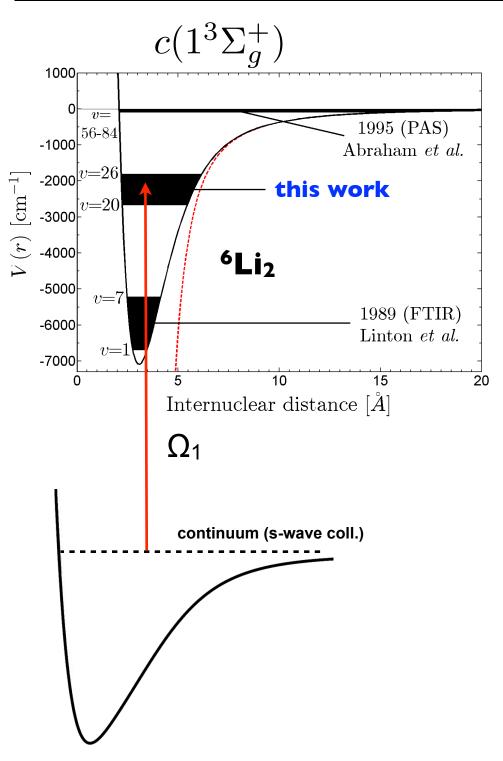


When locked to comb:
1) uncertainty on frequency difference < 10 kHz.</li>
2) line width of each Ti:sapphire: ~ 100 kHz (verified by an independent heterodyne measurement)

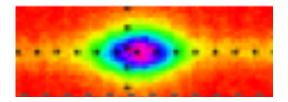


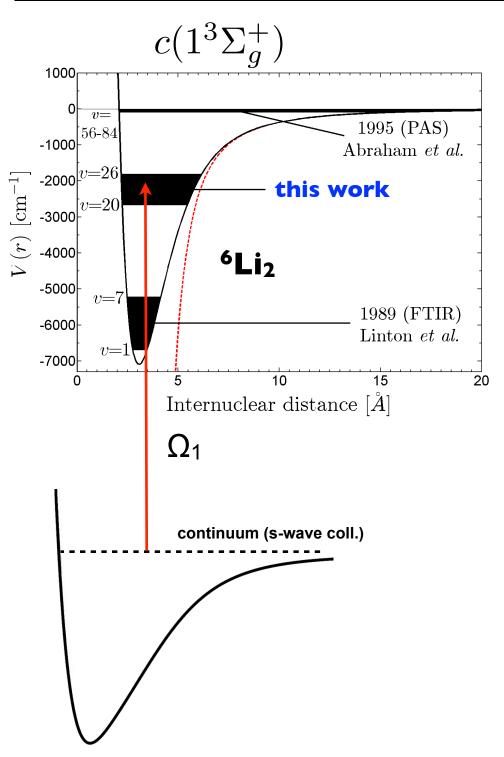




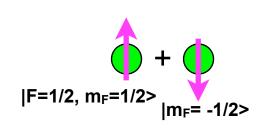


0) To minimize broadening and systematic shifts, we evaporate to very low trap powers and photoassociate a 2-component quantum degenerate Fermi gas  $(T/T_F \sim 0.4)$ 

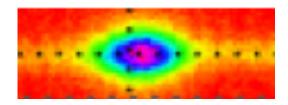


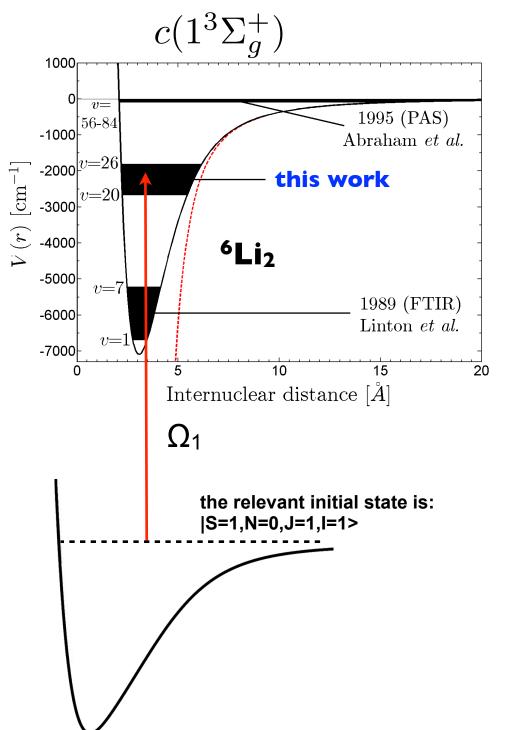


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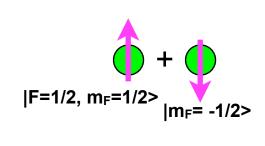


Initial state: S-wave collision: N=0 Total spin = 0 (G = S+I = 0) electronic spin = 0, 1



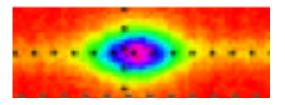


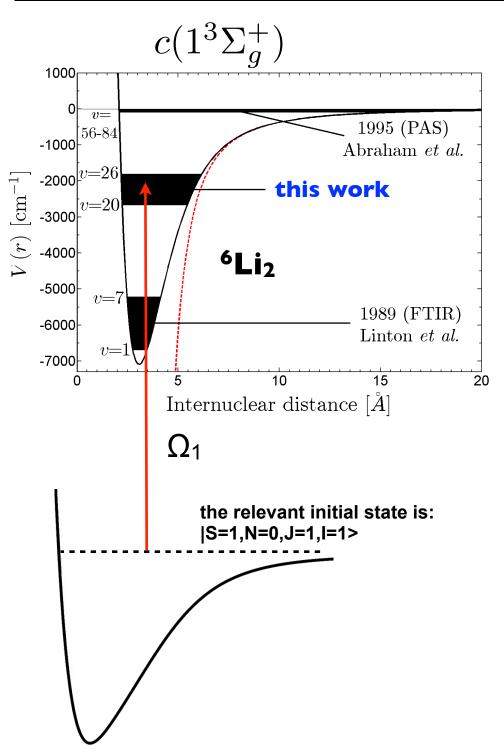
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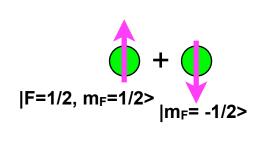
Initial state: S-wave collision: N=0 Total spin = 0 (G = S+I = 0) electronic spin = 0, 1

two states are: |S=0,N=0,J=0,I=0> |S=1,N=0,J=1,I=1>





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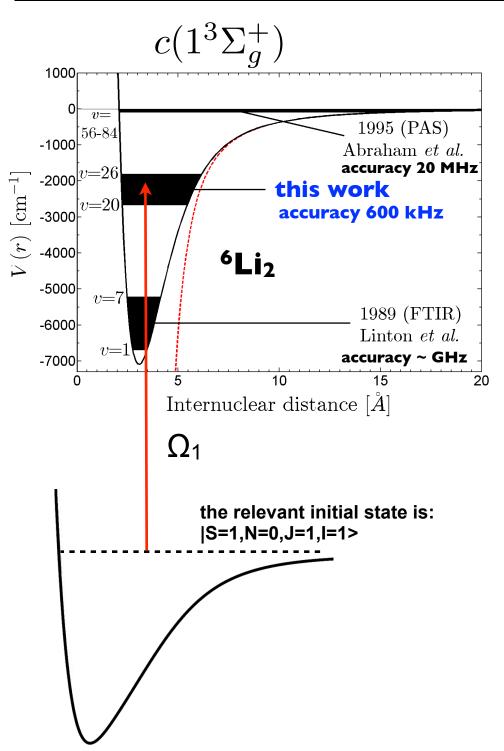
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two states are: |S=0,N=0,J=0,I=0> |S=1,N=0,J=1,I=1>

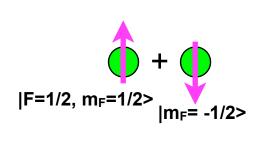
I) We measure 7 levels from v'=20 to v'=26 with an absolute accuracy of +/- 600 kHz (+/- 0.00002 cm-1)

2) For each vibrational level, we observe the N'=1 level AND using a p-wave FR at 187.4 G, we observe the N'=0 and N'=2 rotational levels

3) We also characterized the systematic shifts due to magnetic field, and the residual AC Stark shifts of the PA laser and the trapping laser.



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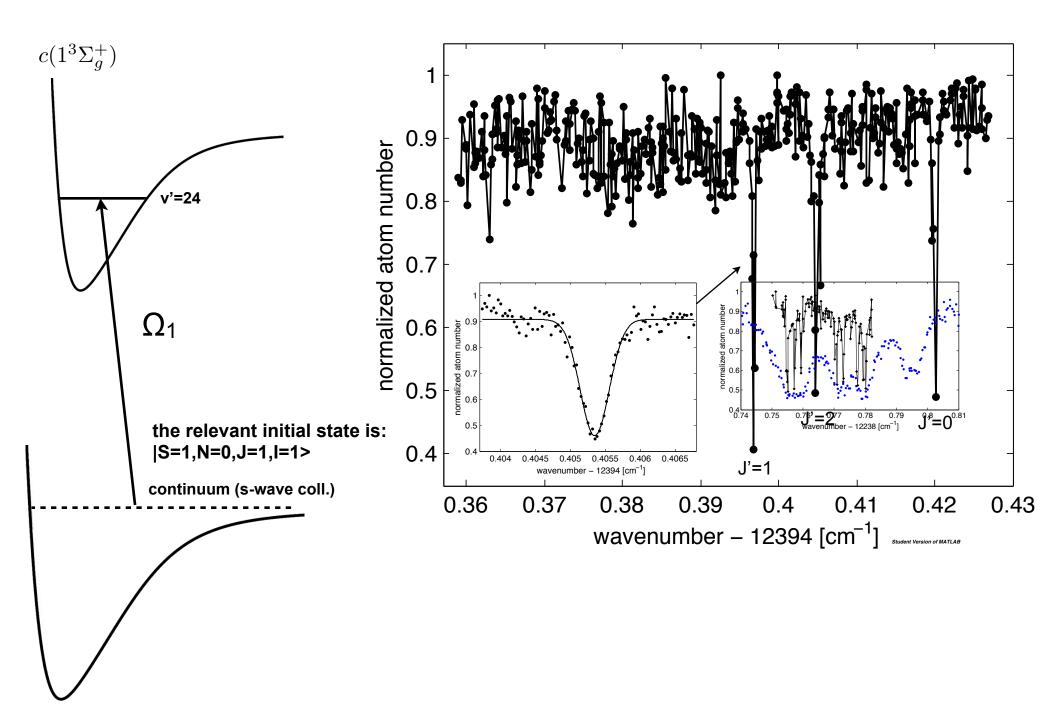
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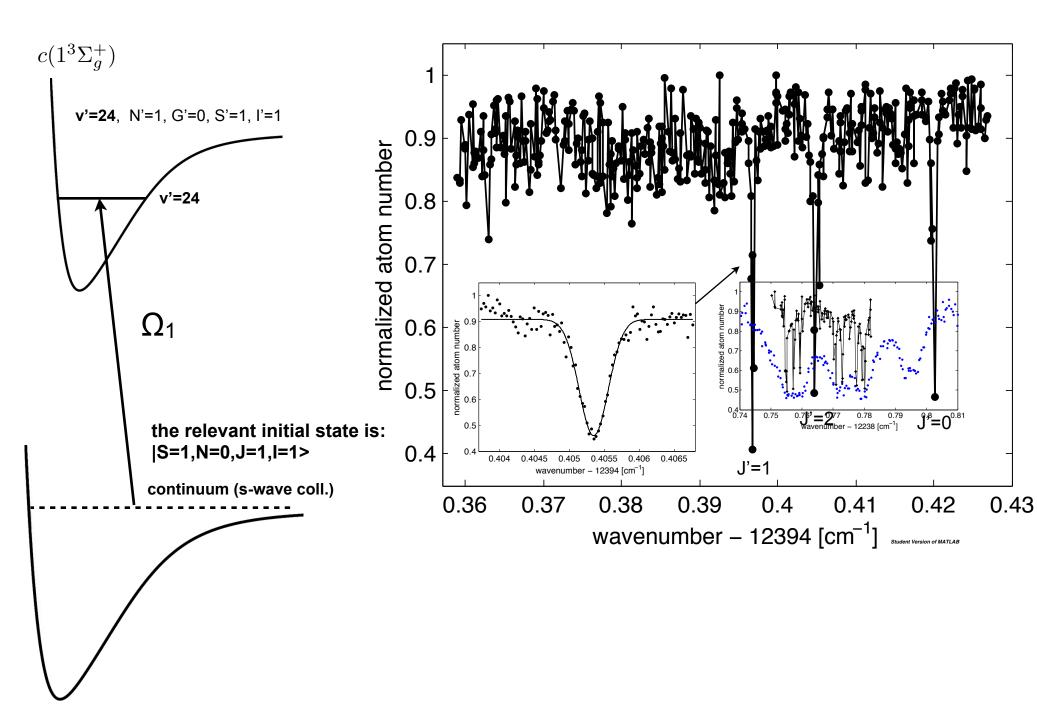
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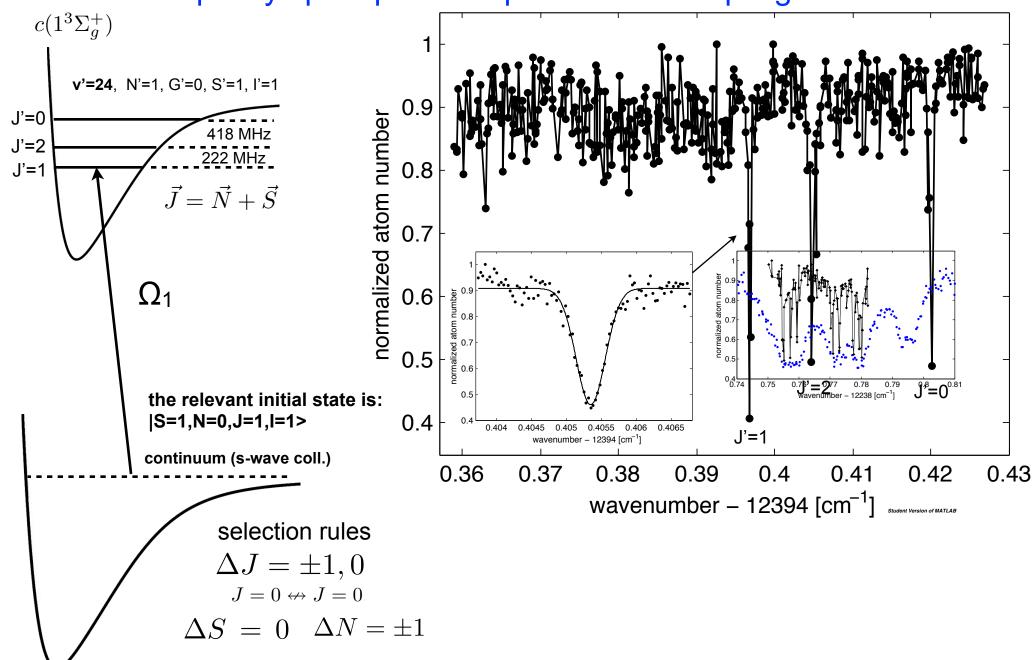
#### We resolve three features for each vibrational level



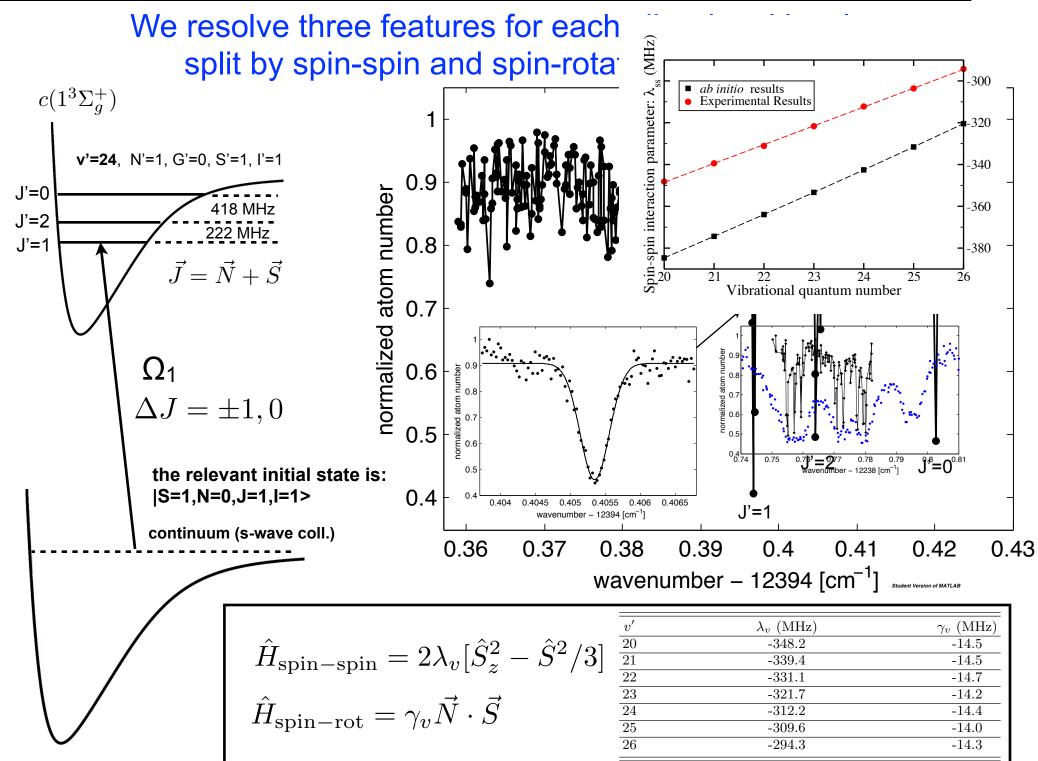
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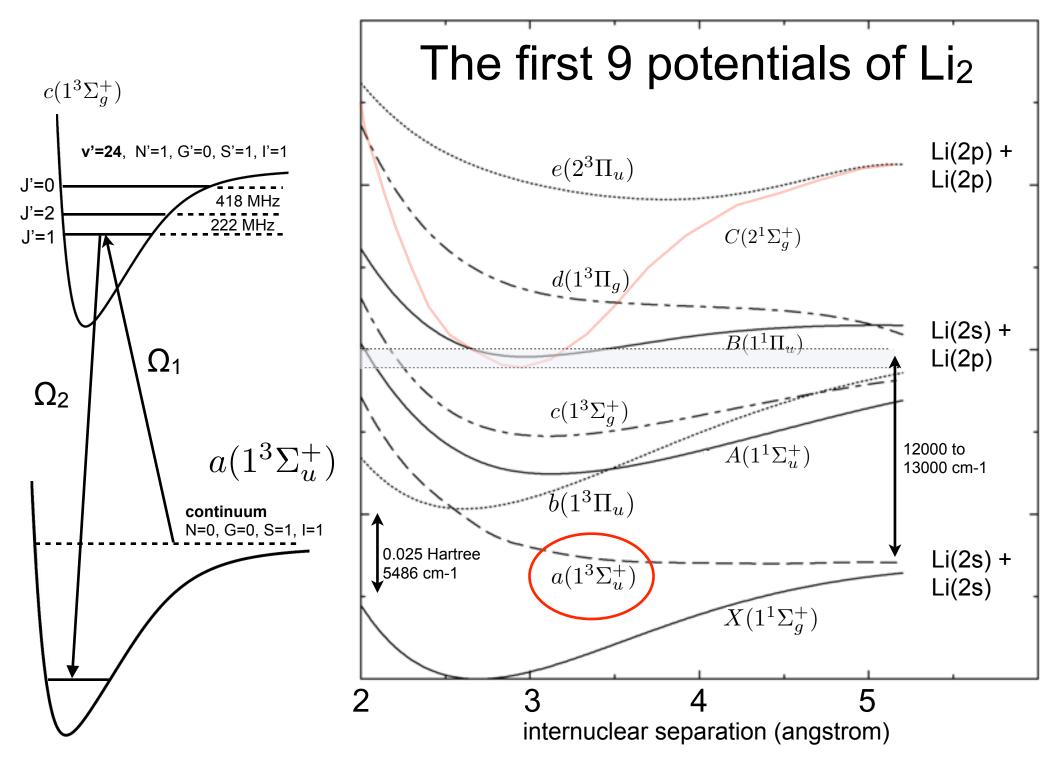
# We resolve three features for each vibrational level split by spin-spin and spin-rotation coupling

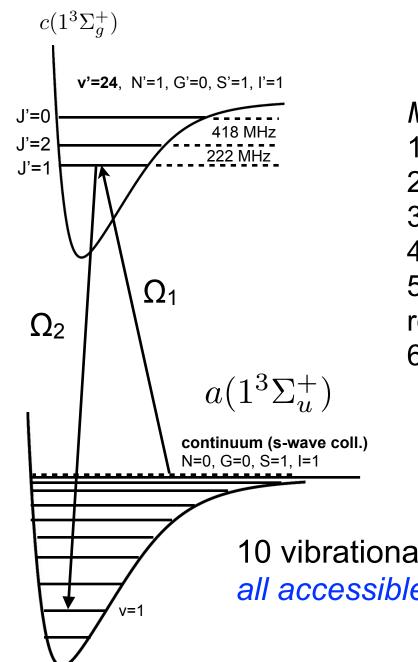


#### 1-color PA spectroscopy results



2-color PA spectroscopy : ground state spectroscopy





Motivations:

1) Technical: we can access with our lasers.

2) It has a magnetic moment (Molecular FRs !)

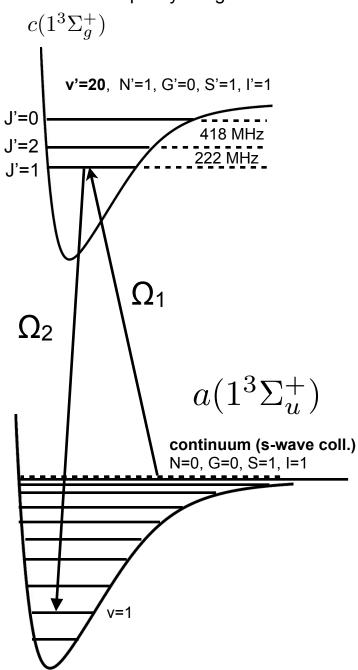
3) Make a BEC of ground state molecules

4) Measure the "Spin blockade"

5) Study collision properties of ultra-cold superrotors (collaboration with Valery Milner)6) Stepping stone for making triplet LiRb

10 vibrational levels *all accessible with our laser system* 

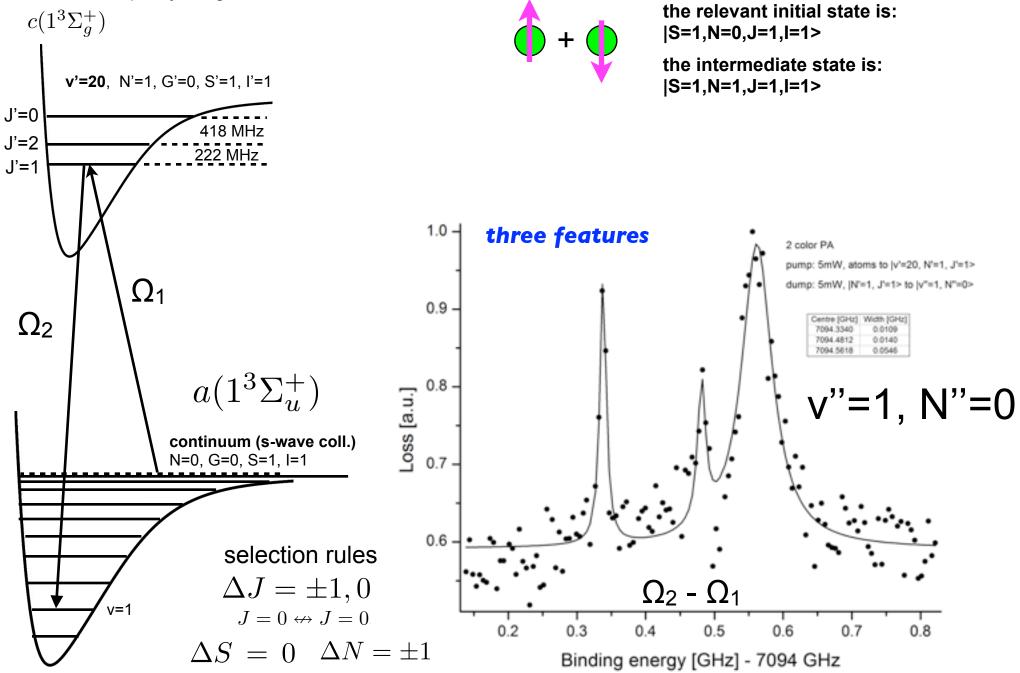
In the data that follows, the loss of atoms due to photo-association induced by  $\Omega 1$  is **suppressed** by the AC Stark shift of the excited state levels induced by  $\Omega 2$ . We specify the excited state v' number and the J' number and we specify the ground state v' number and N' number.

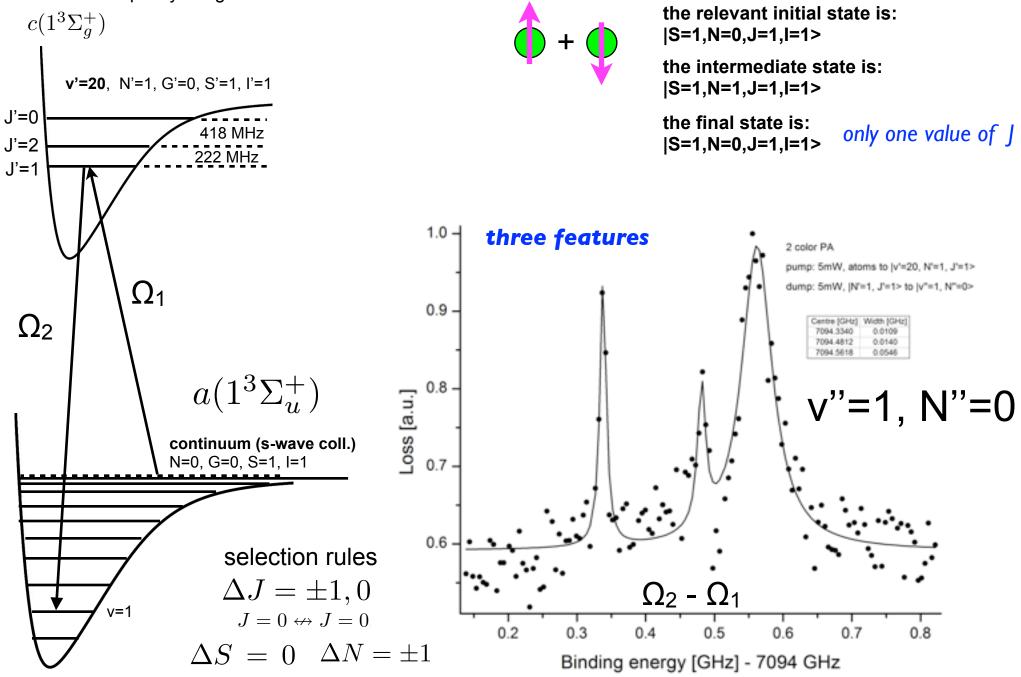


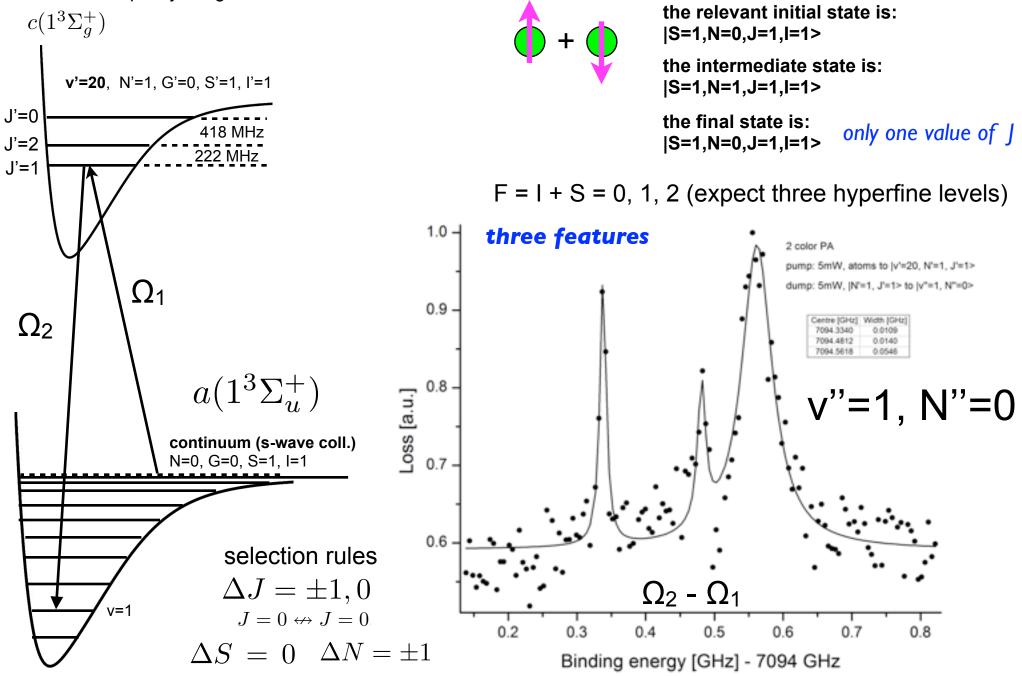
• +

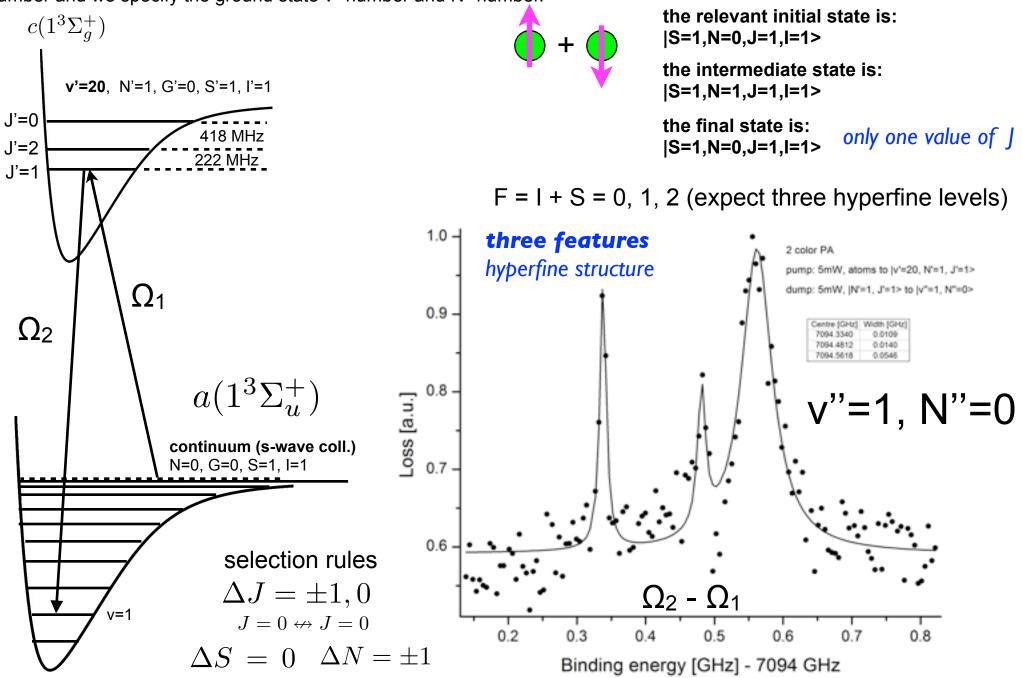
the relevant initial state is: |S=1,N=0,J=1,I=1> the intermediate state is:

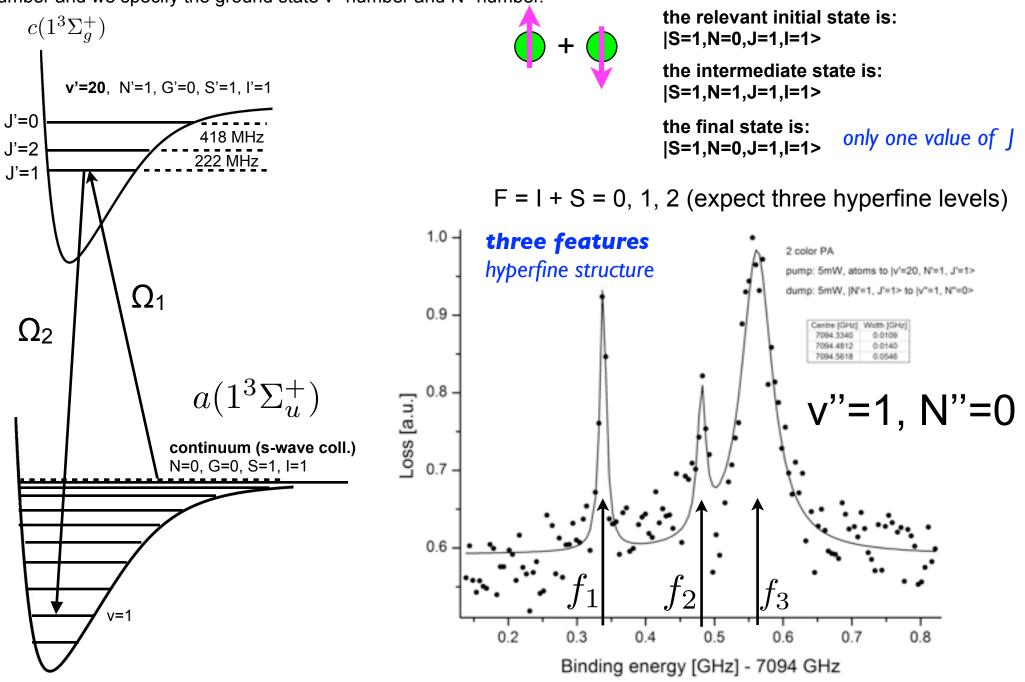
|S=1,N=1,J=1,I=1>



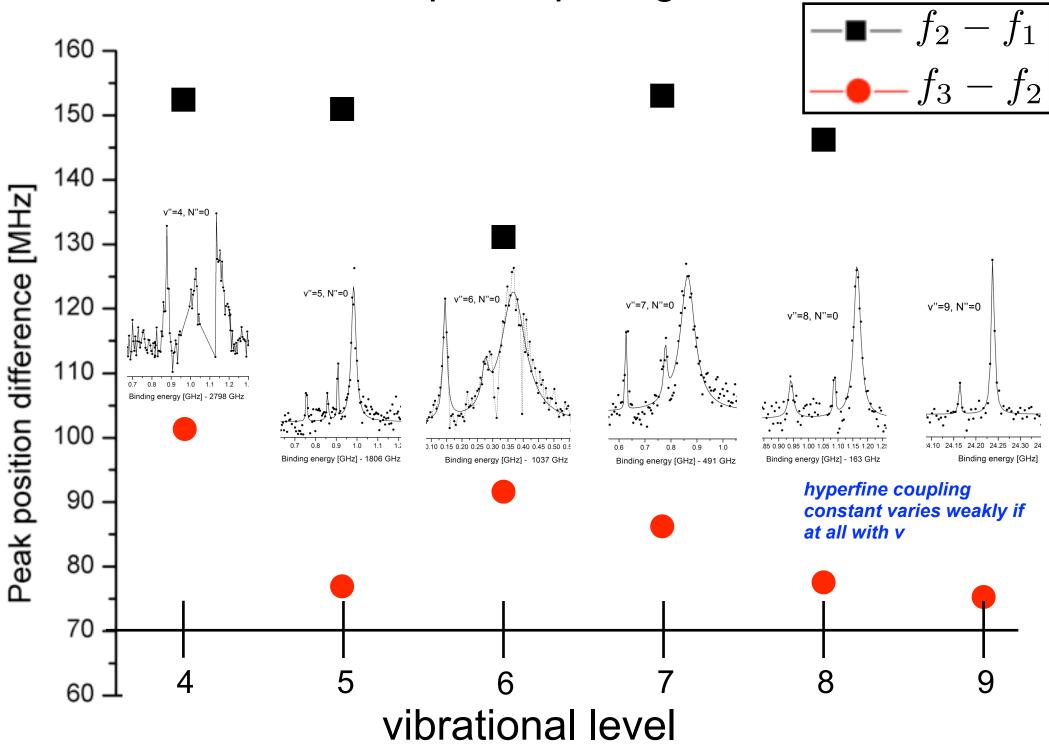




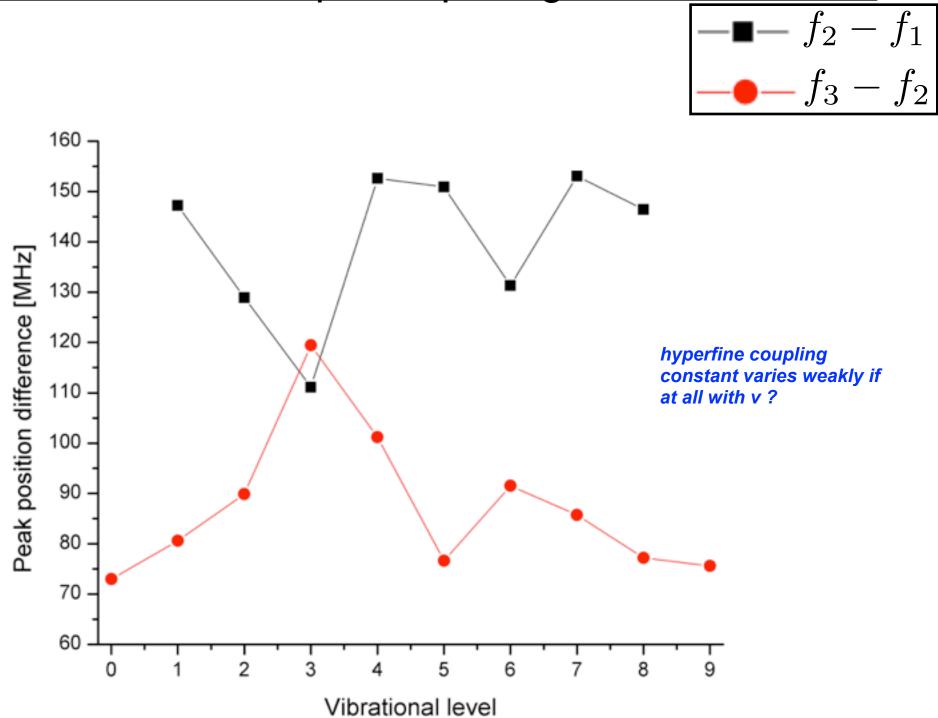


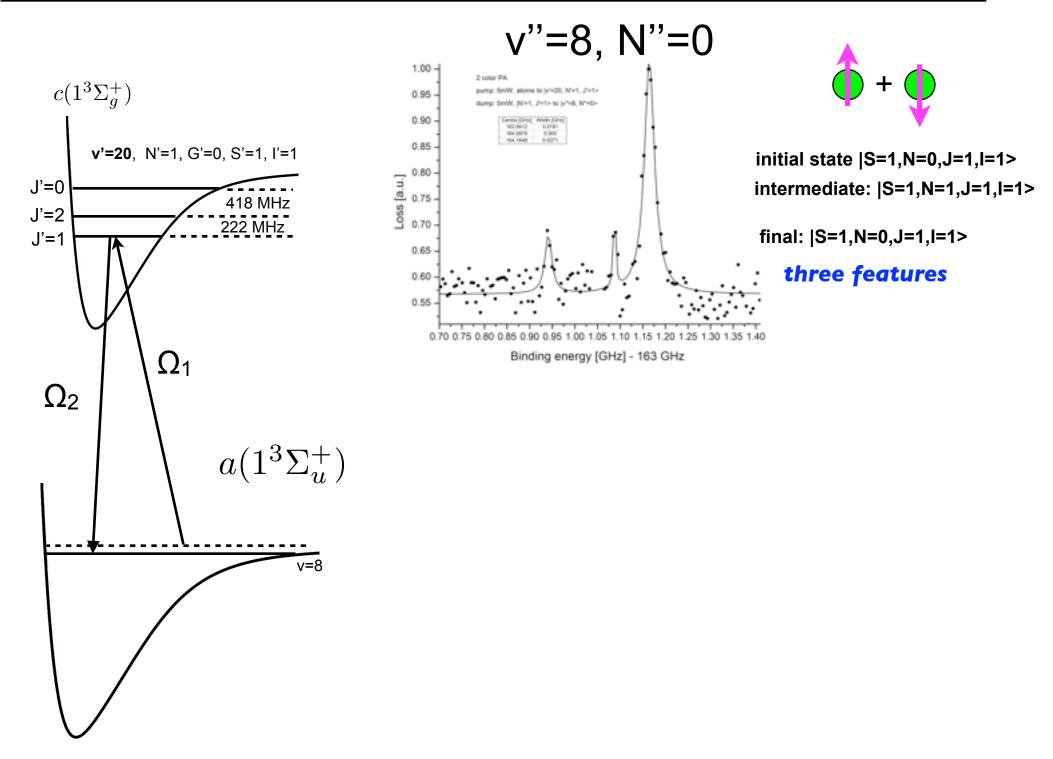


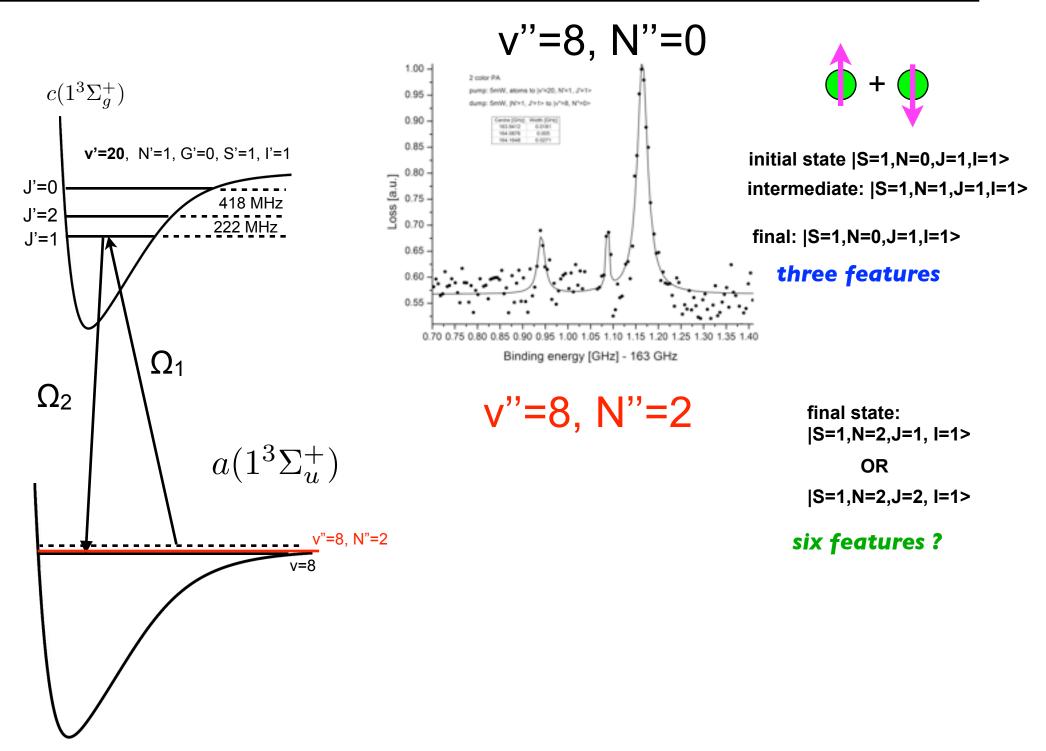
### N=0 peak splittings

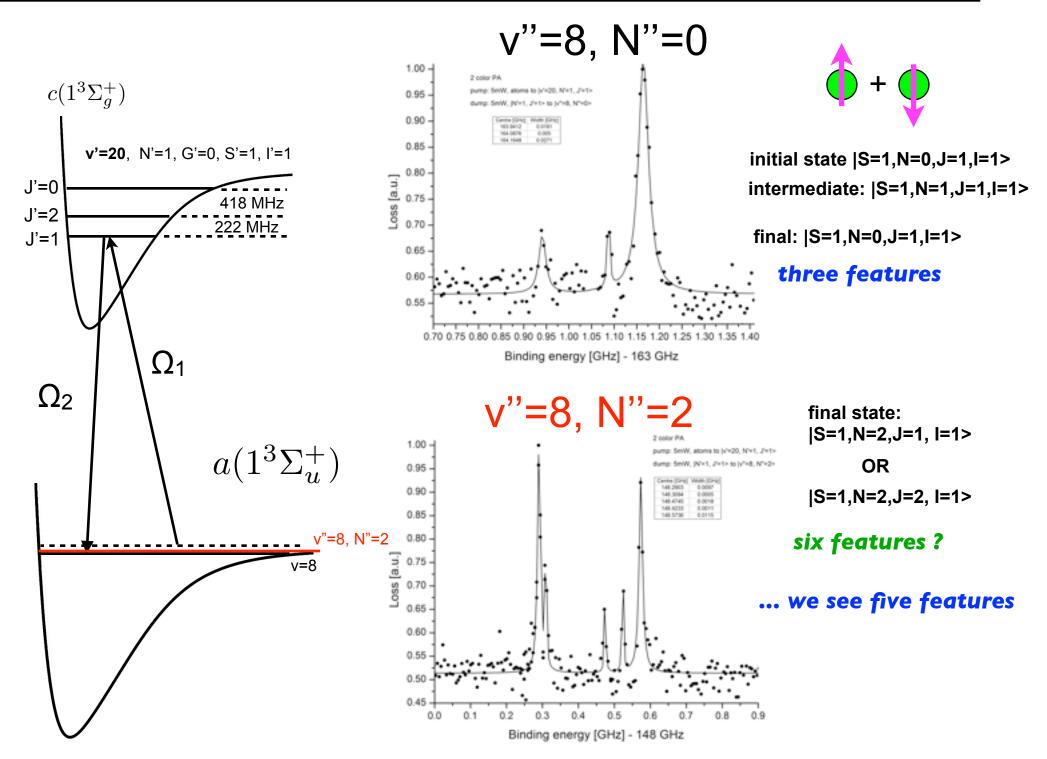


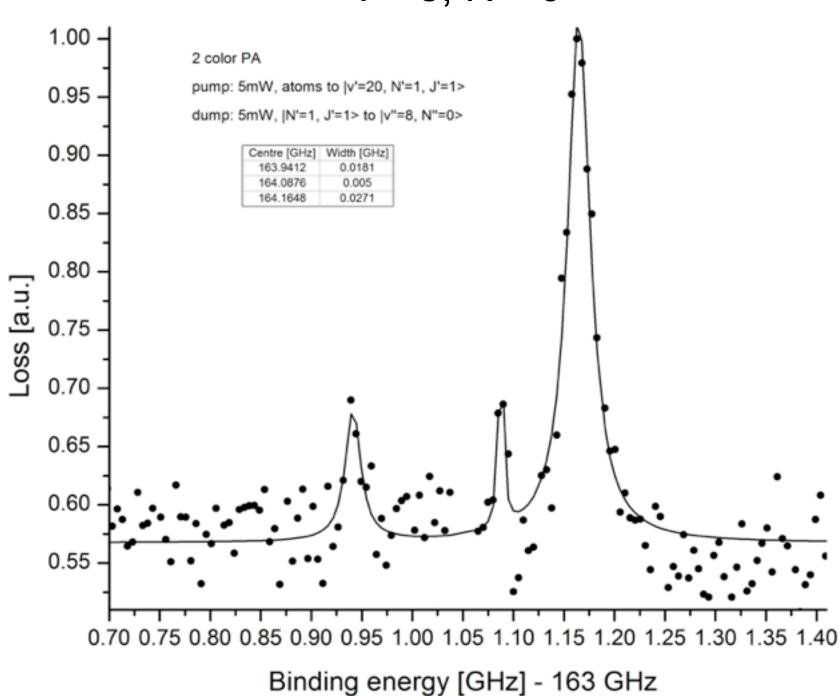
## N=0 peak splittings





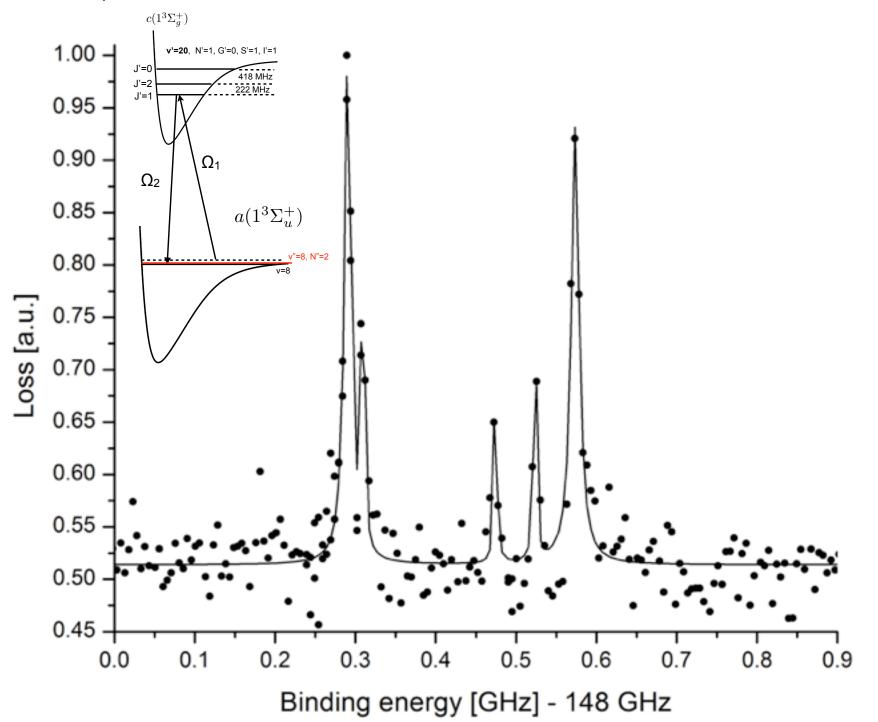


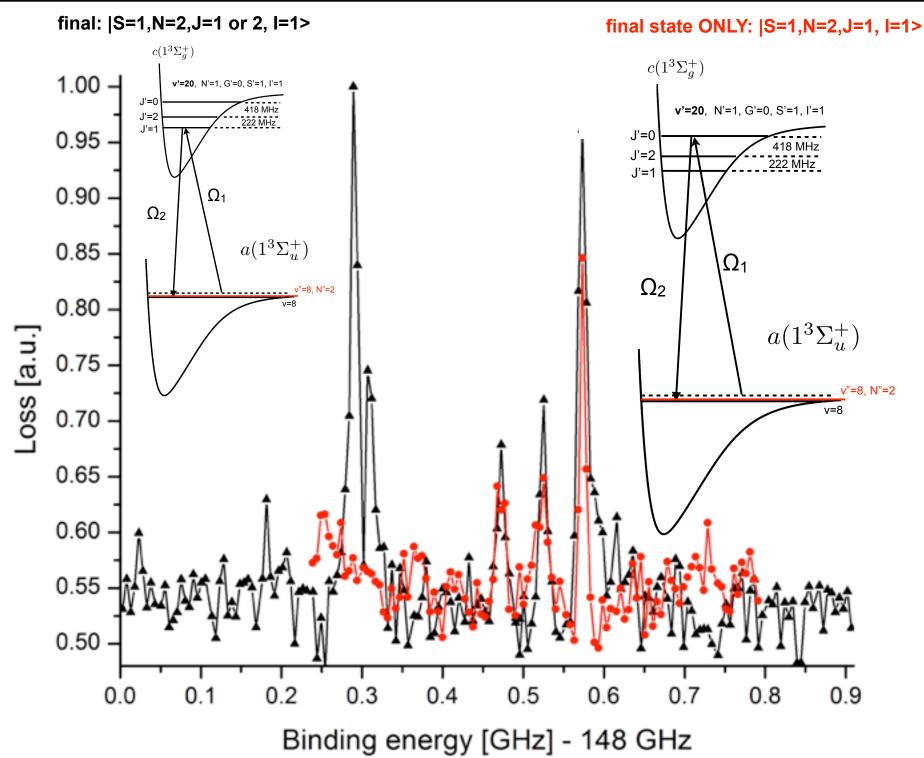




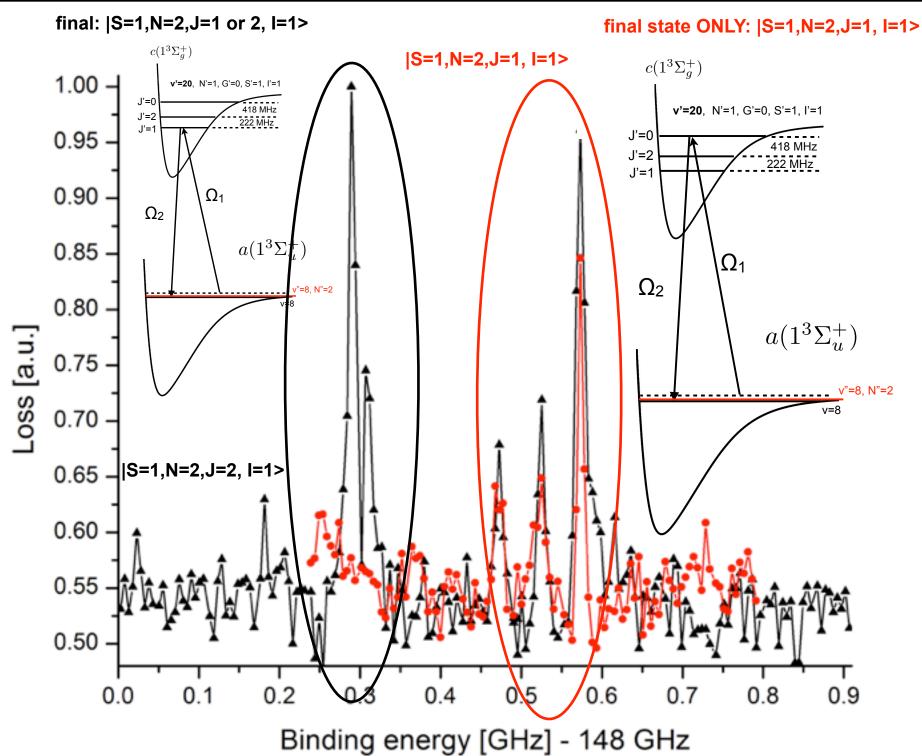
v"=8, N"=0

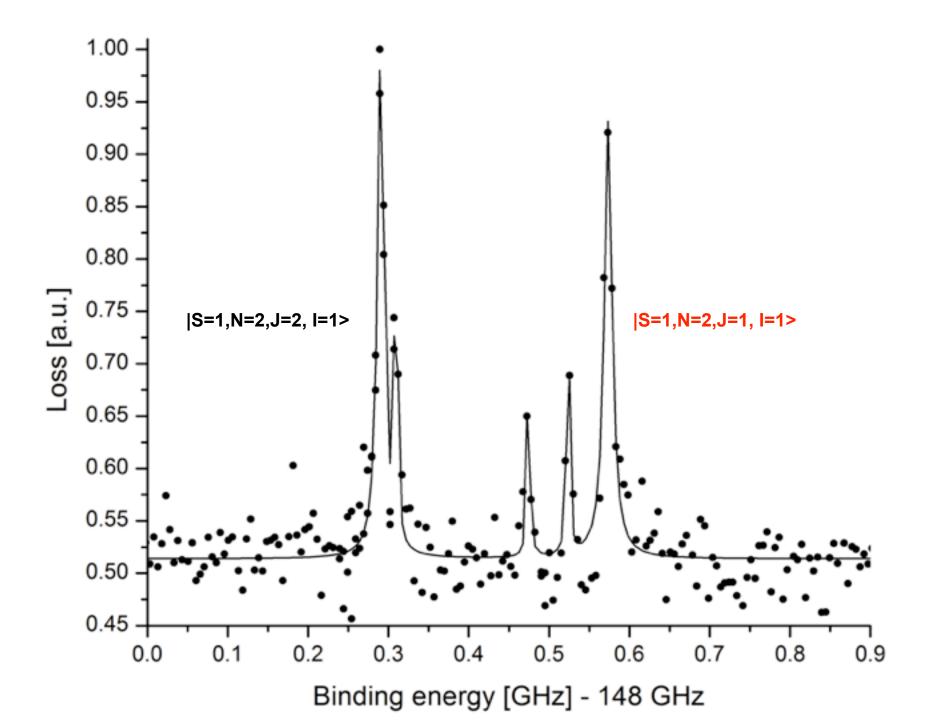
what follows is unchanged and what was presented, but after the talk Mariusz and Will sent me a correction : the data plotted in red were not obtained with  $\Omega$ 1 tuned to the J=0 state, rather it was obtained with  $\Omega$ 1 tuned to the J=2 state! So the conclusions are, as stated, incorrect.

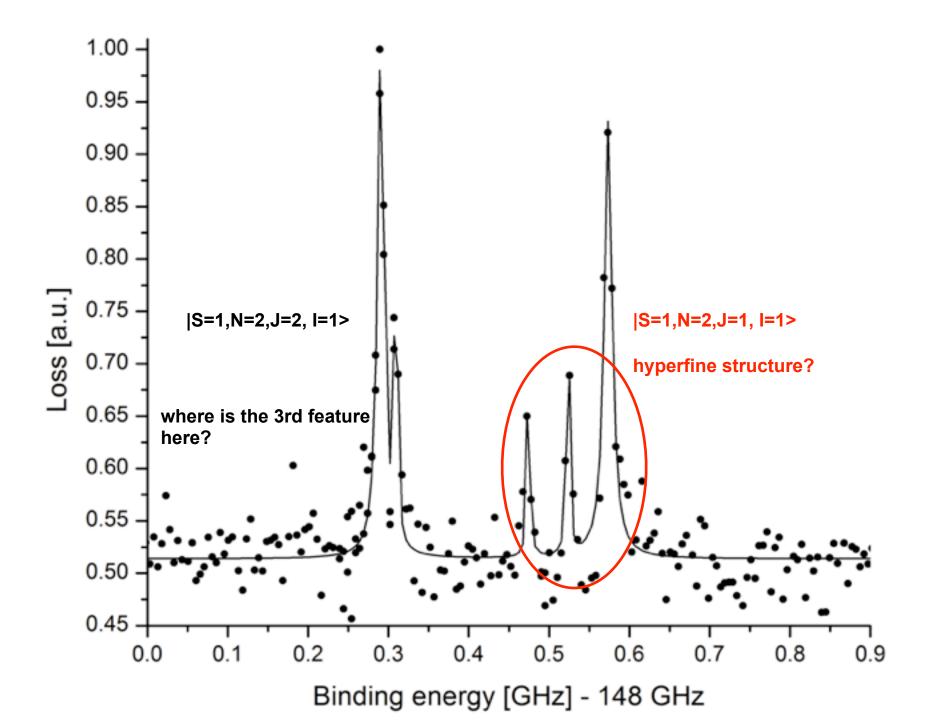


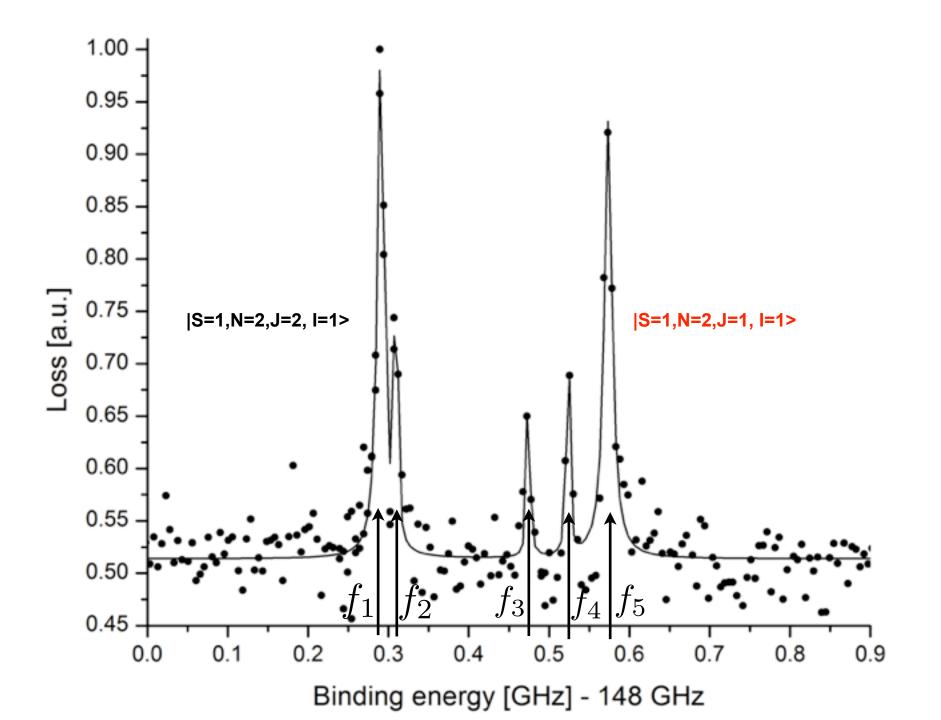


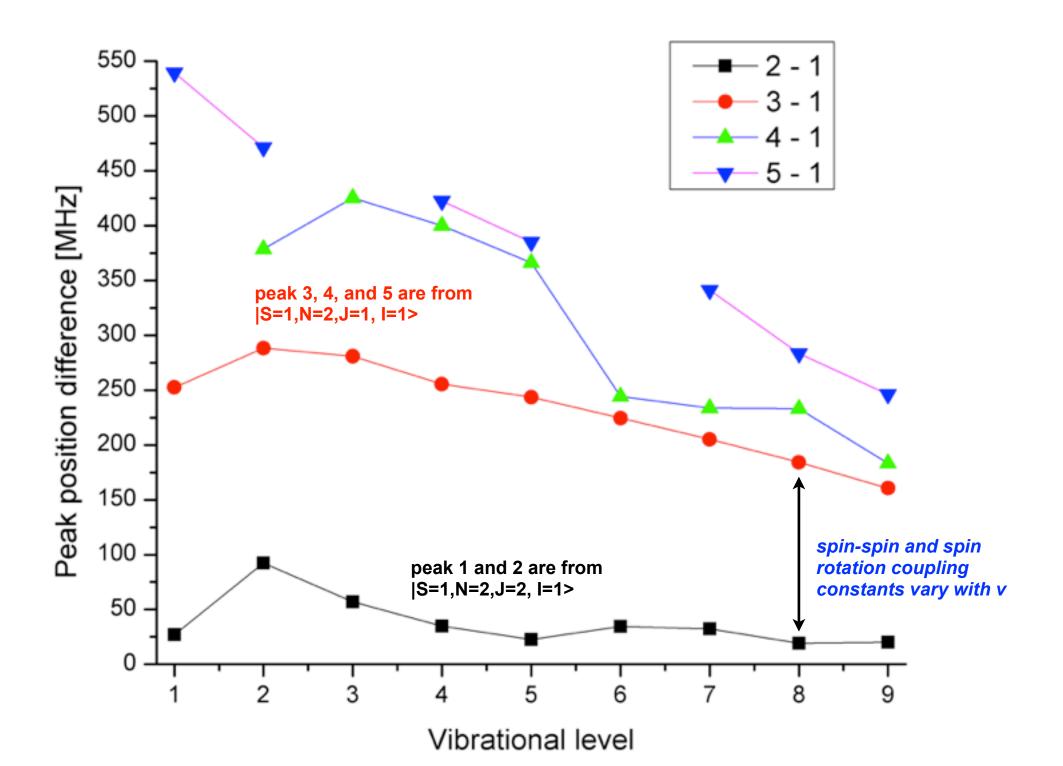
2-color PA spectroscopy results : here  $\Omega_1$  is fixed and  $\Omega_2$  is scanned



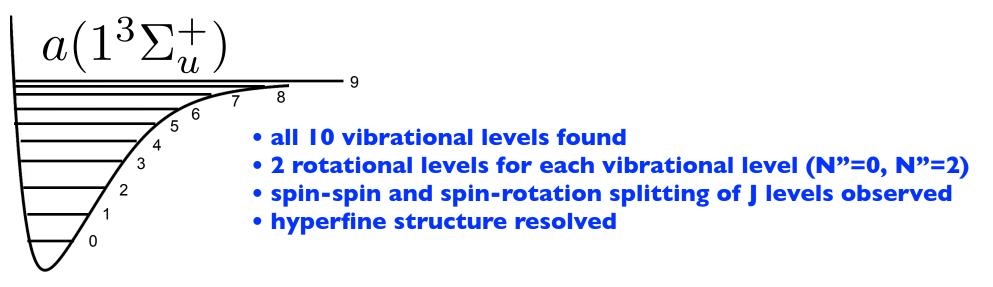








Full characterization of the bound levels of the ground triplet state of <sup>6</sup>Li<sub>2</sub>



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Is this useful? It's the simplest molecule after to H<sub>2</sub>

Full characterization of the bound levels of the ground triplet state of <sup>6</sup>Li<sub>2</sub>

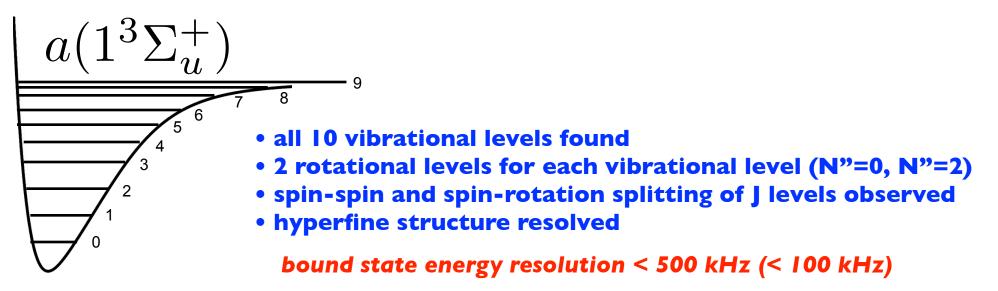


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Next step: STIRAP transfer FR molecules into these states and measure their lifetime

Full characterization of the bound levels of the ground triplet state of <sup>6</sup>Li<sub>2</sub>

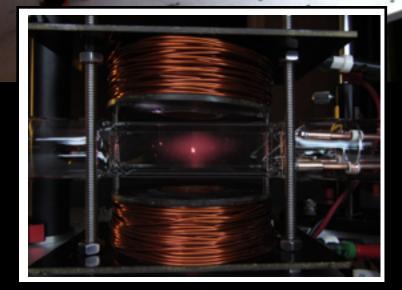


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Is this useful? It's the simplest molecule after to H<sub>2</sub>

Next step: STIRAP transfer FR molecules into these states and measure their lifetime

## Rb+H apparatus: H beam collides with laser cooled Rb atoms



Collaboration with Takamasa Momose (UBC CHEM)

## A new twist on Feshbach resonances: polar collision + electric field

PRL 96, 123202 (2006)

1

PHYSICAL REVIEW LETTERS

week ending 31 MARCH 2006

#### **Controlling Collisions of Ultracold Atoms with dc Electric Fields**

R. V. Krems\*

Department of Chemistry, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada

PHYSICAL REVIEW A 75, 032709 (2007)

Electric-field-induced Feshbach resonances in ultracold alkali-metal mixtures

Z. Li and R. V. Krems\*

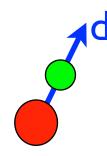
Department of Chemistry, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1

PHYSICAL REVIEW A 79, 042711 (2009)

Effects of electric fields on heteronuclear Feshbach resonances in ultracold <sup>6</sup>Li-<sup>87</sup>Rb mixtures

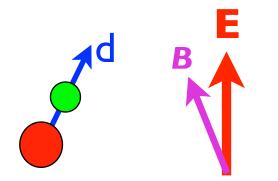
Z. Li<sup>1</sup> and K. W. Madison<sup>2</sup>

## polar collision



A heteronuclear collision complex has an instantaneous electric dipole moment

### polar collision + electric field



A heteronuclear collision complex has an instantaneous electric dipole moment

... and this electric dipole is coupled to an external electric field

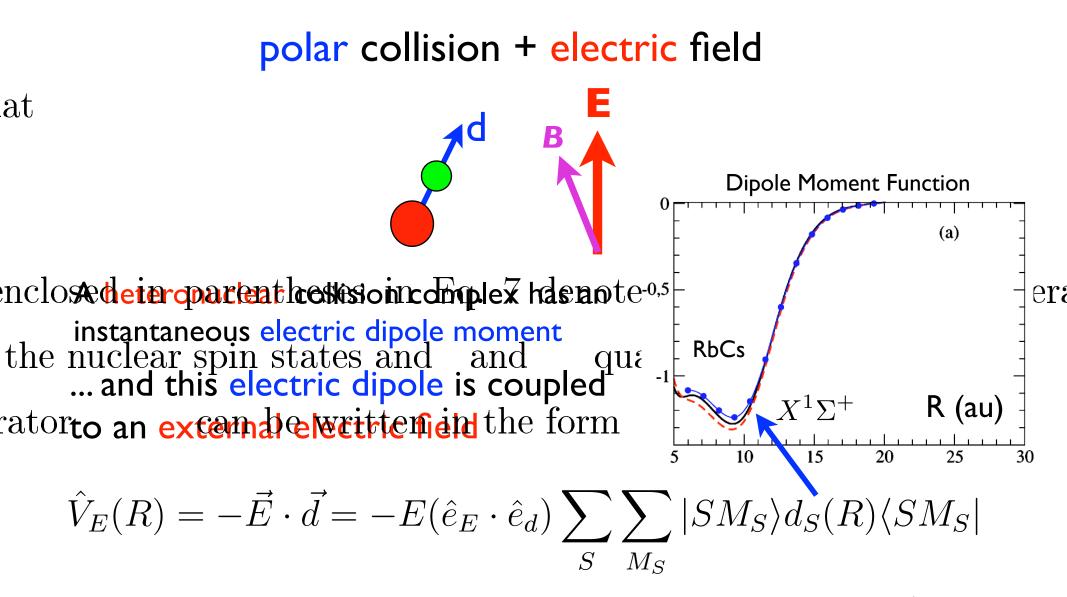
### polar collision + electric field

at

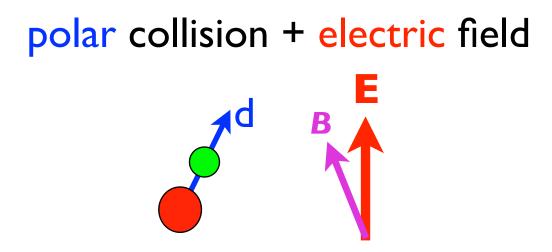
enclose dein contract the solution of the second se

$$\hat{V}_E(R) = -\vec{E} \cdot \vec{d} = -E(\hat{e}_E \cdot \hat{e}_d) \sum_S \sum_{M_S} |SM_S\rangle d_S(R) \langle SM_S|$$

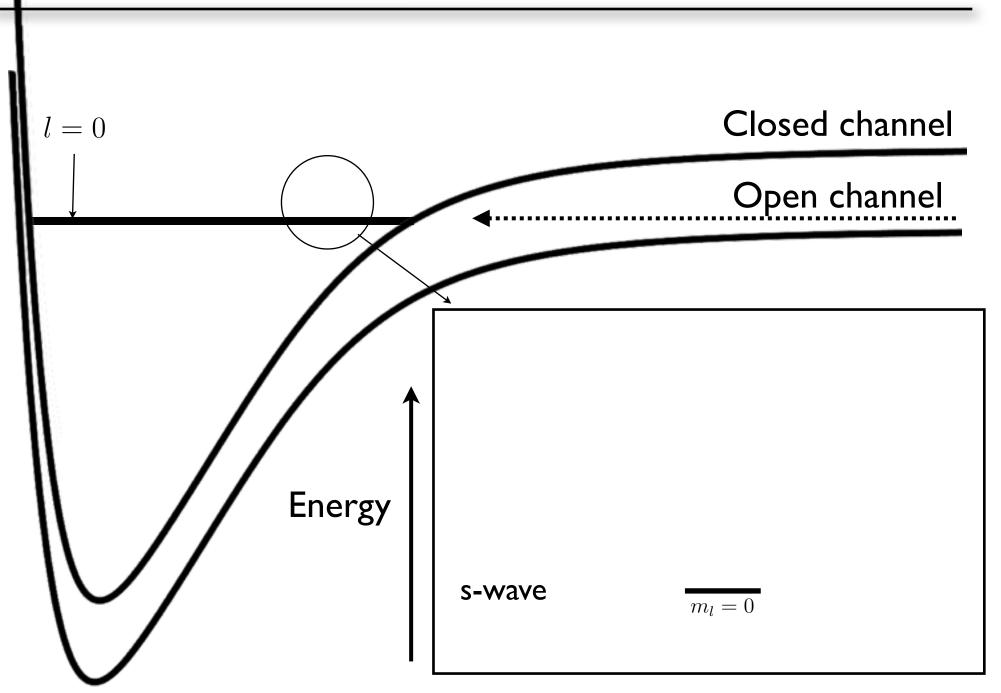
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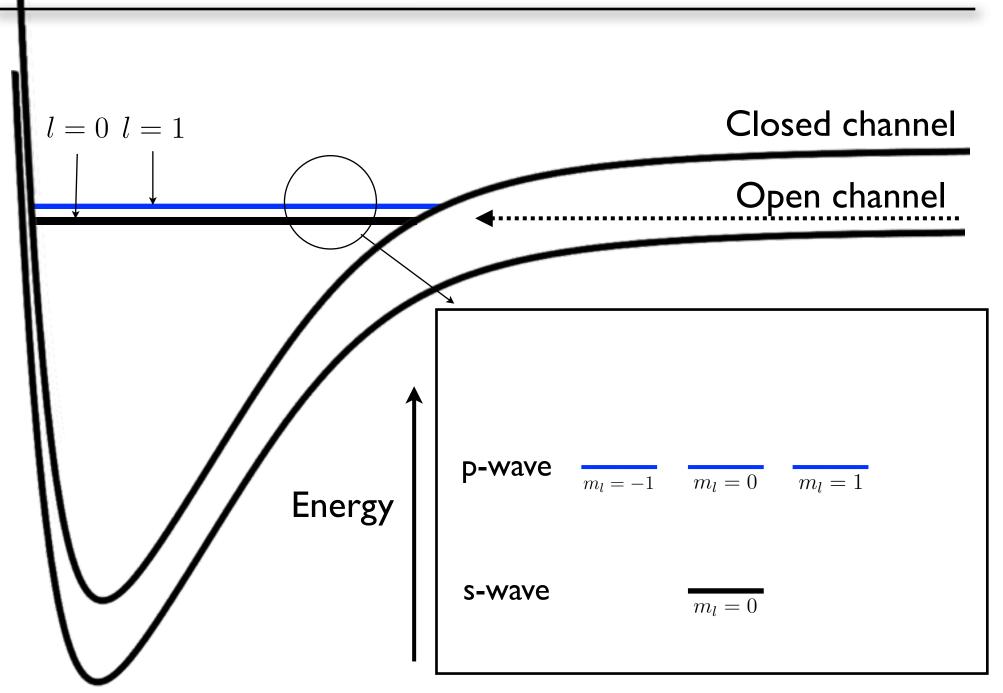


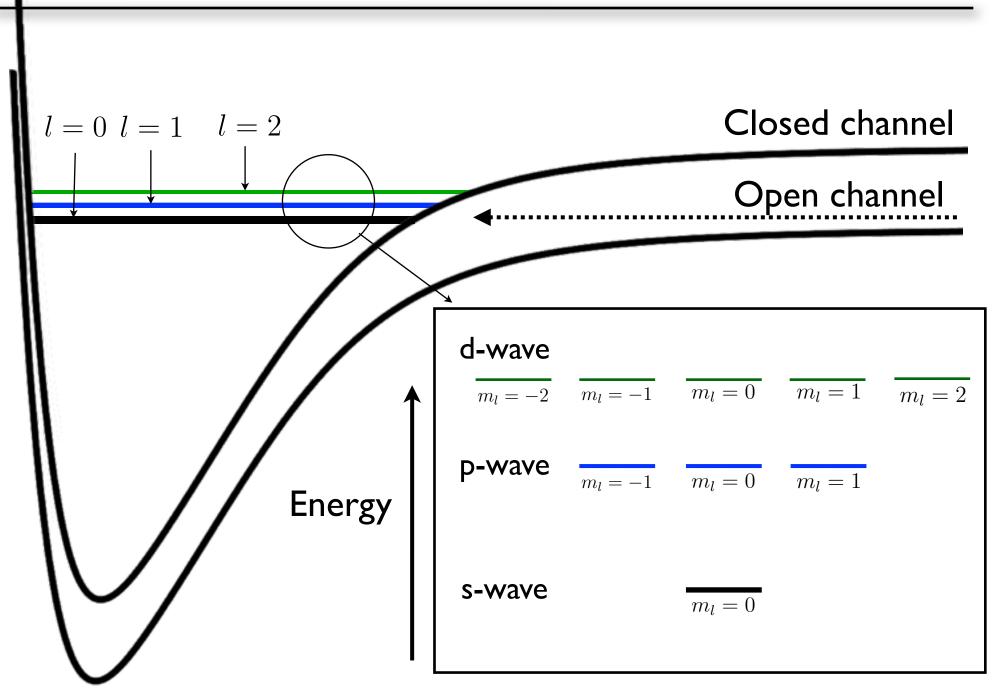
nd this person four less different nertial mertatest ric field than di

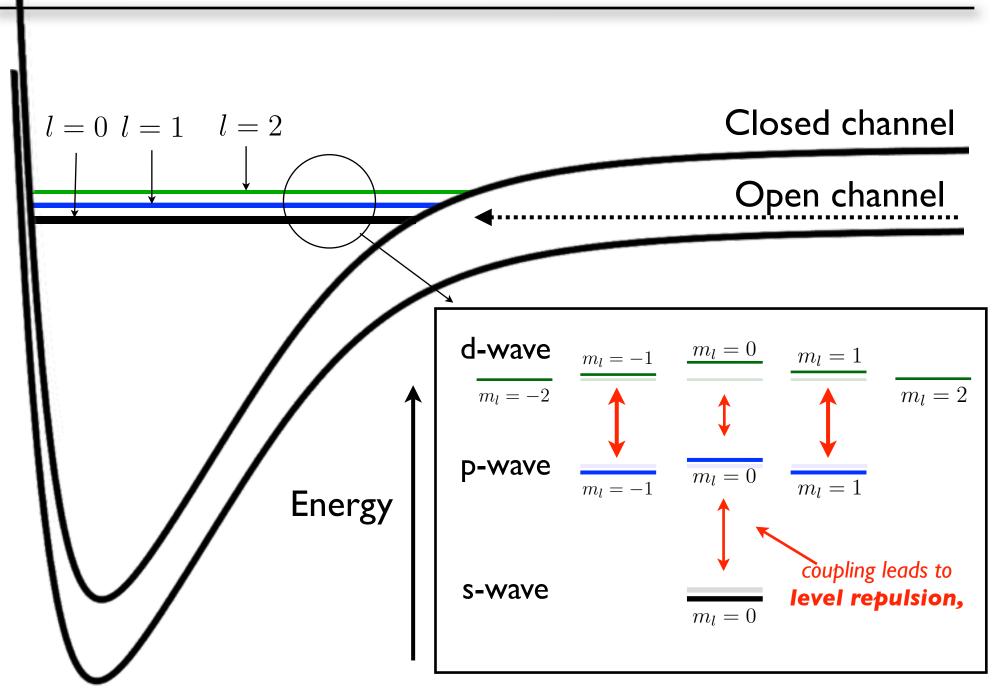


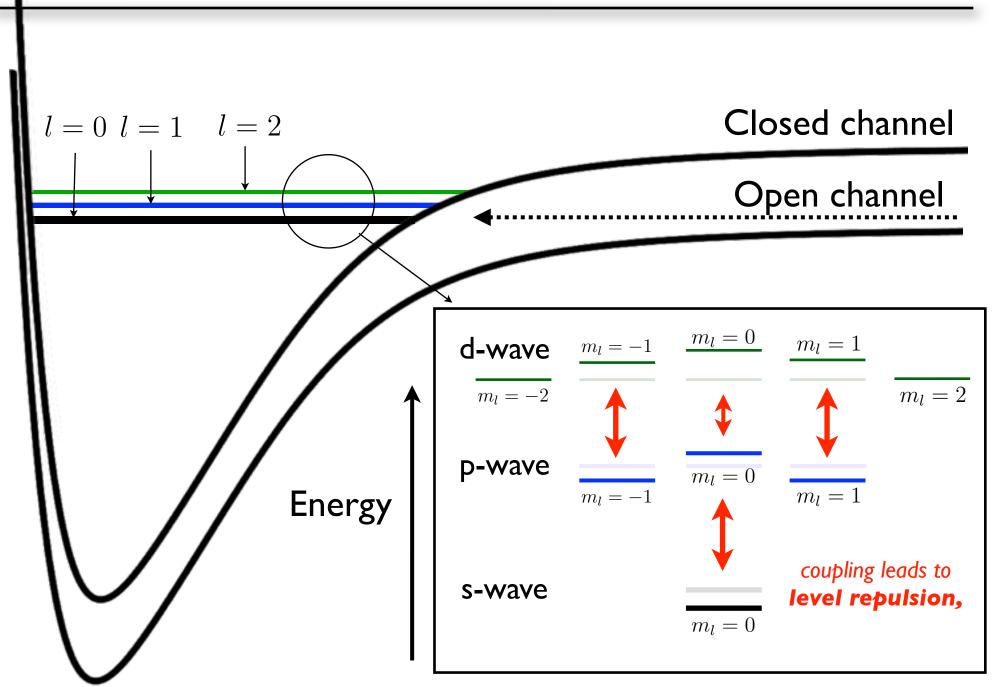
- induce new Feshbach resonances mixing of partial waves
- shift position of intrinsic resonances bound state level repulsion
- split resonances into 1+1 multiplets tunable anisotropic interactions

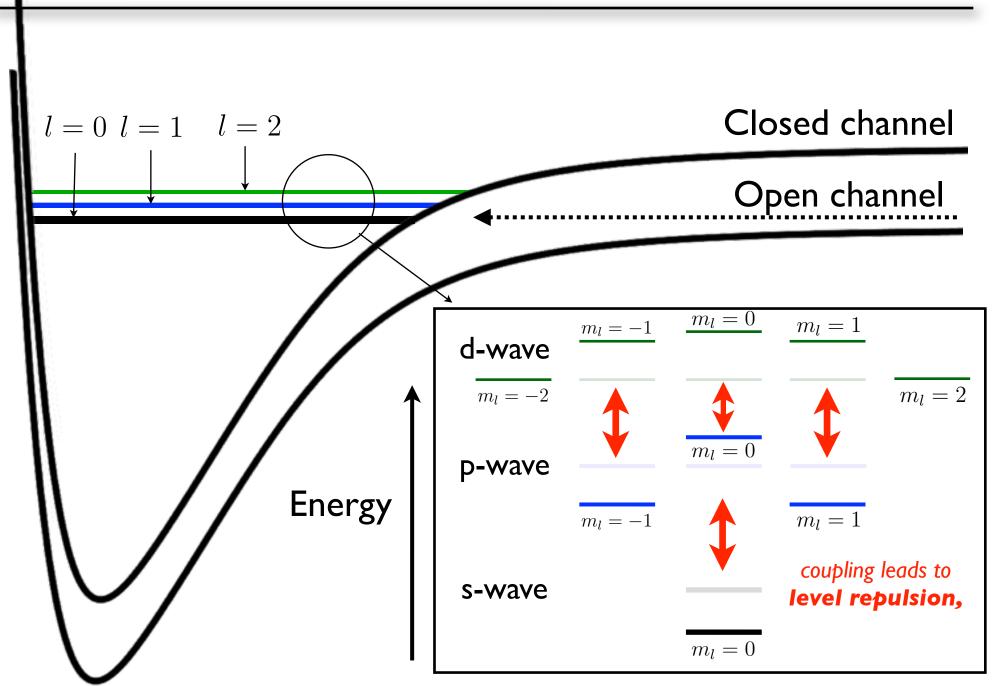


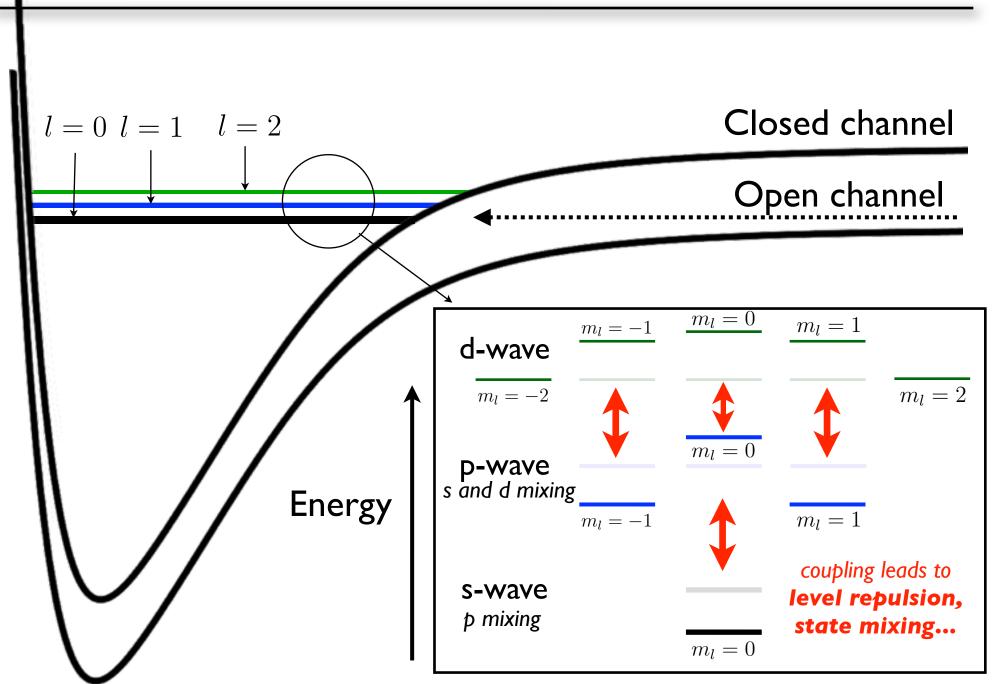


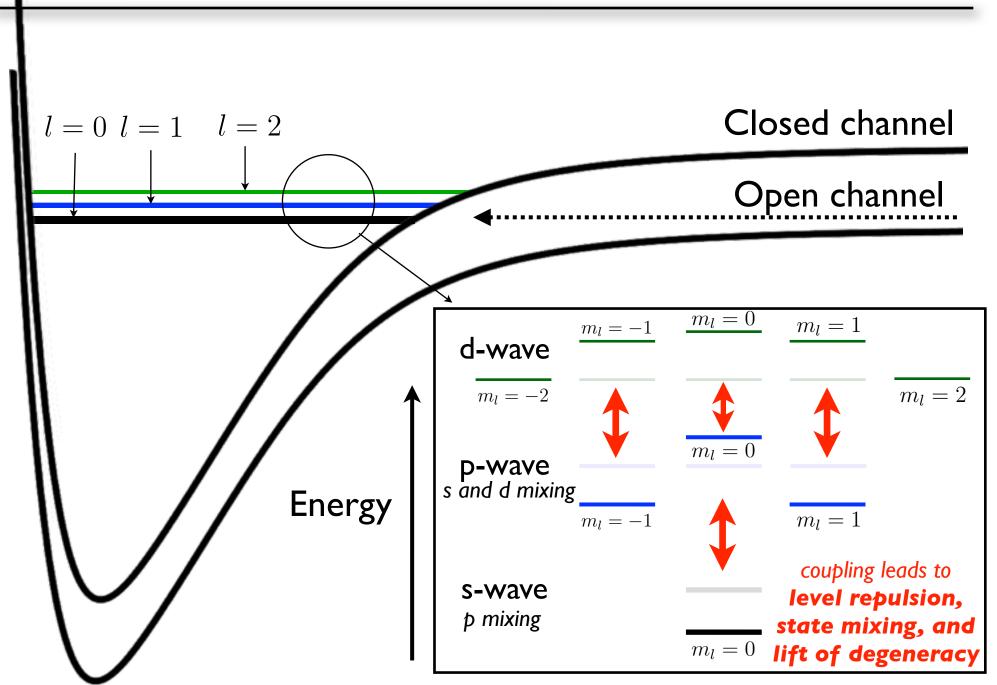




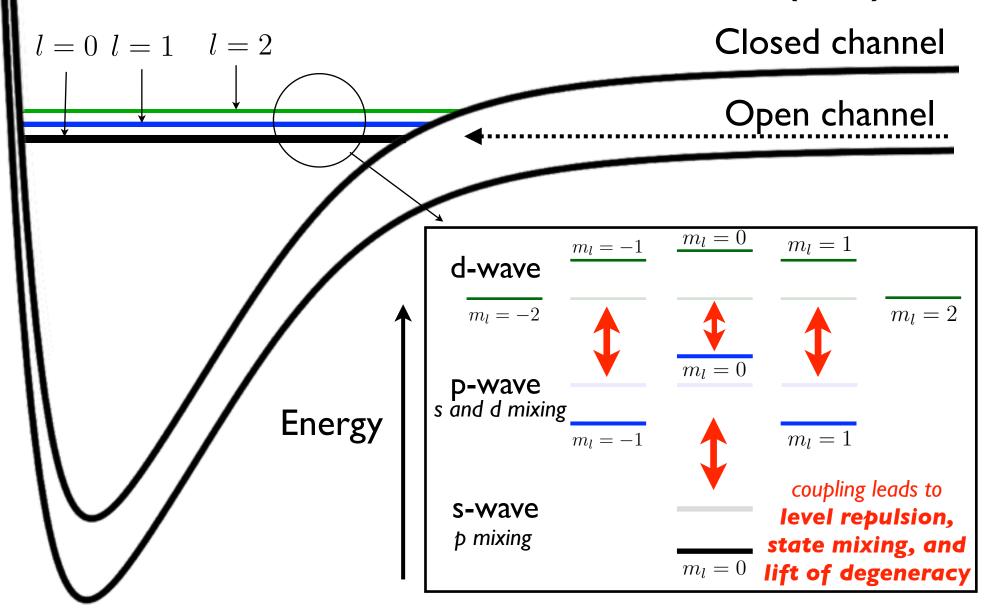








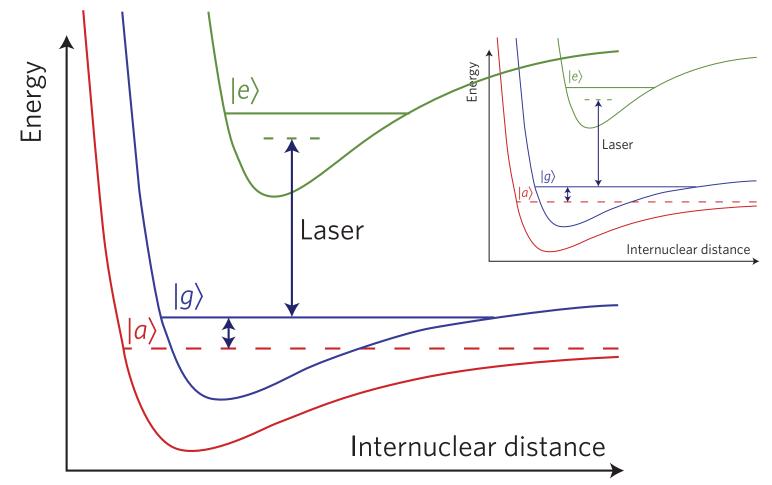
Effects of electric fields on heteronuclear Feshbach resonances in ultracold 6Li-87Rb mixtures, PRA 79, 042711 (2009).





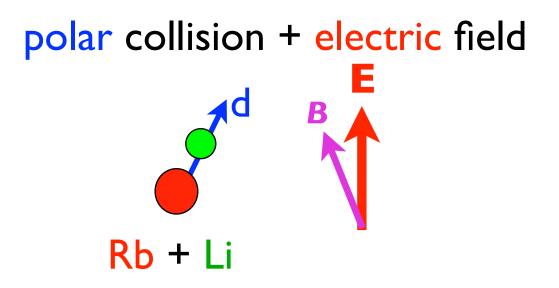
## **Control of a magnetic Feshbach resonance** with laser light

Dominik M. Bauer, Matthias Lettner, Christoph Vo, Gerhard Rempe and Stephan Dürr\*



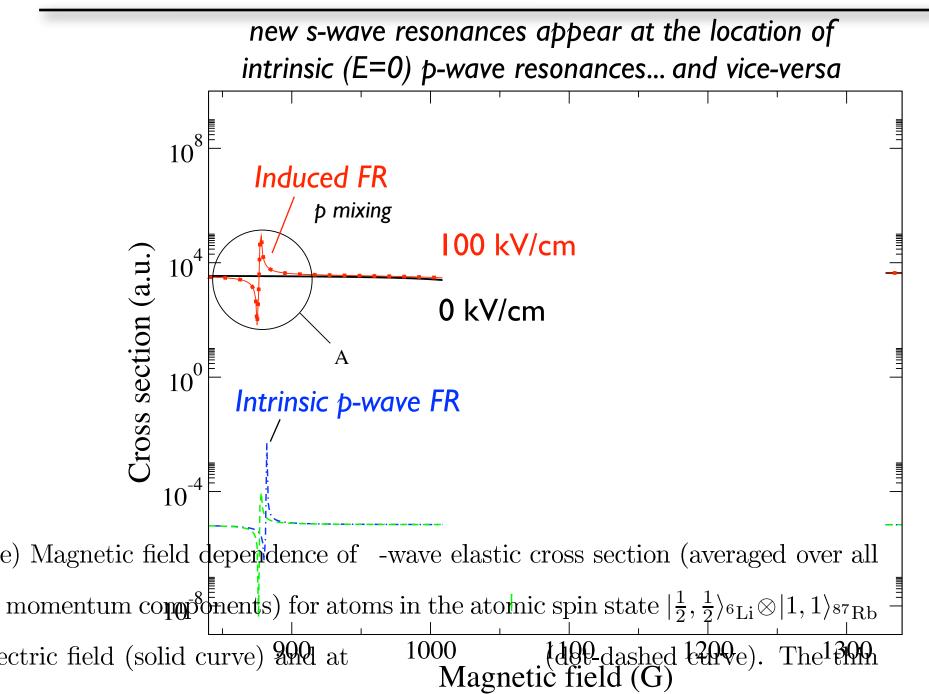
### A new twist on Feshbach resonances:

Effects of electric fields on heteronuclear Feshbach resonances in ultracold 6Li-87Rb mixtures, PRA 79, 042711 (2009).

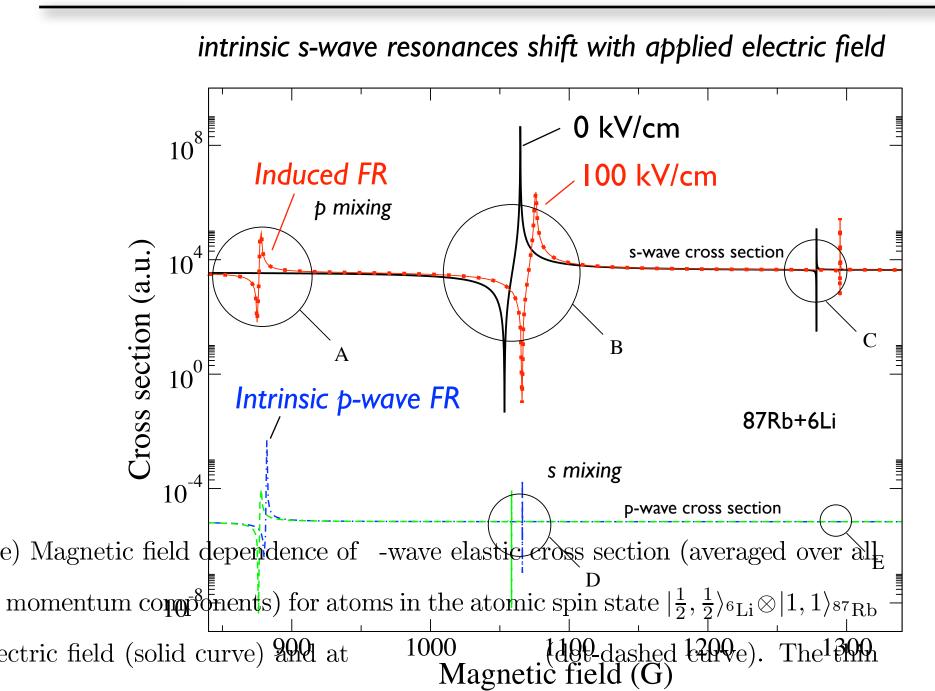


- shift position of intrinsic Feshbach resonances bound state level repulsion
- induce new Feshbach resonances mixing of partial waves
- split resonances into 1+1 multiplets tunable anisotropic interactions

## A new twist on Feshbach resonances: Induced resonances

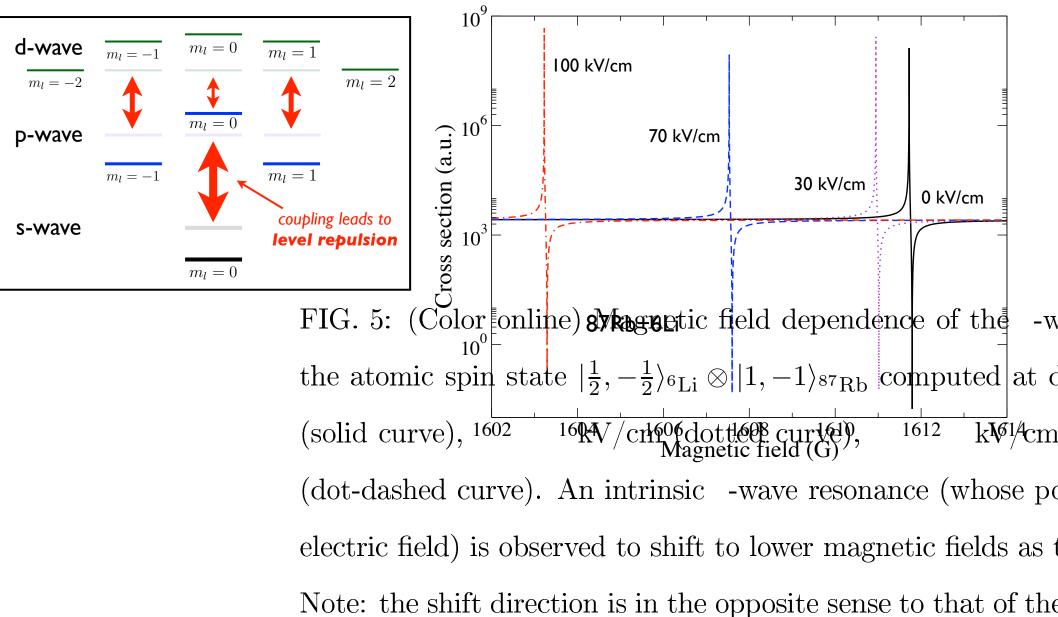


## A new twist on Feshbach resonances: shift of resonances



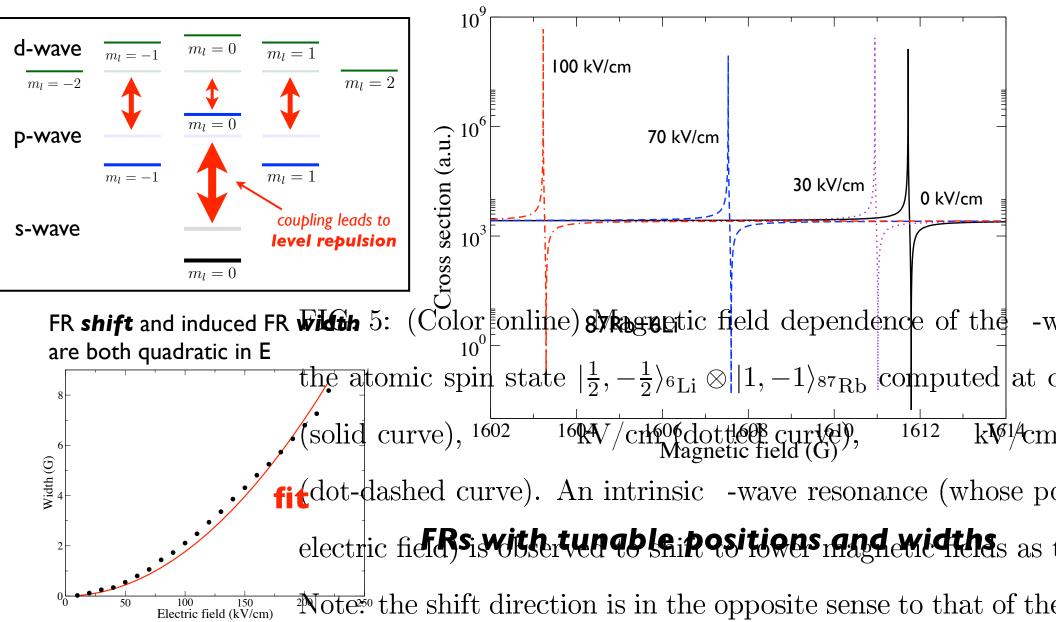
## Shift of resonances:

intrinsic (E=0) resonances shift in position as magnitude of electric field increased



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intrinsic (E=0) resonances shift in position as magnitude of electric field increased

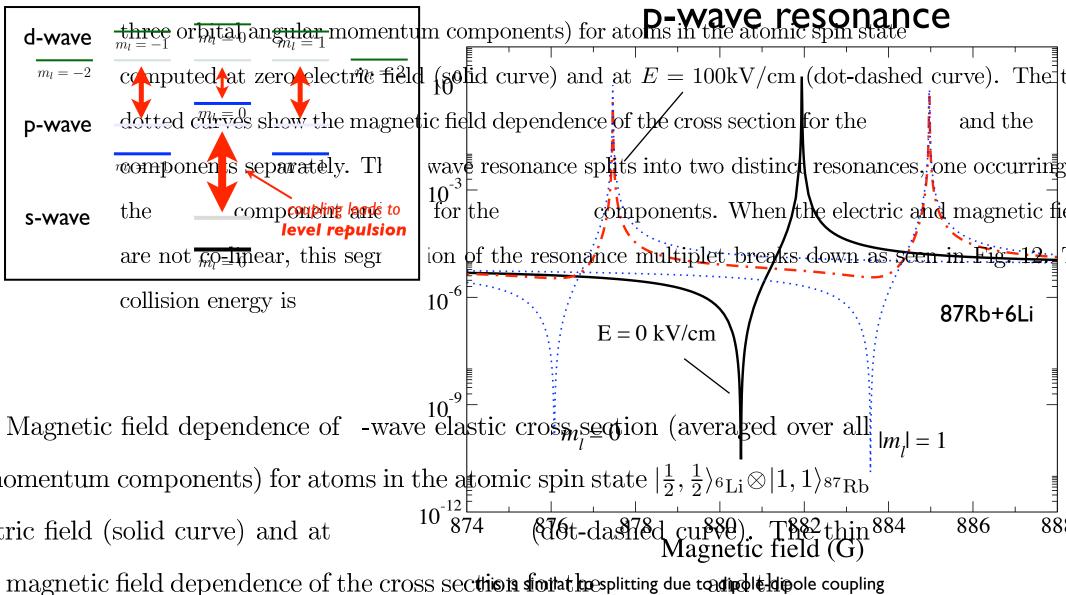


## Splitting of resonances:

#### partial wave resonances split into

#### 1+1 distinct resonances

FIG. 8: (Color online) Magnetic field dependence of -wave elastic cross section (averaged over

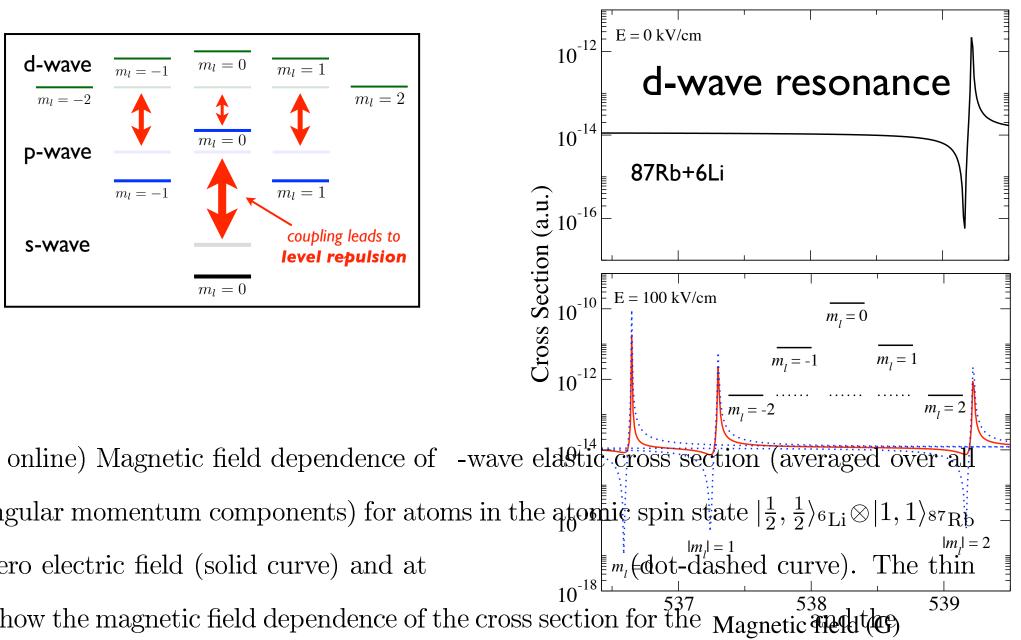


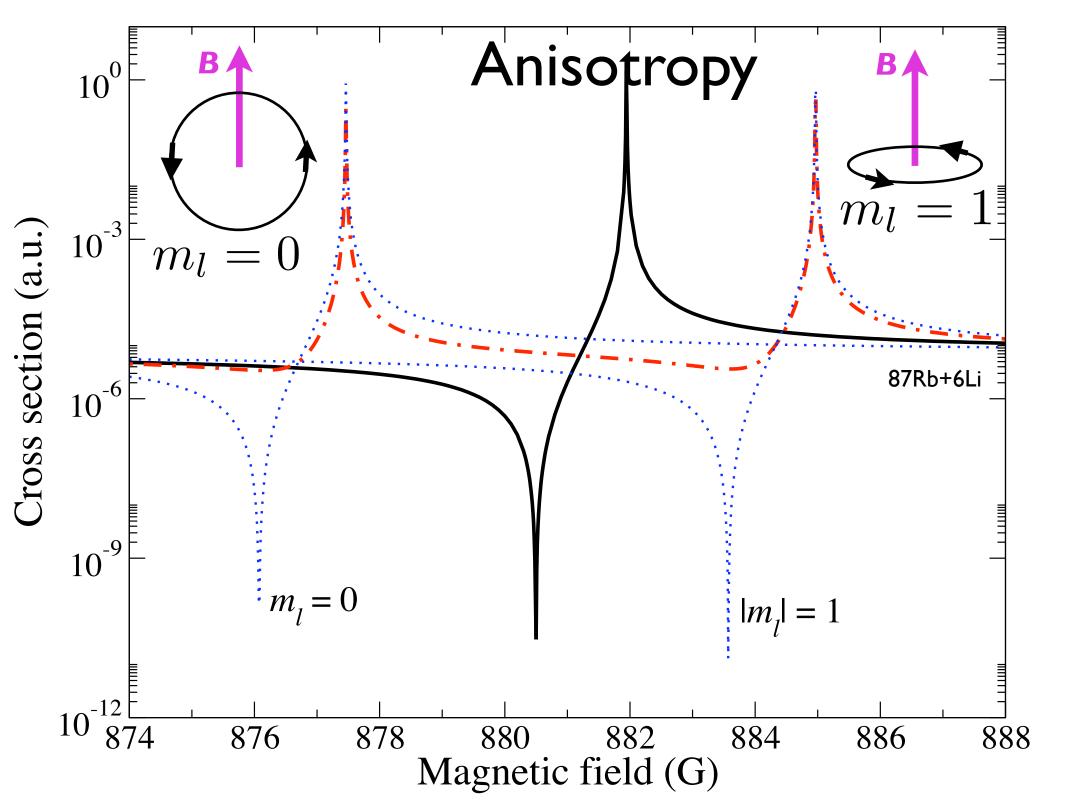
Regal, Ticknor, Bohn, Jin, PRL **90**, 053201 (2003), and PRA **69**, 042712 (2004).

## Splitting of resonances:

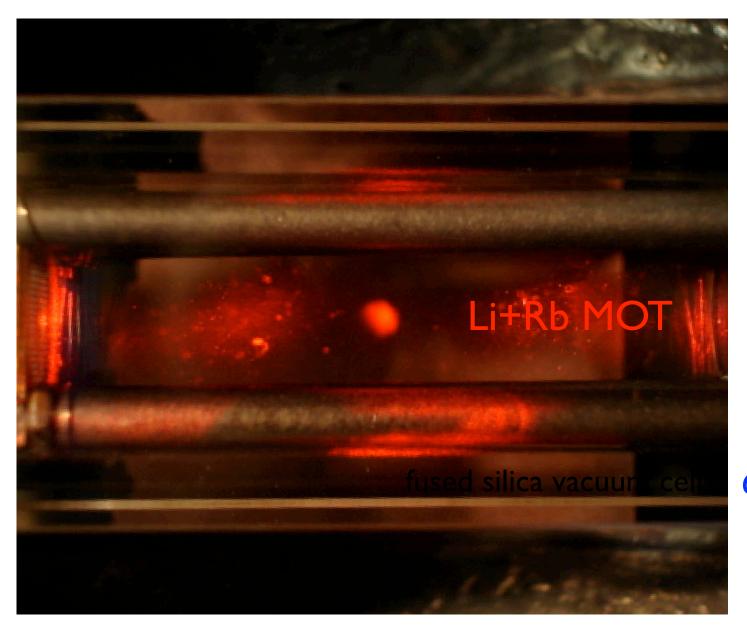
partial wave resonances split into

1+1 distinct resonances





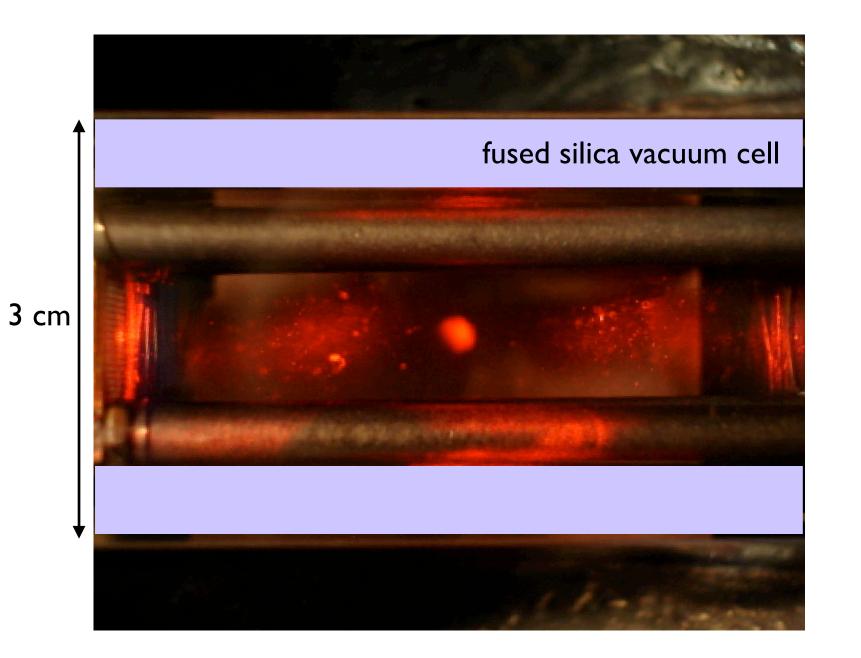
## Experimental challenge: adding the E field



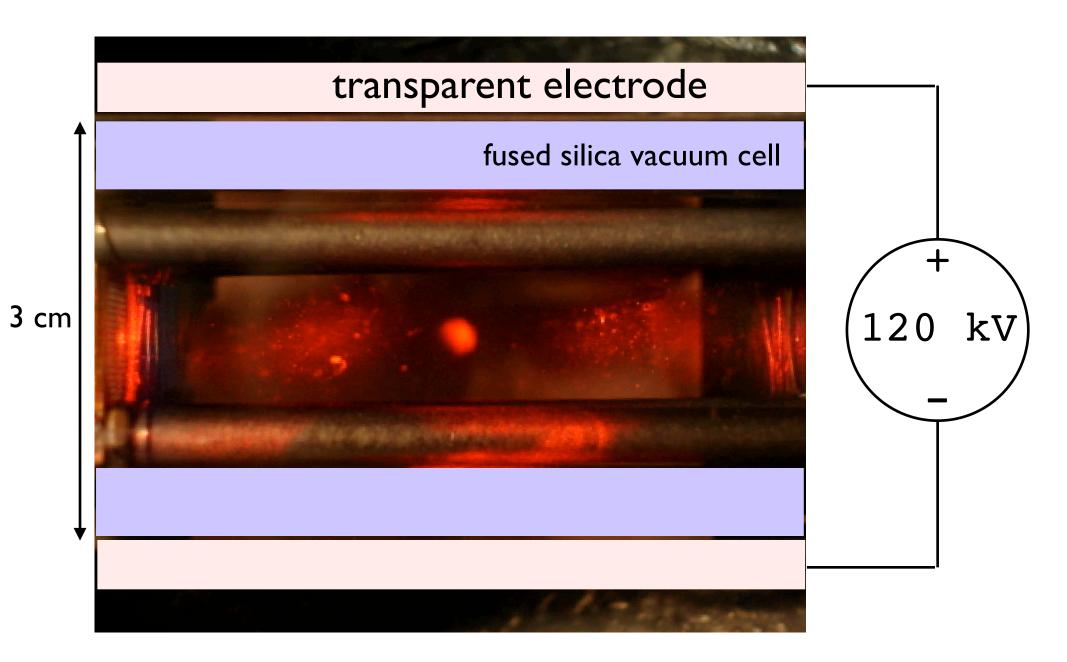
we want a field of about 30 kV/cm

how to add electrodes while keeping good optical access?

## Experimental challenge: adding the E field



### Experimental challenge: adding the E field



high voltage coax

transparent indium tin oxide coated glass slide inside a glass sandwich

#### with epoxy filling



#### **Status:**

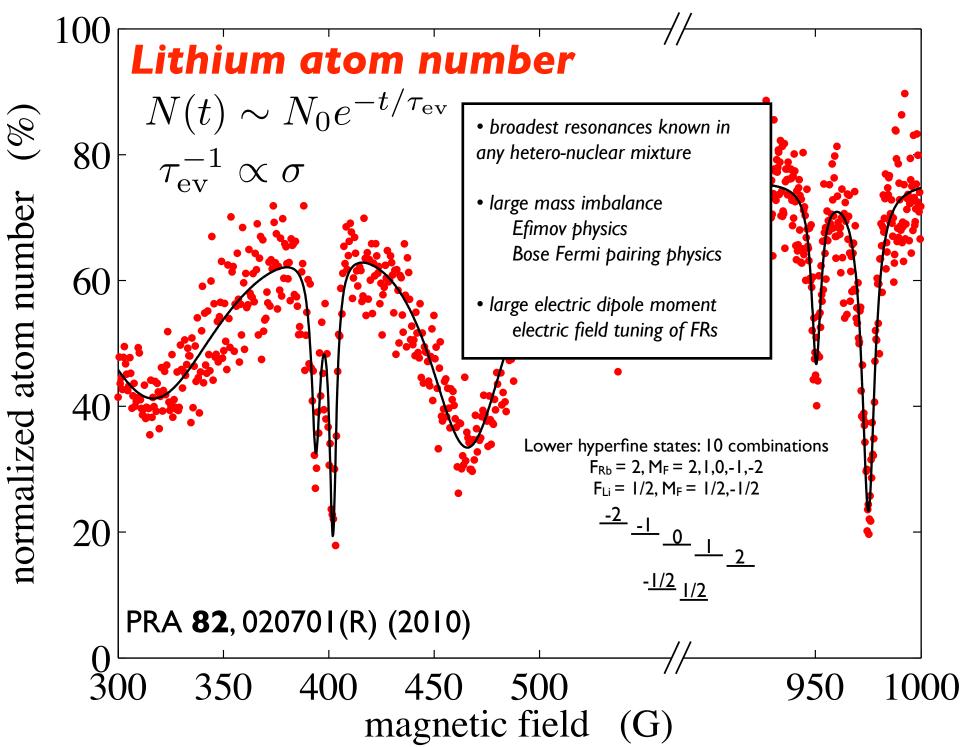
# We have generated and verified fields of 18kV/cm and have another factor of 2 in voltage.

#### **Mysteries:**

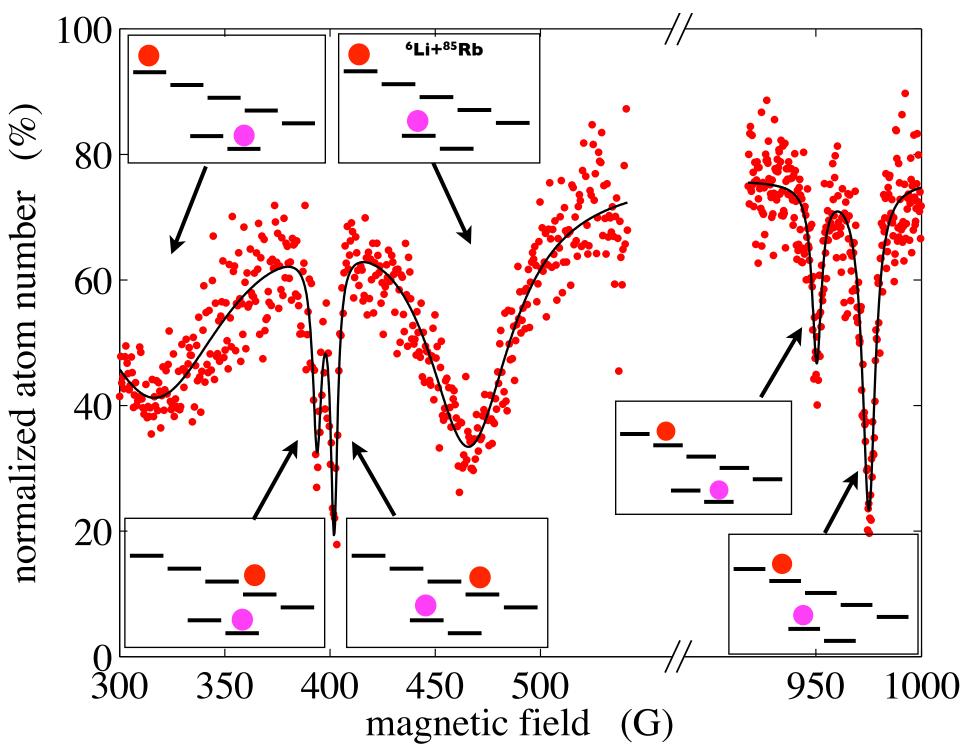
- I) Field peculiarities (evidence of shielding)
- 2) Trap loss associated with energizing plates

### Feshbach resonances in <sup>6</sup>Li+<sup>85</sup>Rb mixtures the strength of resonances

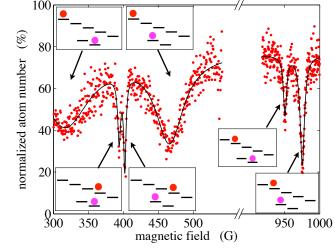
#### Feshbach resonances in <sup>6</sup>Li+<sup>85</sup>Rb mixtures



Feshbach resonances in <sup>6</sup>Li+<sup>85</sup>Rb mixtures



#### Feshbach resonances in <sup>6</sup>Li+<sup>85</sup>Rb mixtures



effective range: 
$$r_{\rm e} = \hbar^2 / (2m_{\rm R}|a_{\rm bg}|\mu_{\rm rel}\Delta B)$$
  
resonance strength:  $E_{\rm res} = \hbar^2 / (2m_{\rm R}r_{\rm e}^2)$ 

TABLE II. The calculated characteristics of seven large FRs for stable Fermi-Bose mixtures of <sup>6</sup>Li-<sup>85</sup>Rb and <sup>6</sup>Li-<sup>87</sup>Rb. The background scattering length  $a_{bg}$  and effective range of the resonance  $r_e$  are given in units of the Bohr radius,  $a_0$ . The value for  $\mu_{rel}$ , the difference in the magnetic moments of the closed channel (molecule) and the open-channel threshold, is given in units of the Bohr magneton  $\mu_B = 9.27400915(23) \text{ J T}^{-1}$ . For each FR, the magnetic fields at which the mixture is energetically stable with respect to two-body spin relaxation is provided. In some cases, because of nearby resonances, we can only provide an approximate lower bound on the resonance width.

Atomic states	$B_0$	$\Delta B$	$\mu_{ m rel}$	$a_{ m bg}$	r <sub>e</sub>	Stability
$ f,m_f\rangle \otimes  f,m_f\rangle$	(G)	(G)	$(\mu_{ m B})$	$(a_0)$	$(a_0)$	(G)
			<sup>6</sup> Li- <sup>85</sup> Rb			
$ rac{1}{2},rac{1}{2} angle\otimes 2,2 angle$	40.7	>40	1.66	-14.9	<231	ground state
$ rac{1}{2},-rac{1}{2} angle\otimes 2,1 angle$	402.5	27.3	1.58	-14.9	358	≥149
$ rac{1}{2},-rac{1}{2} angle\otimes 2,0 angle$	643.7	61.0	1.34	-14.9	189	≥141
$ rac{1}{2},-rac{1}{2} angle\otimes 2,-1 angle$	961.3	75.6	1.81	-14.7	113	≥133
$ rac{1}{2},-rac{1}{2} angle\otimes 2,-2 angle$	466.7	>100	0.58	-14.8	<264	$\geqslant 0$
			<sup>6</sup> Li- <sup>87</sup> Rb			
$ rac{1}{2},rac{1}{2} angle\otimes 1,1 angle$	1065.0	11.5	2.36	-19.0	442	ground state
$ \frac{1}{2}, -\frac{1}{2}\rangle \otimes  1,1\rangle$	1108.6	11.0	2.36	-19.0	463	≥75

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