

# Lecture 2

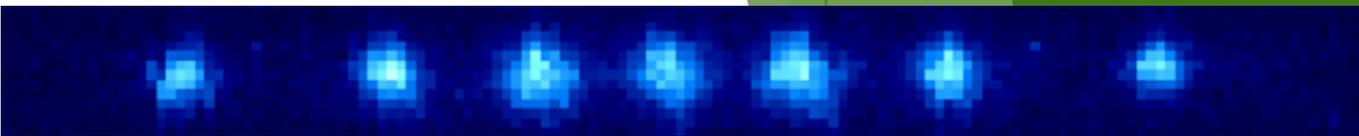


UNIVERSITY OF AMSTERDAM



Towards quantum impurity physics  
with atoms and ions

Rene Gerritsma



## Lecture 2

- ▶ Can we get colder?
- ▶ Spin dynamics
- ▶ Controlling interactions: Rydbergs
- ▶ Quantum chemistry: Trapped ions interacting with Feshbach dimers
- ▶ Conclusions

# Crossover to quantum regime

Type of motion	$E_{\text{kin}}/k_B (\mu\text{K})$	$E_{\text{col}}/k_B (\mu\text{K})$
Radial secular ion	$2 \times 21(9)$	1.4(0.6)
Intrinsic micromotion	$2 \times 21(9)$	1.4(0.6)
Axial secular ion	65(18)	2.2(0.4)
Excess micromotion	44(13)	1.5(0.4)
<b>Total ion energy</b>	<b>193(42)</b>	<b>6.6(1.4)</b>
Atom temperature	$3/2 \times 2.3(0.4)$	3.3(0.6)
<b>Total collision energy</b>	—	<b>9.9(2.0)</b>

Measurement of all types of motion

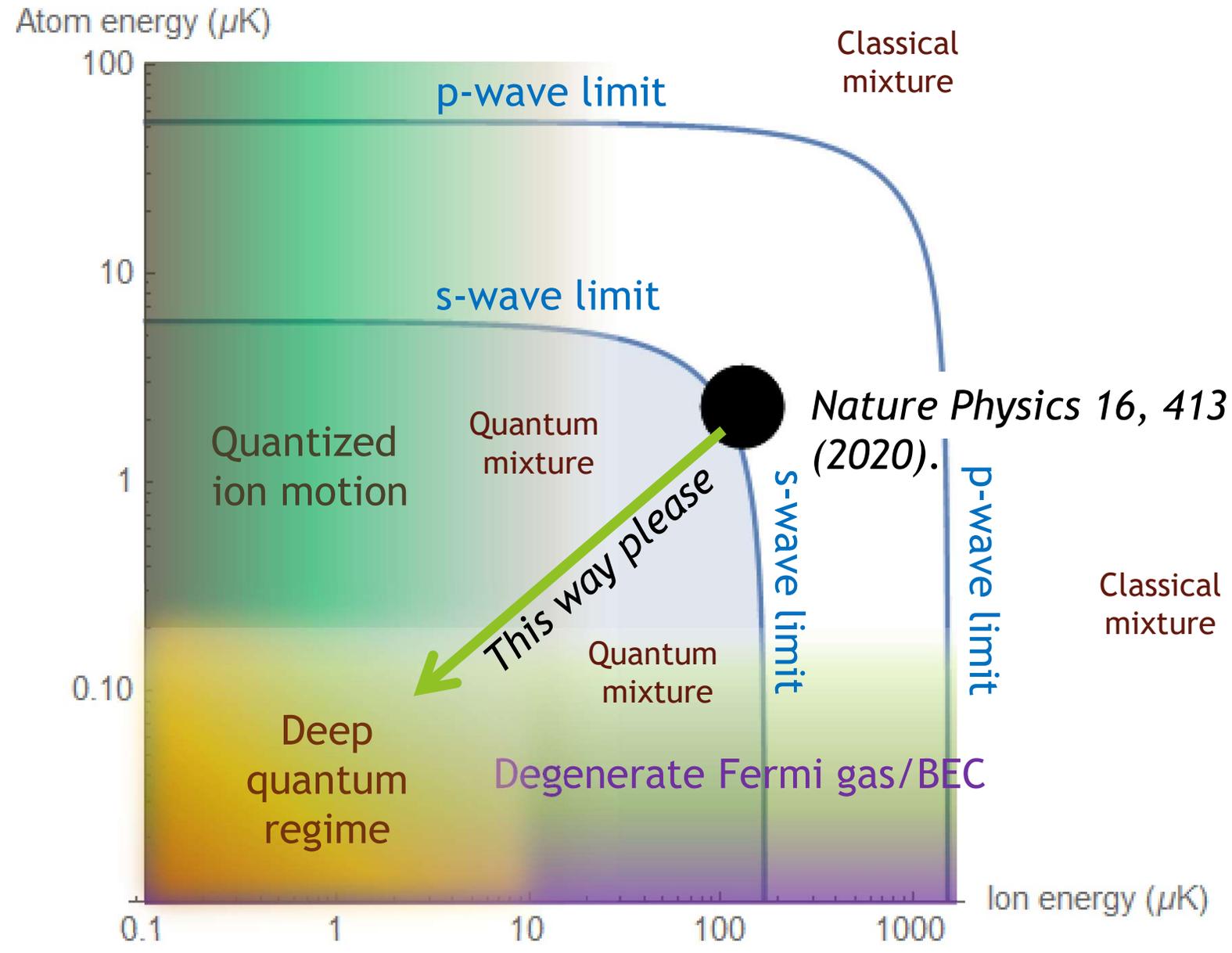
$$E_{\text{col}} = 1.15(23) \times E_s$$


Coldest results

Crossover into quantum regime, can we get colder?

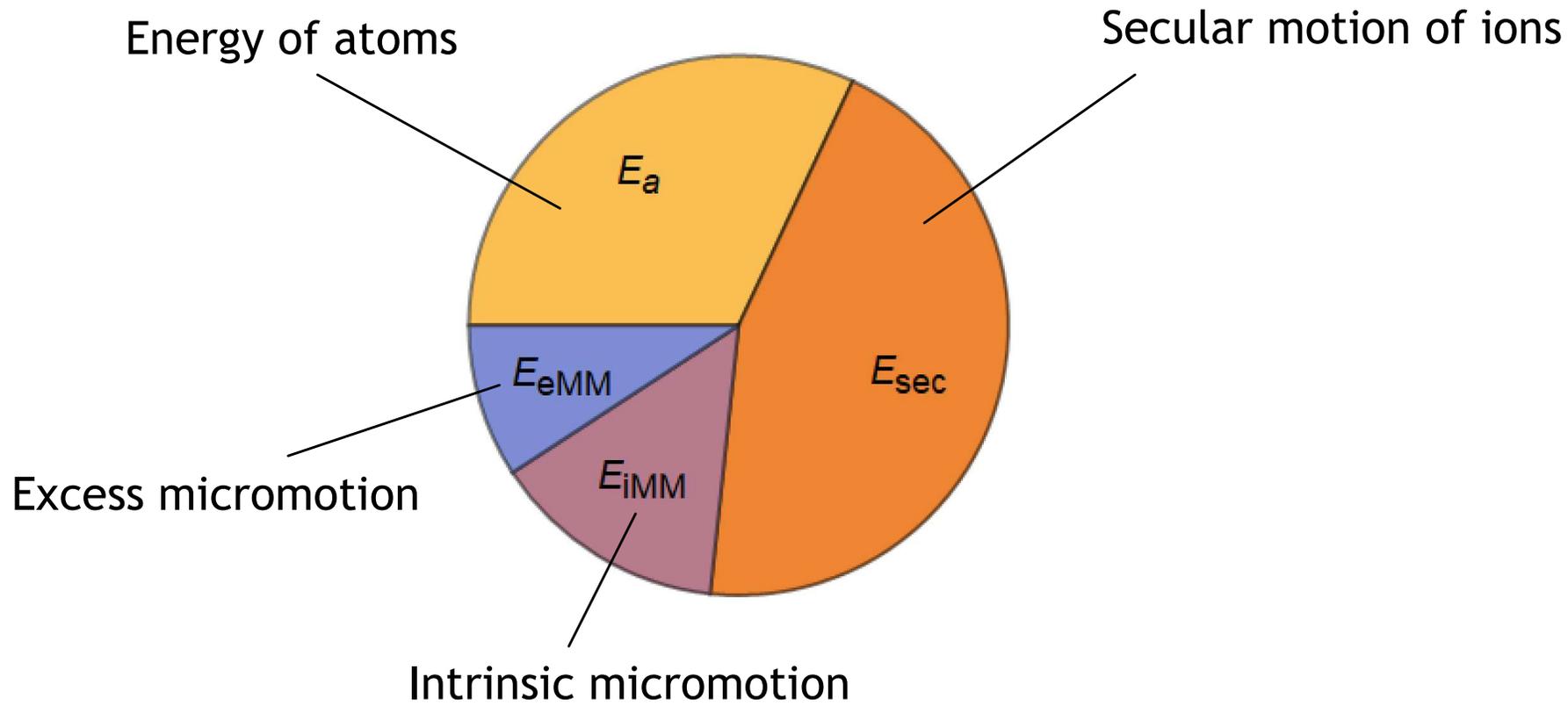
T. Feldker et al., [Nature Physics, 16, 413-416 \(2020\)](#).

# Prospects for getting colder



# Prospects for getting colder

## Collision energy

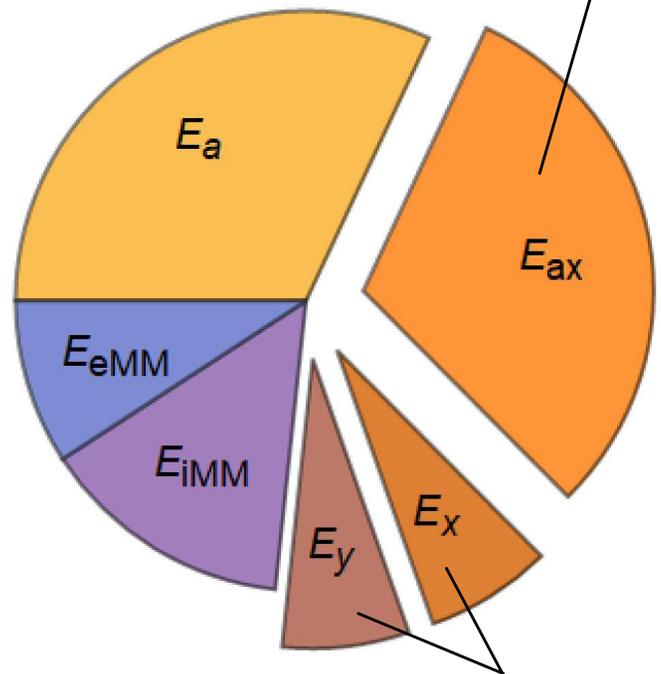


Experimentally determined collision energy

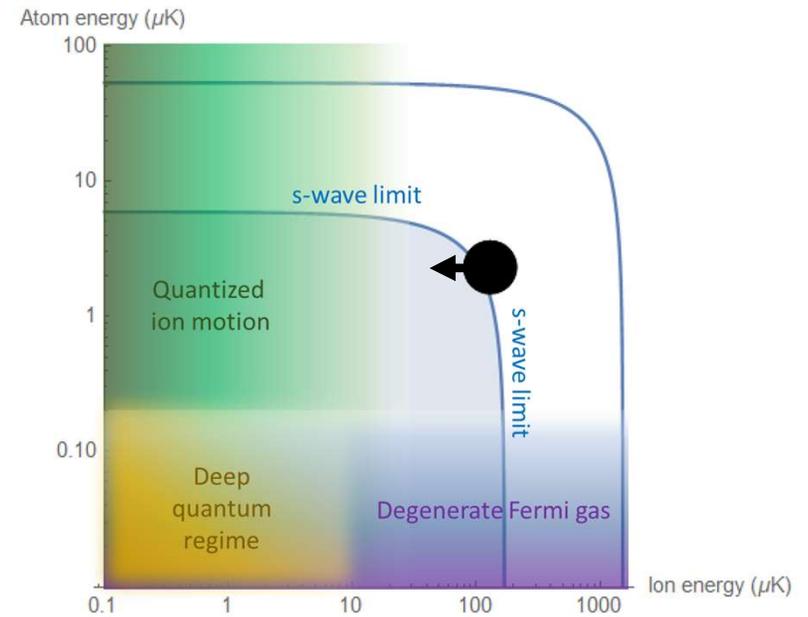
# Prospects for getting colder

Collision energy

Axial motion of ions  
 → Background heating  
 ~ 200  $\mu\text{K/s}$



Radial motion of ions  
 → Background heating  
 ~ 85  $\mu\text{K/s}$

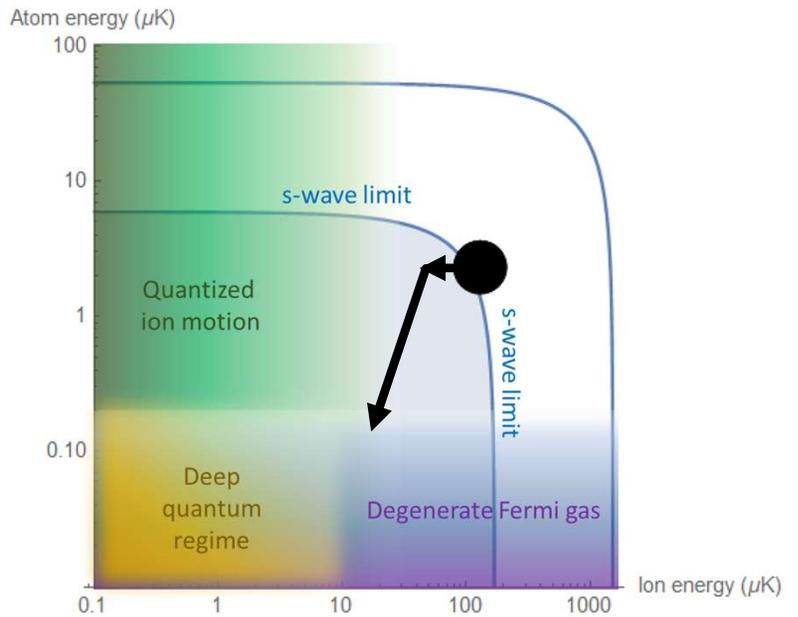
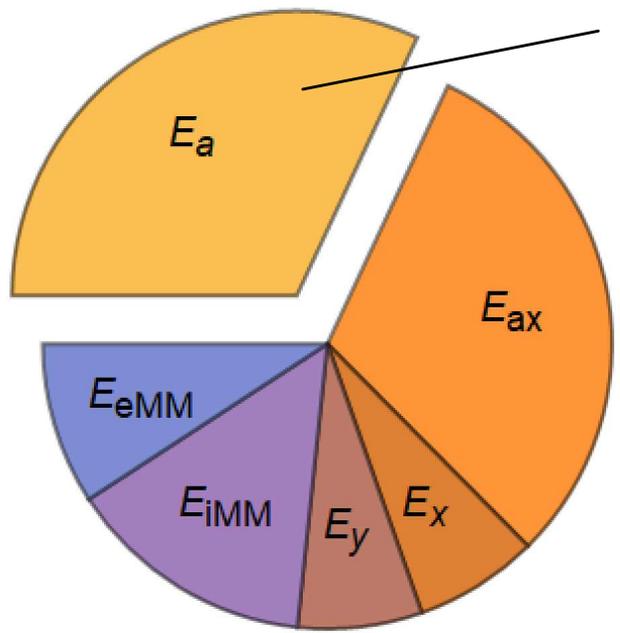


- Denser gas eliminates background heating limits
  - Faster repetition of experiments reduces overestimation
- } factor 2?

# Prospects for getting colder

Collision energy

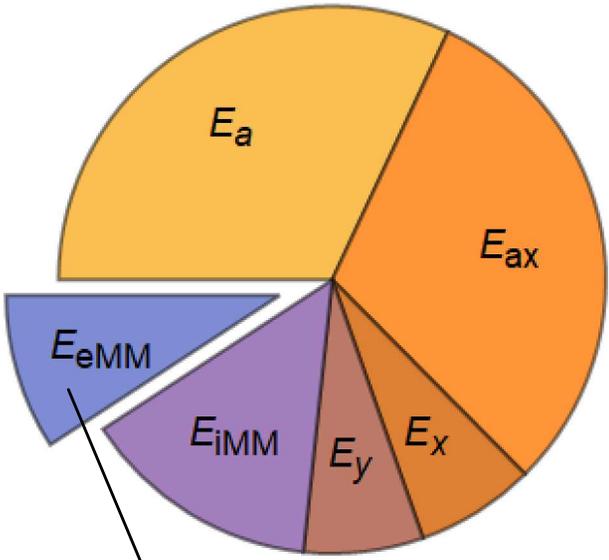
Make colder atoms!  
 → More efficient evaporation  
 → Need denser gas



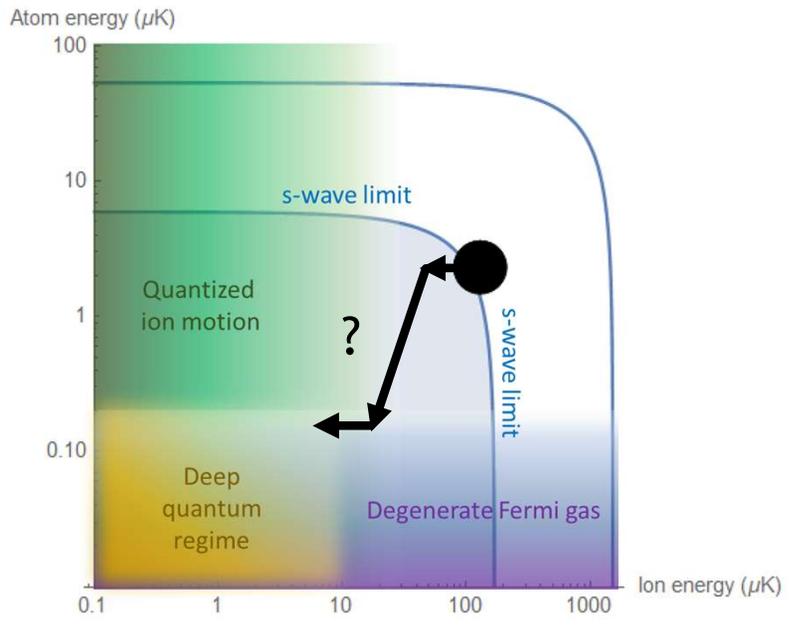
→ Colder gas eliminates atomic energy → another factor of 2?

# Prospects for getting colder

Collision energy



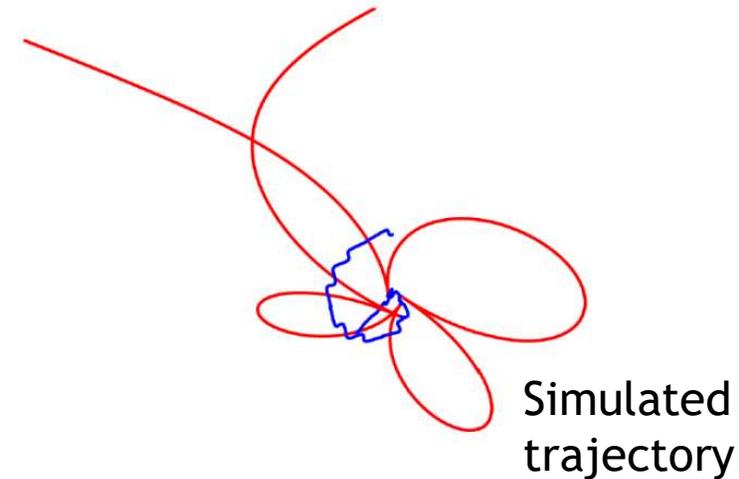
Better excess micromotion compensation



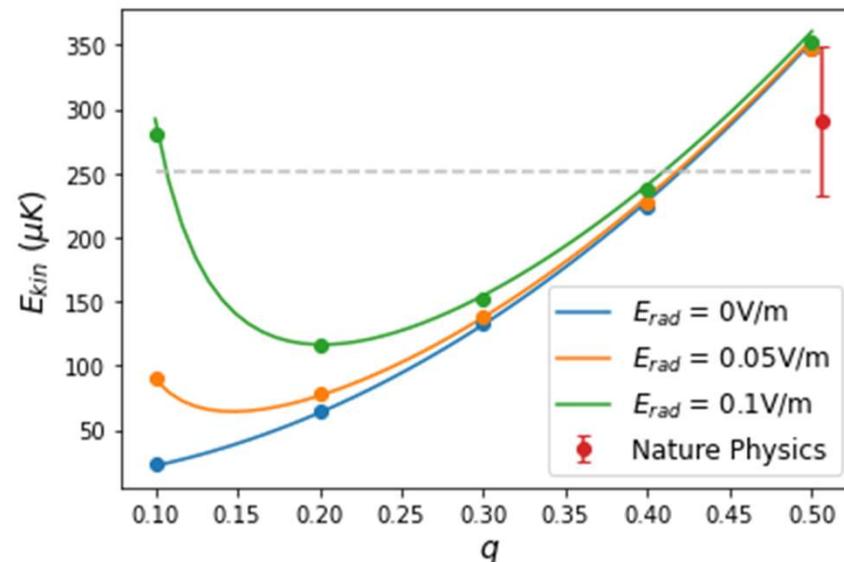
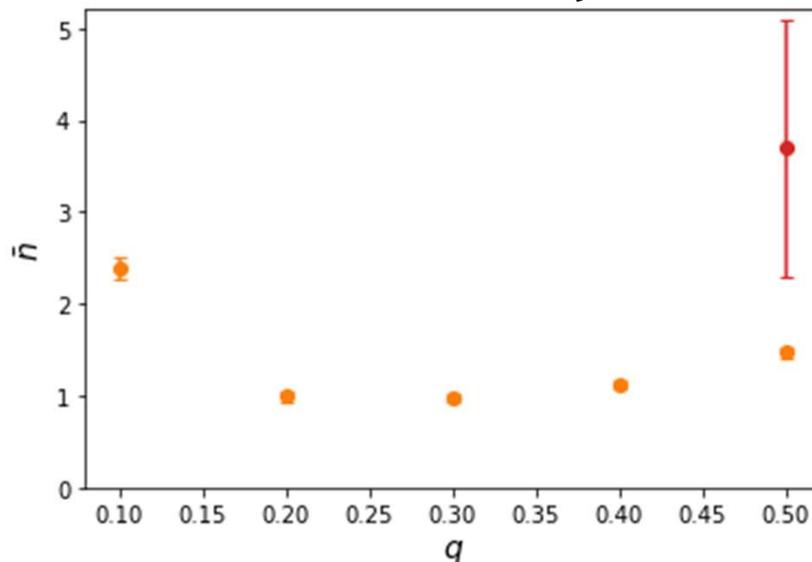
→ Simulations suggest another factor of 2 within reach

# Simulations: Parameter optimization of trap voltage

- ▶ Optimal  $q$  depends on excess micromotion
  - ▶ Measure micromotion -> select  $q$
- ▶ Can feasibly decrease ion temperature by factor 2
- ▶ Can also decrease  $\bar{n}$  through choice of  $q$



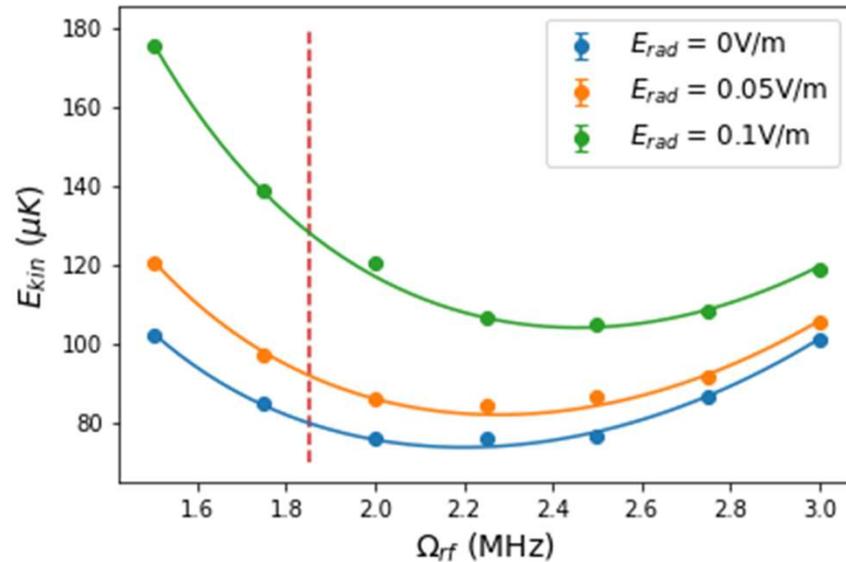
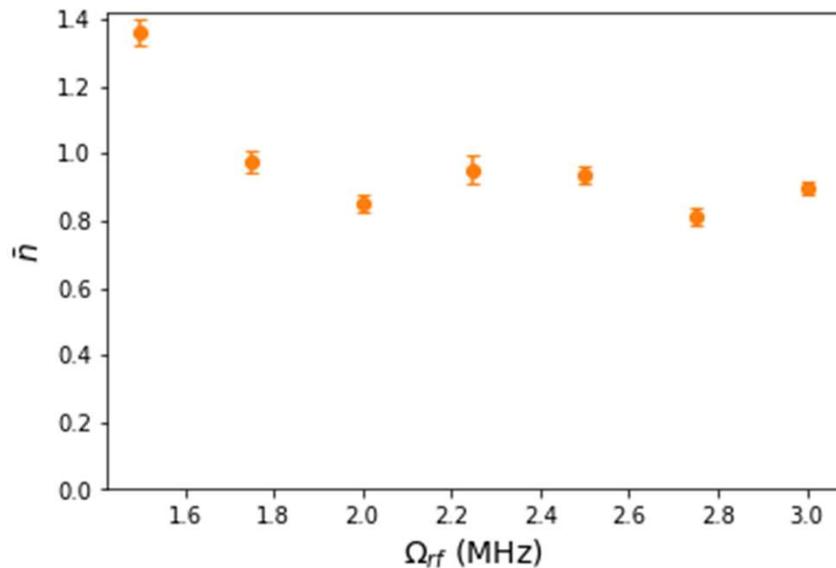
## Classical molecular dynamics simulations



$$T_a = 2\mu K$$
$$\Omega_{rf} = 2MHz$$

# Simulations: Parameter optimization of Paul trap drive freq.

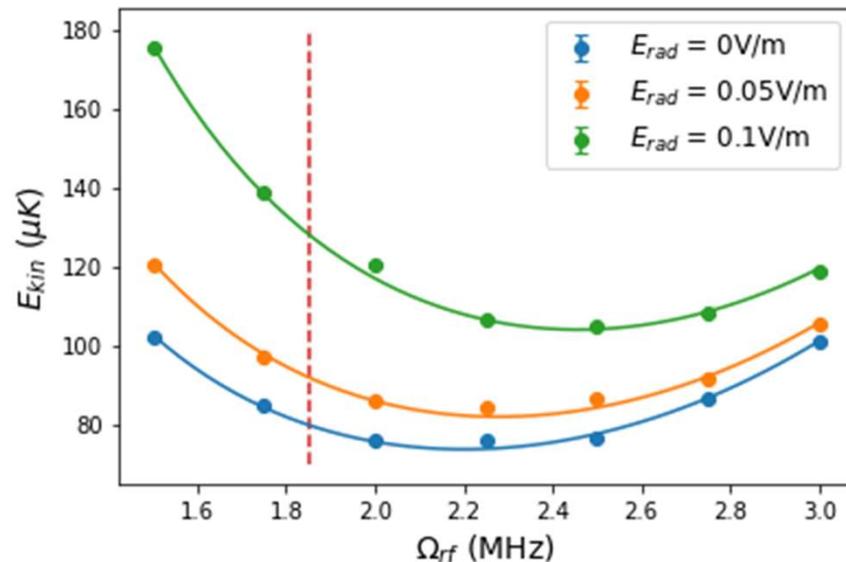
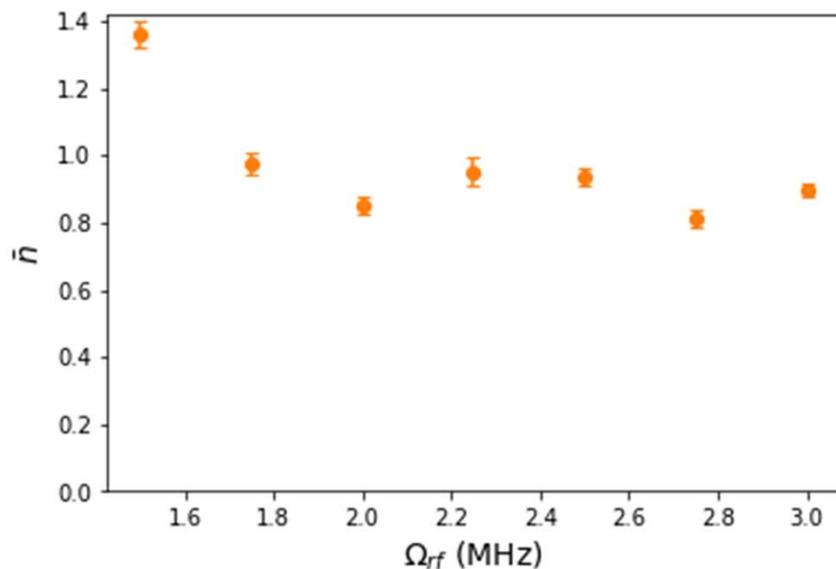
- Optimal  $\Omega_{rf}$  also depends on excess micromotion



$T_a = 2\mu\text{K}$   
 $q = 0.219$

# Simulations: Parameter optimization of Paul trap drive freq.

- Optimal  $\Omega_{rf}$  also depends on excess micromotion



- The simulations show that  $\bar{n} \sim 1$  are possible:  
Buffer gas cooling is competitive w.r.t. sub-Doppler cooling?  
→ What will be the role of quantum effects?

# Interactions in quantum regime

Type of motion	$E_{\text{kin}}/k_{\text{B}}(\mu\text{K})$	$E_{\text{col}}/k_{\text{B}}(\mu\text{K})$
Radial secular ion	$2 \times 21(9)$	1.4(0.6)
Intrinsic micromotion	$2 \times 21(9)$	1.4(0.6)
Axial secular ion	65(18)	2.2(0.4)
Excess micromotion	44(13)	1.5(0.4)
<b>Total ion energy</b>	<b>193(42)</b>	<b>6.6(1.4)</b>
Atom temperature	$3/2 \times 2.3(0.4)$	3.3(0.6)
<b>Total collision energy</b>	—	<b>9.9(2.0)</b>

Measurement of all types of motion

$$E_{\text{col}} = 1.15(23) \times E_{\text{s}}$$

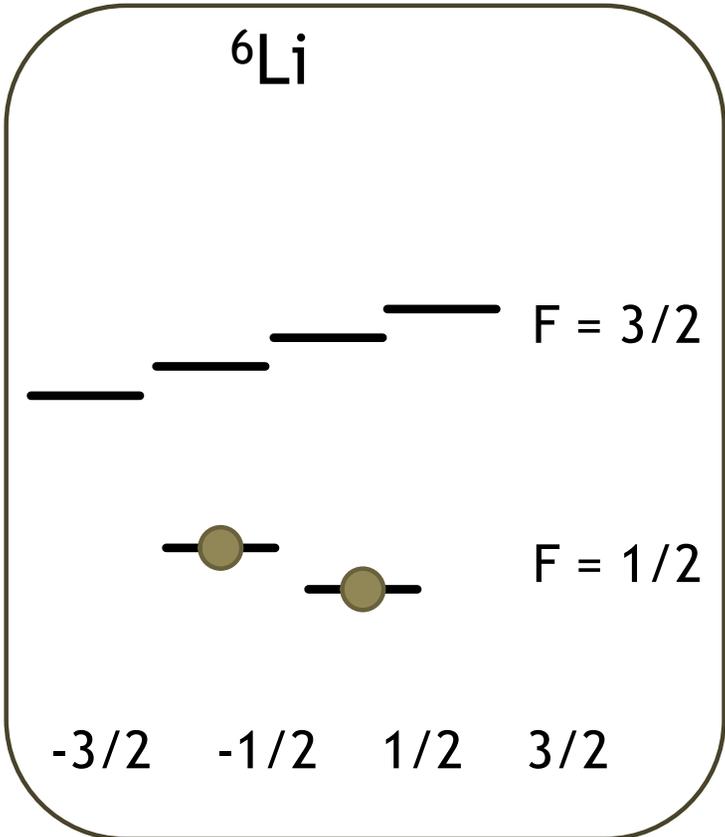
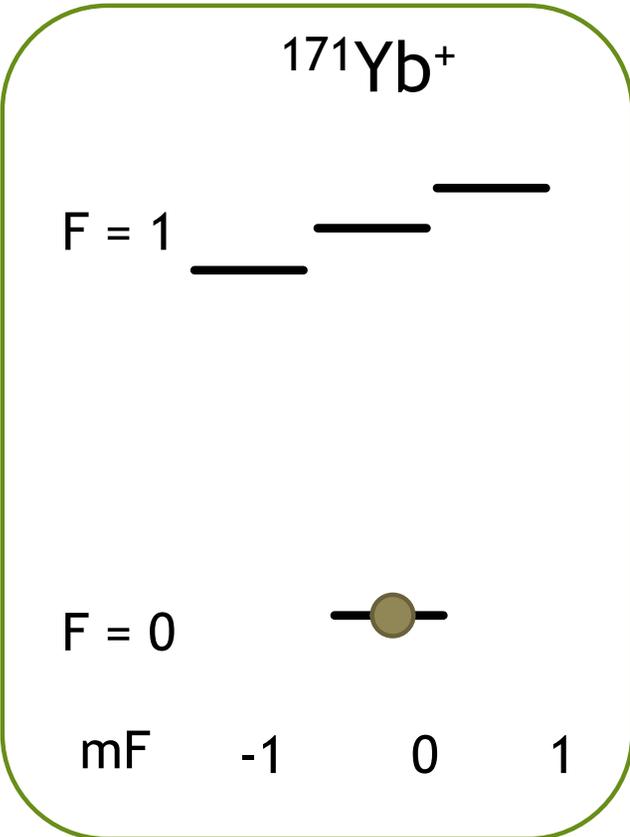

Coldest results

So can we measure something ‘quantum’ about it?

T. Feldker et al., [Nature Physics, 16, 413-416 \(2020\)](#).

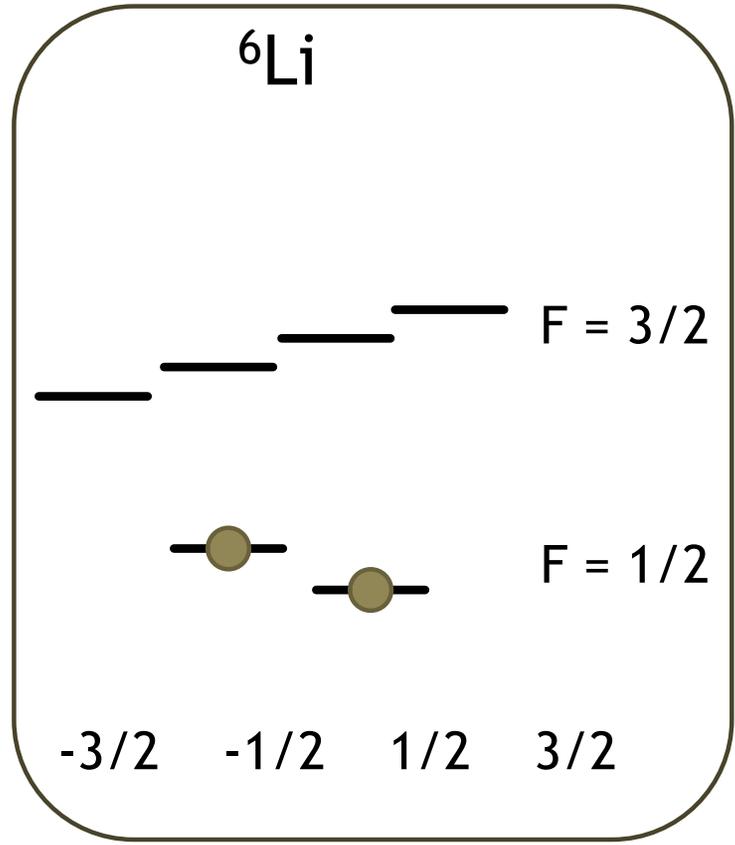
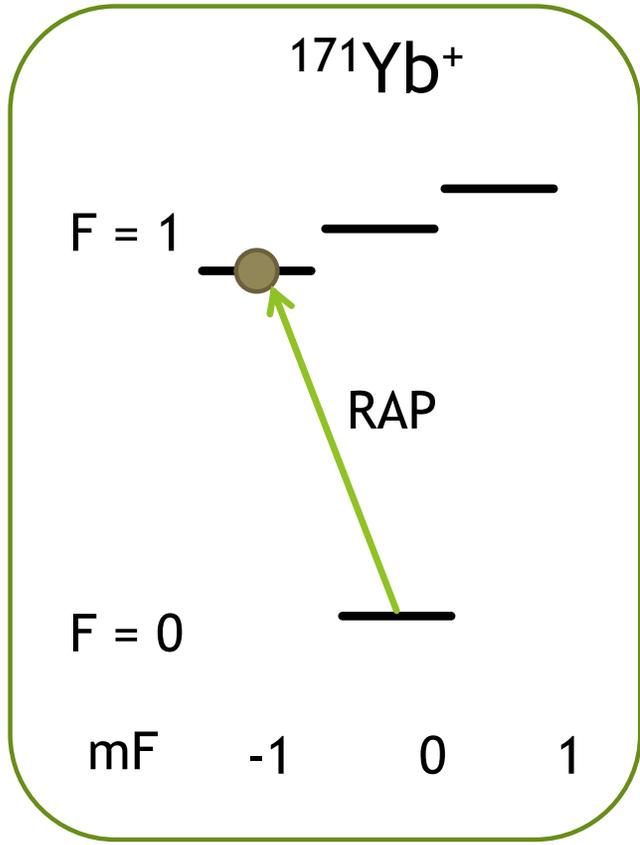
# Quantum effects in atom-ion collisions?

- Spin exchange rates
- Prepare spin in ion after buffer gas cooling, detect spin flip



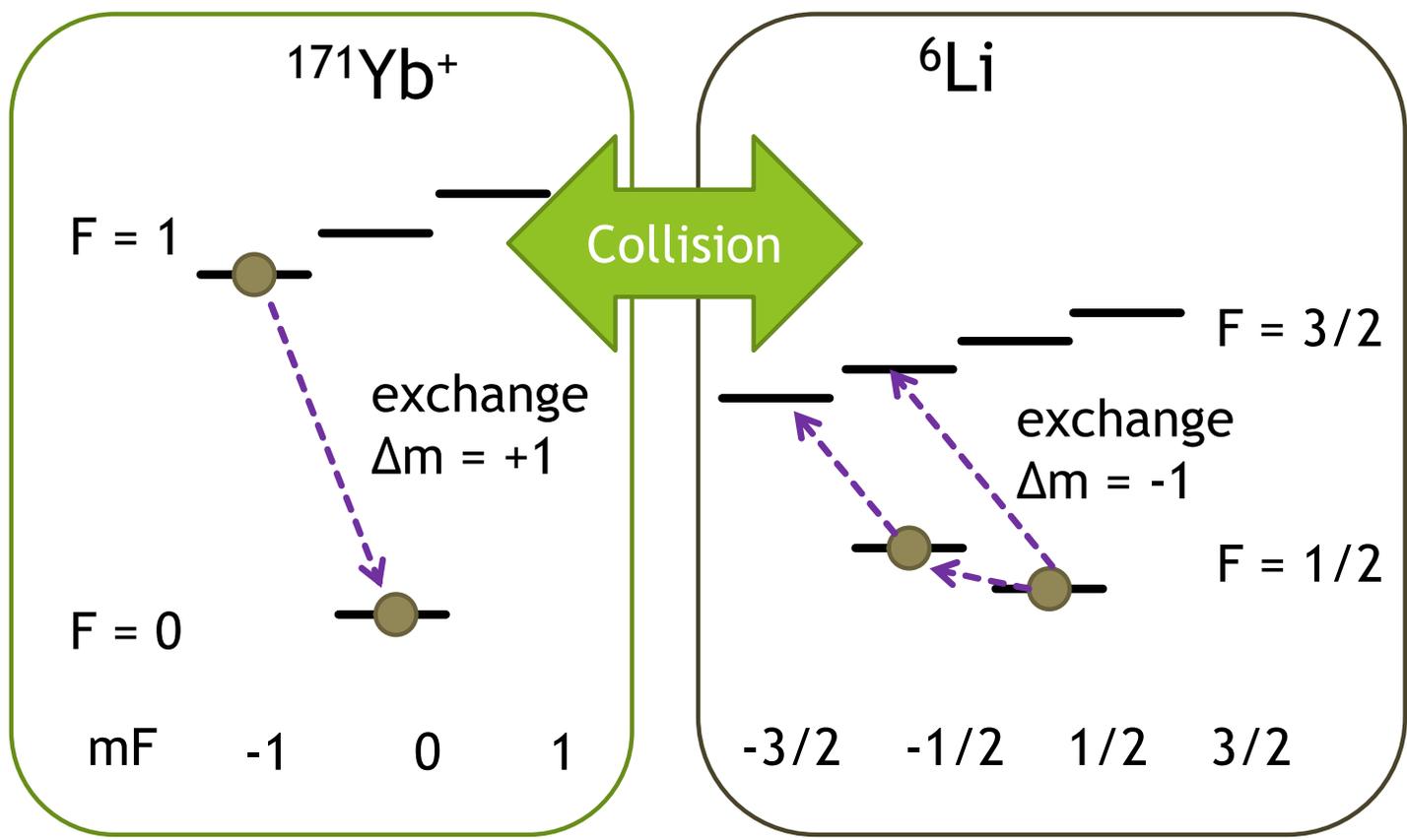
# Quantum effects in atom-ion collisions?

- Spin exchange rates
- Prepare spin in ion after buffer gas cooling, detect spin flip



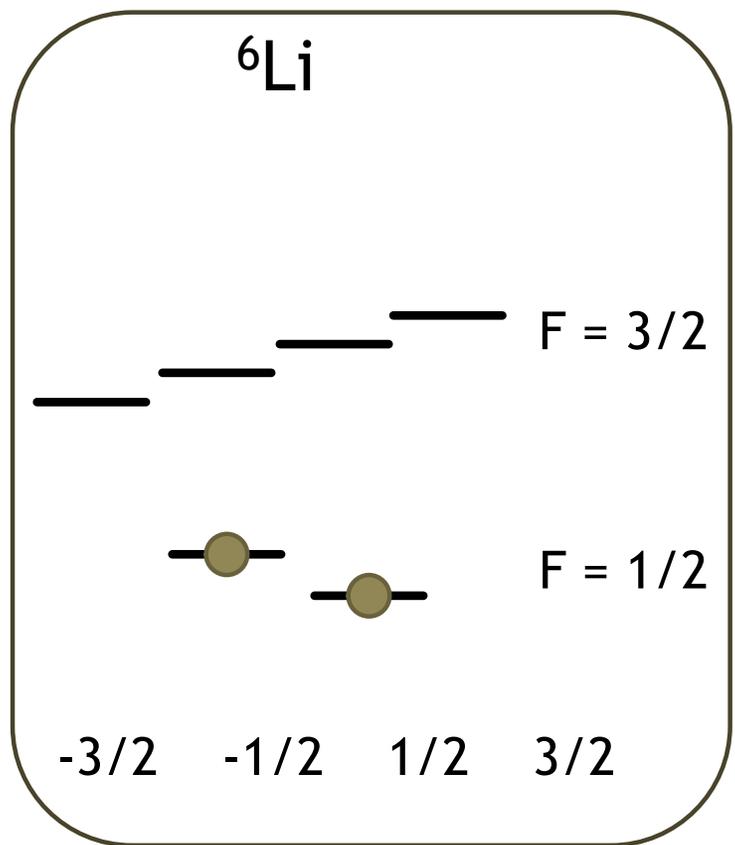
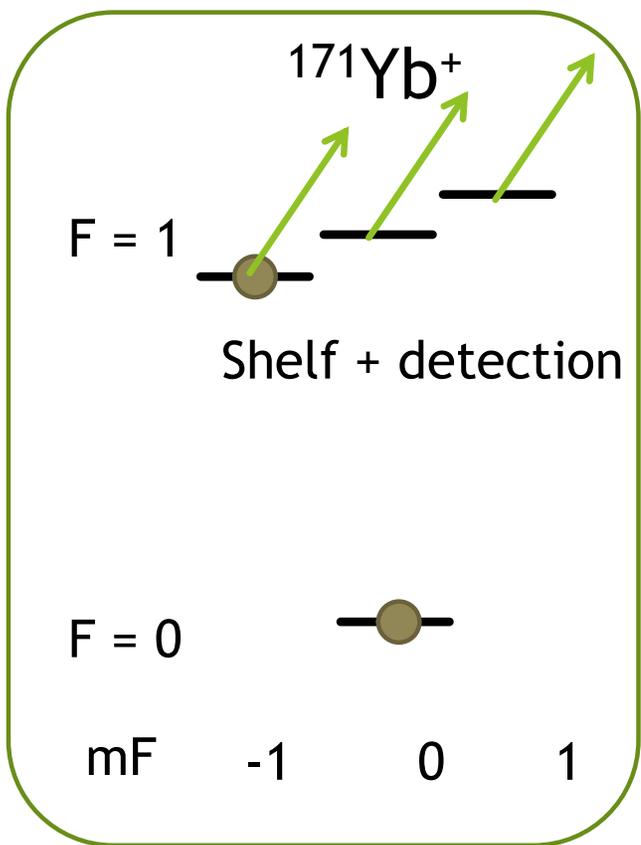
# Quantum effects in atom-ion collisions?

- Spin exchange rates
- Prepare spin in ion after buffer gas cooling, detect spin flip



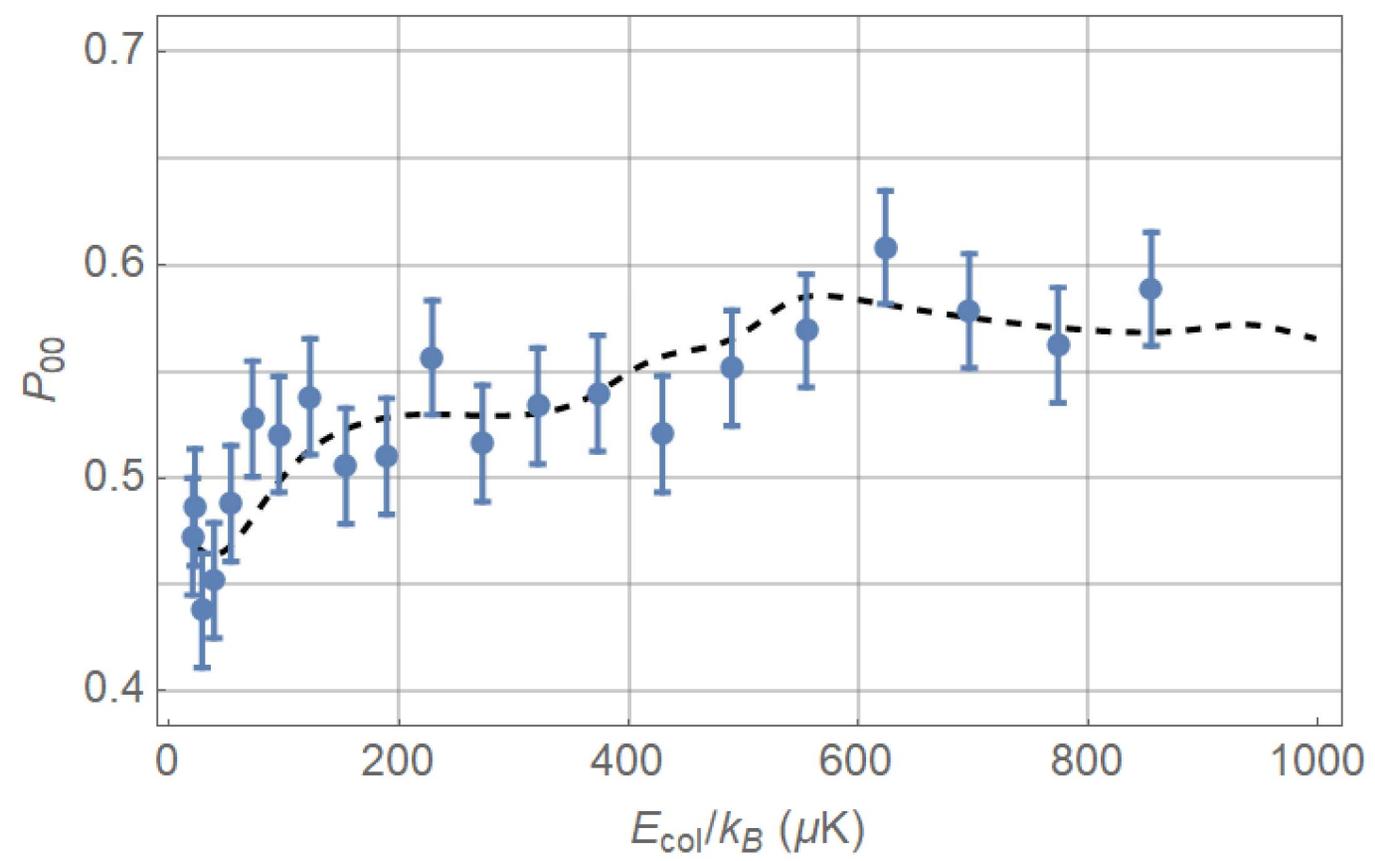
# Quantum effects in atom-ion collisions?

- Spin exchange rates
- Prepare spin in ion after buffer gas cooling, detect spin flip



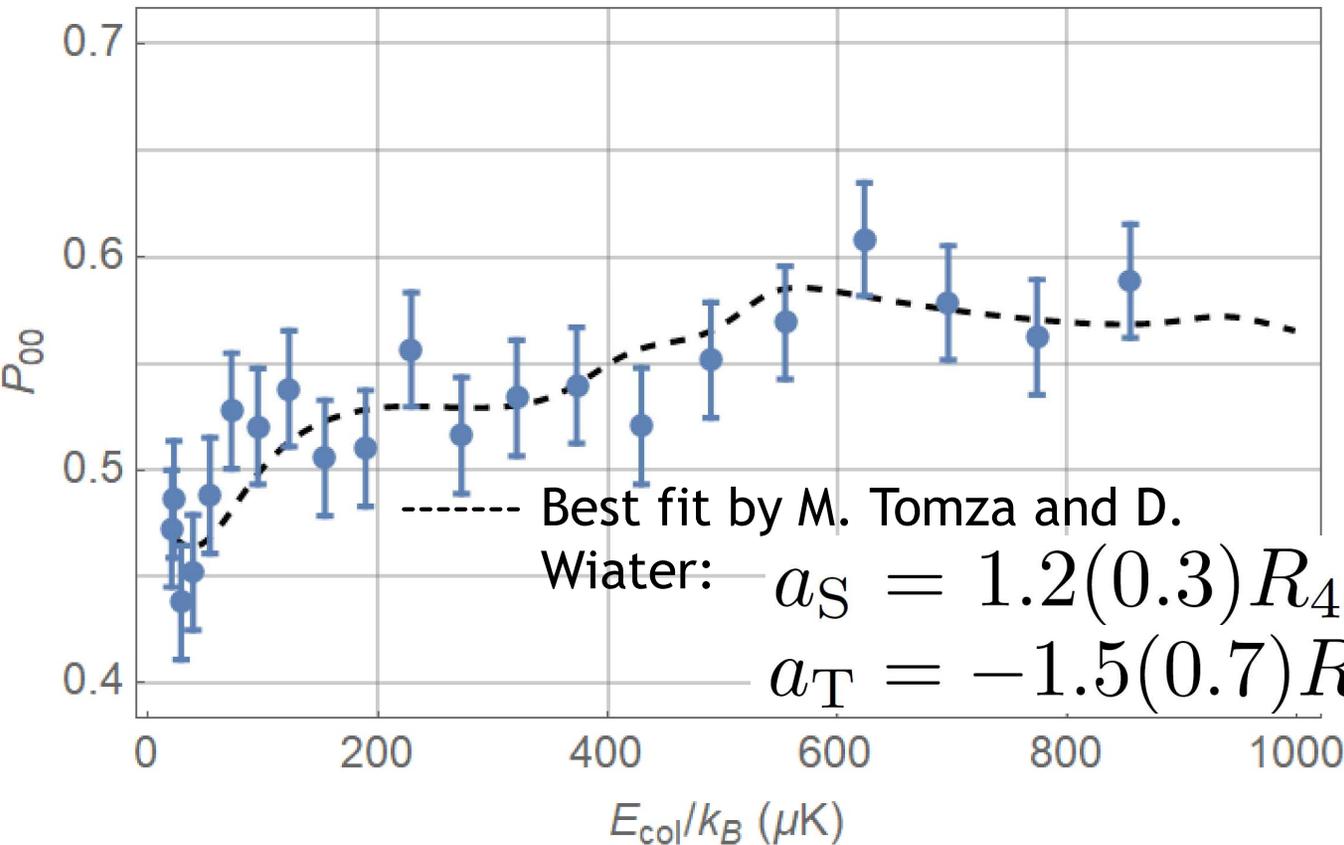
# Quantum effects in atom-ion collisions?

→ Scan collision energy via radial excess MM



# Quantum effects in atom-ion collisions?

→ Scan collision energy via radial excess MM

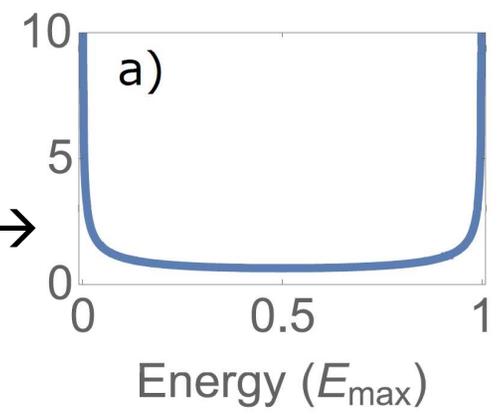
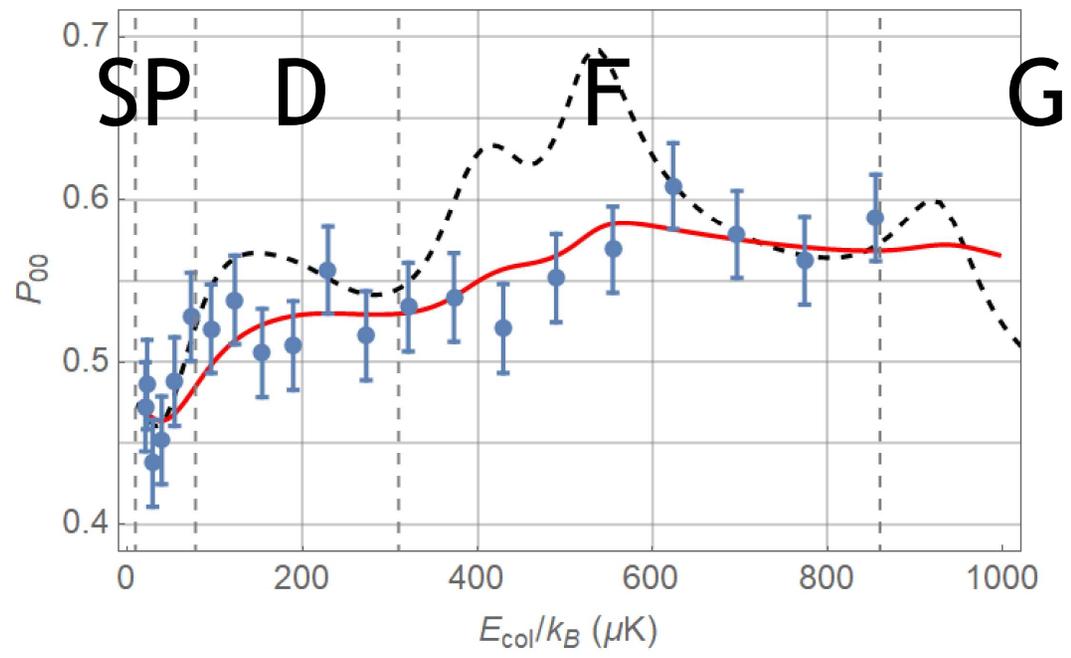
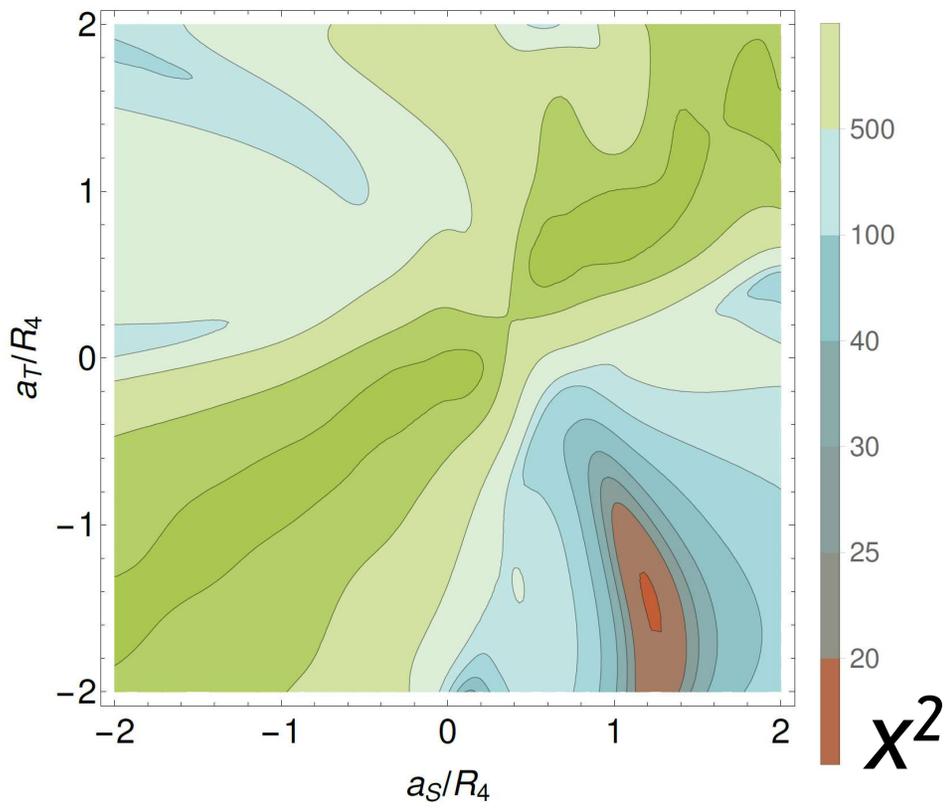


$$\left. \begin{aligned} a_S &= 1.2(0.3)R_4 \\ a_T &= -1.5(0.7)R_4 \end{aligned} \right\} \text{Scattering lengths}$$

$$R_4 = 1320 a_0$$

# Estimates on scattering lengths

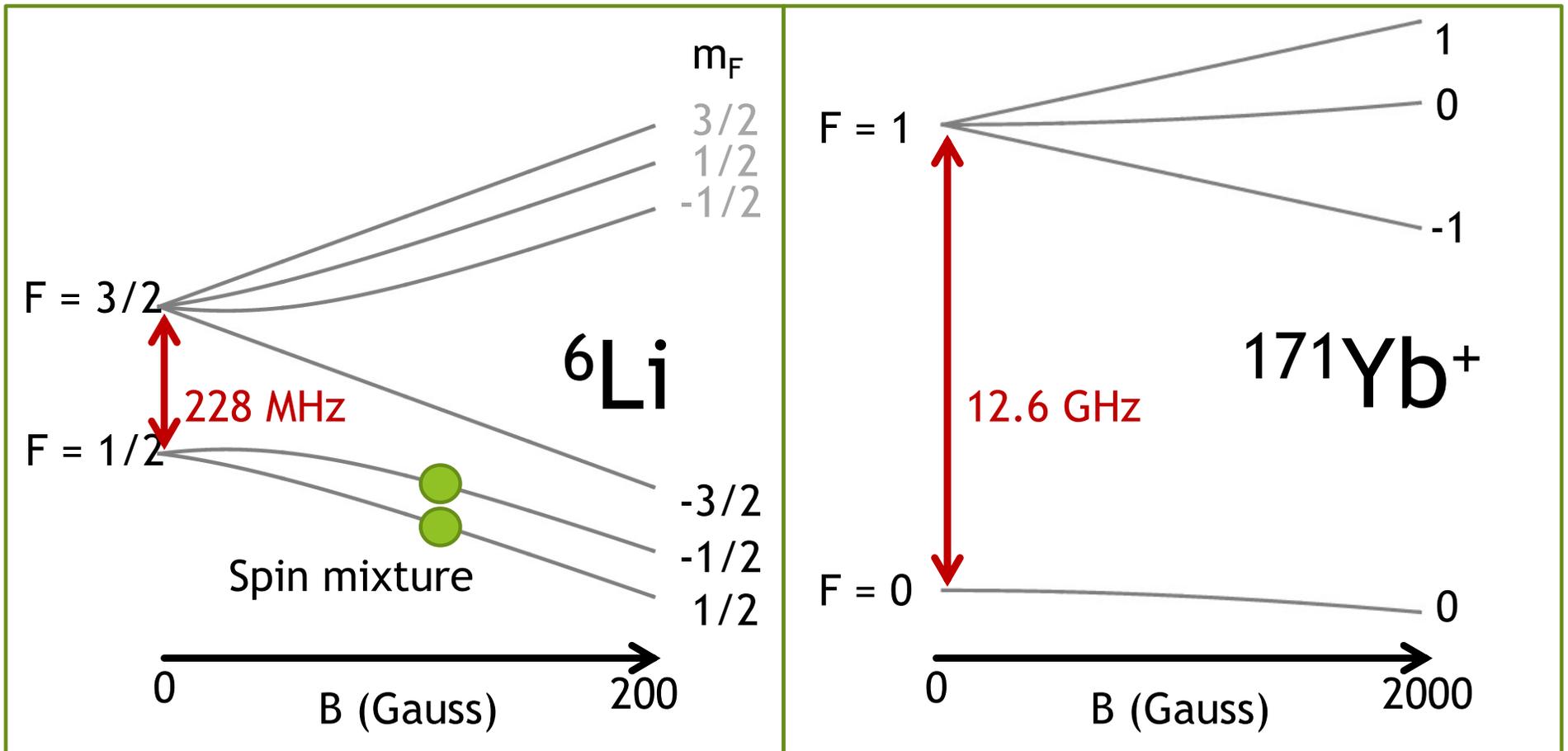
Work by M. Tomza and D. Wiater



Energy distribution →

Note: almost every collision results in spin-exchange!

# Candidates for Feshbach in Yb<sup>+</sup>/<sup>6</sup>Li



**Spin-exchange:**  $|1, -1\rangle_{ion} |1/2, 1/2\rangle_{atom} \longleftrightarrow |1, 0\rangle_{ion} |1/2, -1/2\rangle_{atom}$   
 $B < 15 \text{ G}, \nu = -1 \quad \rightarrow \quad \text{low field, strong resonance}$

**Motion (<sup>174</sup>Yb<sup>+</sup>):**  $|1/2, -1/2\rangle_{ion} |1/2, 1/2\rangle_{atom} \longleftrightarrow |1/2, 1/2\rangle_{ion} |1/2, -1/2\rangle_{atom}$   
 $B < 10 \text{ G}, \nu = -1 \text{ or } B = 10\text{-}50 \text{ G for } \nu = -2$



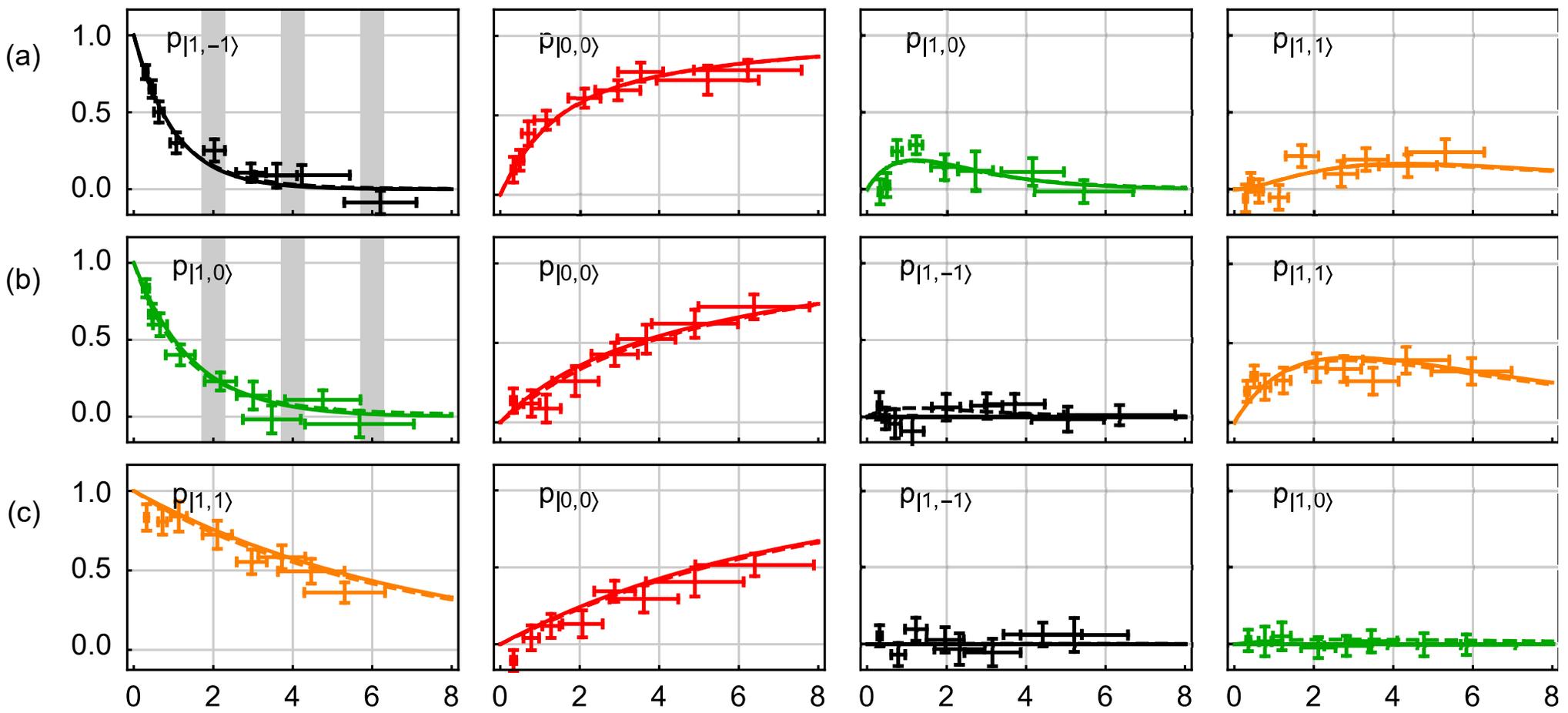
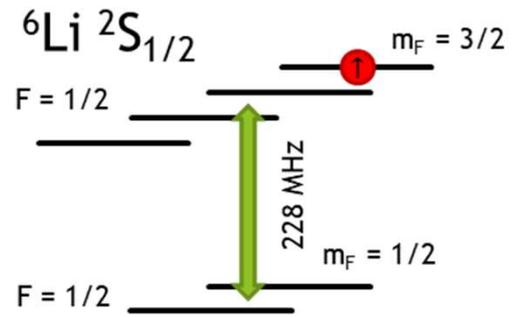
# Spin dynamics in atom-ion mixtures

→ Things are a bit different than in neutral mixtures....

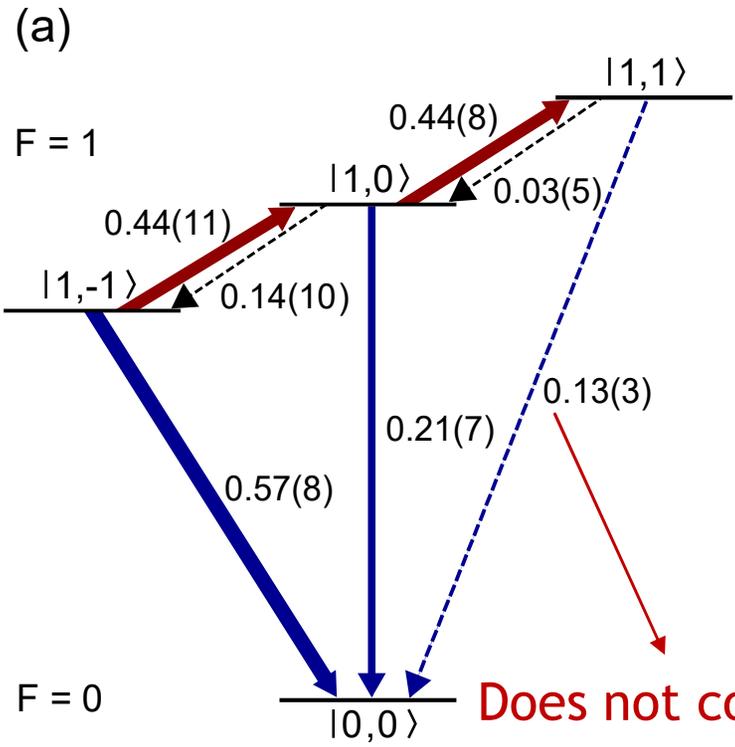
From: L. Ratschbacher, C. Sias, L. Carcagni, J. M. Silver, C. Zipkes, and M. Köhl  
Phys. Rev. Lett. 110, 160402 (2013).

# Spin dynamics of $^{171}\text{Yb}^+$

These results are for 600  $\mu\text{K}$  atoms in the  $\left| \begin{smallmatrix} 3 & 3 \\ 2 & 2 \end{smallmatrix} \right\rangle$  stretched state

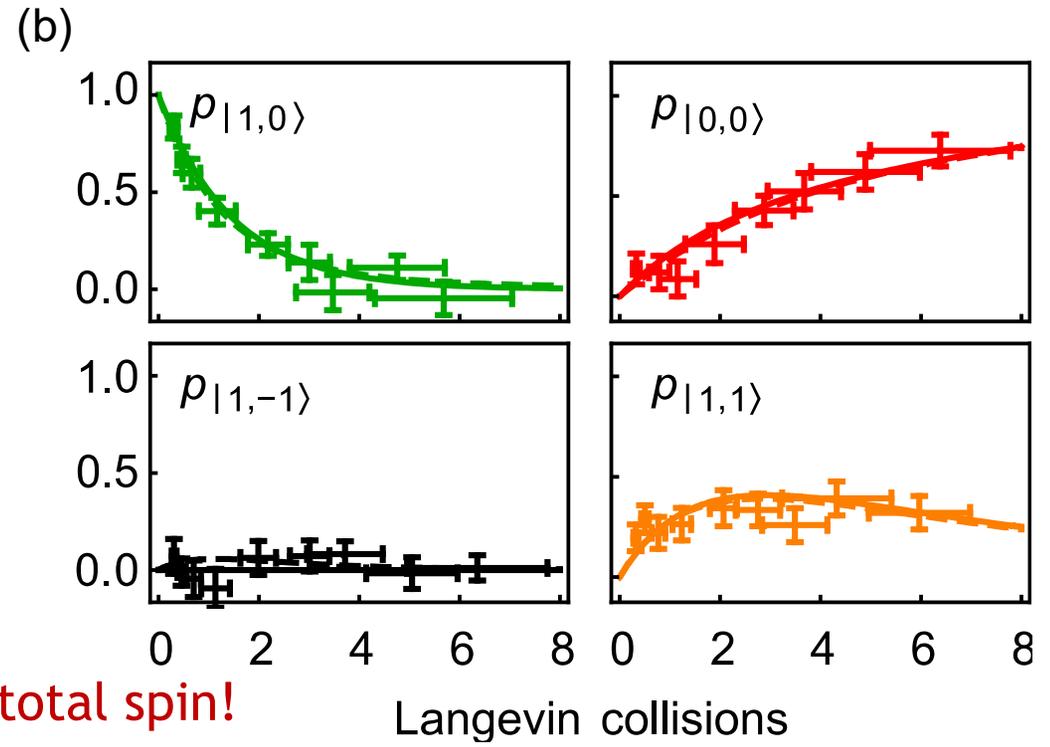


# Spin dynamics of $^{171}\text{Yb}^+$



Does not conserve total spin!

$^{171}\text{Yb}^+ \ ^2S_{1/2}$  hyperfine ground states and transition rates in units of the Langevin rate

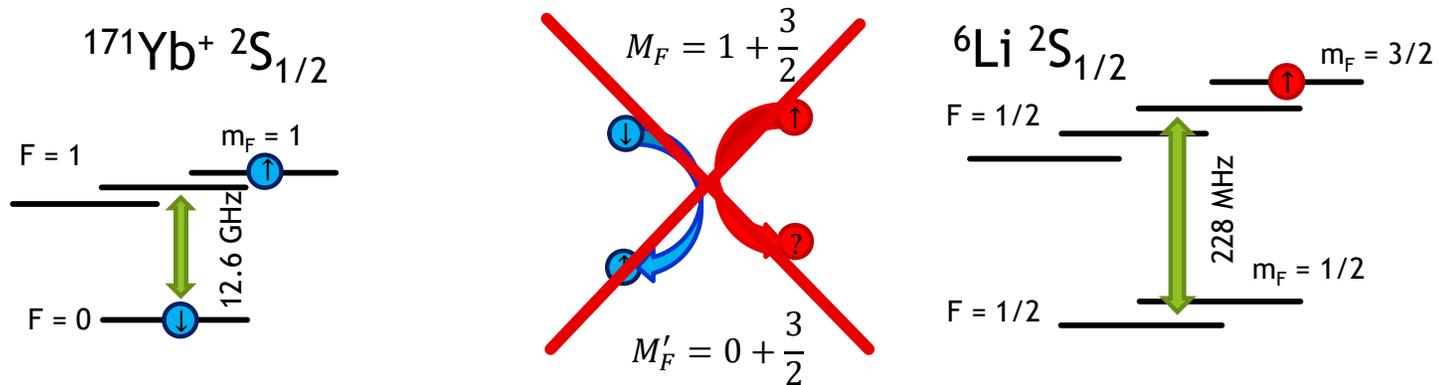


Population dynamics for starting in the  $^{171}\text{Yb}^+ \ ^2S_{1/2} \ |1,0\rangle$  state

- ▶ Almost every Langevin collision flips the Spin when in  $|1, -1\rangle$

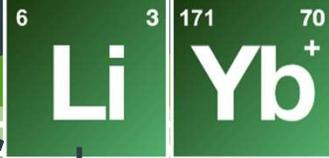
# Spin exchange and relaxation

- Hyperfine qubit in  $^{171}\text{Yb}^+ + {}^6\text{Li}$ :



These states should be protected by spin and energy conservation

→ But they are not, what is happening?



# Previous Work on Rb-Yb<sup>+</sup> and Rb-Sr<sup>+</sup>

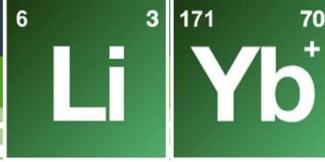
L. Ratschbacher et al., Phys. Rev. Lett. **110**, 160402 (2013)

T. Sikorski et al., Nature Communications. **9**, 920 (2018)

Rb in stretched state  $|1,1\rangle_a$   
Yb ion in either  $|^{1/2}, ^{1/2}\rangle_i$  or  $|^{1/2}, -^{1/2}\rangle_i$

Yb<sup>+</sup> is in a mixed state after interaction  
→ Spin relaxation dominates exchange  
→ total spin is not conserved!

Similar results in Rb-Sr<sup>+</sup>: Exchange is 5 times faster than relaxation



# Mechanism

Second order spin-orbit coupling T. V. Tscherbul et al., Phys. Rev. Lett. **117**, 143201 (2016)

Causes effective spin-spin interaction  
Made worse by crossing of potential lines and heavy ions  
→ qubits in atomic gases seems not sustainable

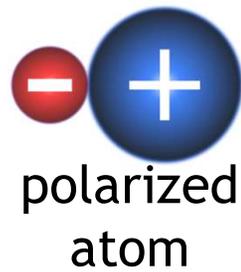
# Controlling the interactions between atoms and ions

- ▶ Feshbach resonances
- ▶ Rydberg dressing

↑ The group of Tobias Schaetz observed Feshbach resonances between  ${}^6\text{Li}$  and  $\text{Ba}^+$  Nature 600, 429-433 (2021).

# Controlling the interactions

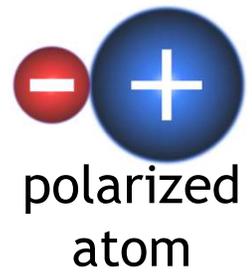
→ Interaction between atoms and ion proportional to polarizability



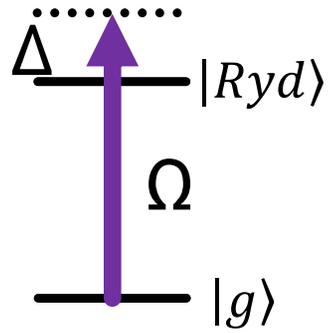
$$V_{a,i}(r) = -\frac{C_4}{2 r^4}$$

# Controlling the interactions

→ Interaction between atoms and ion proportional to polarizability



$$V_{a,i}(r) = -\frac{C_4}{2 r^4}$$

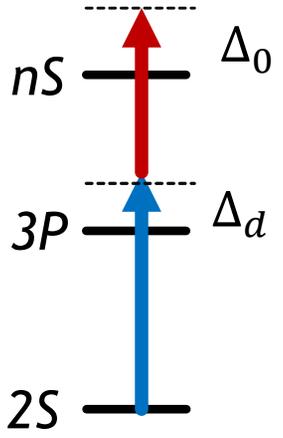


**Rydberg dressing: Polarizability scales as  $n^7$**   
 Can be many orders of magnitude larger even for weak dressing

# Rydberg dressing and ions

→ Weakly couple atom to Rydberg state → increased range and strength of potential, but not limited by Rydberg lifetime

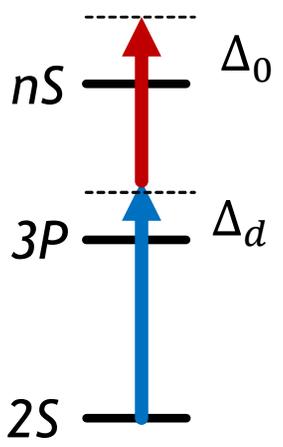
$$H_{3-level} = \begin{pmatrix} 0 & \hbar\Omega_d(\mathbf{r}_a) & \hbar\Omega \\ \hbar\Omega_d(\mathbf{r}_a) & -\hbar\Delta_d & 0 \\ \hbar\Omega & 0 & -\hbar\Delta_0 - \frac{C_4^{|R\rangle}}{R^4} \end{pmatrix}$$



# Rydberg dressing and ions

→ Weakly couple atom to Rydberg state → increased range and strength of potential, but not limited by Rydberg lifetime

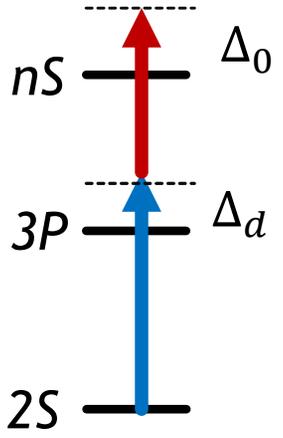
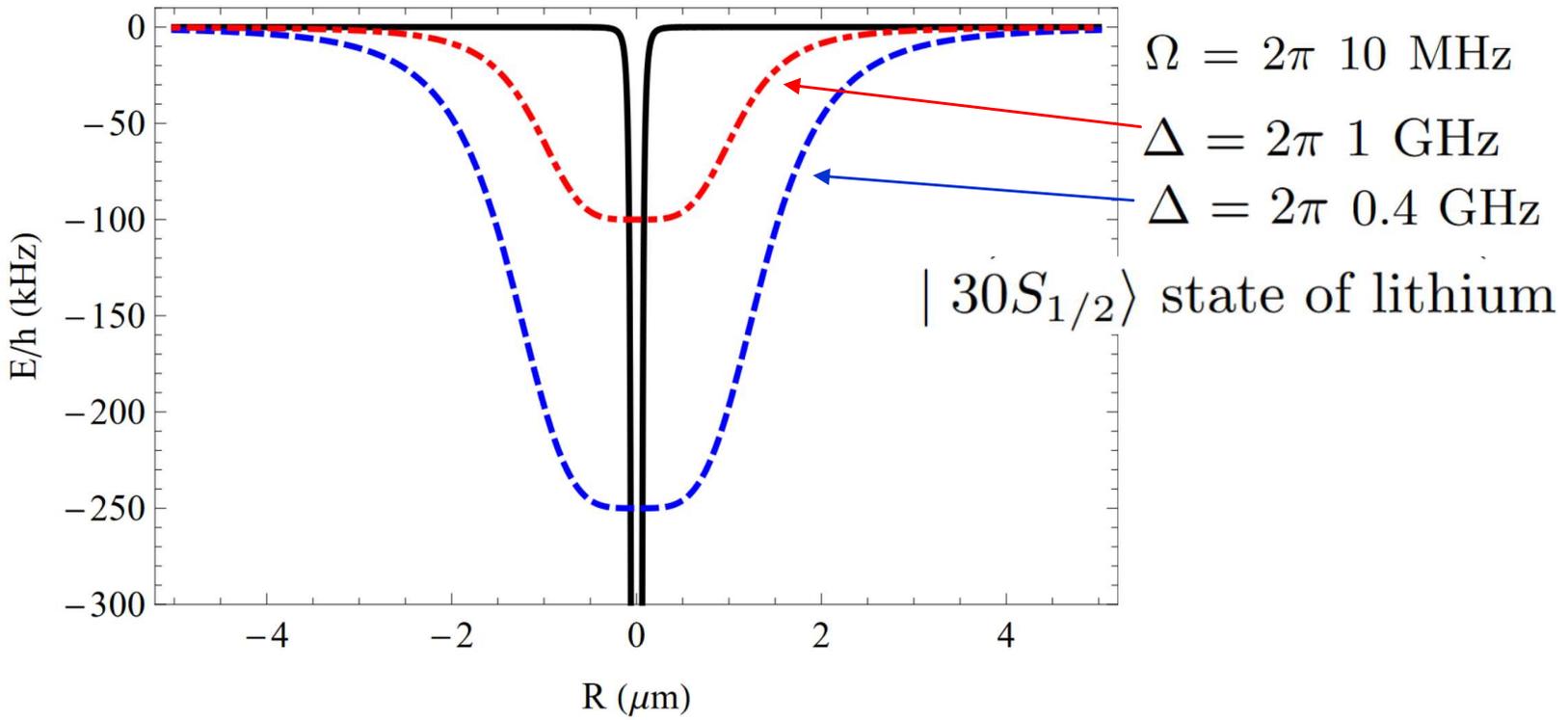
$$H_{3-level} = \begin{pmatrix} 0 & \hbar\Omega_d(\mathbf{r}_a) & \hbar\Omega \\ \hbar\Omega_d(\mathbf{r}_a) & -\hbar\Delta_d & 0 \\ \hbar\Omega & 0 & -\hbar\Delta_0 - \frac{C_4^{|R|}}{R^4} \end{pmatrix}$$



Neglect ground state atom-ion interaction

Rydberg polarizability

# Rydberg dressing and ions



$$V(R) = -\frac{AR_w^4}{R^4 + R_w^4} \quad \leftarrow \text{Adiabatic potential}$$

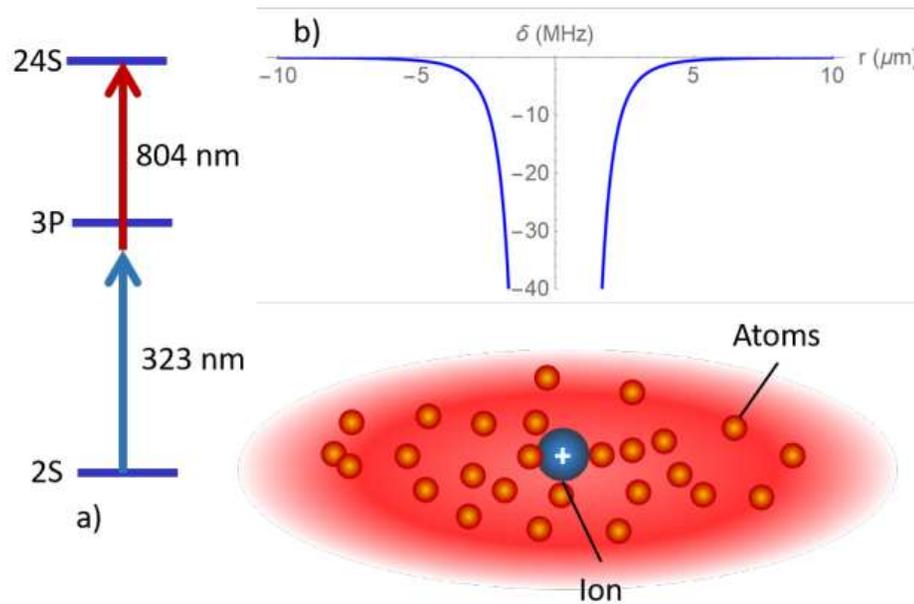
$$A = \hbar\Omega^2 / \Delta_0$$

$$R_w = (C_4^{|R\rangle} / \hbar\Delta_0)^{1/4}$$

PRA 94, 013420 (2016)

# Let's try it: start with Rydberg excitation

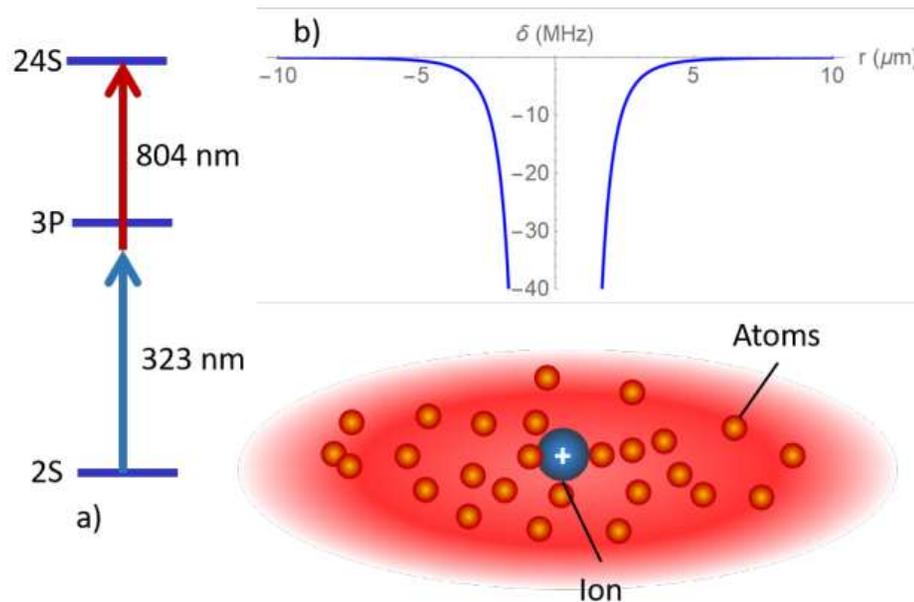
- Two photon Rydberg excitation to  $24S_{1/2}$
- Image atoms and ions



Polarizability of  $24S$  state is about  $10^8$  times larger than for the ground state

# Exciting Rydbergs

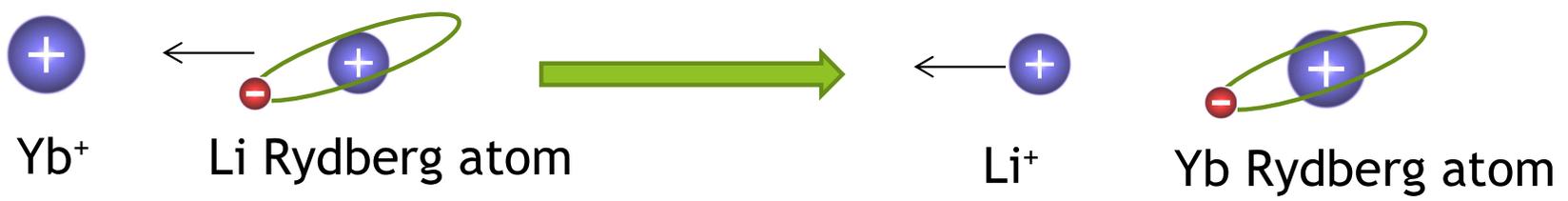
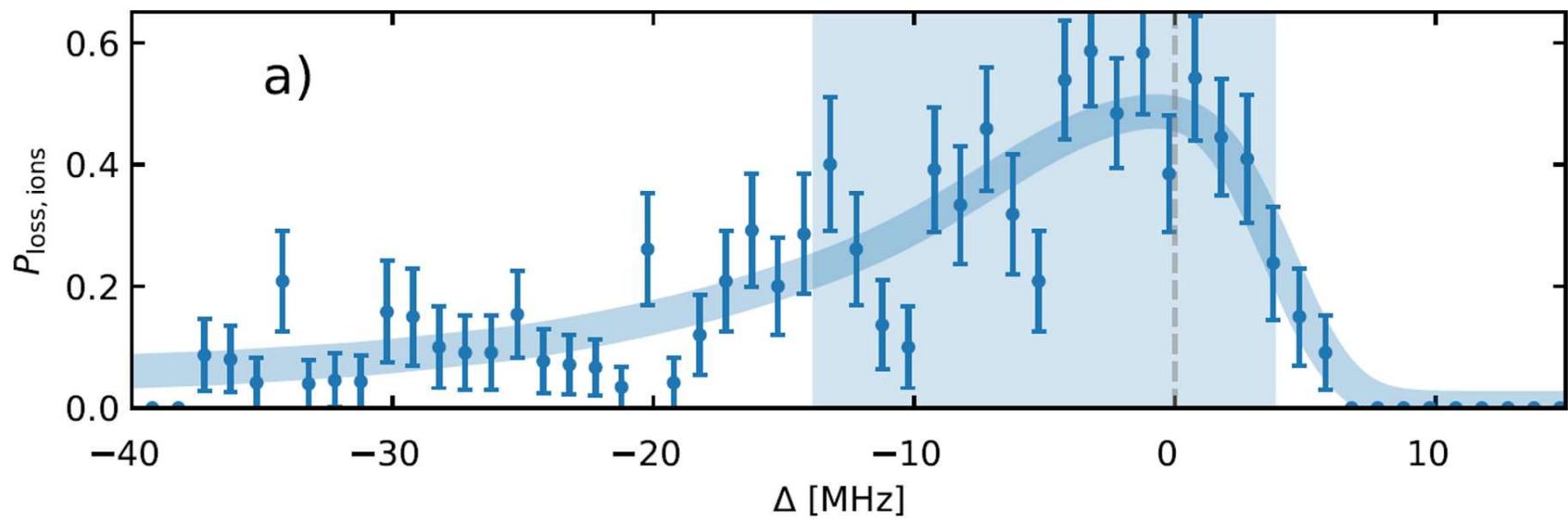
- Two photon Rydberg excitation to  $24S_{1/2}$
- Image atoms and ions: Losses?



Polarizability of  $24S$  state is about  $10^8$  times larger than for the ground state

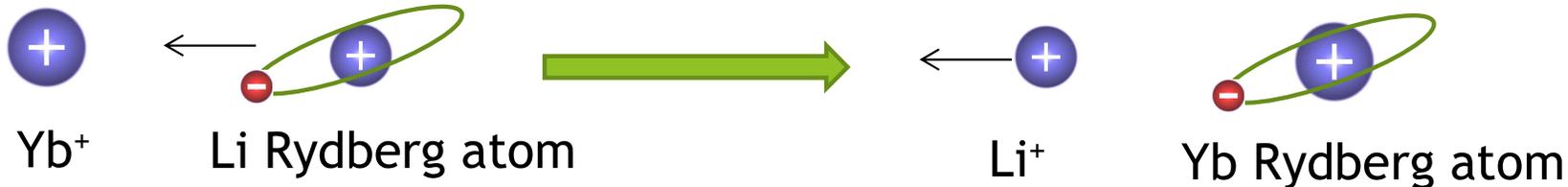
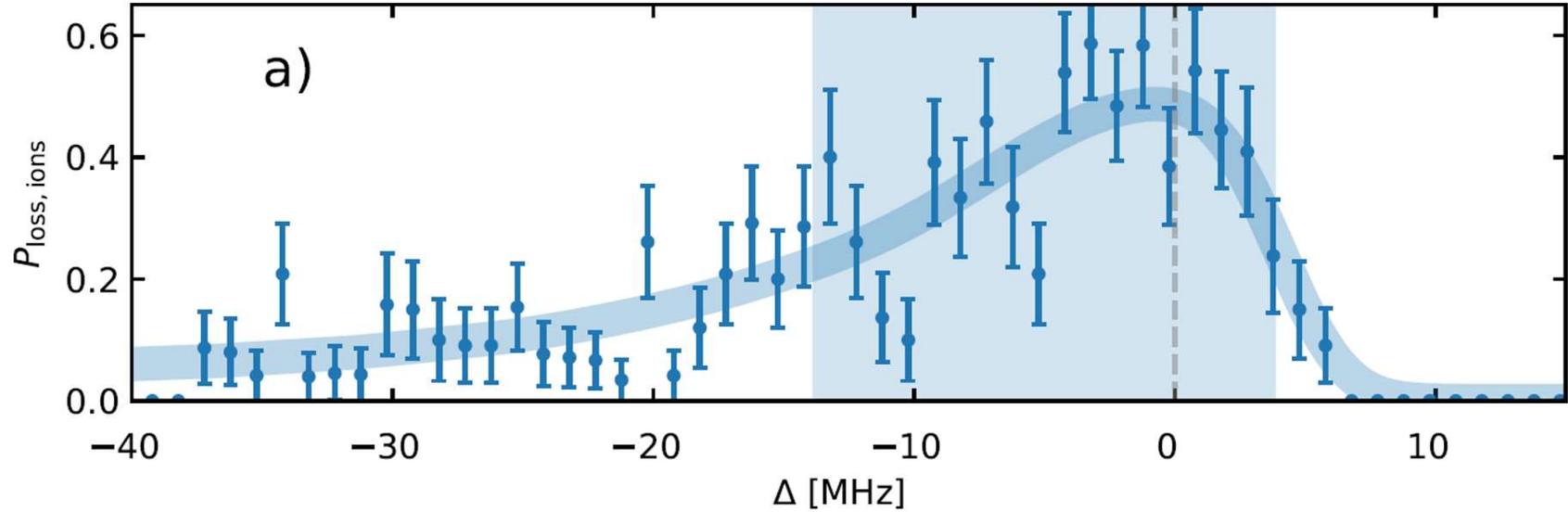
# Rydberg atom-ion interactions

Ion loss spectrum for 20  $\mu$ s excitation pulse



# Rydberg atom-ion interactions

Ion loss spectrum for 20  $\mu$ s excitation pulse



**Ion loss exceeds Langevin collision rate for ground state atoms by factor  $\approx 10^3$   
 We have boosted the interaction strength!**

# Repulsive interactions

- We boosted the interactions 😊, but we lose our ions ☹️
- We should use repulsive interactions: Prevent charge transfer



Unfortunately in Li, transitions to such states are not allowed

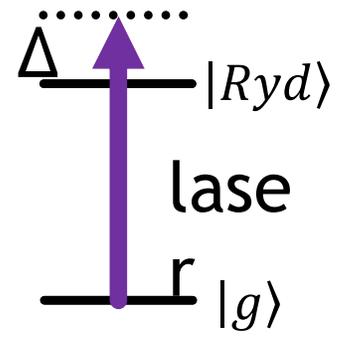
# Repulsive interactions

- We boosted the interactions 😊, but we lose our ions ☹️
- We should use repulsive interactions: Prevent charge transfer

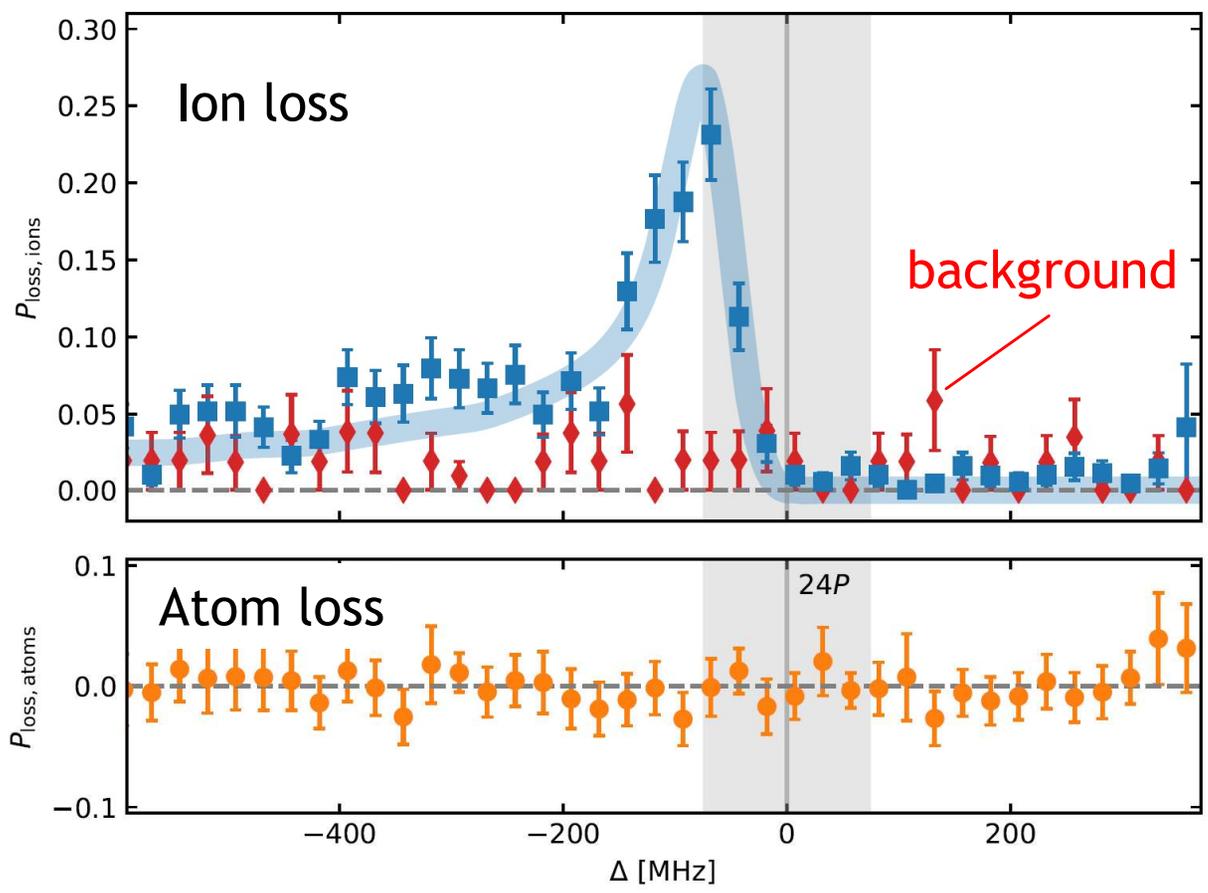
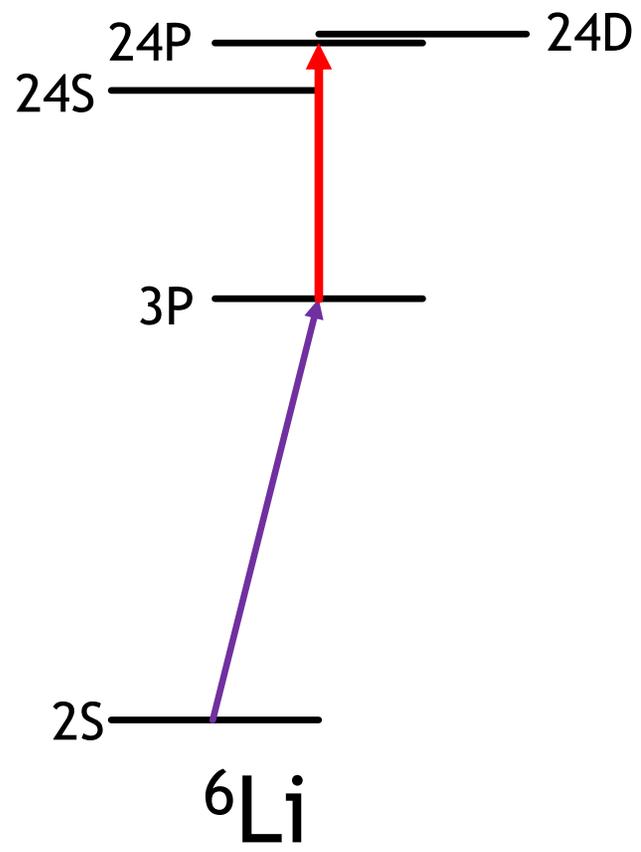


Unfortunately in Li, transitions to such states are not allowed

Unless of course, the atom is in a strong electric field

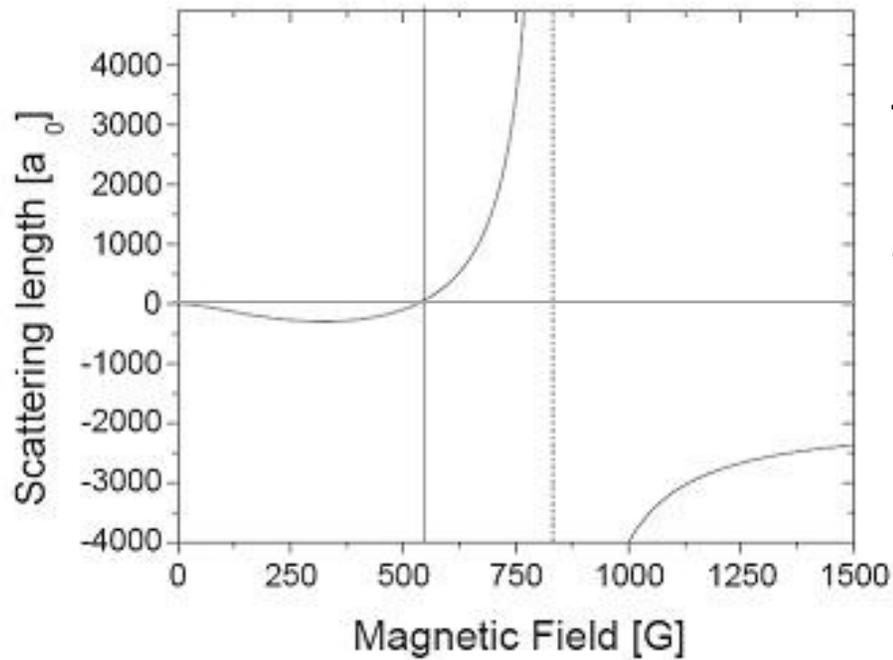


# Excitation on a dipole forbidden transition in the field of a single ion: first attempt



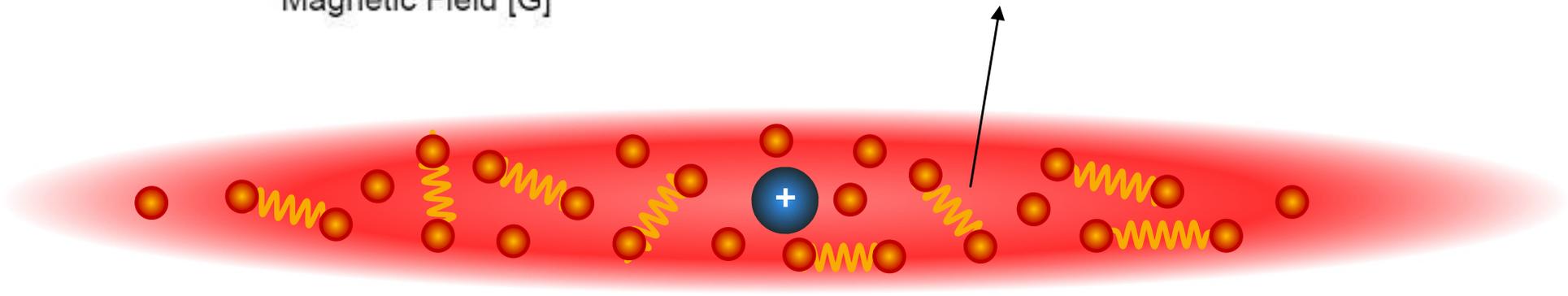
Note: The P state has the wrong sign of the polarizability so we still lose ions  
 Prospect: Engineer repulsive interaction

# Now for some chemistry

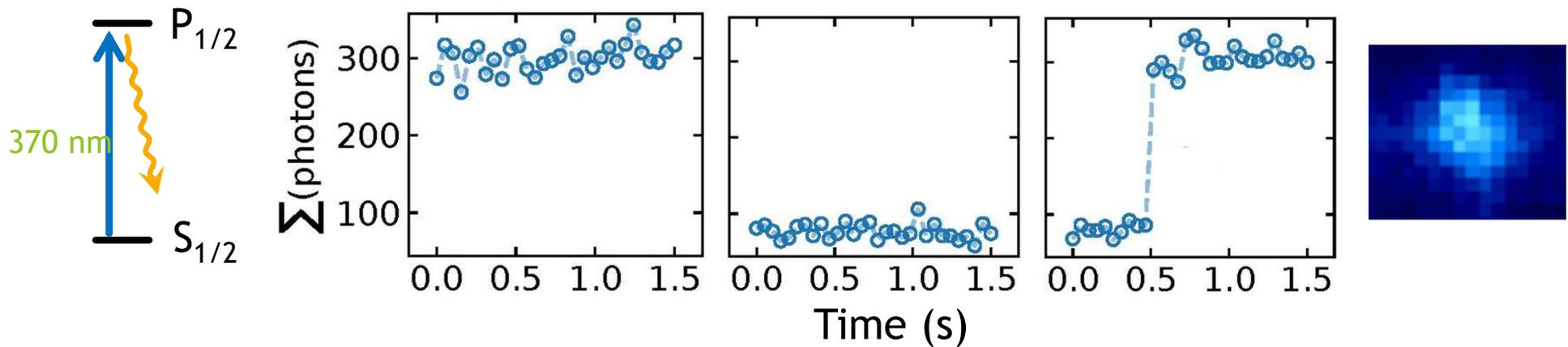


←  ${}^6\text{Li}$  Feshbach resonances  
Taken from R. Grimm:  
Proceedings of the International School  
of Physics "Enrico Fermi"

Trace amounts of  $\text{Li}_2$  dimers  
Due to  $\text{Li} + \text{Li}' + \text{Li} \rightleftharpoons \text{Li}_2 + \text{Li}$



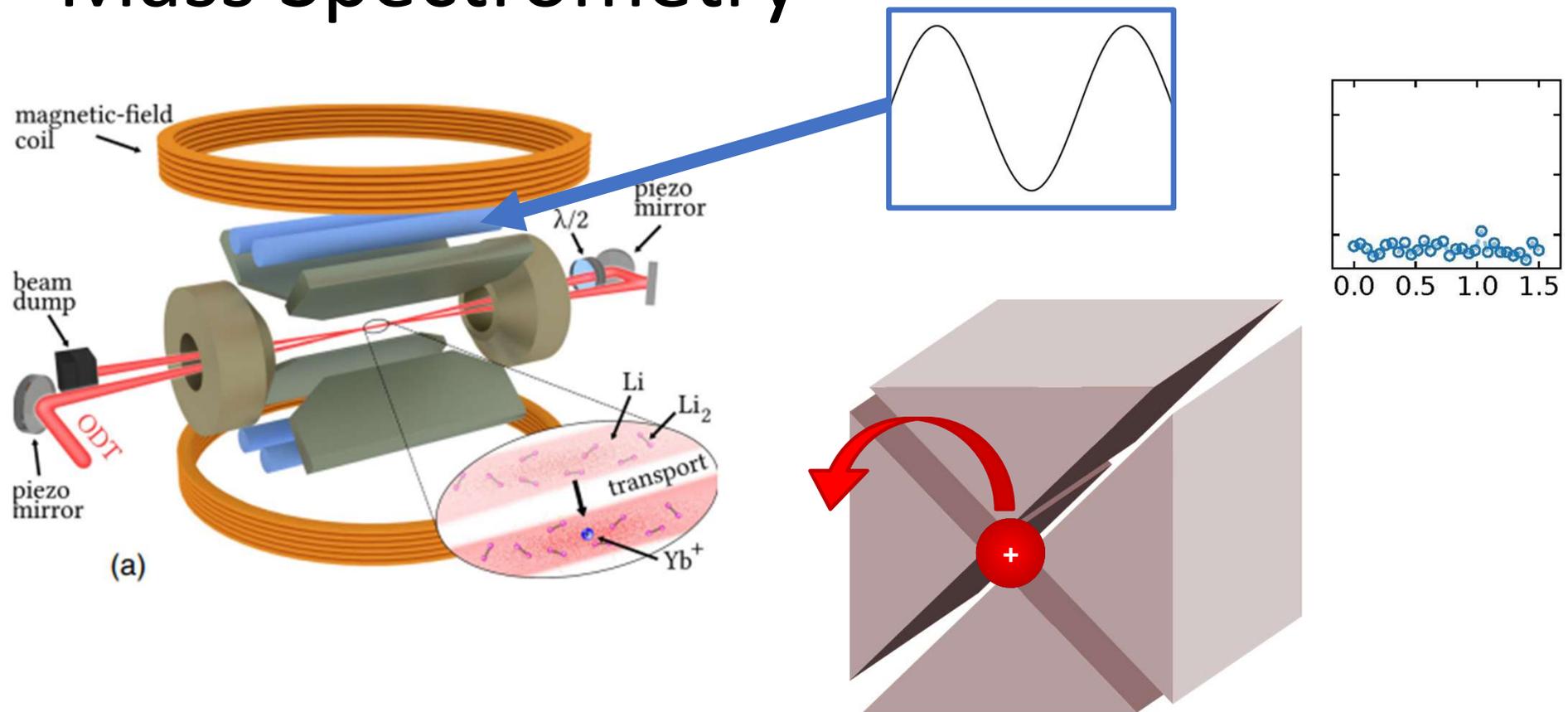
# Ion in a bath of Feshbach Dimers



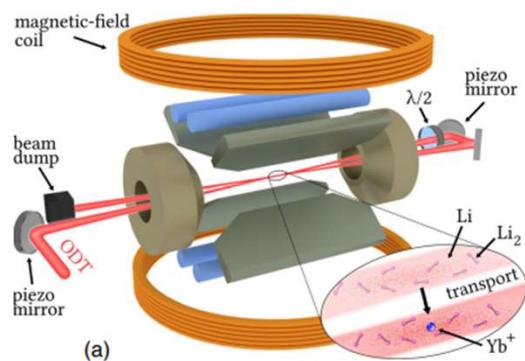
$\text{LiYb}^+$



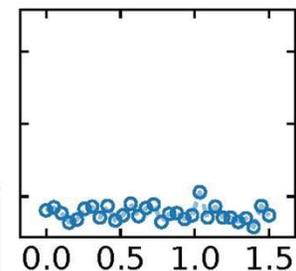
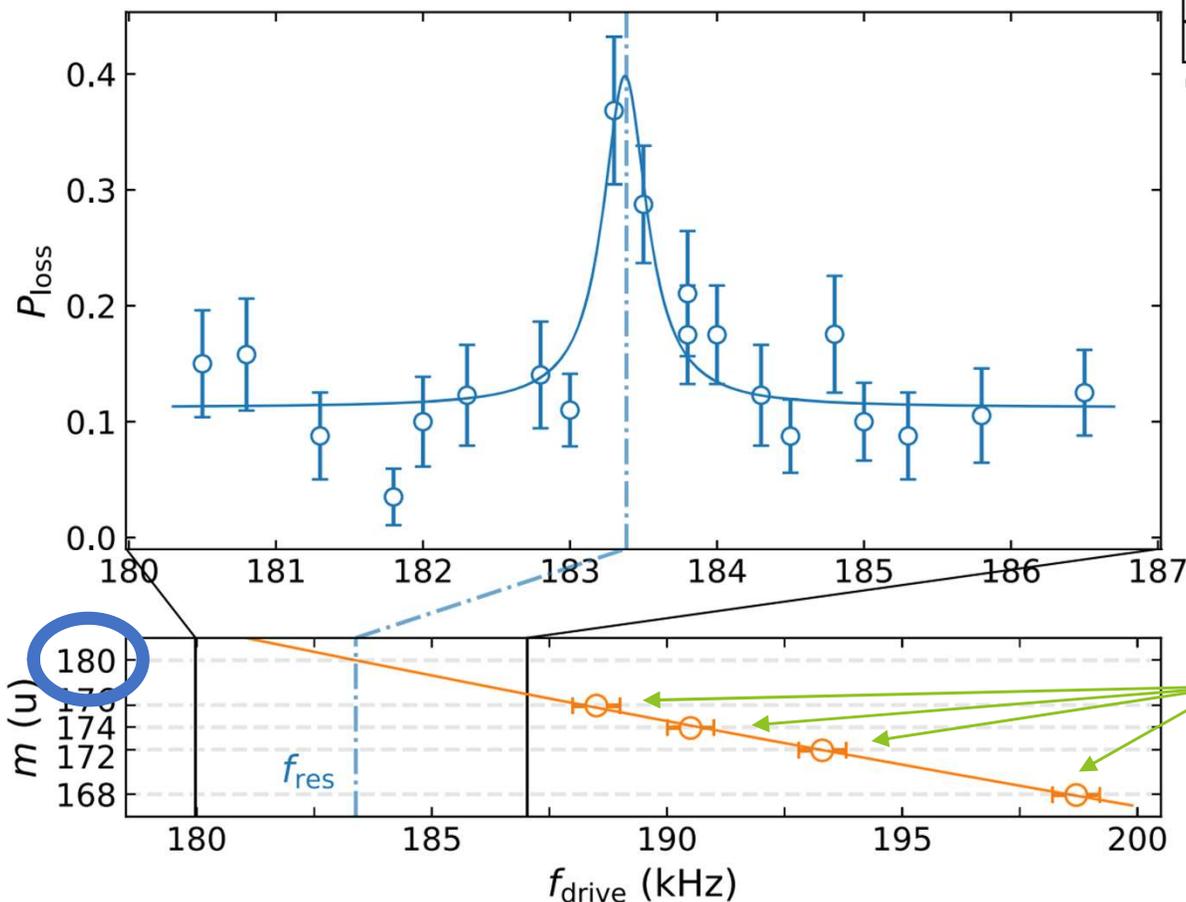
# Mass Spectrometry



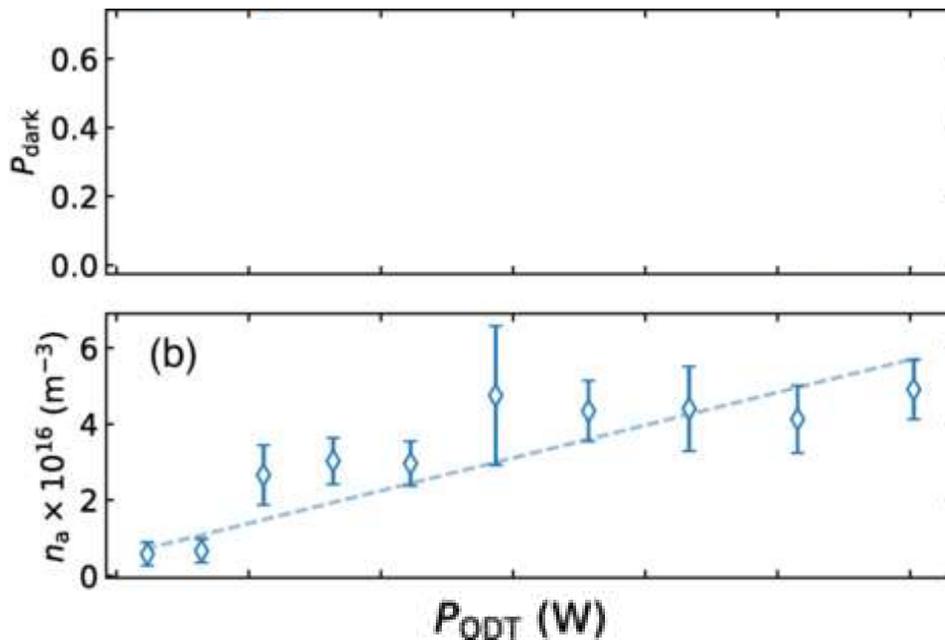
# Mass Spectrometry



LiYb<sup>+</sup>



Calibrate with Yb<sup>+</sup> isotopes



Change  $P_{ODT}(W)$

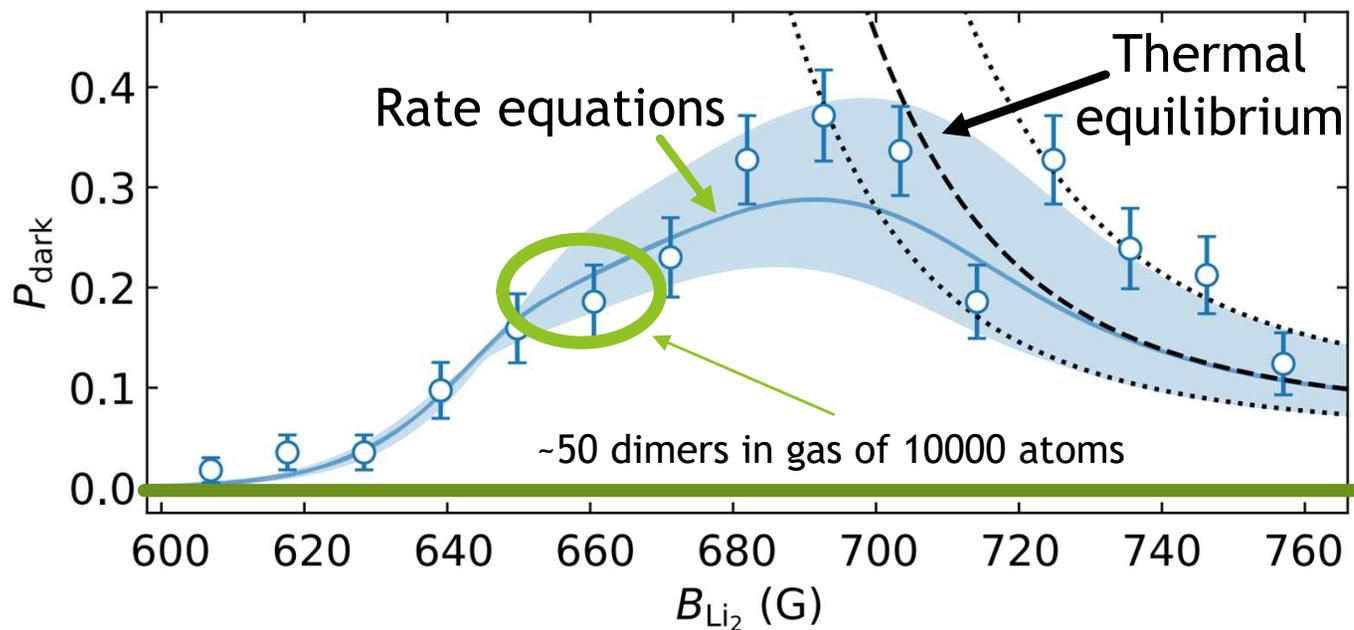


Change in atom density



Change in  $\text{LiYb}^+$  formation?

# Dimer Density

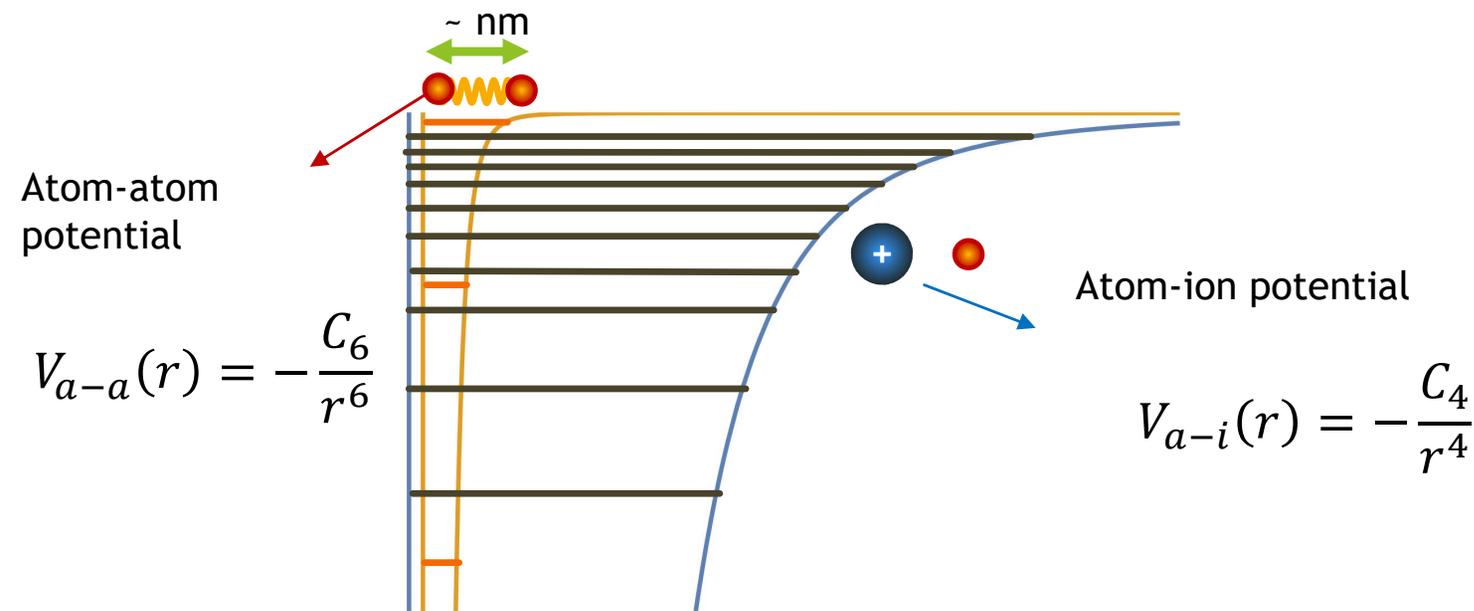


Change B (G)  
↓  
Change in dimer density  
↓  
Change in LiYb<sup>+</sup> formation

→ No fit parameters, but we assume all dimer-ion collisions lead to dark ions

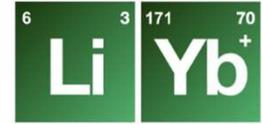
Theory based on: Jochim et al., Science **302** (2003);  
Chin and Grimm, PRA **69** (2004);

# Density of states



- Density of states much larger for atom-ion potential
- Expect molecular ions to be formed

# Feshbach dimers



← Taken from  
Chin et al., RMP 82, 1225 (2010).

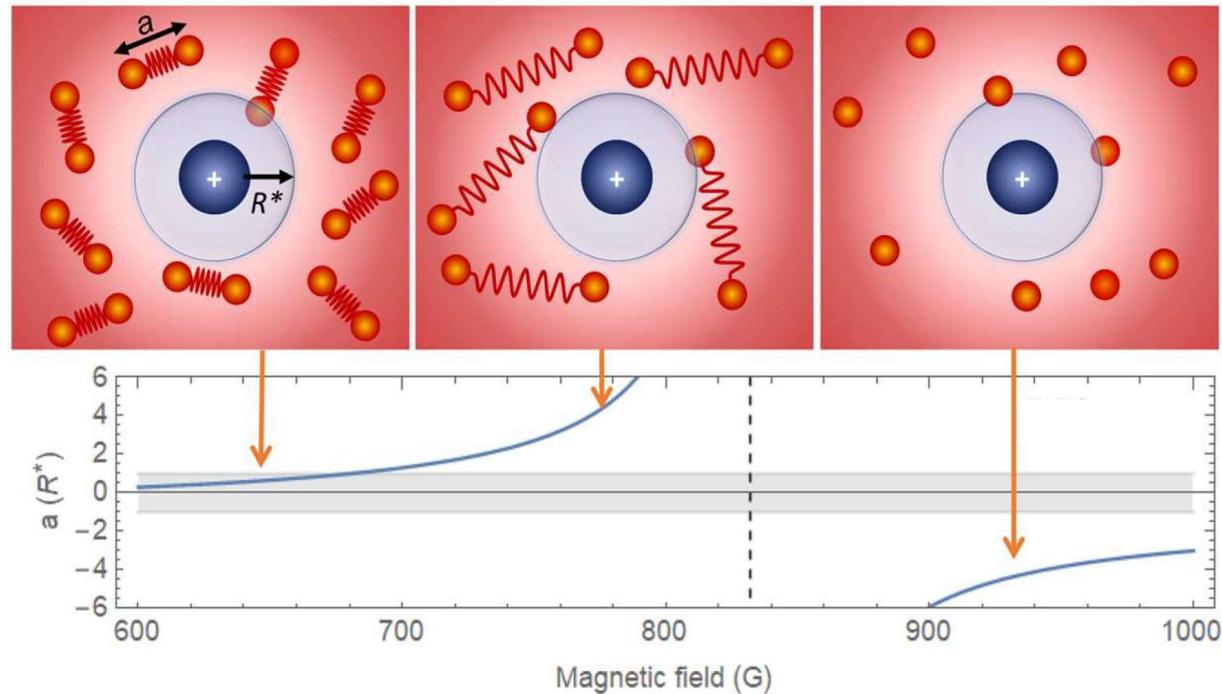
Li<sub>2</sub> dimers created by  
three-body recombination



Up until now, we ramp the B-field to 0...

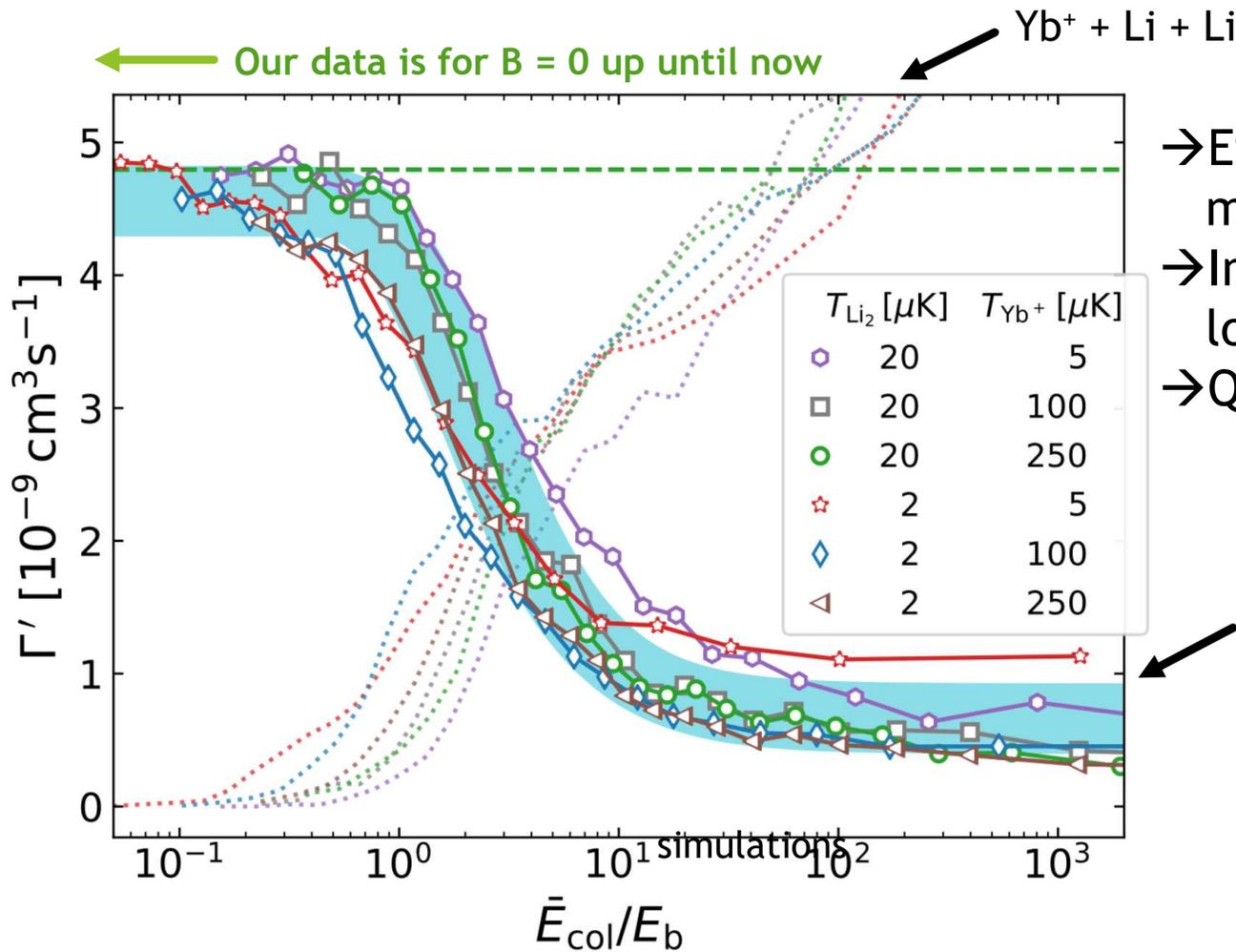


# Trapped ions in a bath of Feshbach dimers



- Tune size of Feshbach dimers with magnetic field
- Interesting crossover of length scales:  $E^*_{\text{atom-ion}} = E_{\text{binding Li-Li}}$  @  $B = 704$  G
- Crossover from atom-ion to molecule-ion collisions

# Theory



- Efficient creation of molecular ions!
- Impurity physics on BEC side: losses?
- Quantum effects?

Classical theory by:  
H. Hirlzer and Jesús Pérez-Ríos

# Summary

- ▶ Plenty of interesting physics to explore with atoms and ions!
- ▶ We introduced the atom-ion interaction potential
- ▶ We introduced ion trapping
- ▶ We explored micromotion-induced heating and what to do about it
- ▶ We now have two systems,  $\text{Yb}^+/\text{}^6\text{Li}$  and  $\text{Ba}^+/\text{}^6\text{Li}$  that have reached the crossover into the quantum regime
- ▶ Tomorrow: Some quantum chemistry and controlling interactions between atoms and ions