RIKEN SNP Seminar

Ultracold AMO experiment for quantum few-body and many-body

Atomic, Molecular, and Optical

Osaka City University, NITEP

Munekazu Horikoshi

June 22 (Monday), 14:00 – 15:00 by Zoom

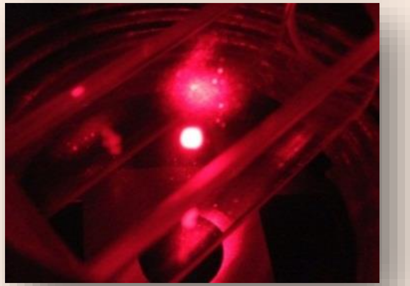
Contens

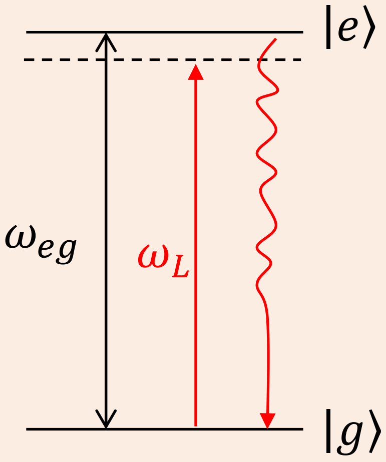
- Background of Ultracold AMO physics
- Road from complex molecular potentials to Universal Feshbach molecules
- Absorption spectroscopy of Feshbach molecules

Ultracold AMO Physics has developed quantum physics

AMO

Laser cooling of atoms

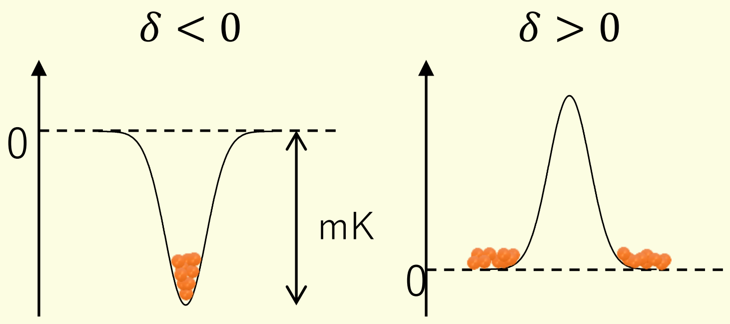




Absorption and Emission

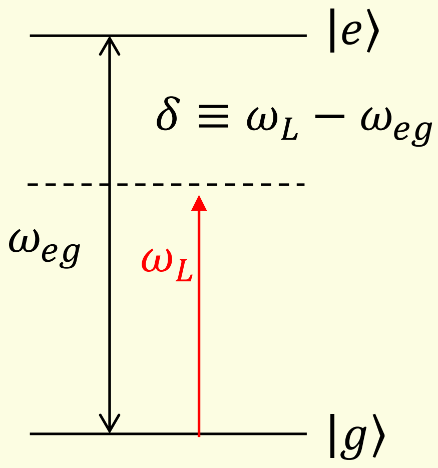
AMO

Optical potential



Attractive potential

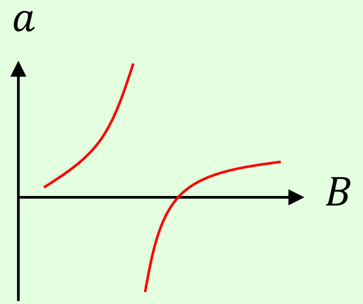
Repulsive potential

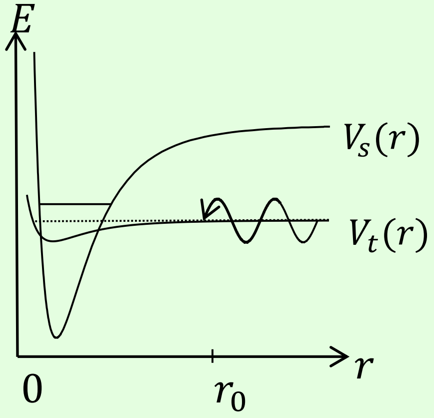


Energy shift in the light

AMO

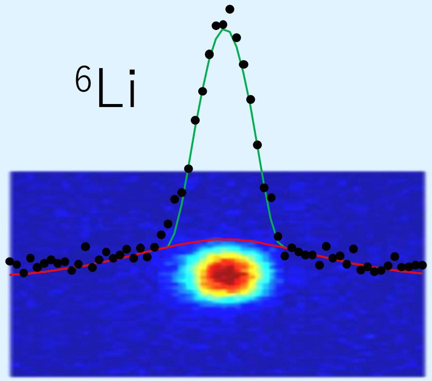
Feshbach resonance



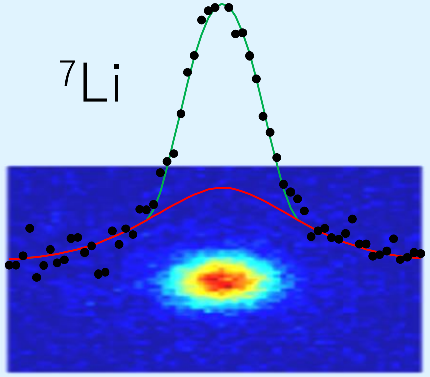


Coupling between molecular potentials

AMO



Fermi Superfuid



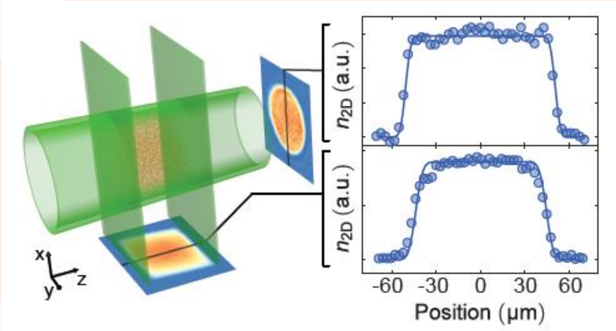
Molecular Bose-Einstein Condensate

Recent Ultracold AMO Physics

AMO

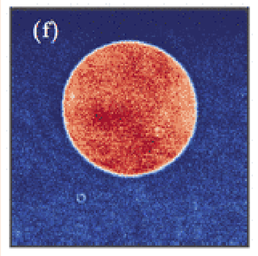
Various trap configurations

3D box potential



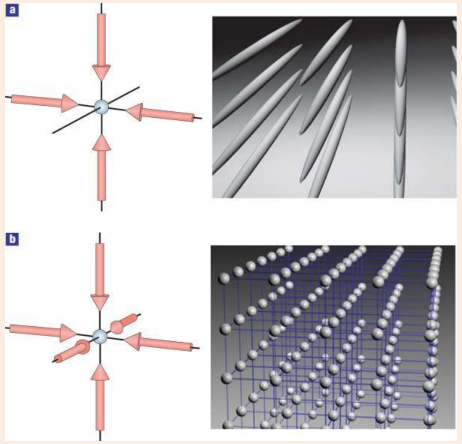
B. Mukherjee, PRL. 118, 123401 (2017)

2 D sheet potential



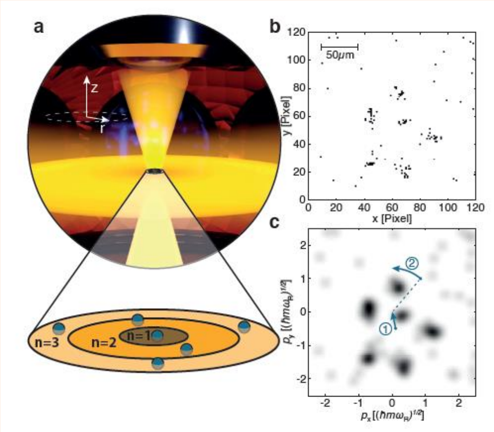
K. Hueck, Phys. Rev. Lett. 120, 060402 (2018)

Periodic potential



I. Bloch Nature Physics 1, 23 (2005)

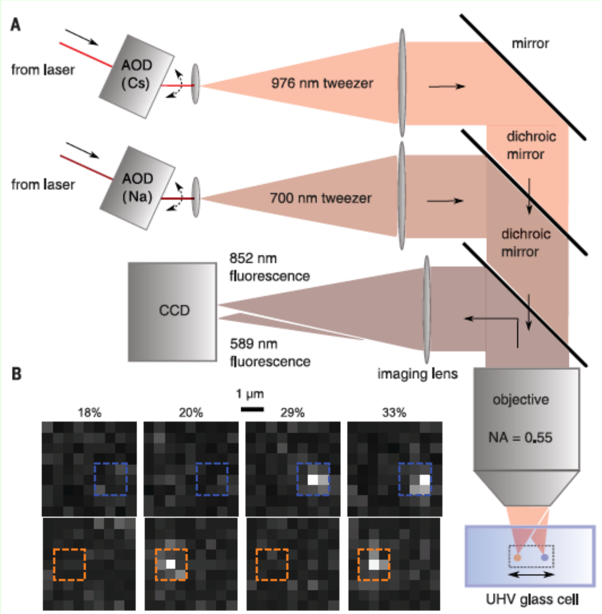
2D shell structure



Marvin Holten, arXiv:2005.03929

AMO

Optical tweezer

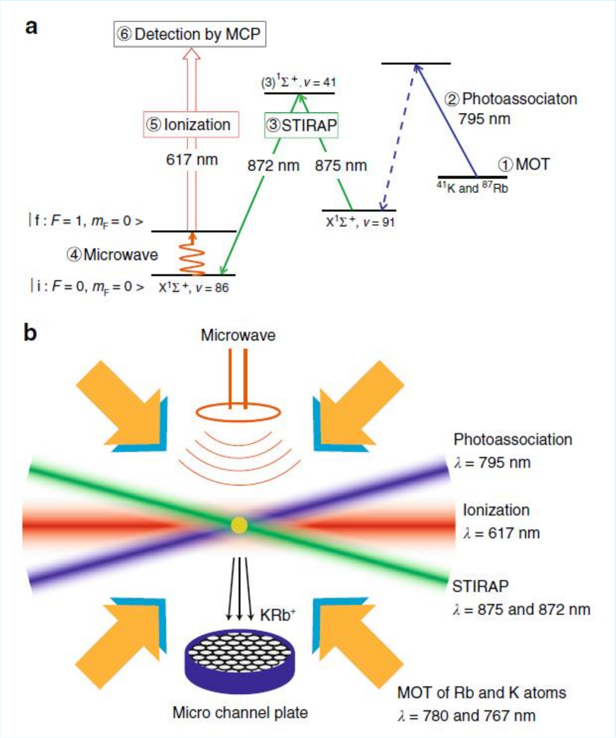


Chemical reaction

L. R. Liu, *Science* 360, 900 (2018)

AMO

Coherent transfer and precision measurement



Electron-to-proton mass ratio

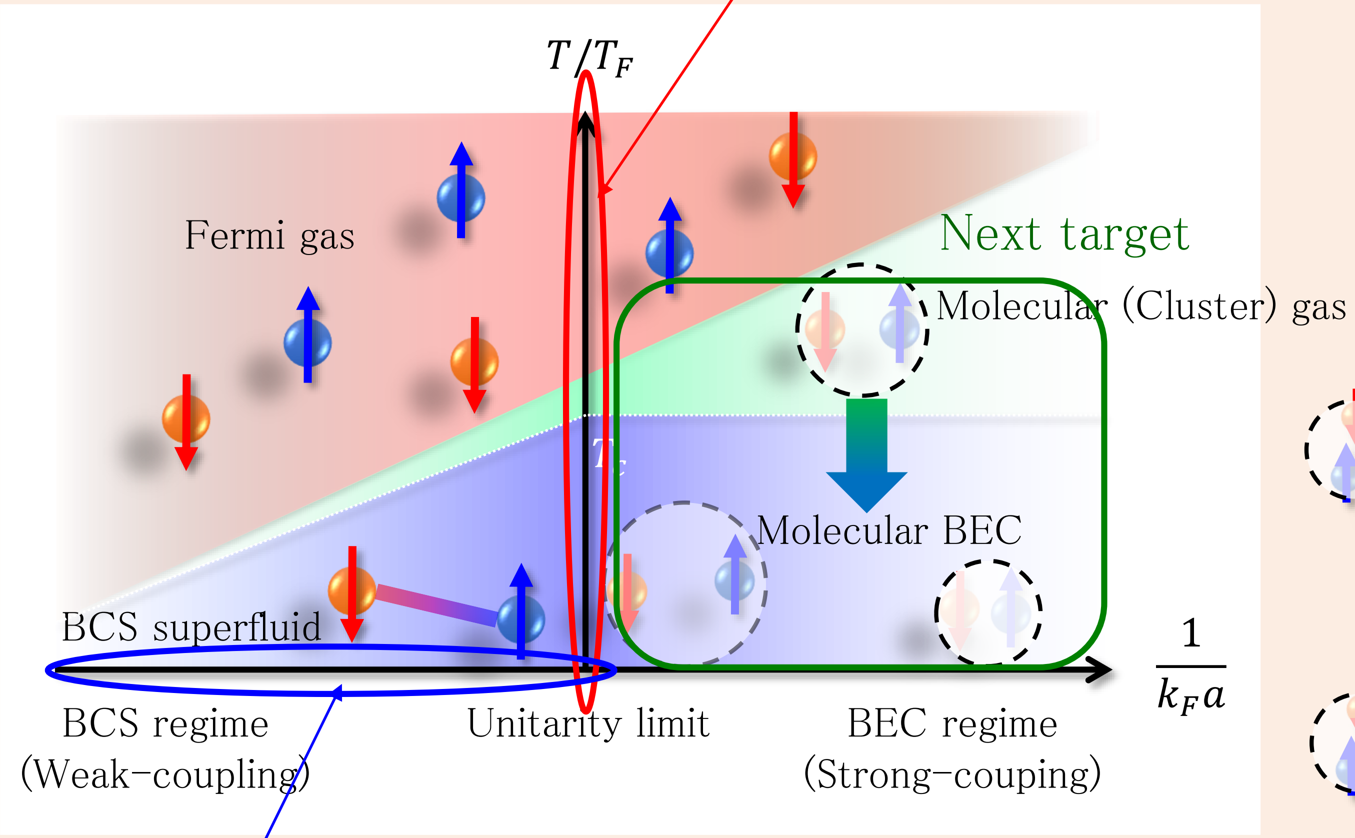
J. Kobayashi, S. Inouye
Nature communications 10, 3771 (2019)

Our interest in Ultracold AMO Physics

AMO

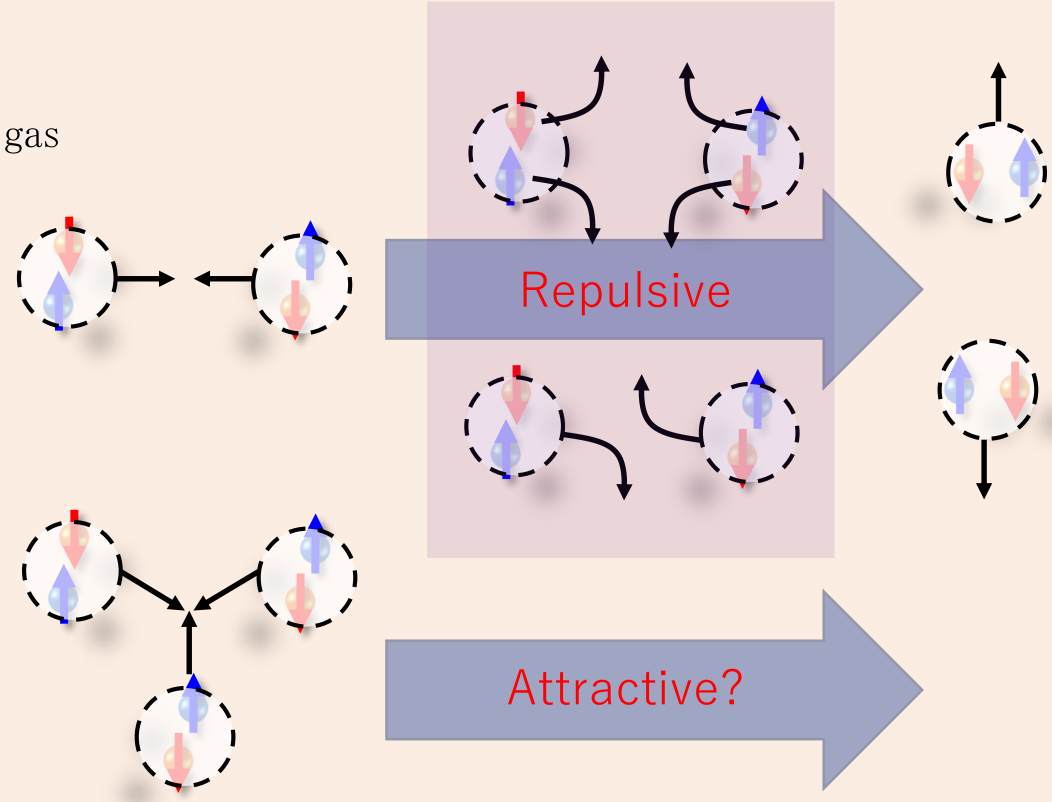
Phase diagram of spin-1/2 fermions

Munekazu Horikoshi, Science 327, 442 (2010)



Munekazu Horikoshi, PRX 7, 041004 (2017)

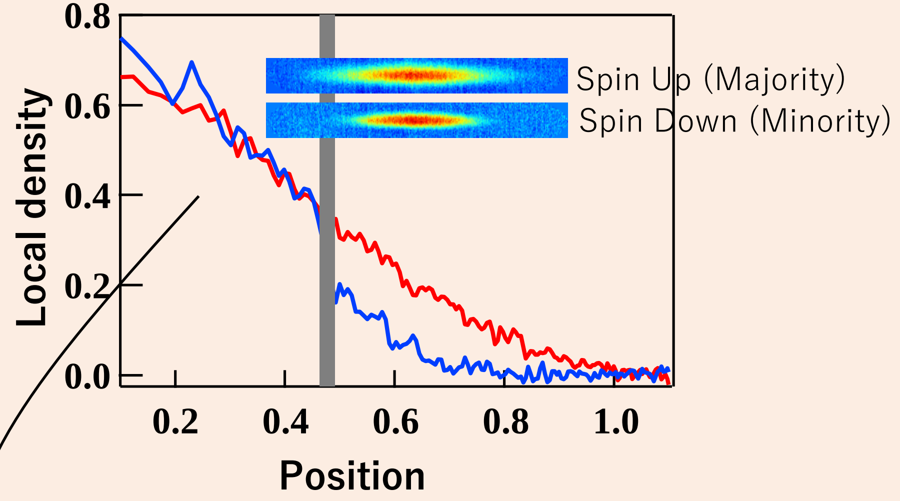
- How physical properties of the many-body system change depending on the size of molecule?
- What is the interactions between clusters?



Our interest in Ultracold AMO Physics

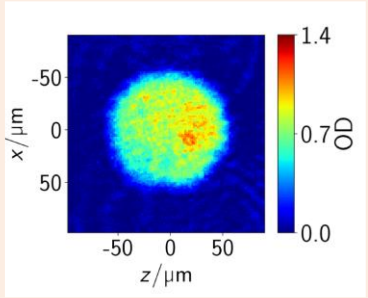
AMO

Spin-imbalanced fermions in a harmonic potential



Rb BEC in a 2D box potential @ OCU

Spin-imbalanced fermions in a box potential



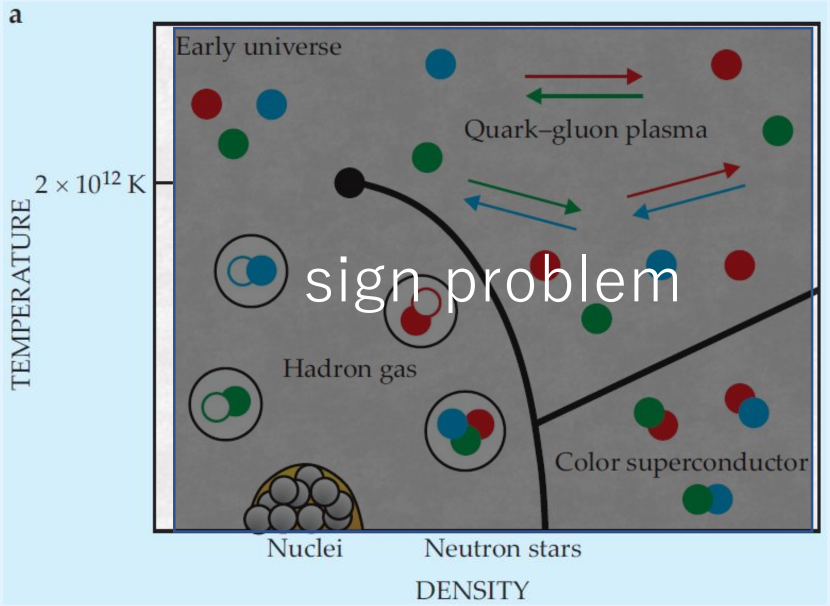
Janek Fleper, Kohei Kato, Shin Inouye, JPS autumn meeting 13aK14-4 (2019)

Quantum simulation

Fermi system with a negative sign problem for Quantum Monte Carlo Calculation

⬍

Development of improved algorithm (complex Langevin method)



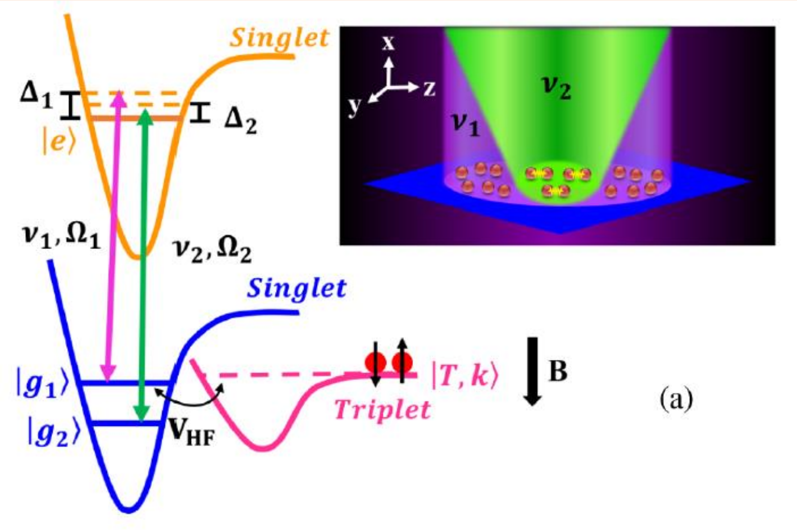
Published in: Carlos A. R. Sá de Melo; *Physics Today* 2008, 61, 45-51.

Our interest in Ultracold AMO Physics

AMO

Optical upgrade of magnetic Feshbach resonance

Independent tuning of scattering length and effective range

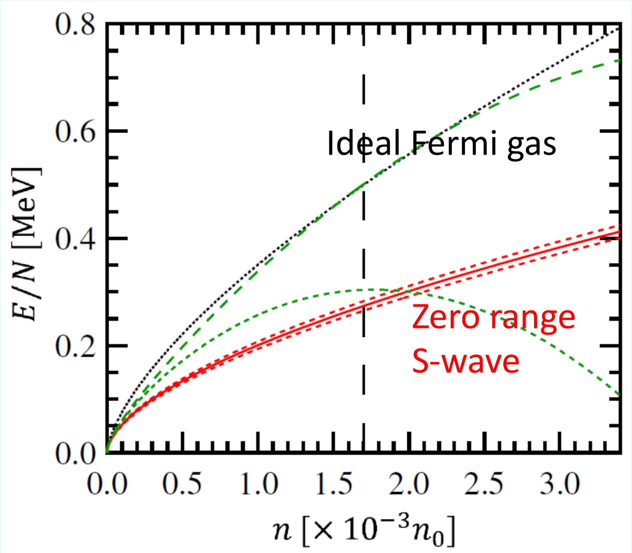


N. Arunkumar, PRL 122, 040405 (2019)
Haibin Wu, Phys. Rev. A 86, 063625 (2012)

Quantum simulation

Neutron matter EOS

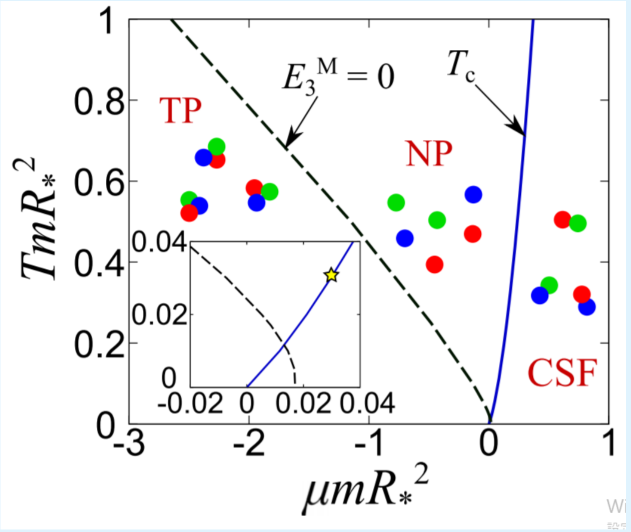
Internal energy per neutron



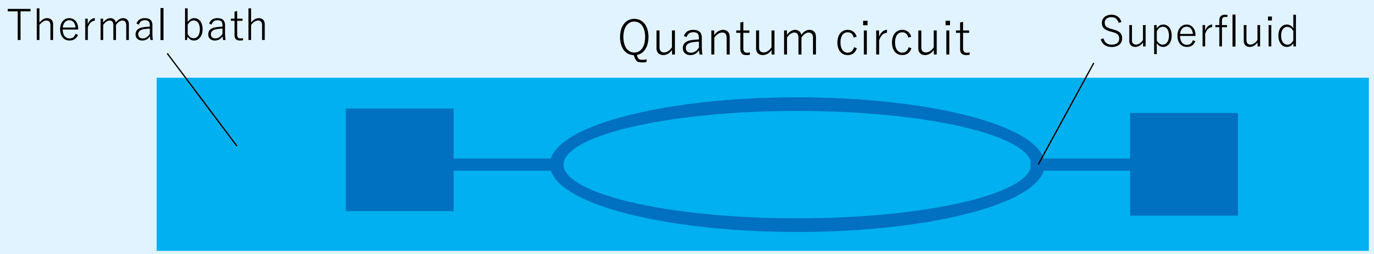
Munekazu Horikoshi, IJMPE 28 (2019)

Three-component fermi system

Phase diagram under $1/a = 0$



Hiroyuki Tajima and Pascal Naidon, New J. Phys. 21 07305 (2019)



Contens

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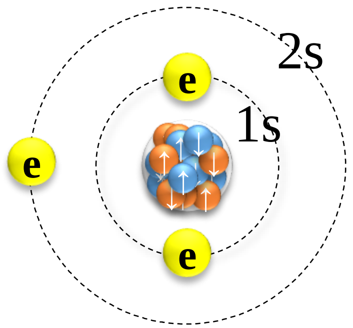
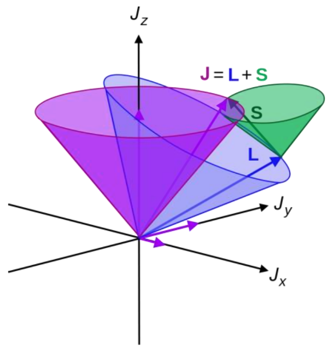
Atomic species we have used

^{6}Li atoms

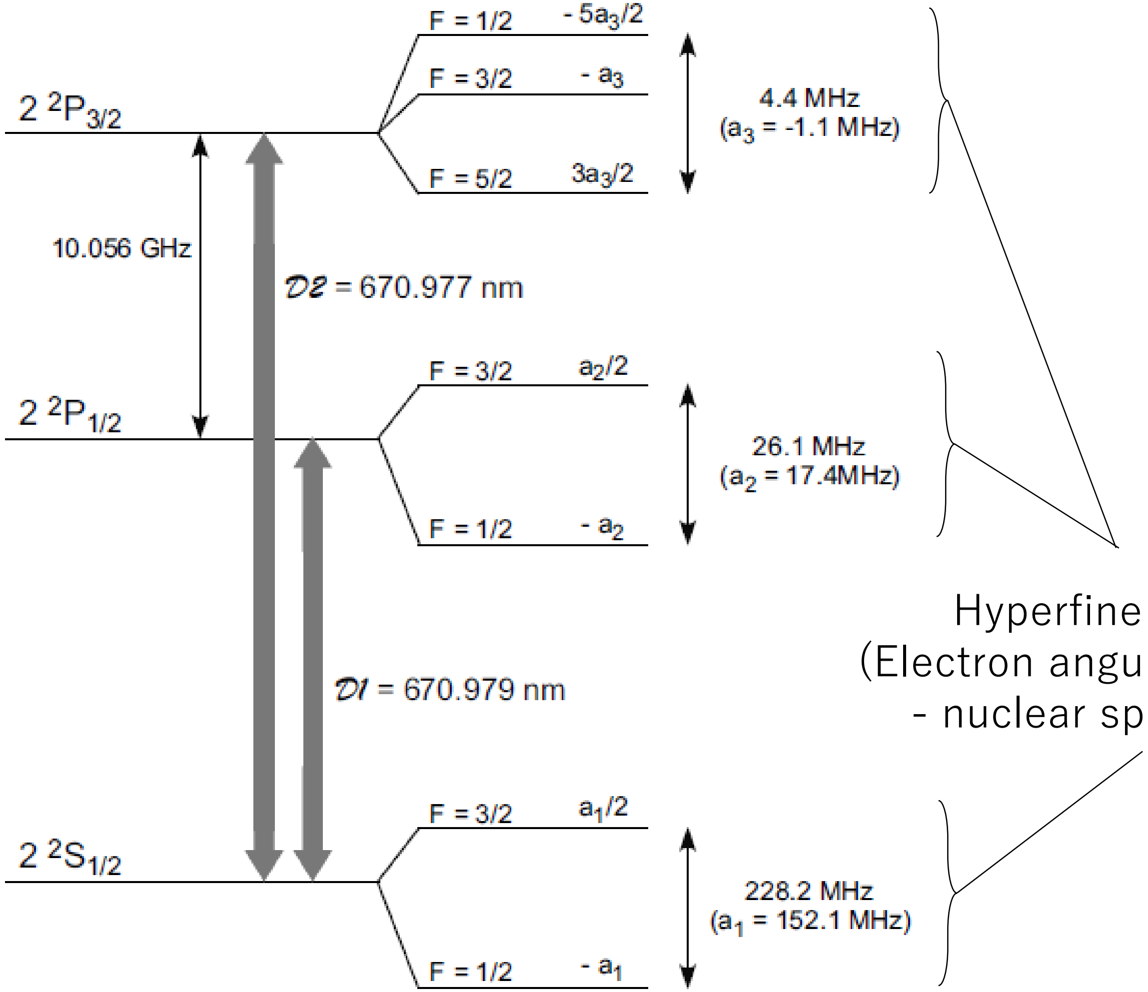




P-orbit : $L = 1$

Fine structure
(Spin-Orbit coupling)

S-orbit : $L = 0$



Hyperfine structure
(Electron angular momentum
- nuclear spin coupling)

Electron spin : $S = 1/2$

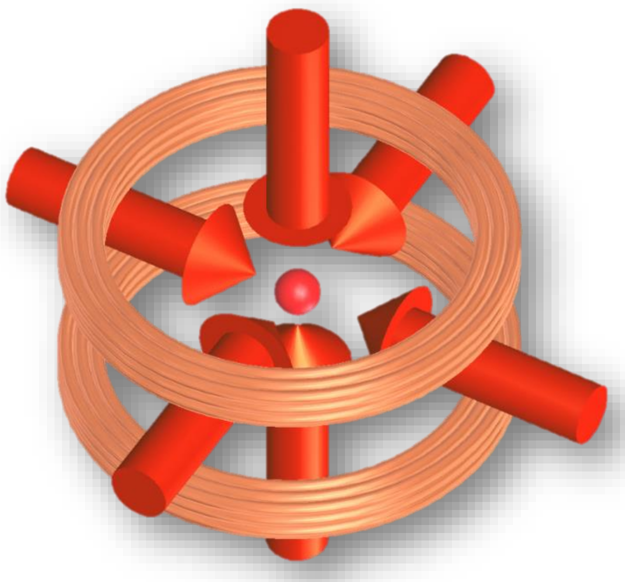
Nuclear spin : $I = 1$

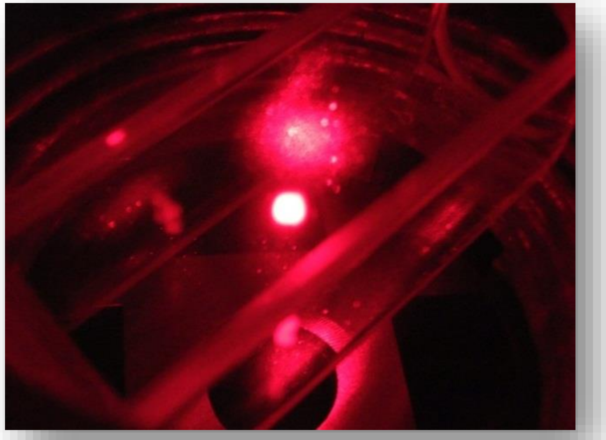
Fermion

Laser cooling of 6Li atom

Magneto-optical trapping

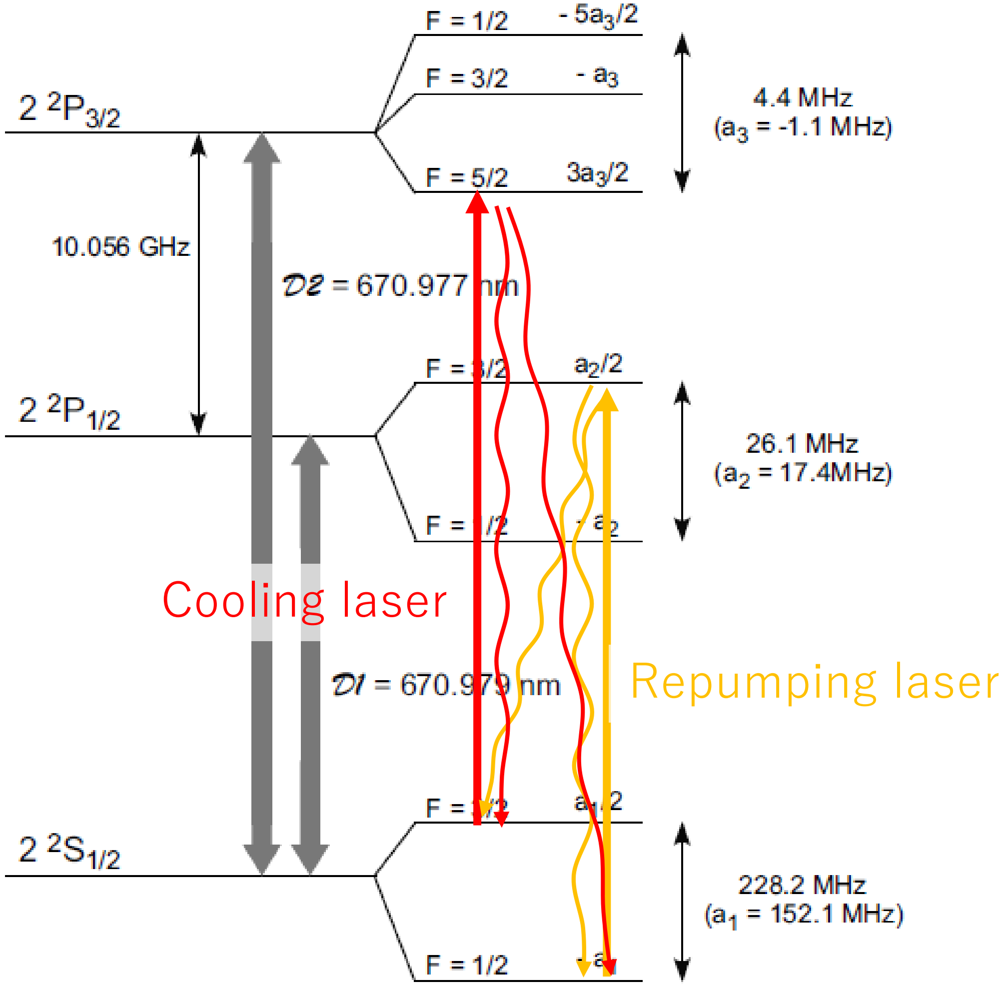
Velocity and position dependent force given by momentum of photons
Doppler effect + Zeeman effect



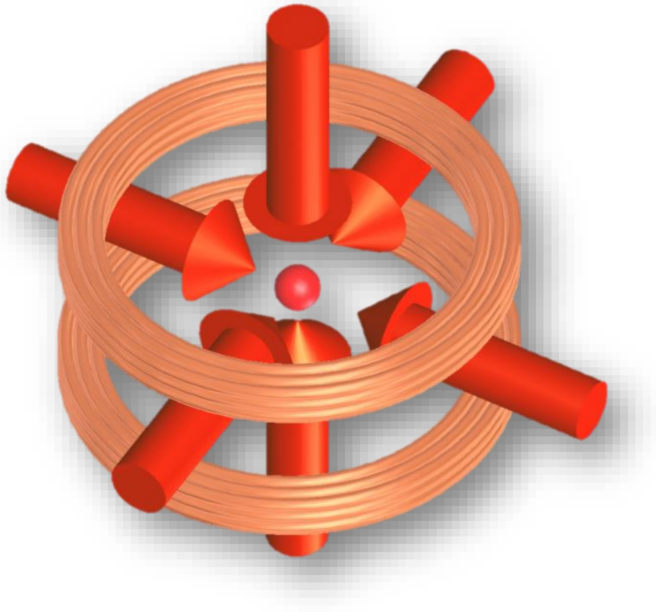


$N \sim 10^8, T \sim 1\mathrm{mK}$

Cooling transition lines



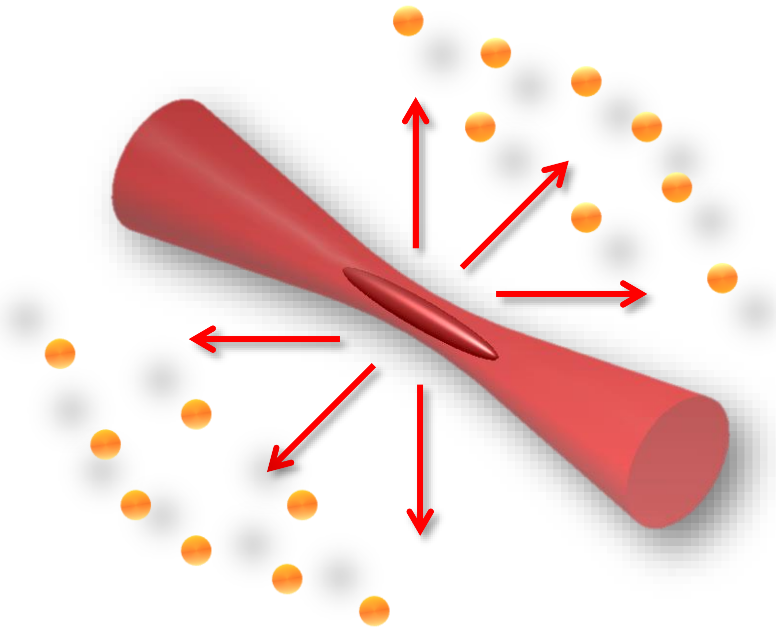
Realization of ultracold atomic gas



Trap cold atoms in an optical trap

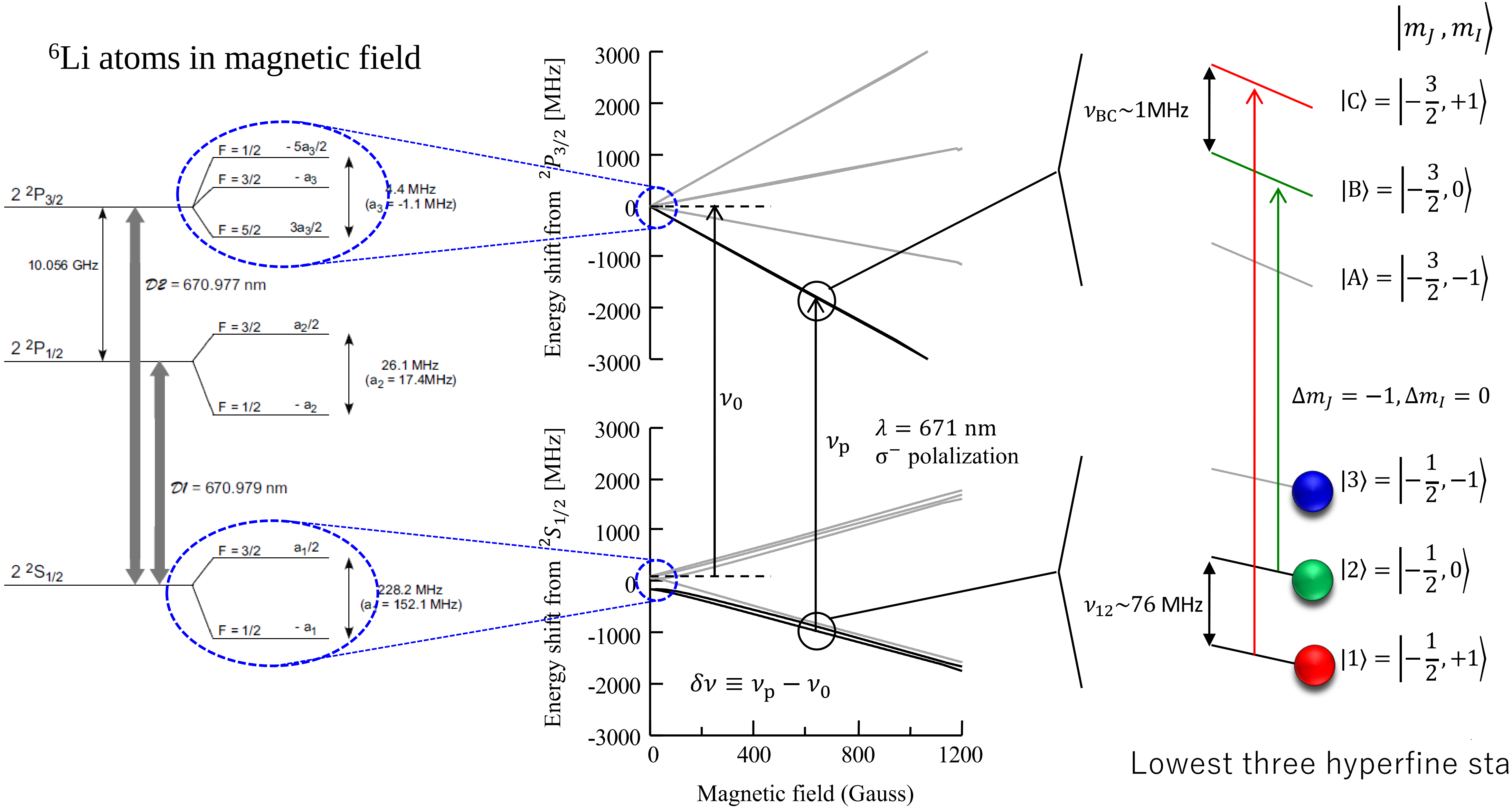
Evaporative cooling

Remove energetic atoms selectivity



$T \sim 100\text{nK}$

Atomic species we have used



Lowest three hyperfine states

Interacting Fermi system under Ultracold temperature

$$\left|m_J = m_S, m_I\right\rangle$$

$$|3\rangle = \left|-\frac{1}{2}, -1\right\rangle$$

$$|2\rangle = \left|-\frac{1}{2}, 0\right\rangle$$

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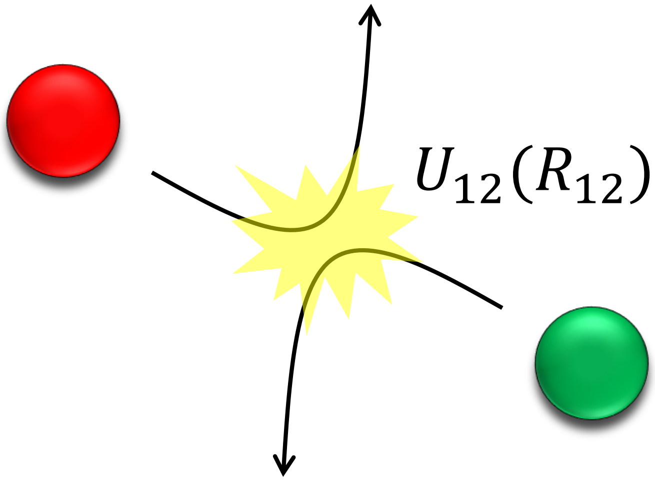

$U_{12}(R_{12})$: detail of particles

How can we enjoy universal physics using such atomic interaction !?

Interaction between two Li atoms : molecular potential

Calculation of the real Li2 potential is challenging problem

Chemical Physics
Volume 323, Issues 2–3, 21 April 2006, Pages 563-573

Calculation of adiabatic potentials of Li_2

P. Jasik, J.E. Sienkiewicz

JCTC Journal of Chemical Theory and Computation — Article
pubs.acs.org/JCTC
J. Chem. Theory Comput. (2014), 10, 1200−1211

First Principle Calculations of the Potential Energy Curves for Electronic States of the Lithium Dimer

Monika Musiał* and Stanisław A. Kucharski

Institute of Chemistry, University of Silesia, Szkolna 9, 40-006 Katowice, Poland

Calculation of the real Li3 potential is more challenging problem

Calculations of long-range three-body interactions for $\mathrm{Li}(2\,^2S) - \mathrm{Li}(2\,^2S) - \mathrm{Li}(2\,^2P)$

Pei-Gen Yan, Li-Yan Tang, Zong-Chao Yan, and James F. Babb
Phys. Rev. A **94**, 022705 – Published 9 August 2016

A diabatic representation of the two lowest electronic states of Li_3

J. Chem. Phys. **140**, 154304 (2014); https://doi.org/10.1063/1.4871014

Elham Nour Ghassemi[1], Jonas Larson[2,3], *and* Åsa Larson[2, a)]

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ELSEVIER
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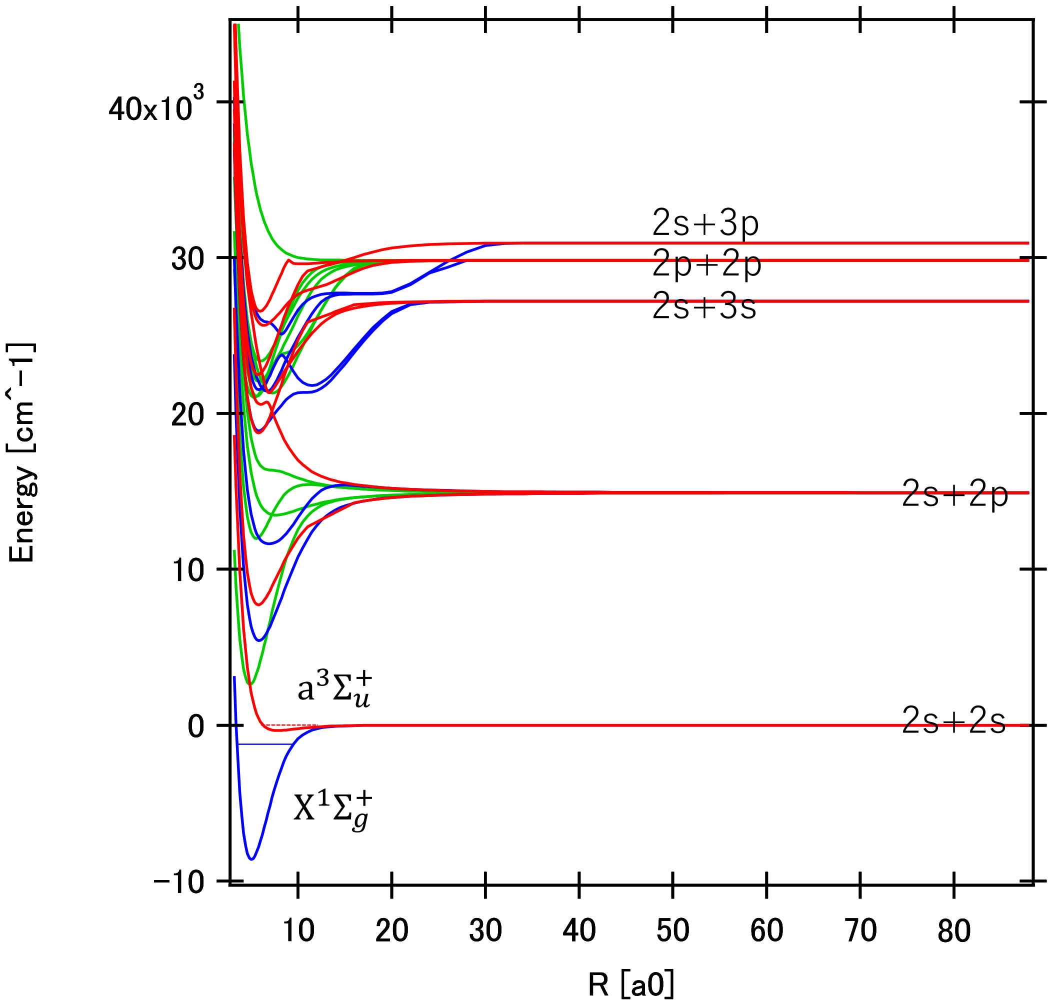
Interaction between two Li atoms : molecular potential

Li_2 molecular potential without considering atomic fine structure



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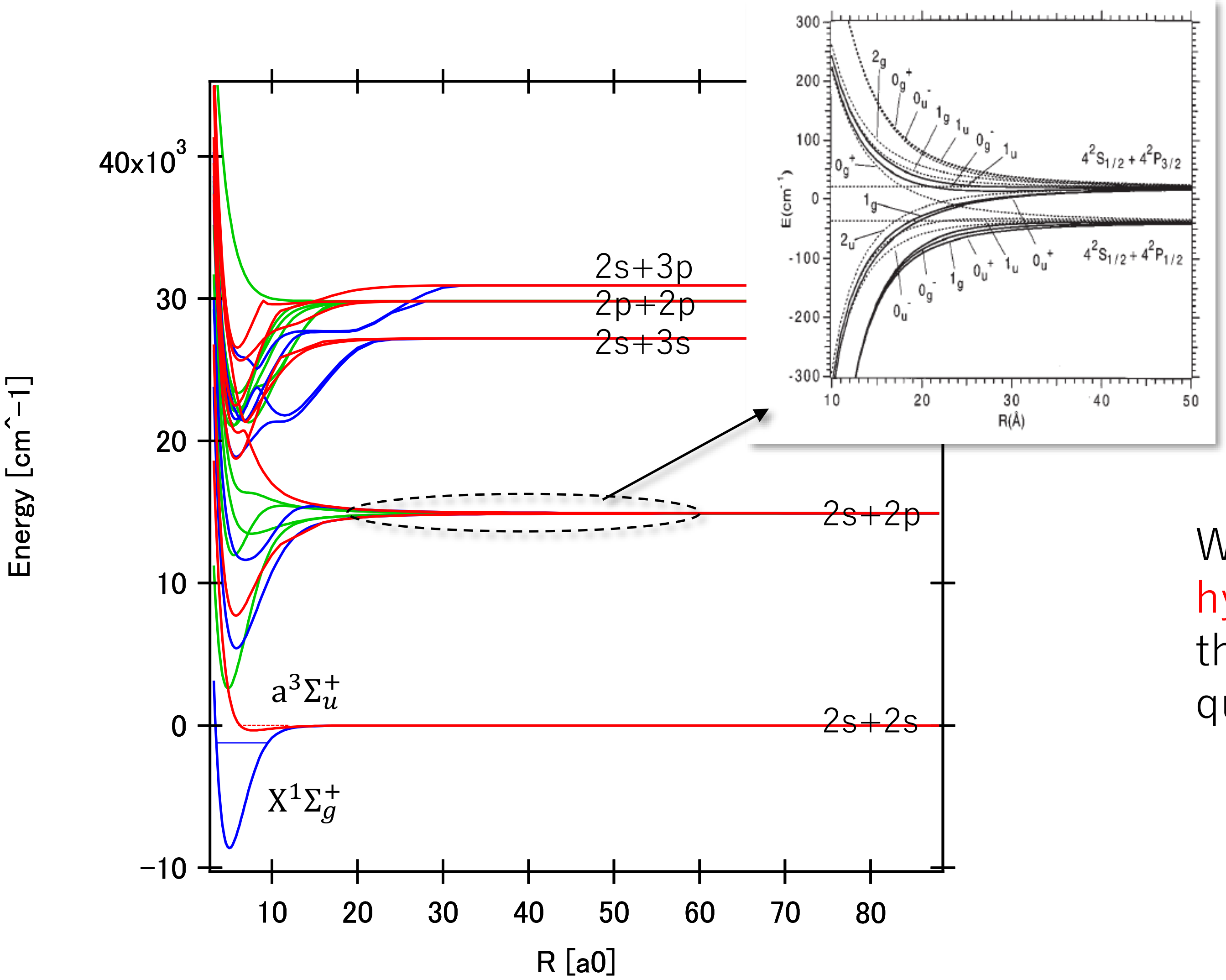


Fine structure (It is for K2, not Li2)

When we include interactions up to hyperfine interactions, the interaction potentials become quite complex

Don't worry !

旅の最後の準備：フェッシュバッハ共鳴による散乱長の制御

$$\left| m_J = m_S, m_I \right\rangle$$

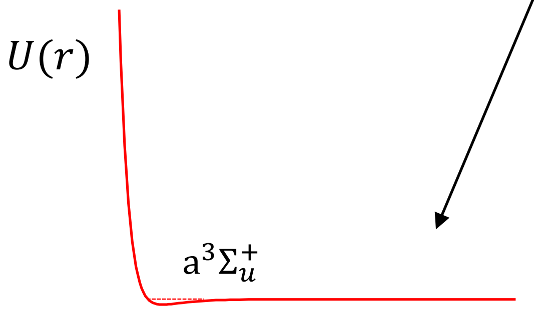
$$|3\rangle = \left| -\frac{1}{2}, -1 \right\rangle$$

$$|2\rangle = \left| -\frac{1}{2}, 0 \right\rangle$$

$$|1\rangle = \left| -\frac{1}{2}, +1 \right\rangle$$

Electric ground state
Combination of them is spin triplet

They interact with this triplet potential

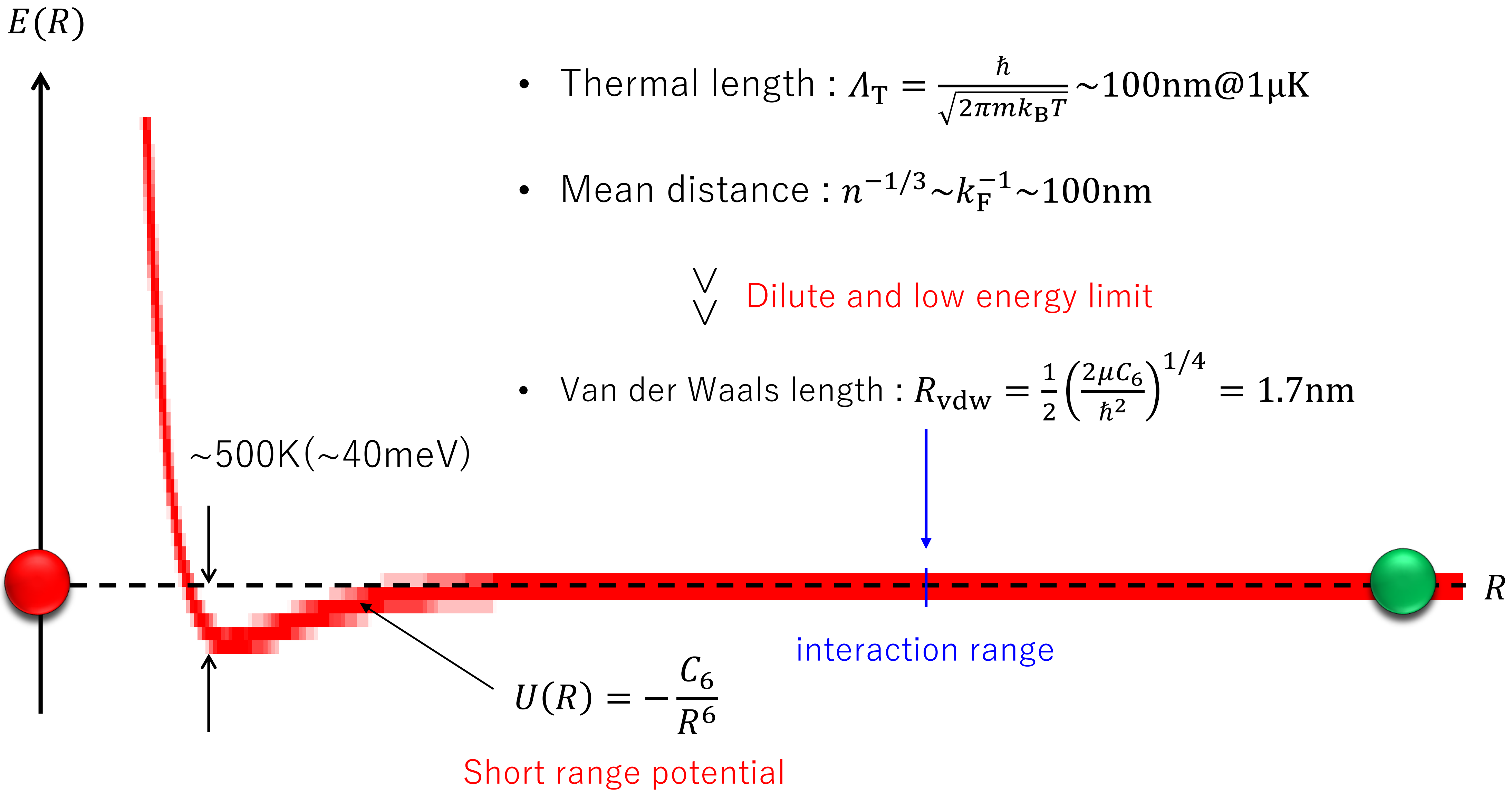


Length scales

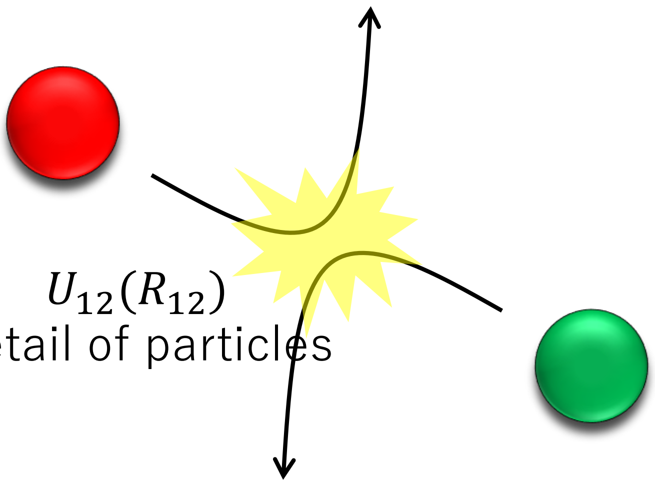
- Thermal length : $\Lambda_{\mathrm{T}} = \frac{\hbar}{\sqrt{2\pi m k_{\mathrm{B}} T}} \sim 100\mathrm{nm}@1\mu\mathrm{K}$
- Mean distance : $n^{-1/3} \sim k_{\mathrm{F}}^{-1} \sim 100\mathrm{nm}$

$\vee$
$\vee$ Dilute and low energy limit

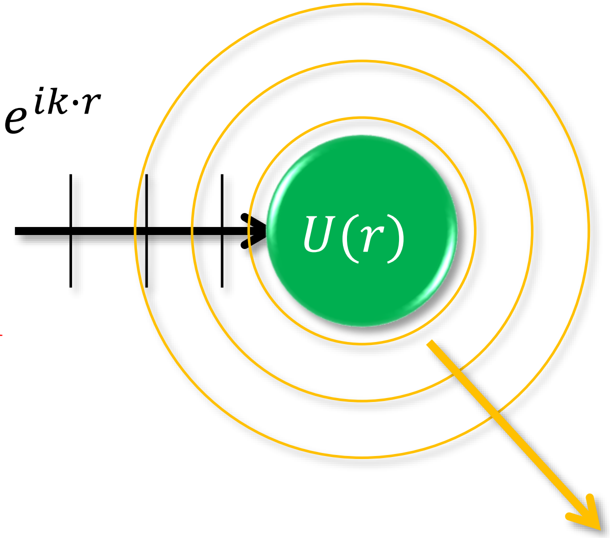
- Van der Waals length : $R_{\mathrm{vdw}} = \frac{1}{2}\left(\frac{2\mu C_6}{\hbar^2}\right)^{1/4} = 1.7\mathrm{nm}$



Principle of universal physics



Incident wave $: e^{ik\cdot r}$



- Short-range potential
- Dilute
- Low energy

Scattering wave $: \psi(r) \xrightarrow{|r_{\uparrow}-r_{\downarrow}| \gg r_0} \frac{C}{kr}\sin(kr+\delta_0)$

Phase shift : $\cot\delta_0 = -\frac{1}{ak} + \frac{1}{2} r_e k$

Origin of universality :

Quantum systems show the exactly same physics when particles have same a, r_e even if they have different $U(r)$

Grand-canonical many-body Hamiltonian :

$$\hat{\mathcal{H}} - \mu\hat{\mathcal{N}} = \sum_{\sigma}\int\left(\frac{\hbar^2}{2m}\nabla\hat{\Psi}_{\sigma}^{\dagger}(r)\nabla\hat{\Psi}_{\sigma}(r) - \mu\right)dr - \frac{\hbar^2}{m}g(a, r_e)\int \hat{\Psi}_{\uparrow}^{\dagger}(r)\hat{\Psi}_{\downarrow}^{\dagger}(r)\hat{\Psi}_{\downarrow}(r)\hat{\Psi}_{\uparrow}(r)dr$$

Feshbach resonance

$$\left|m_J = m_S\,, m_I\right\rangle$$

$$|3\rangle = \left|-\frac{1}{2}, -1\right\rangle$$

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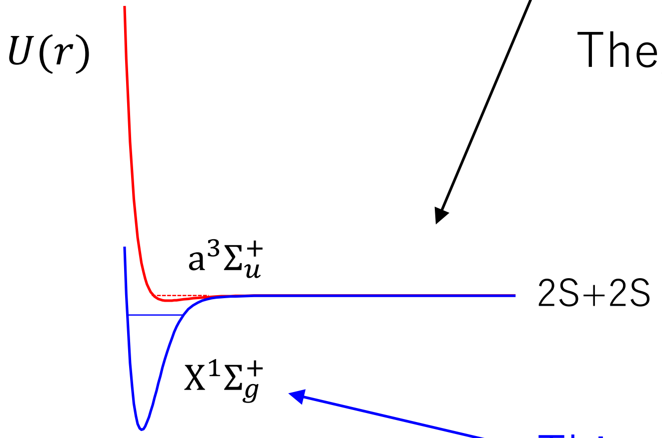
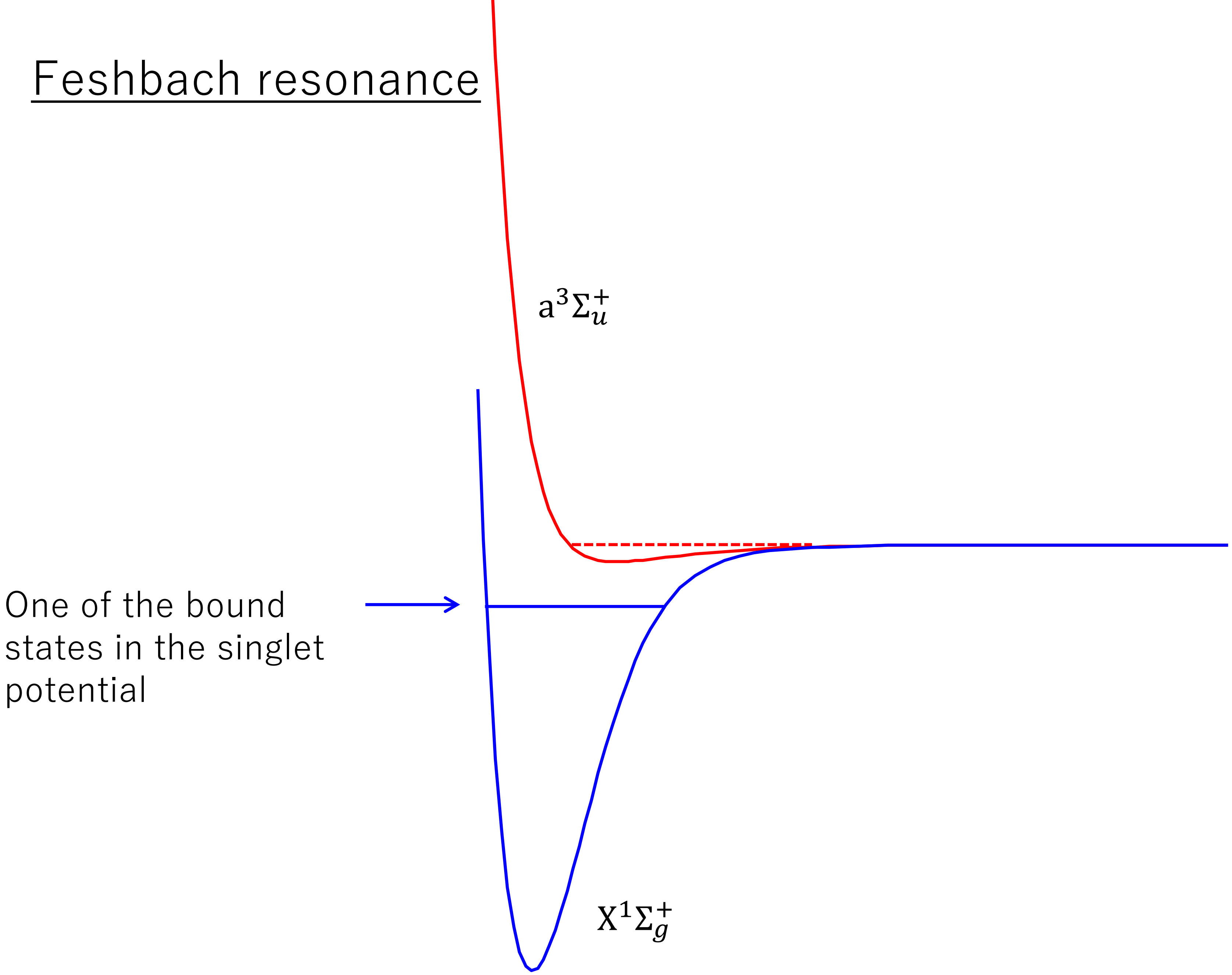
Electric ground state
Combination of them is spin triplet

They interact with this spin triplet potential

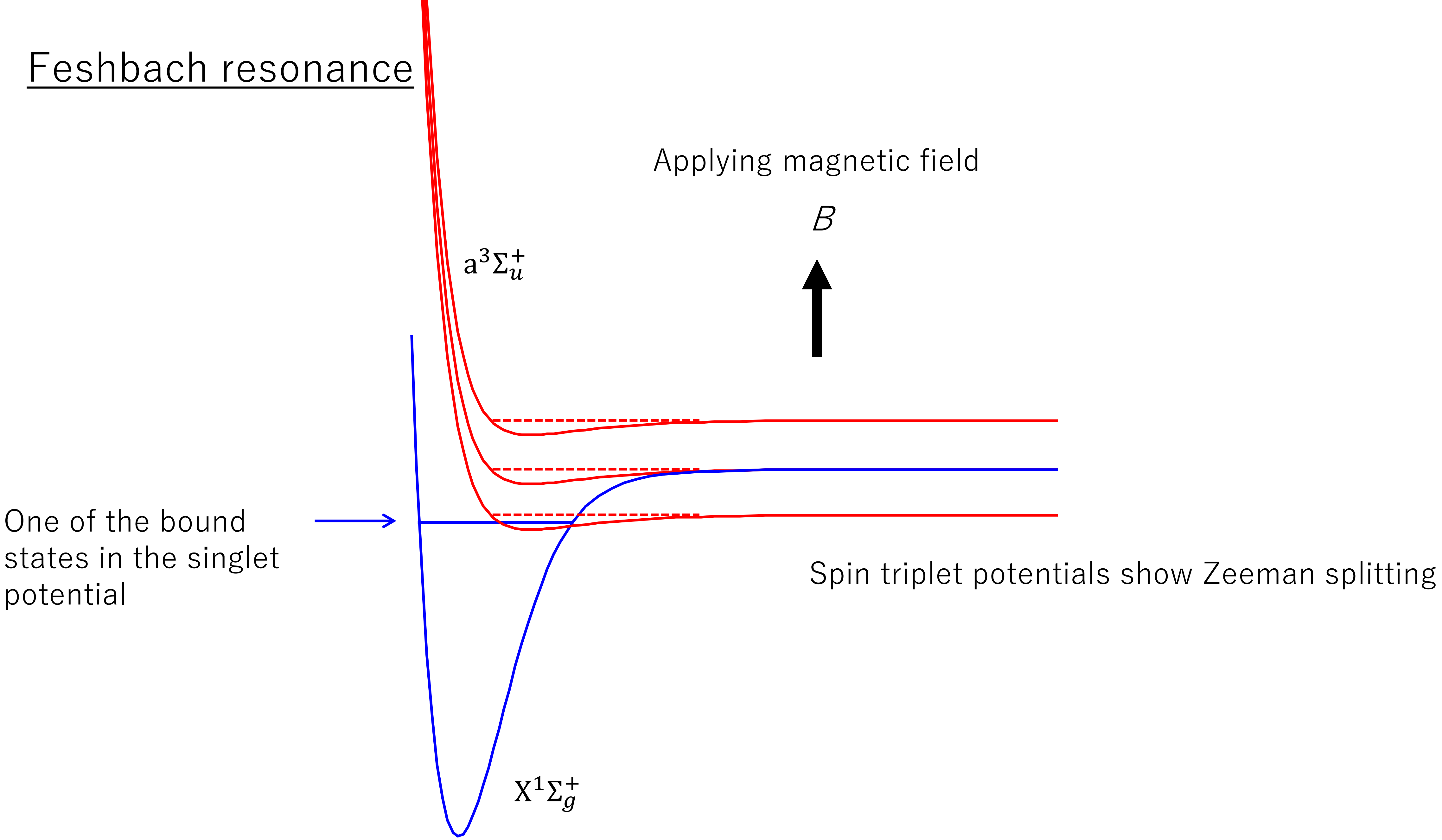


This spin singlet potential gives dramatic effect

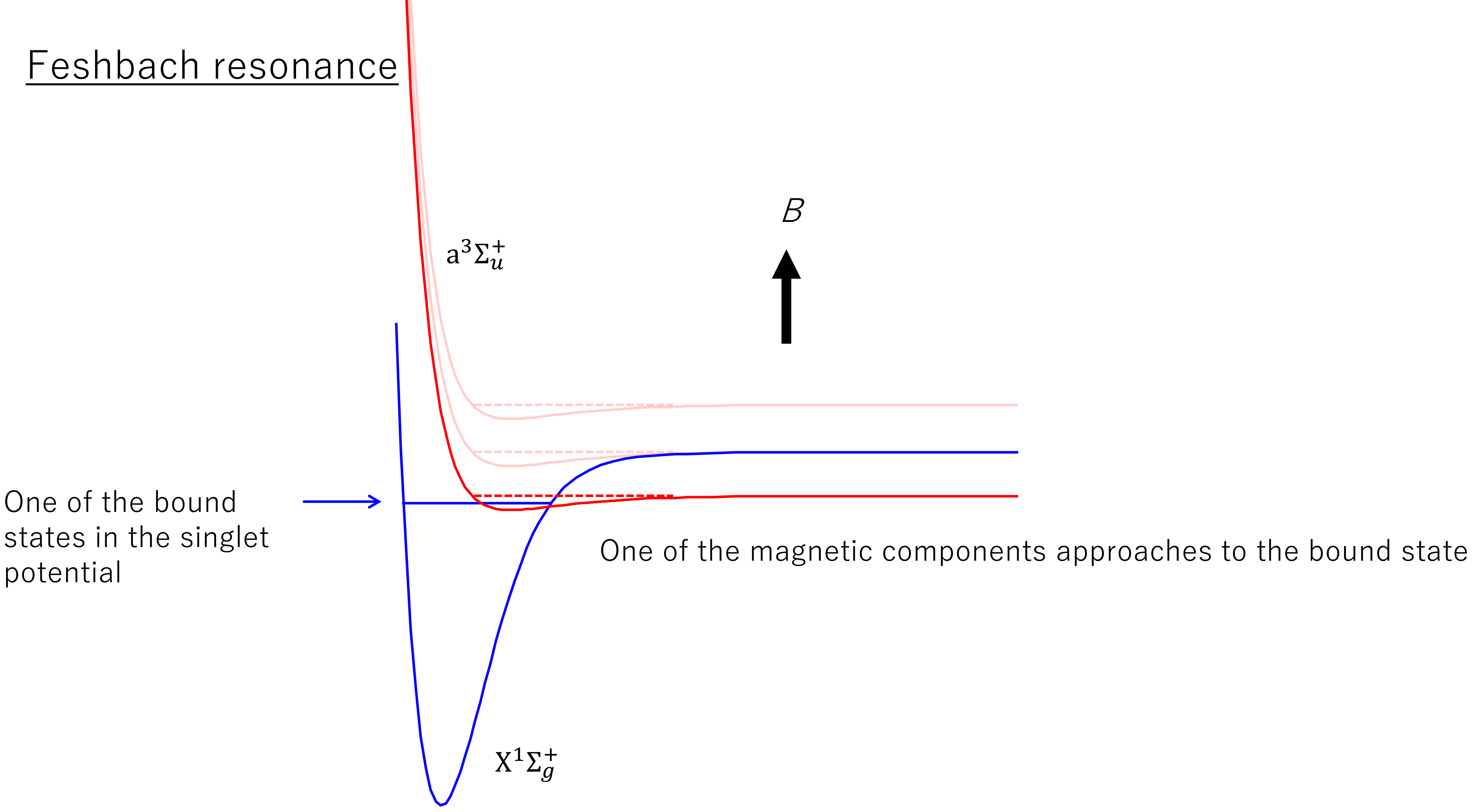
Feshbach resonance



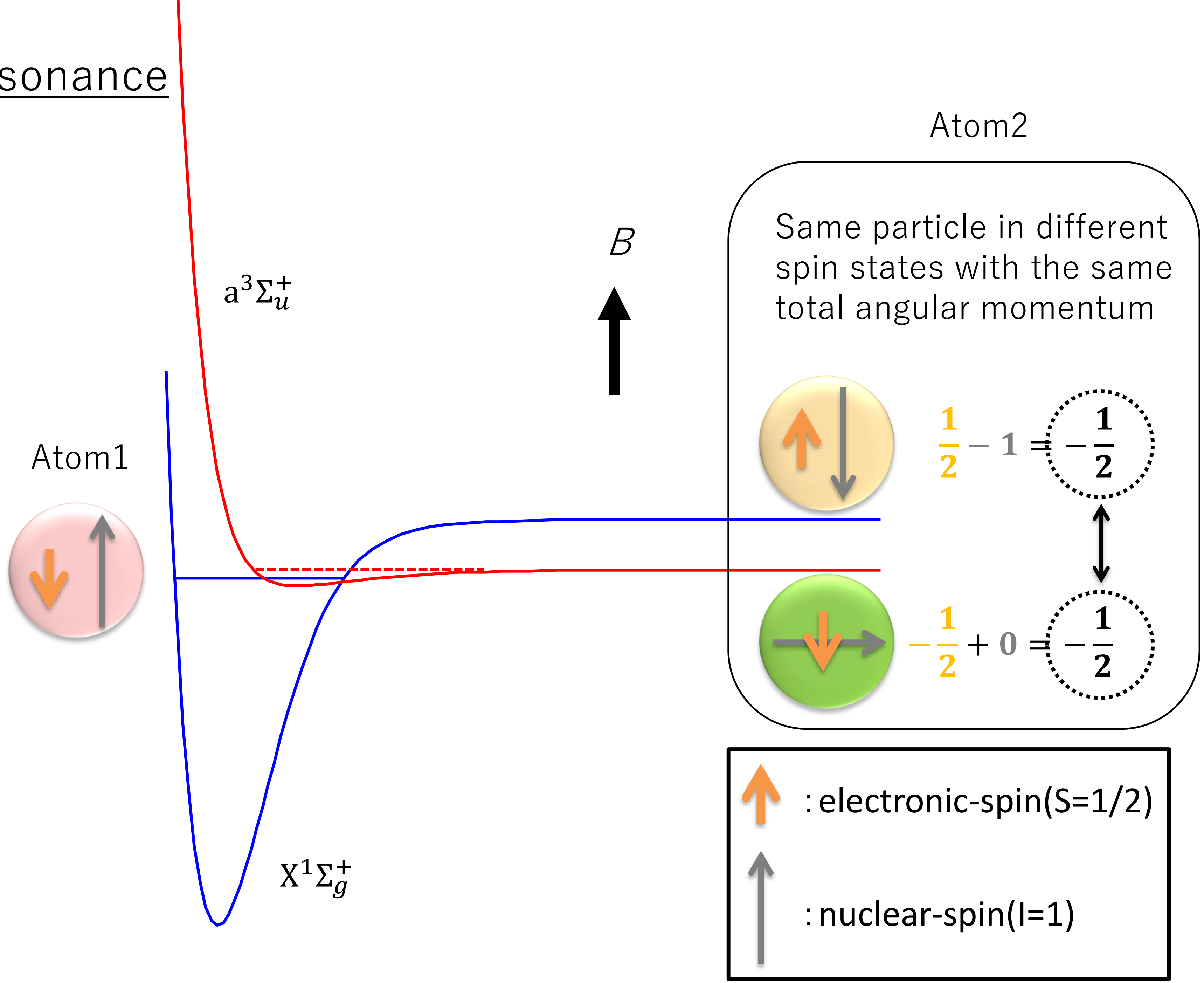
Feshbach resonance



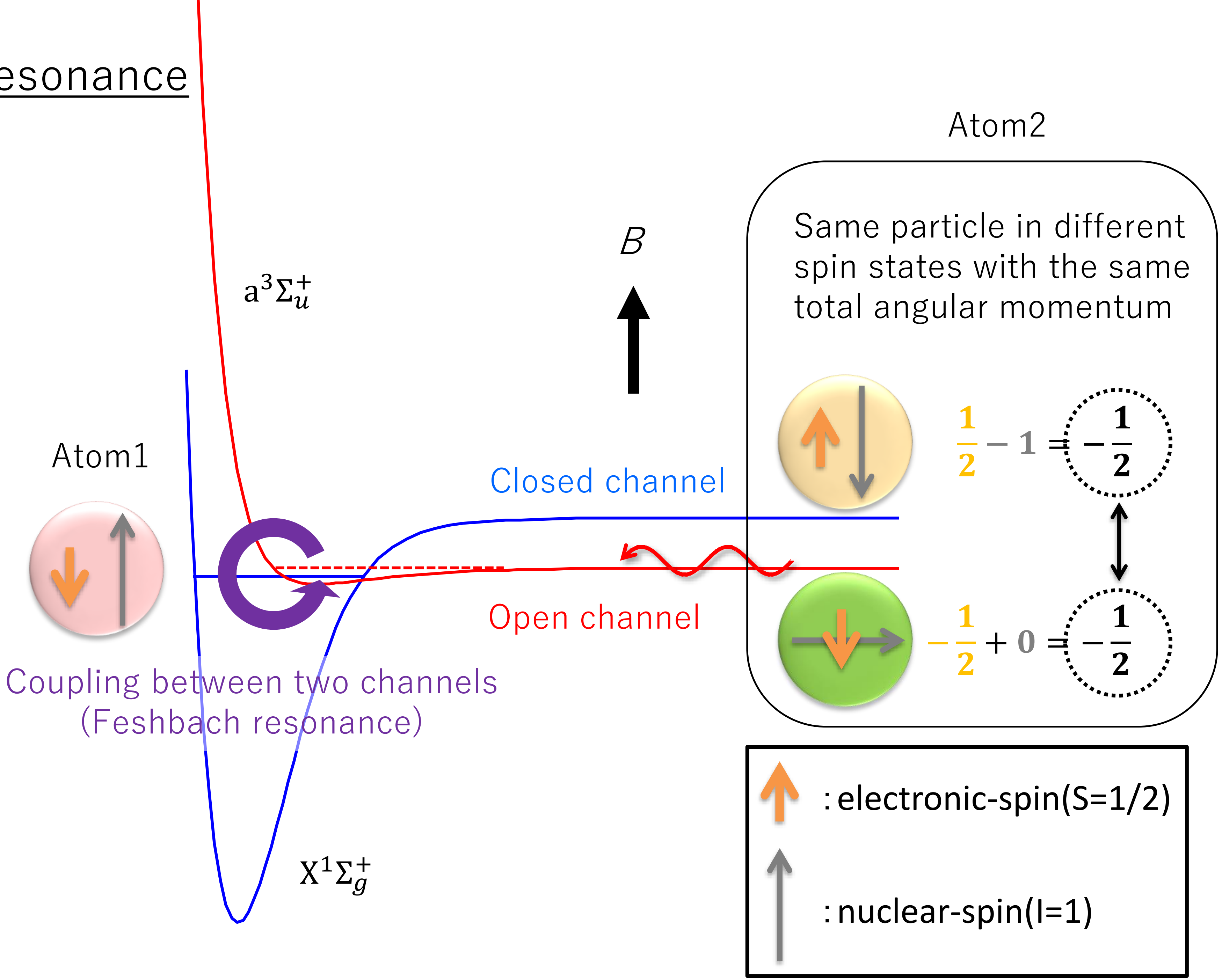
Feshbach resonance



Feshbach resonance



Feshbach resonance



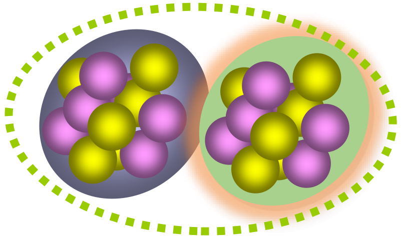
Feshbach resonance in nuclear physics (from presentation by Y. Sakuragi)

Nogami-Imanish model

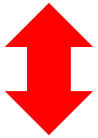
M. Nogami, private comm.(1969)
B. Imanishi, Nucl. Phys. **A125** (1969), 33.

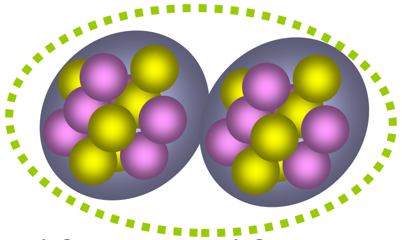
"Feshbach resonance"

Coupling between Internal excitation and external freedom

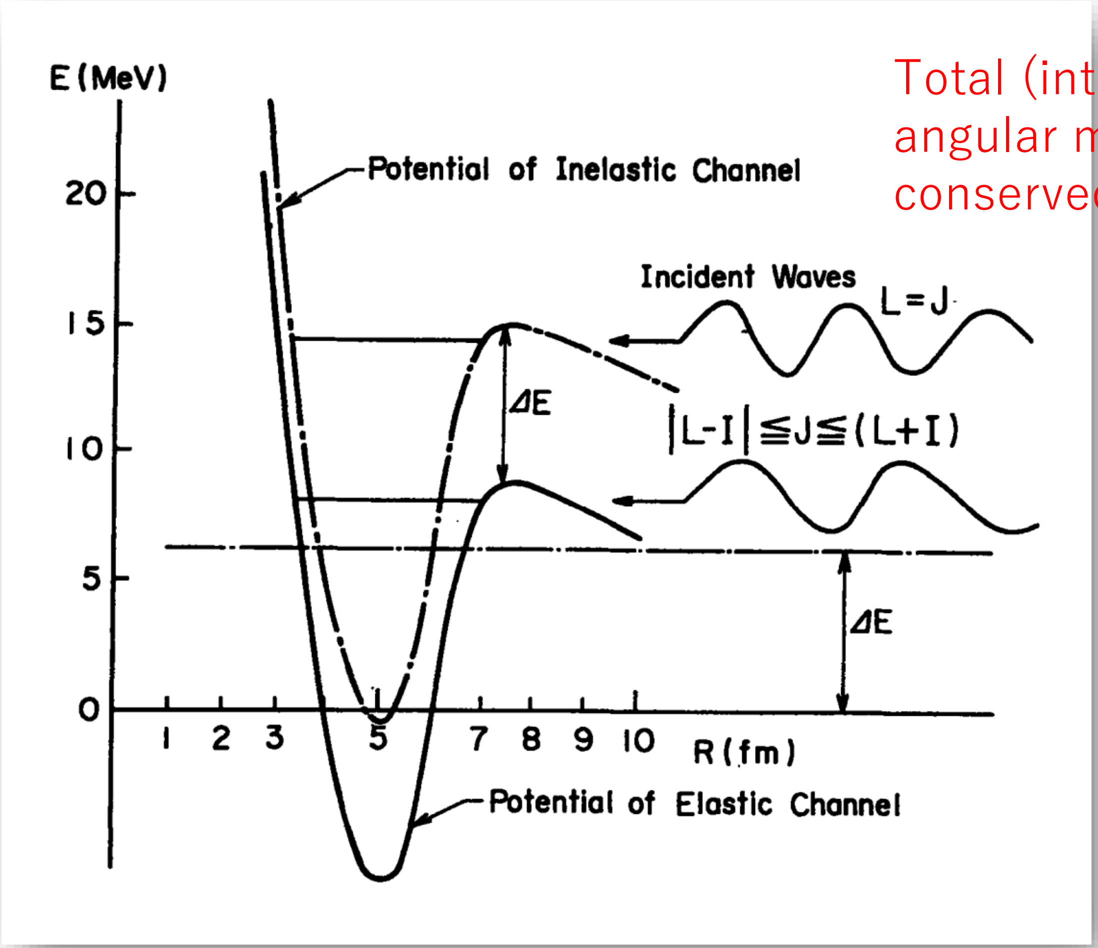


$^{12}C + {}^{12}C^{*}(E_x = \Delta E)$





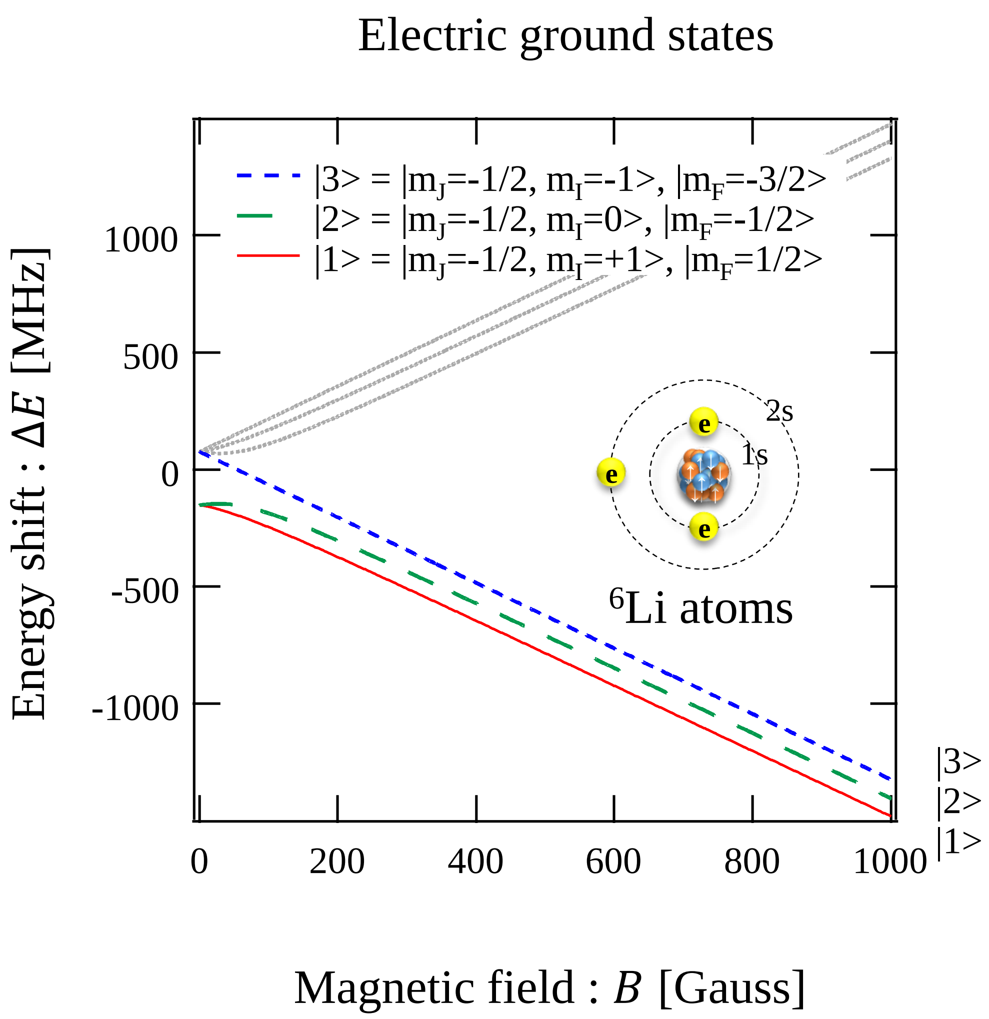
$^{12}C + {}^{12}C$(g.s.)

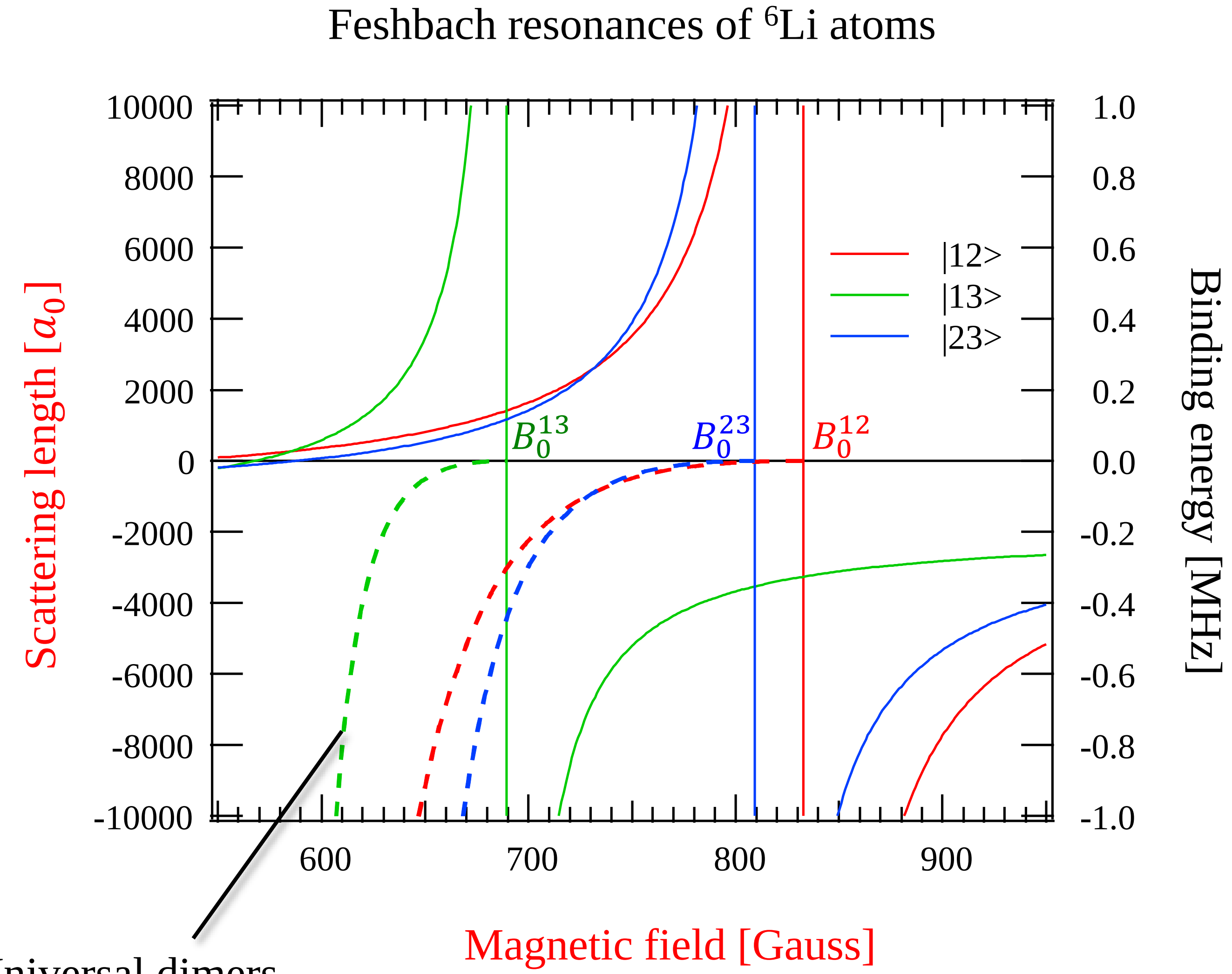


Total (internal+external) angular momentum is conserved

Y. Abe, Y. Kondo, T. Matsuse, *Prpg. Theor. Phys, 68, 303 (1980)*

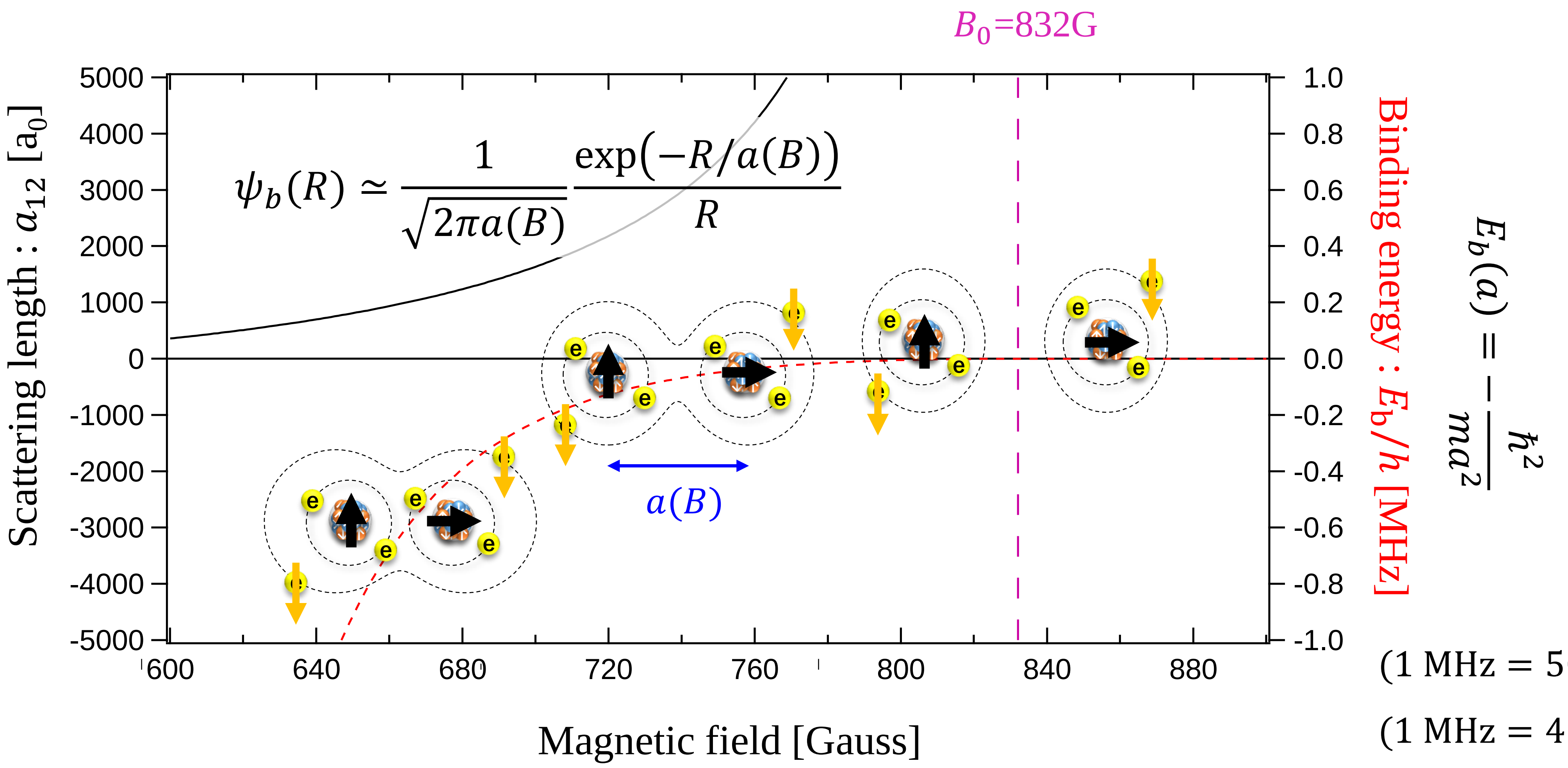
Feshbach resonance of 6Li atoms





Universal dimers
(Feshbach molecules)

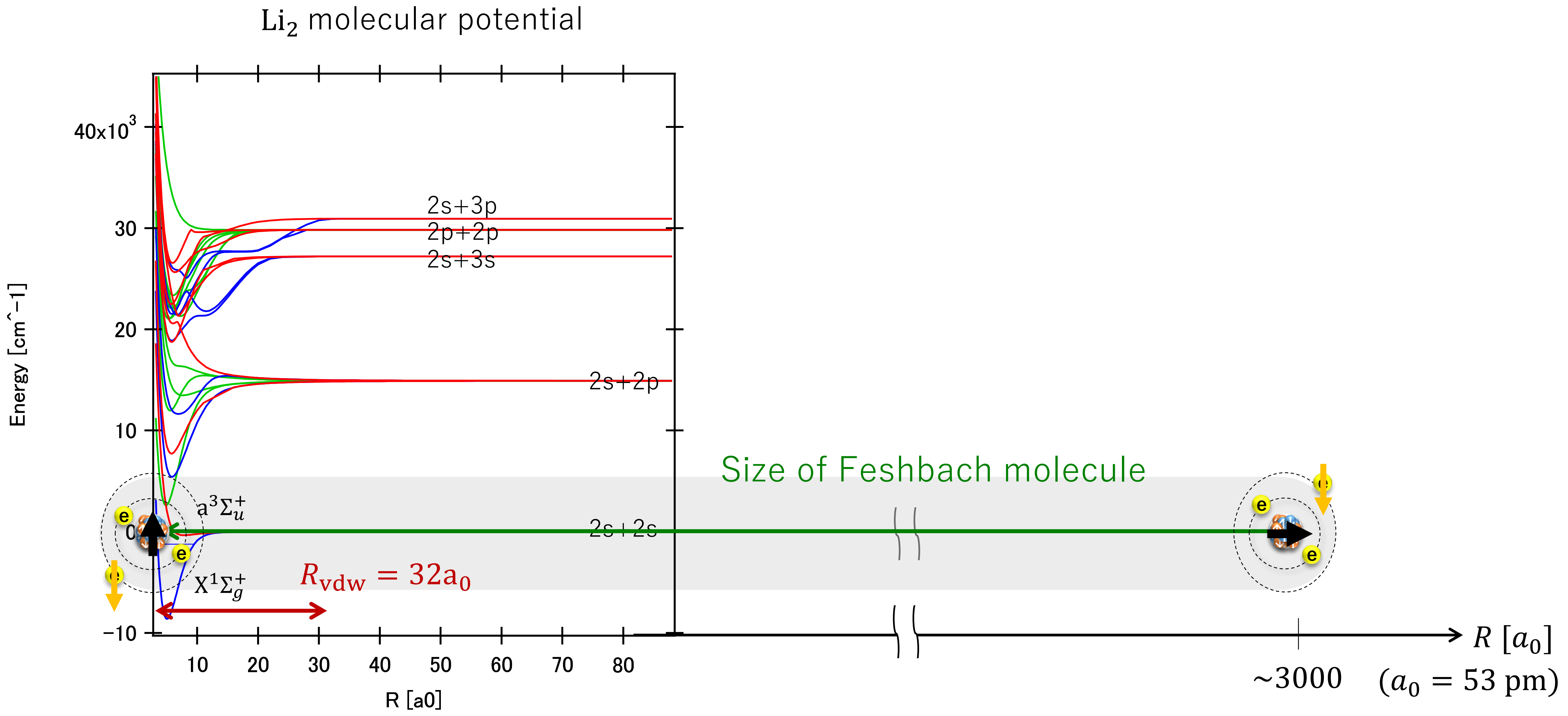
Feshbach resonance between |1⟩ and |2⟩ of ^{6}Li atom



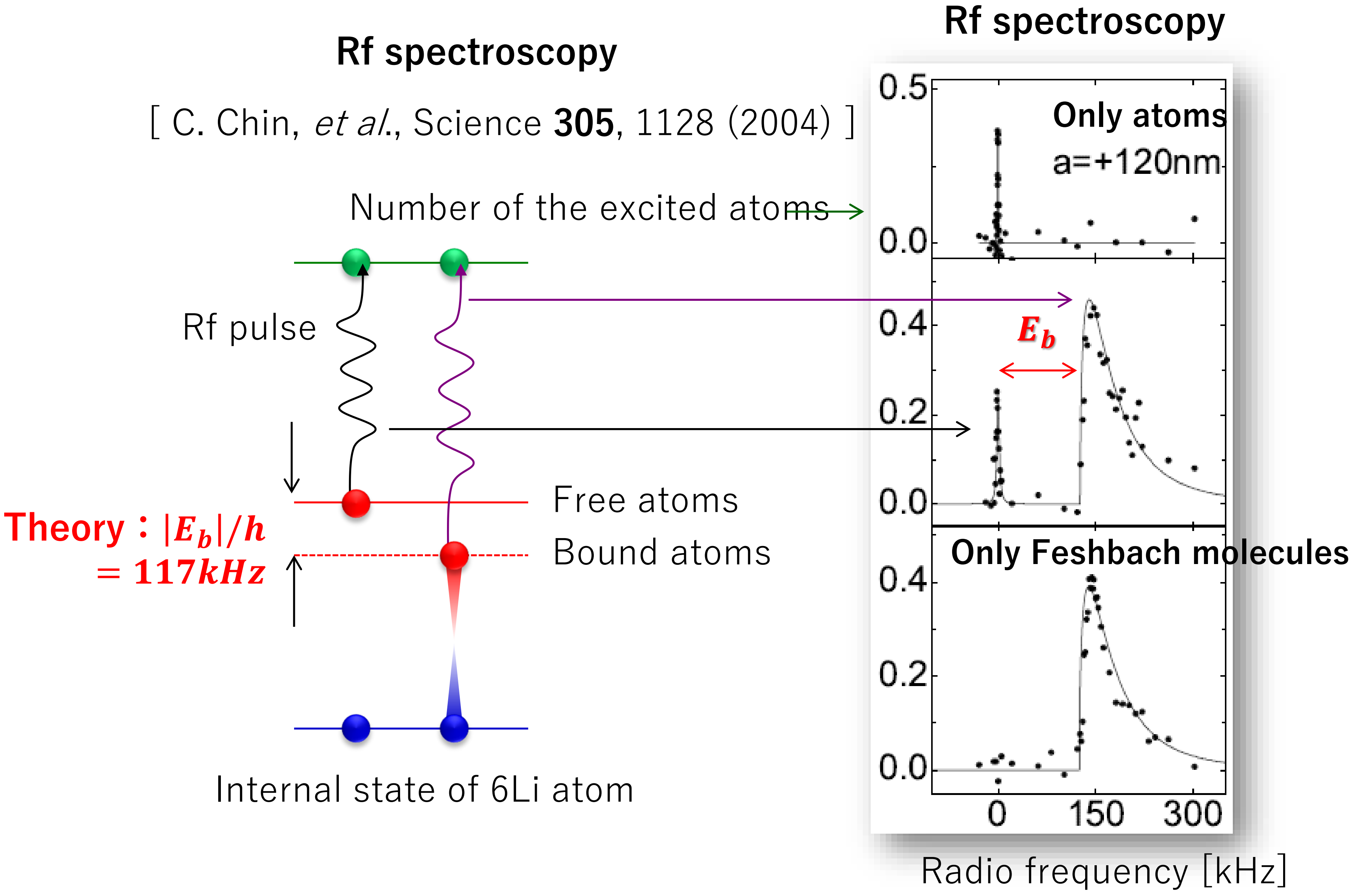
(1 MHz = 50 μK)

(1 MHz = 4 neV)

Size of Feshbach molecules are huge

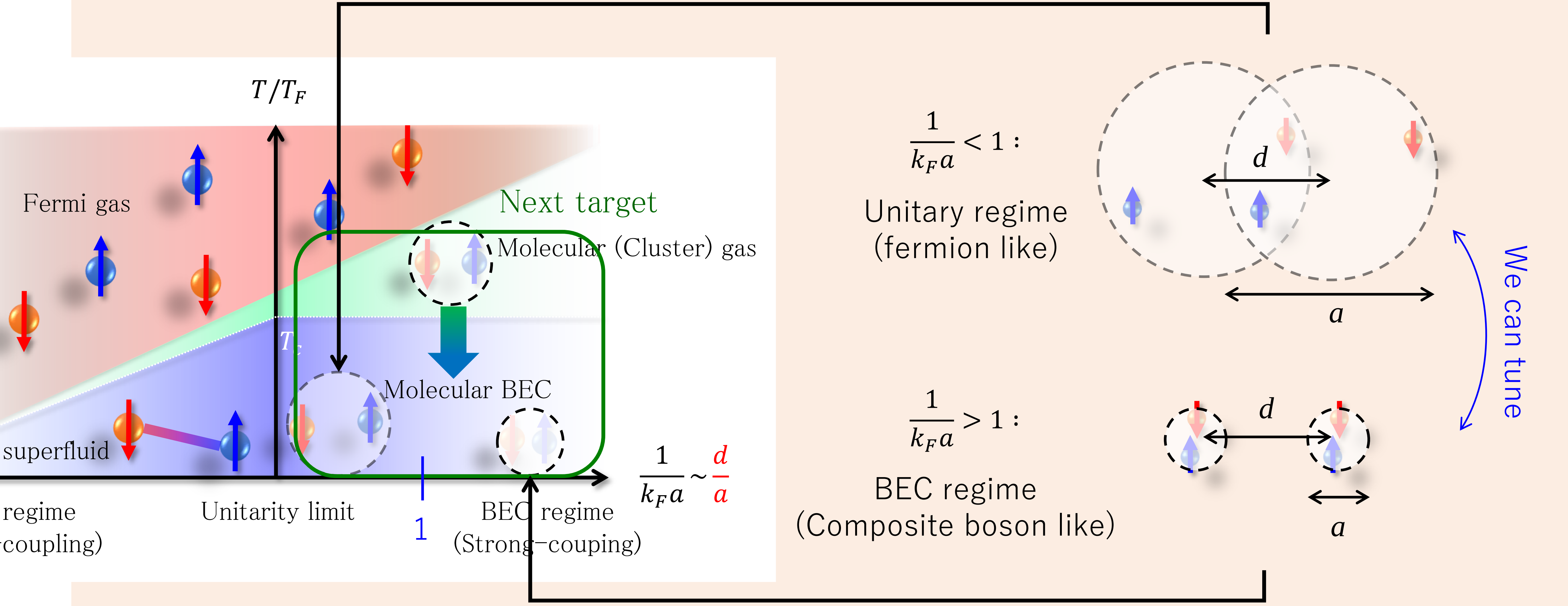


Previous experiment to confirm the Feshbach molecules



Our interest in Ultracold AMO Physics

Ideal condition to study a many-body system of quantum clusters



Contens

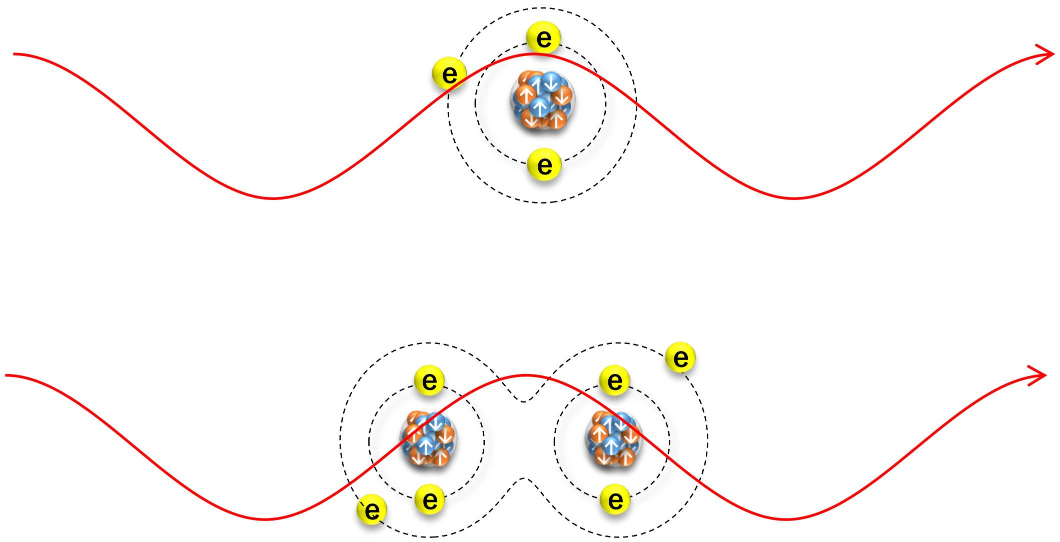
- Background of Ultracold AMO physics
- Road from Complex molecular potentials to Universal Feshbach molecules
- Absorption spectroscopy of Feshbach molecules

Absorption spectroscopy of Feshbach molecules

Motivation

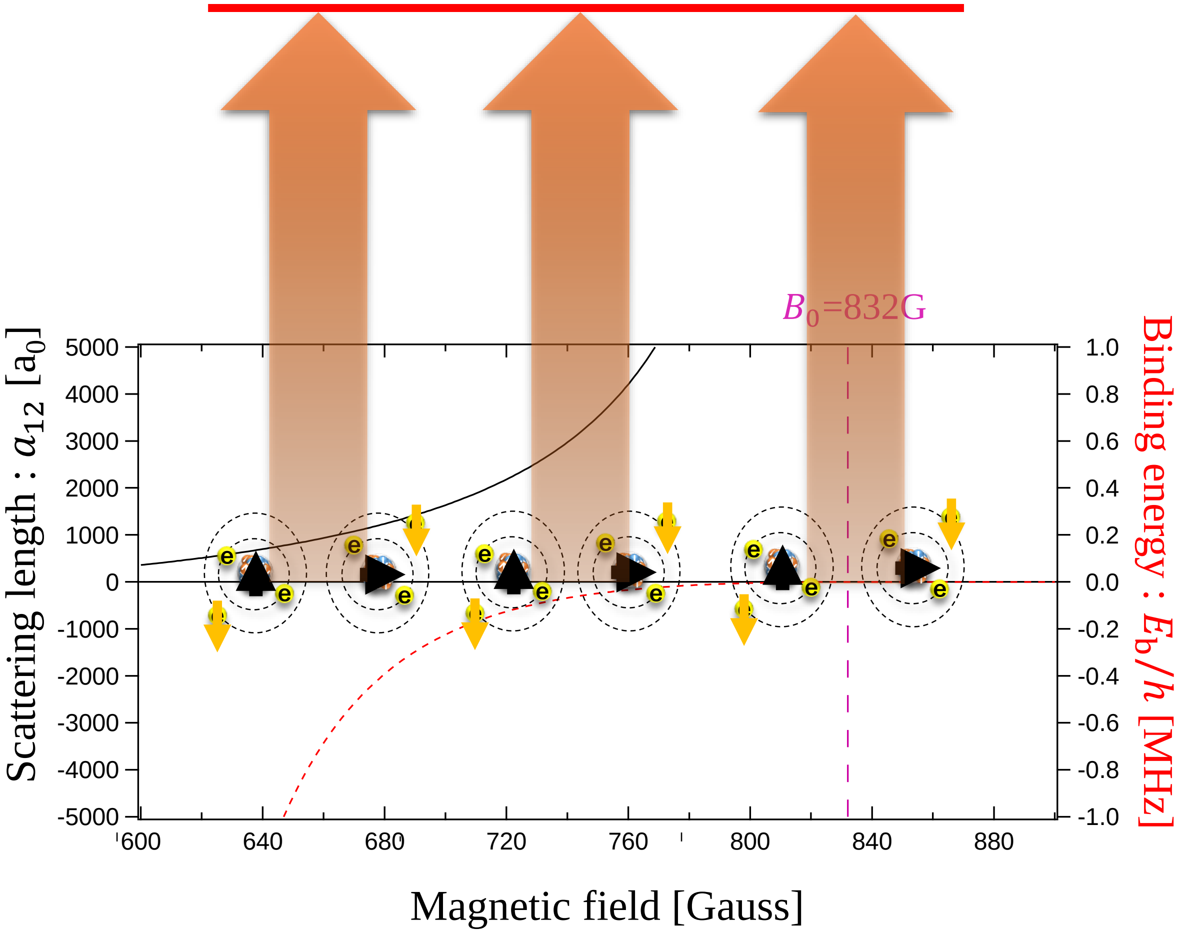
1. How does optical dipole transition change when particles associate clusters?
   Are there some universal rule?

2. Optical response is important for precision measurement of cold atoms.

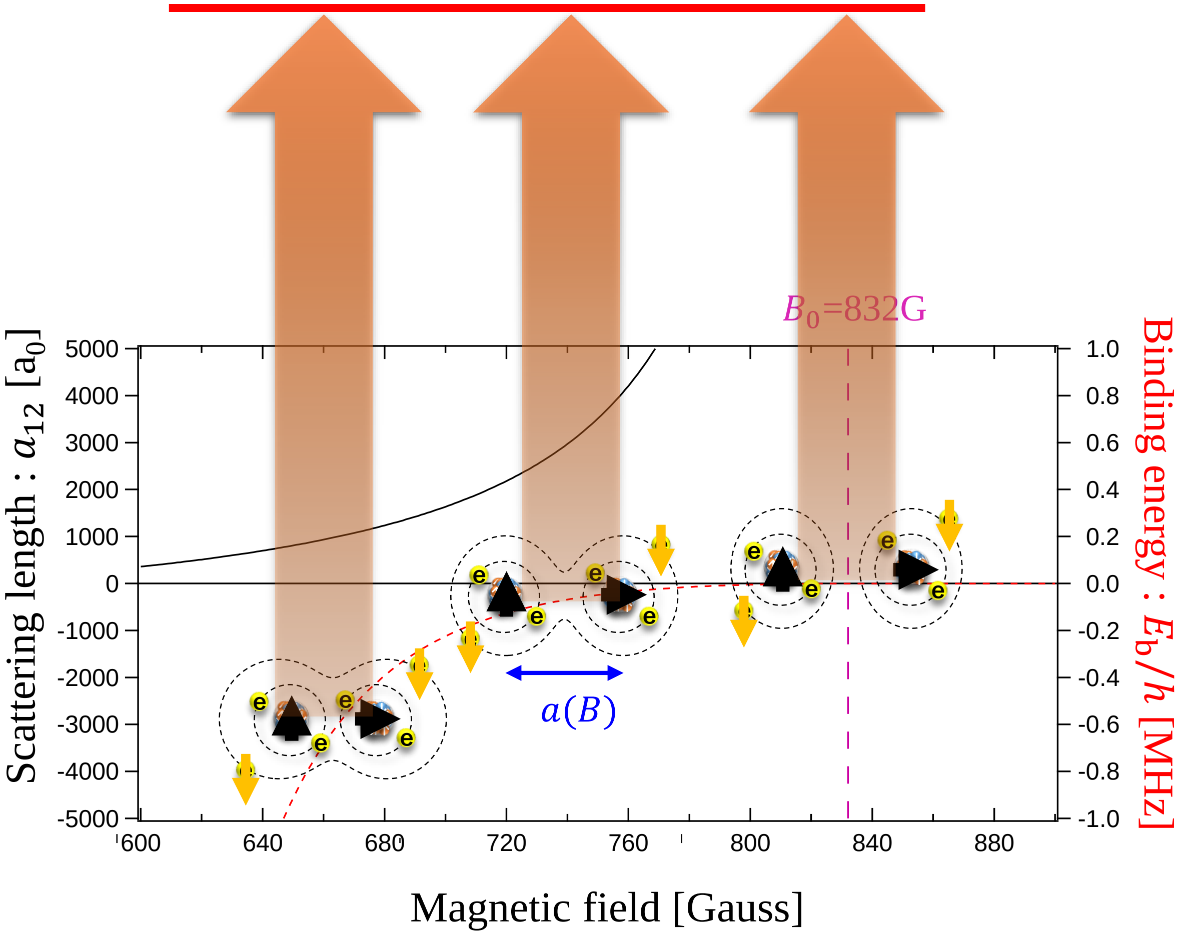


Method

Electronically excited states



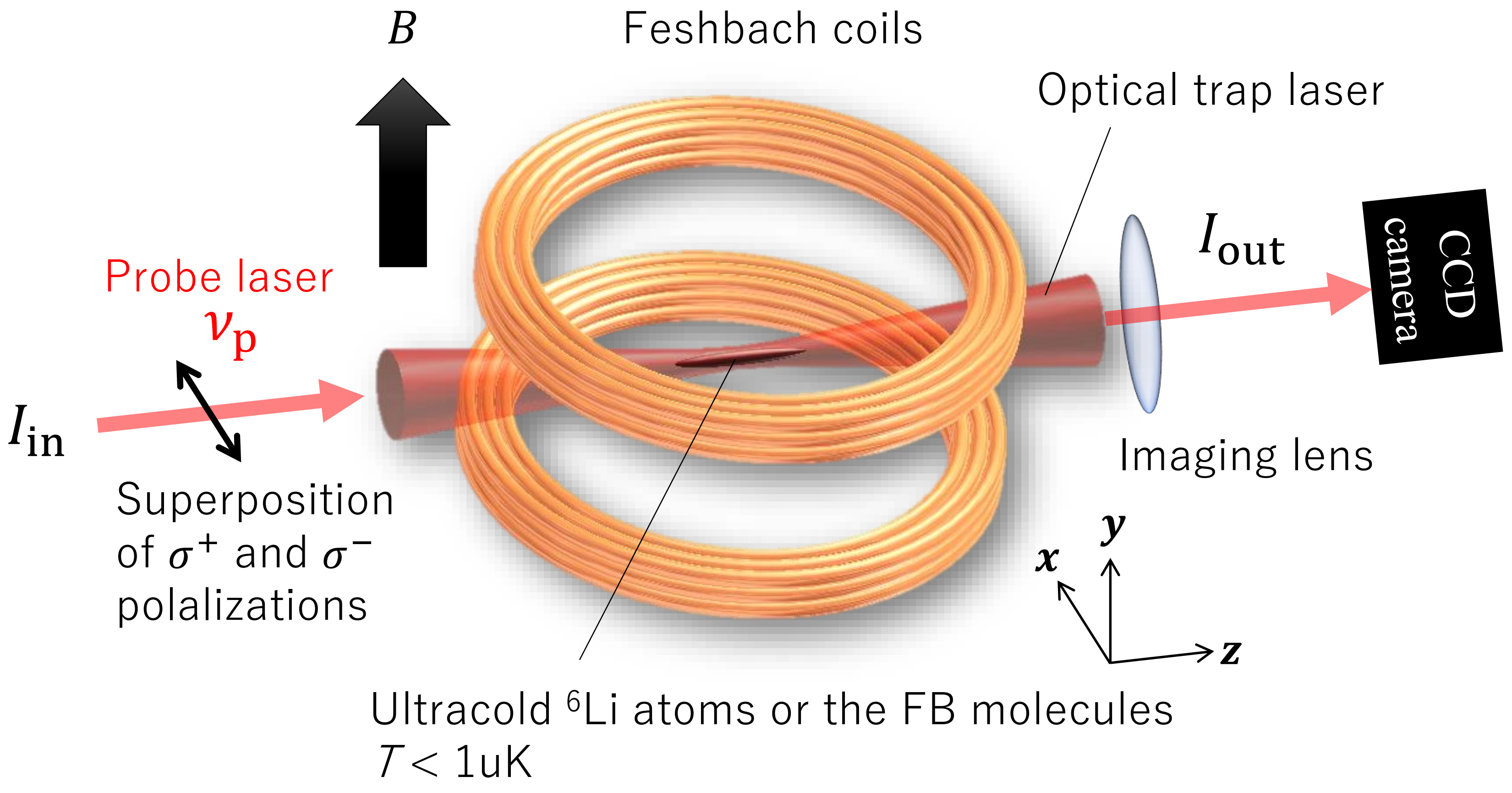
Atoms

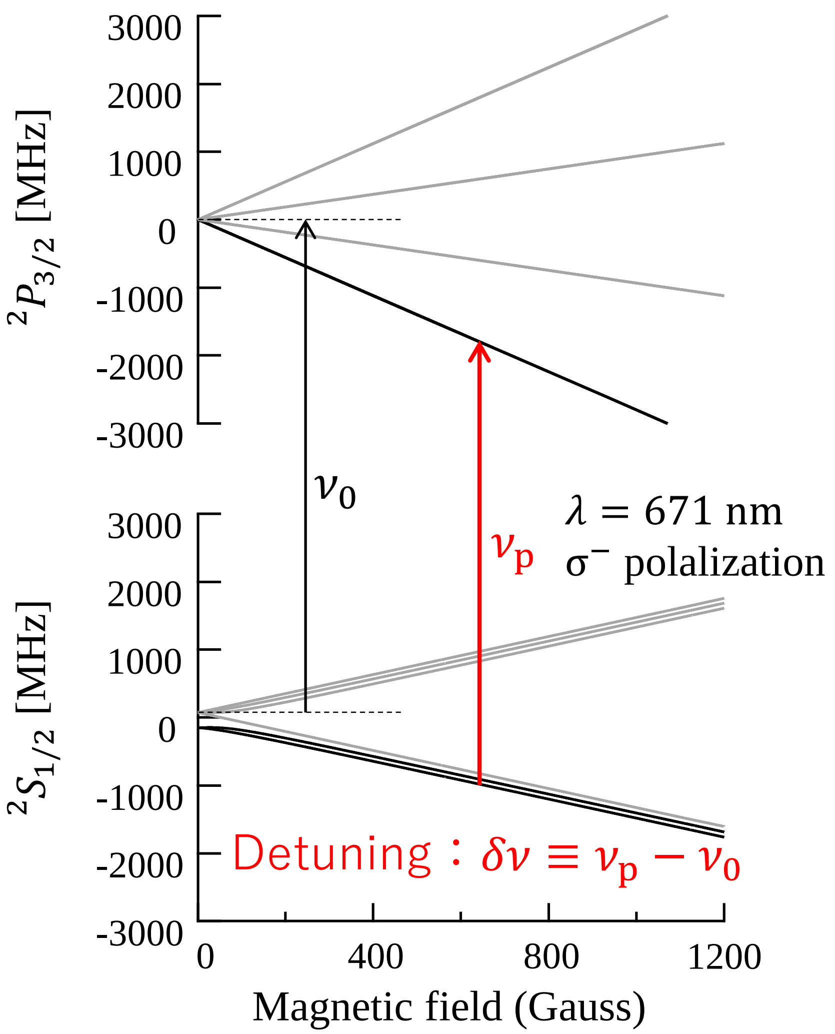


Feshbach molecules

Experimental setup

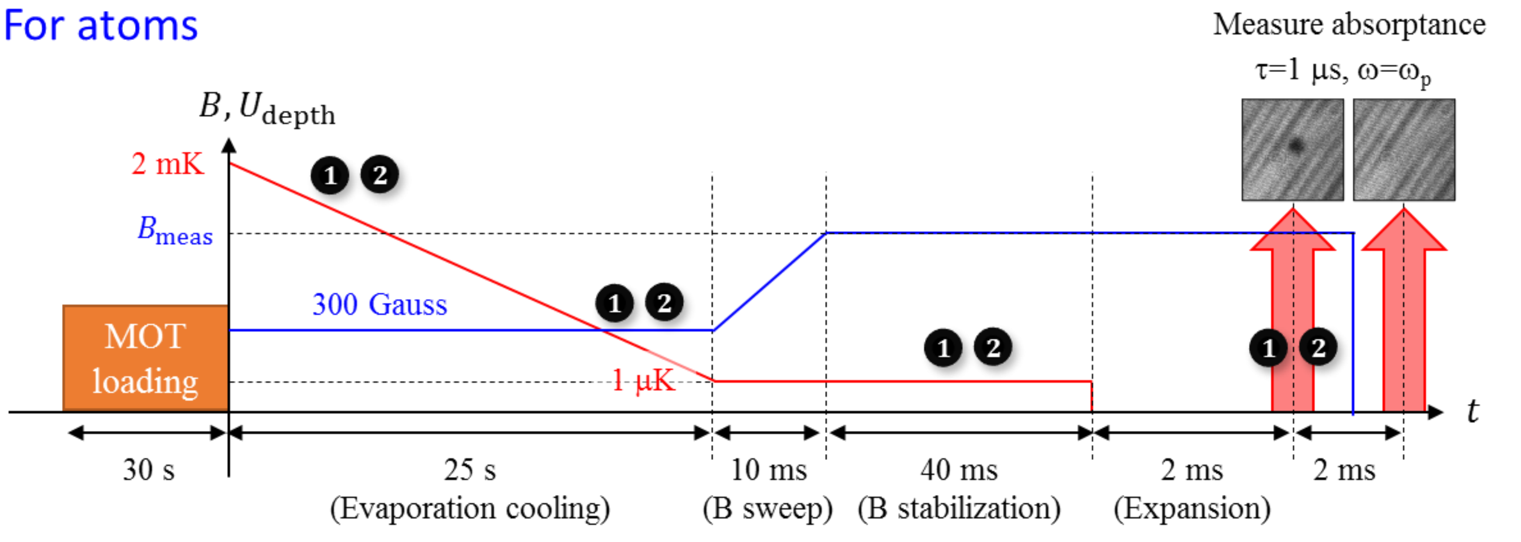
The optical density $(OD = -\log(I_{\mathrm{out}}/I_{\mathrm{in}}))$ is measured as a function of the laser frequency ν_{p} at various magnetic field



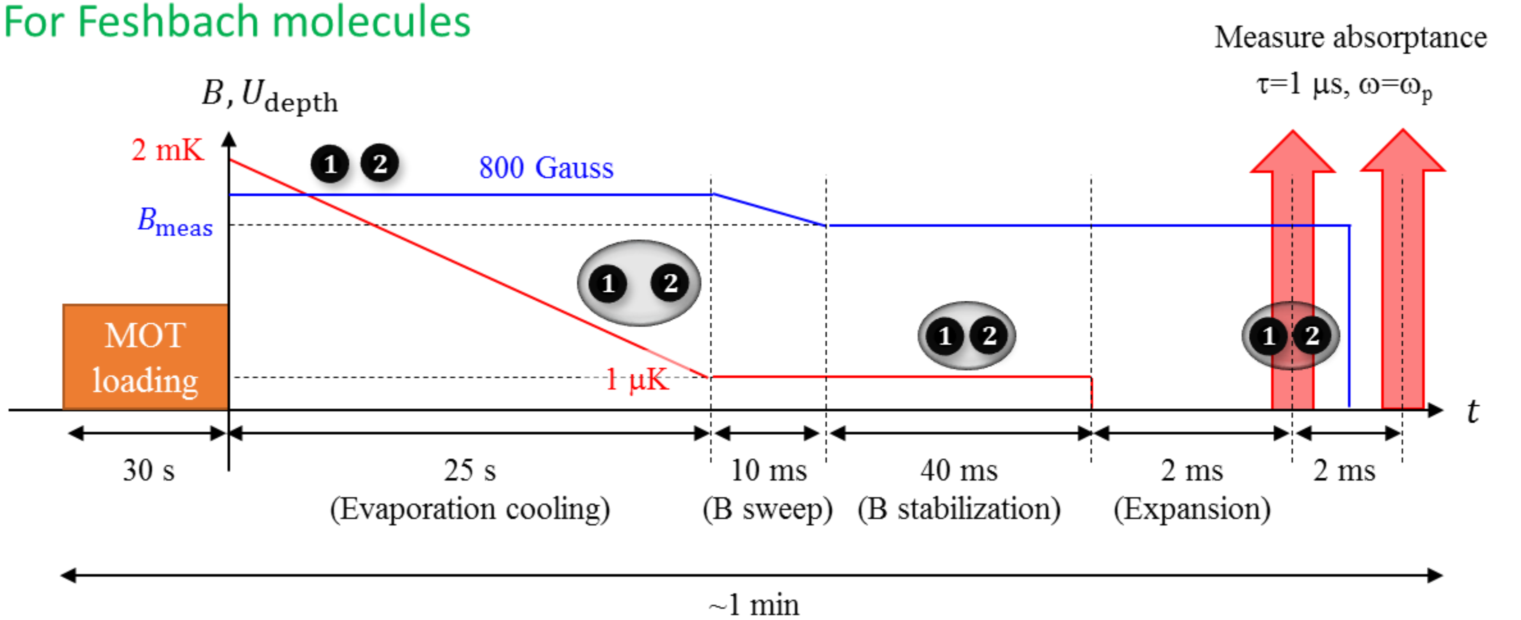


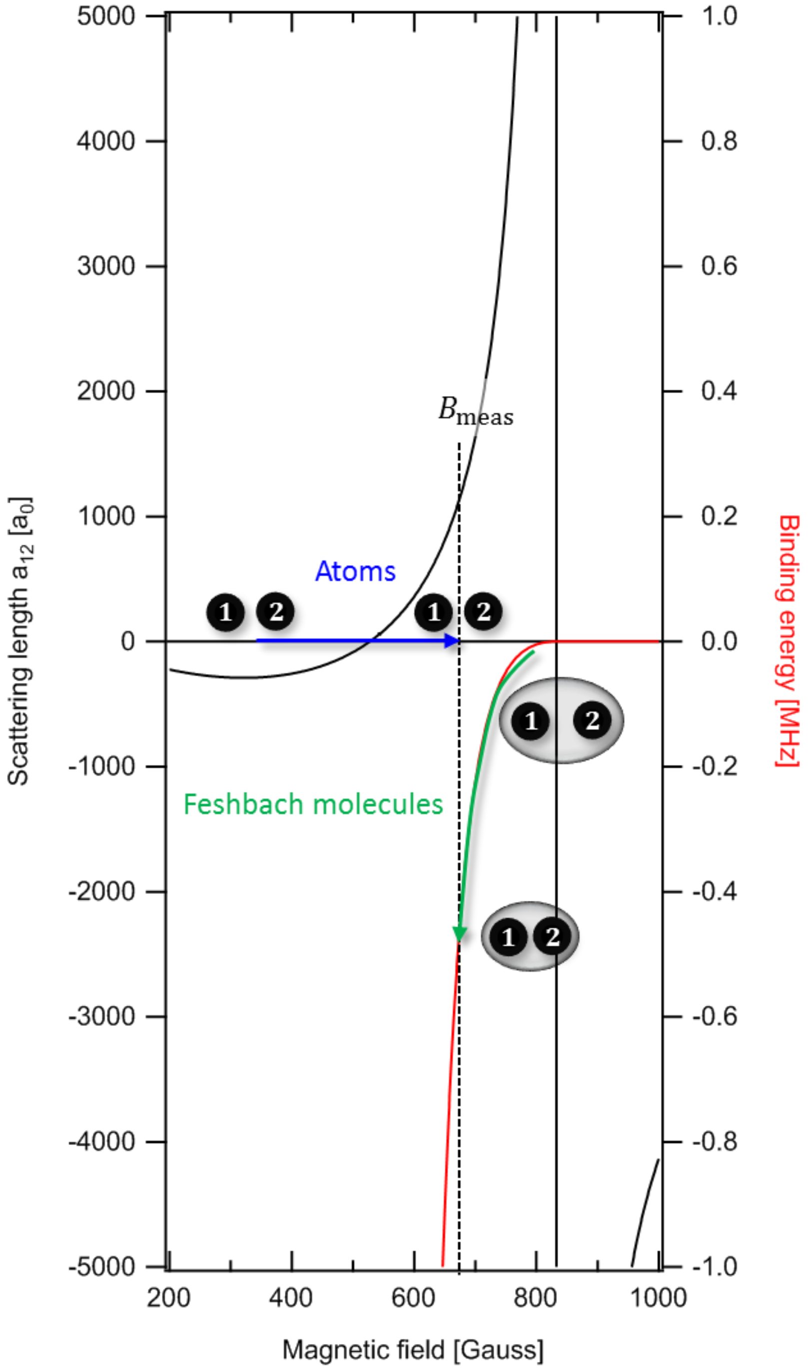
Experimental procedure

For atoms

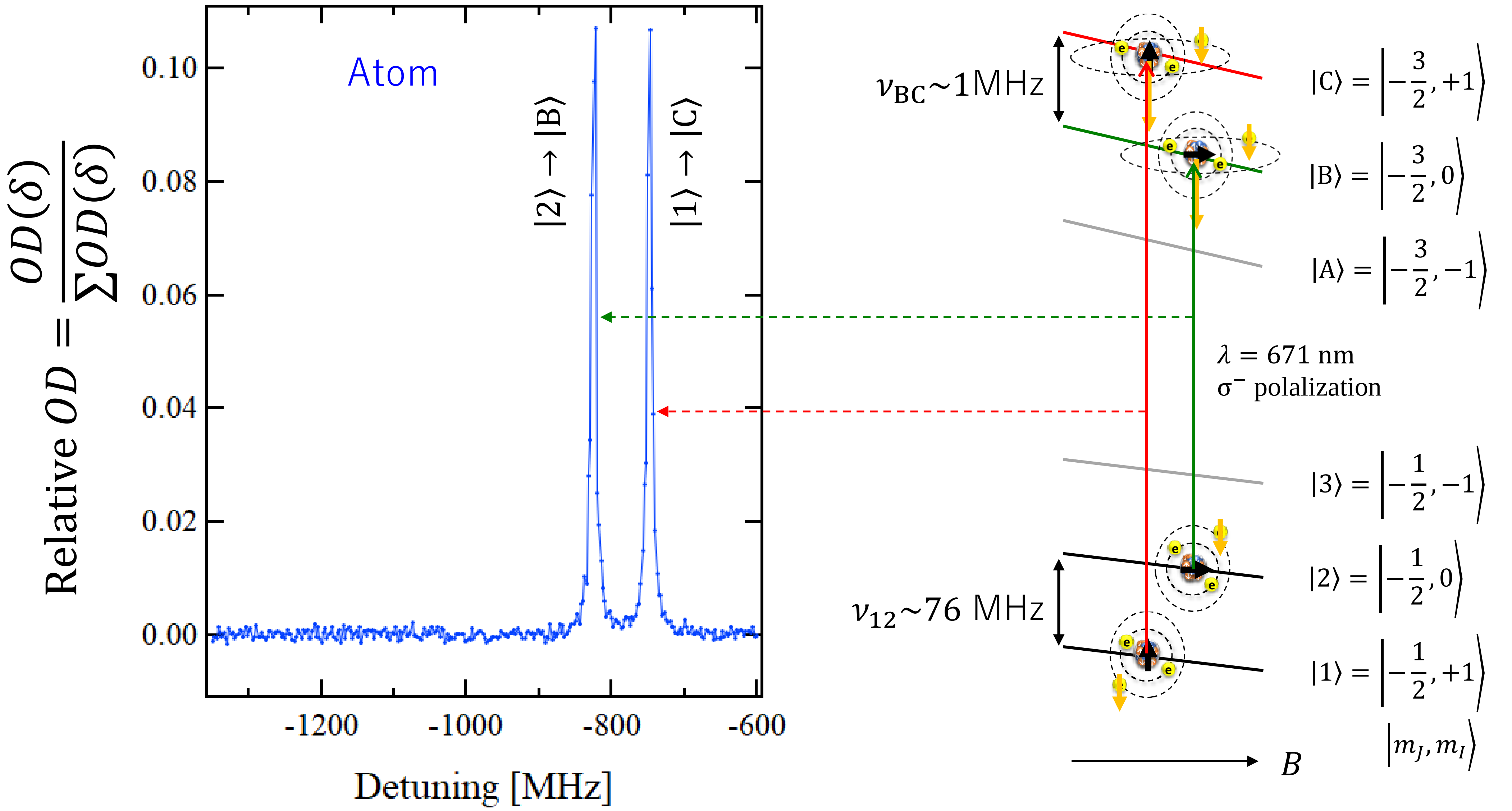


For Feshbach molecules

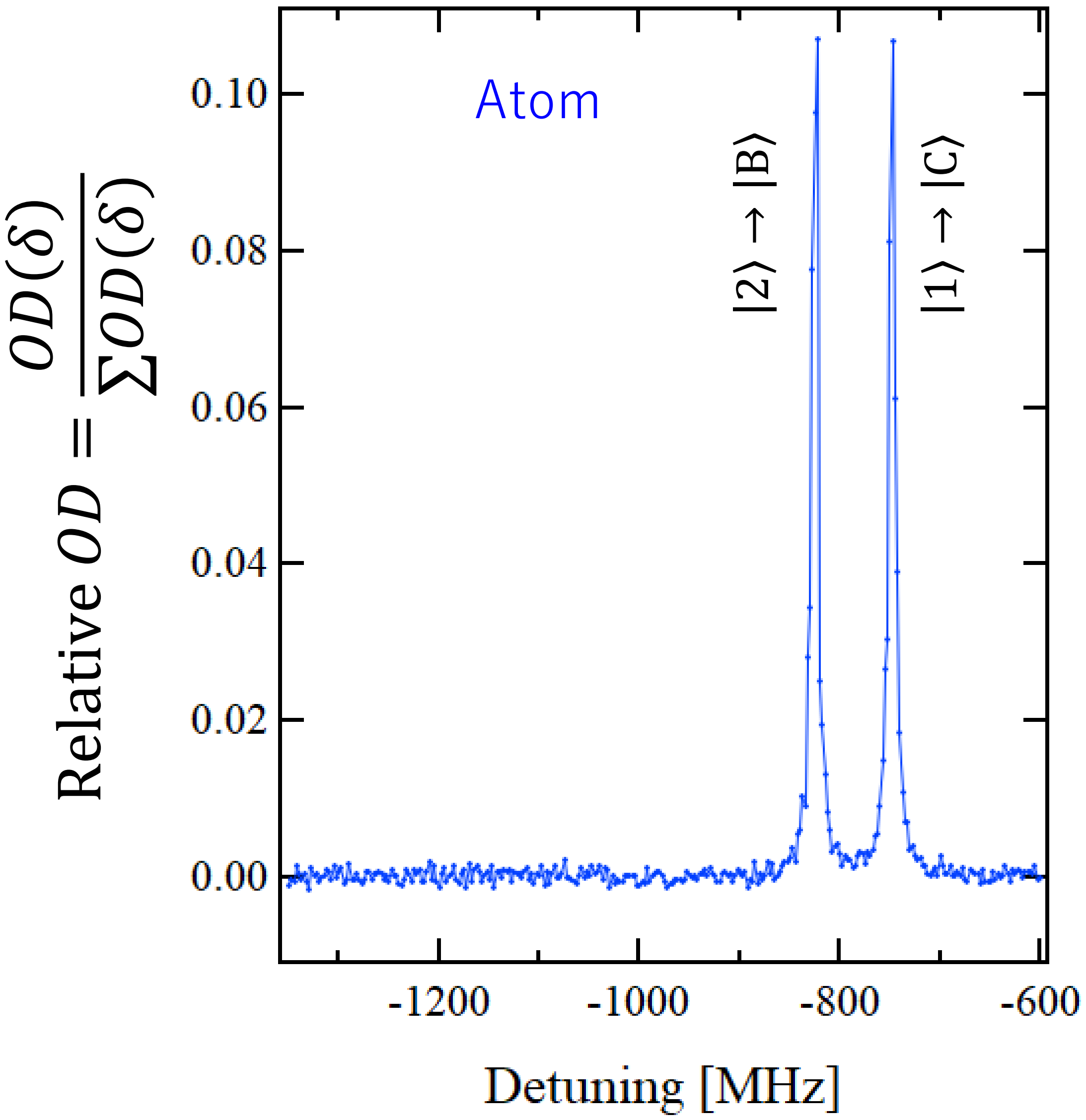


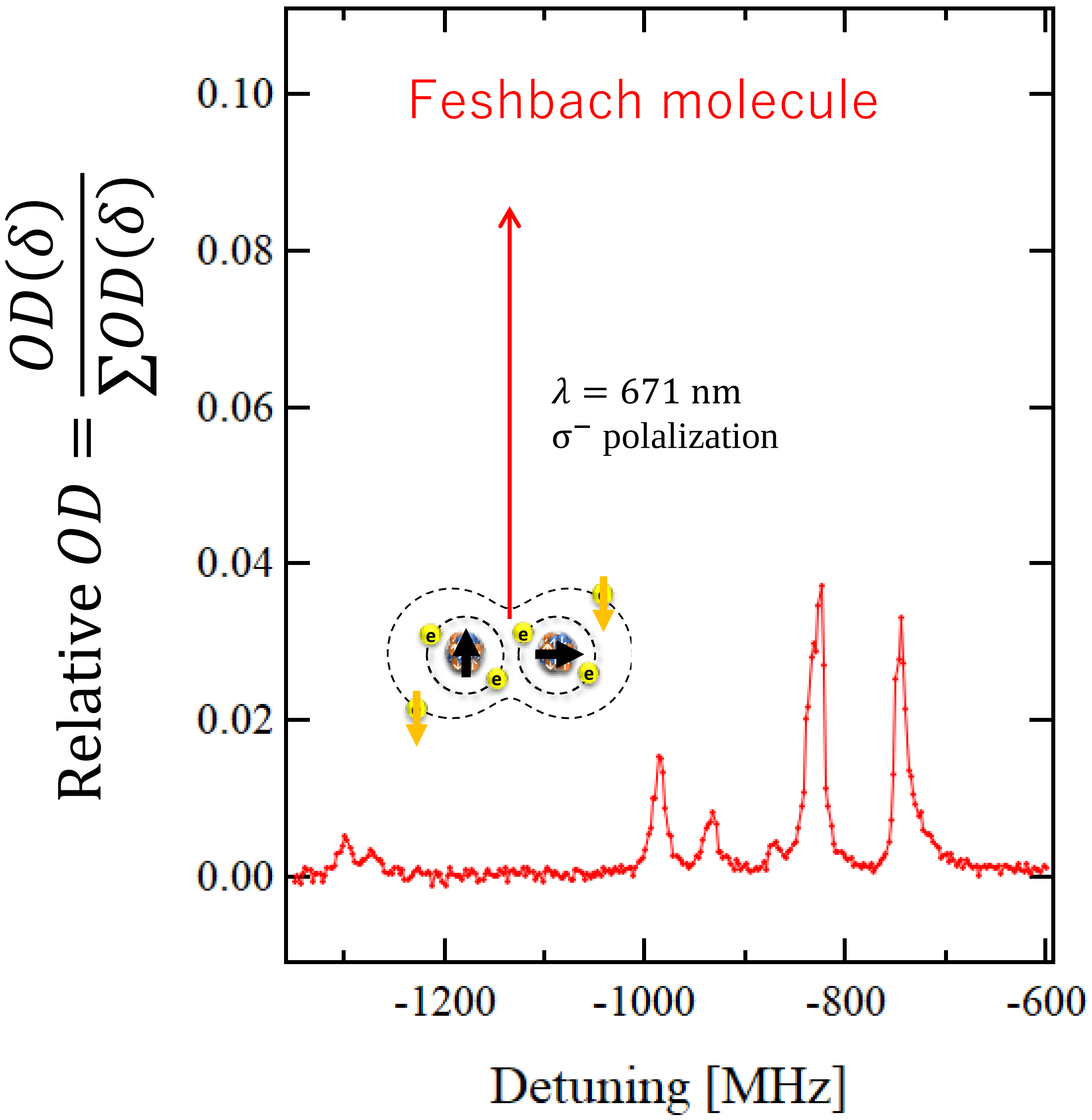


Spectral data @ 650Gauss



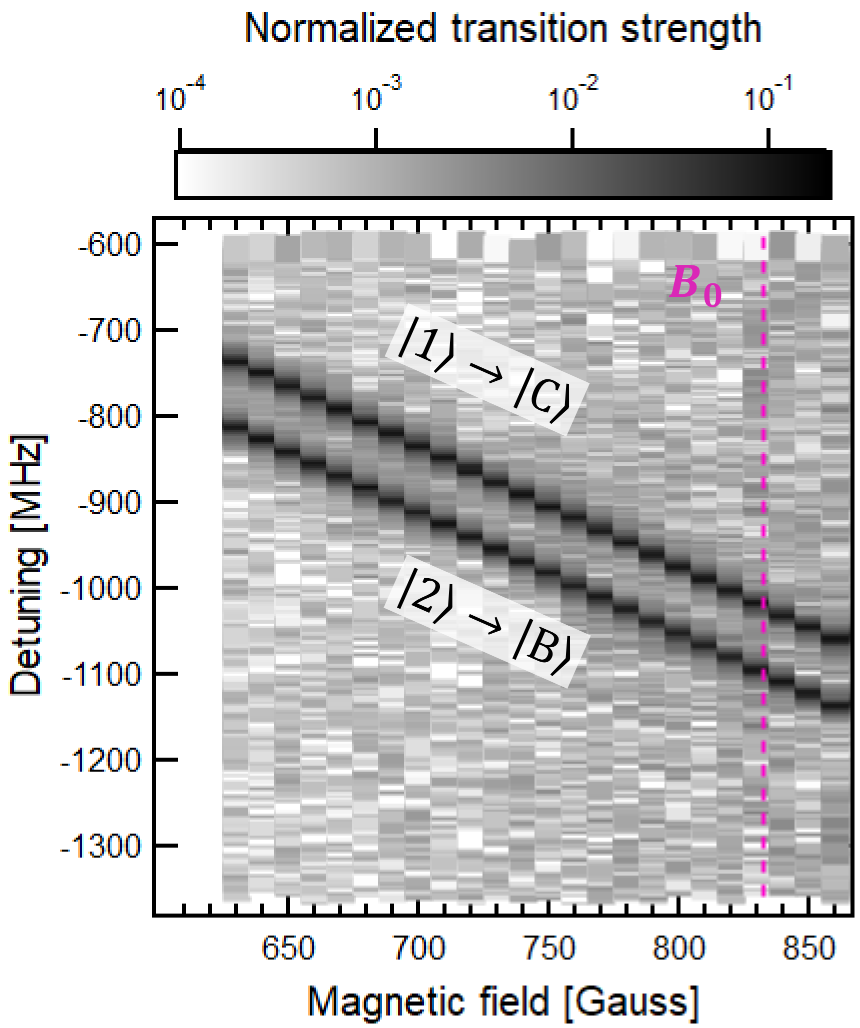
Spectral data @ 650Gauss



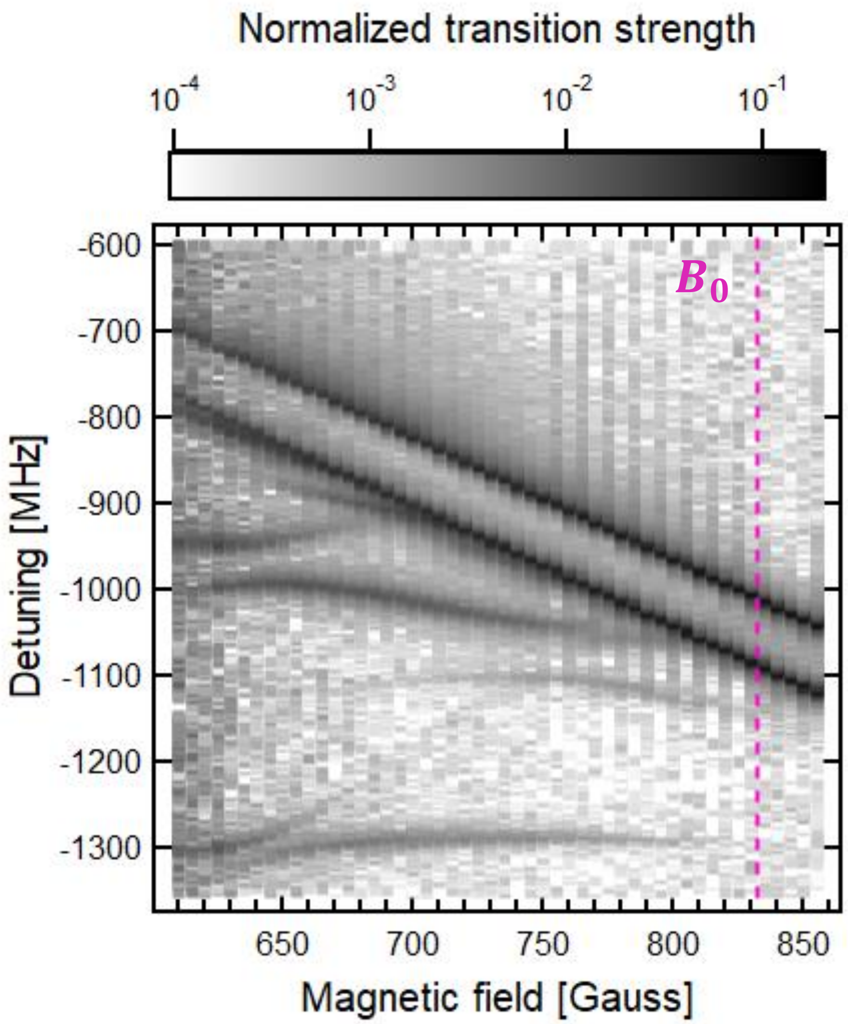


Two-dimensional spectral data

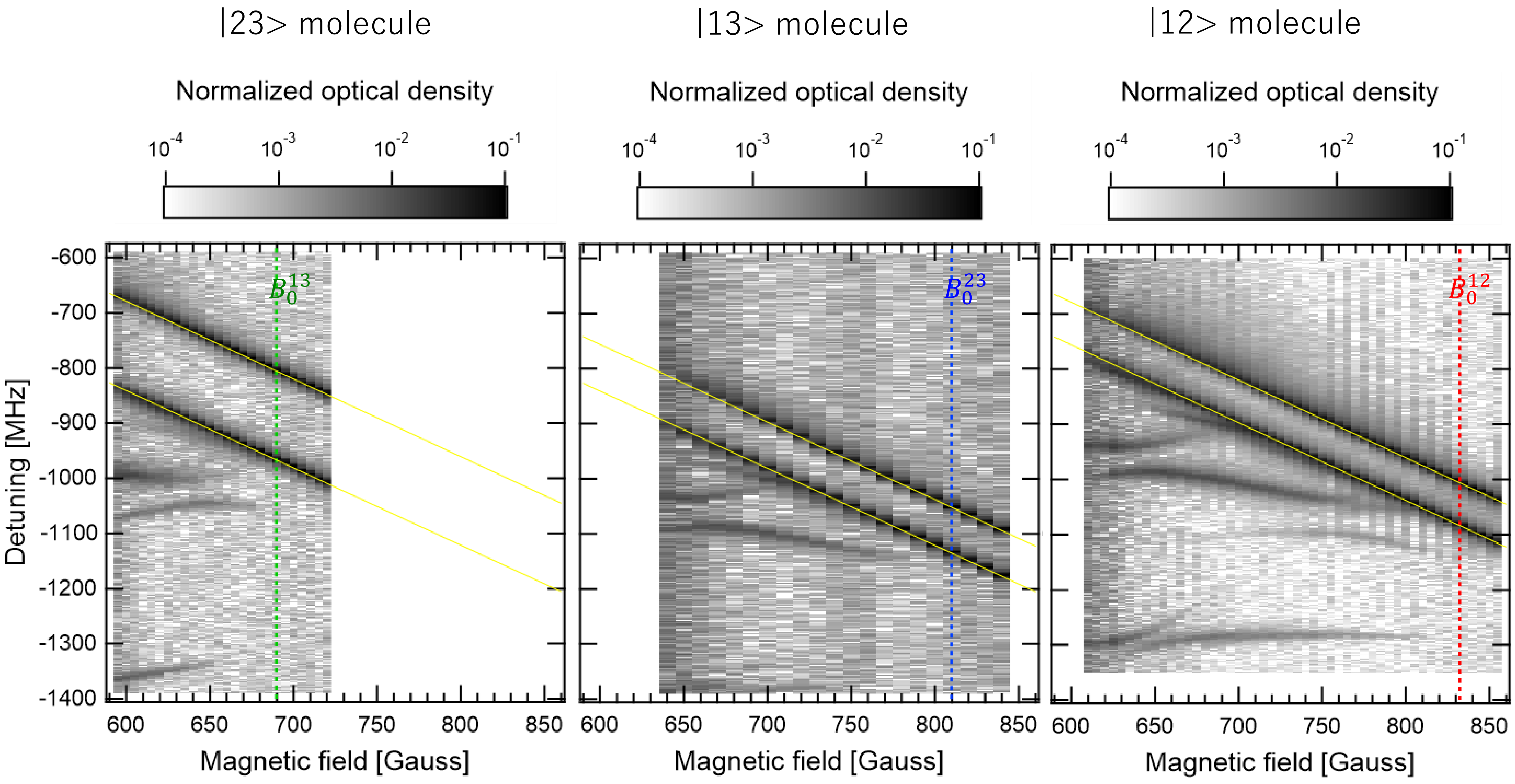
Atom (630~860G, 10G interval)



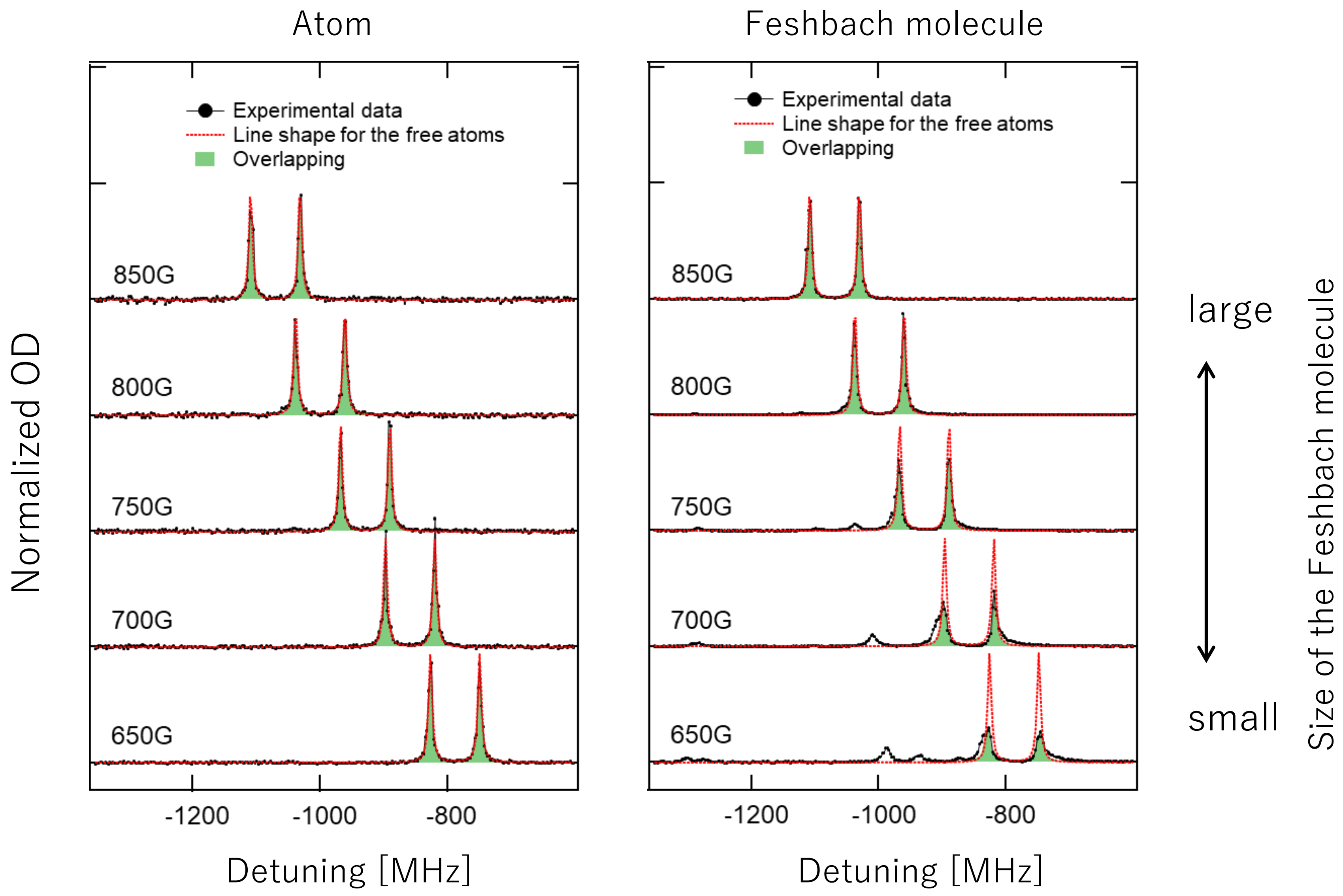
Feshbach molecule (610~855G, 5G interval)



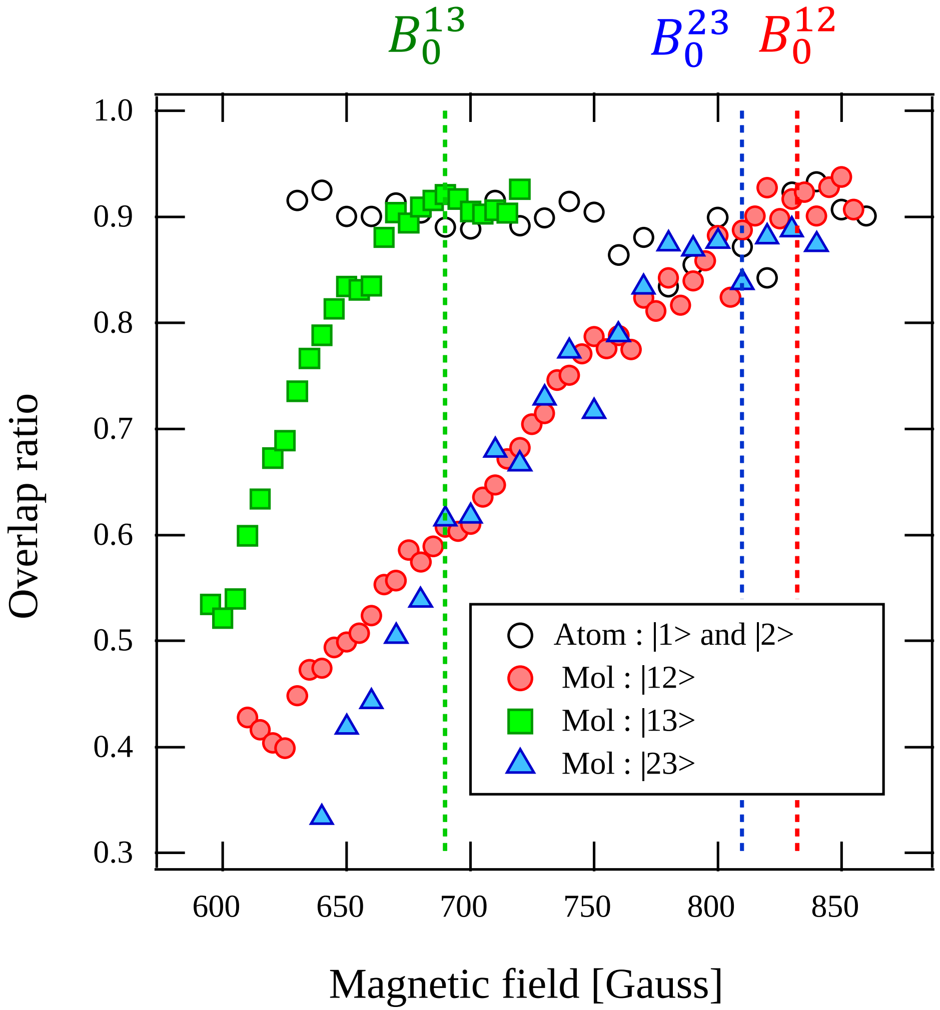
Two-dimensional spectral data

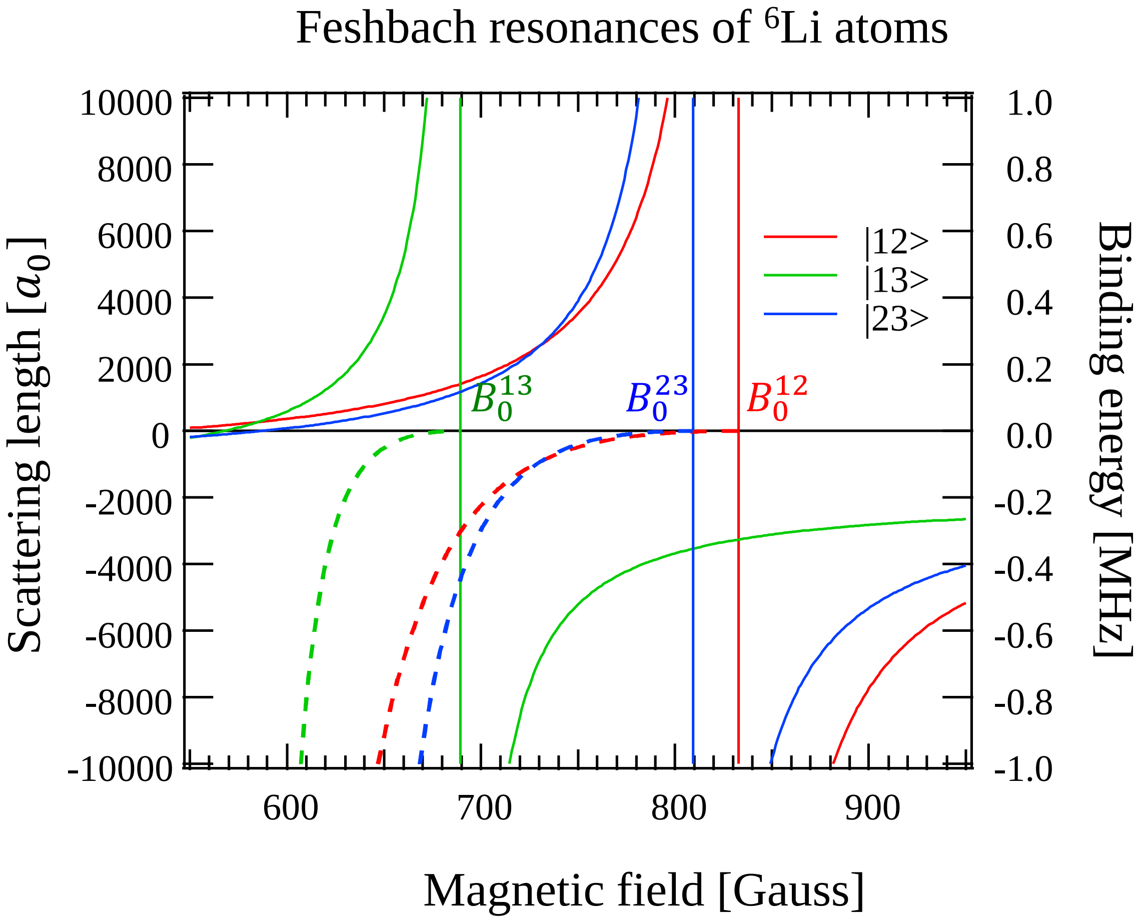


Line shapes at different Feshbach magnetic fields

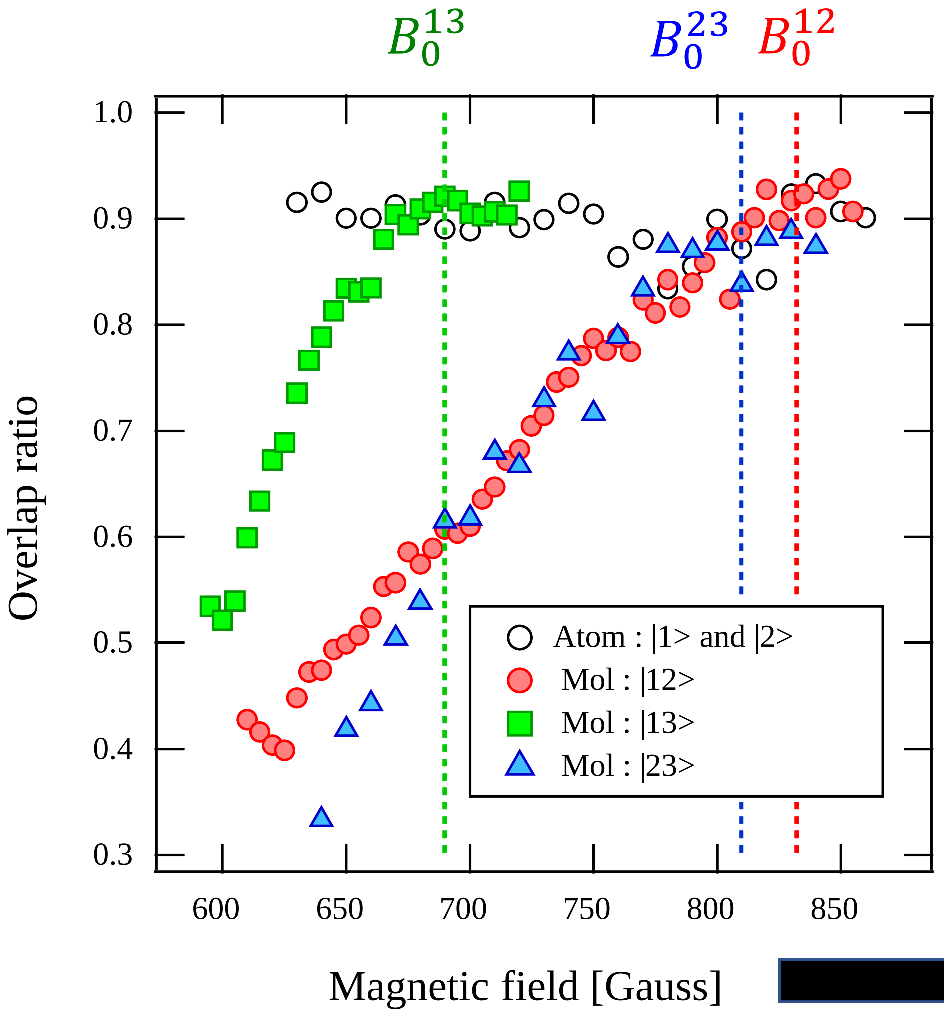


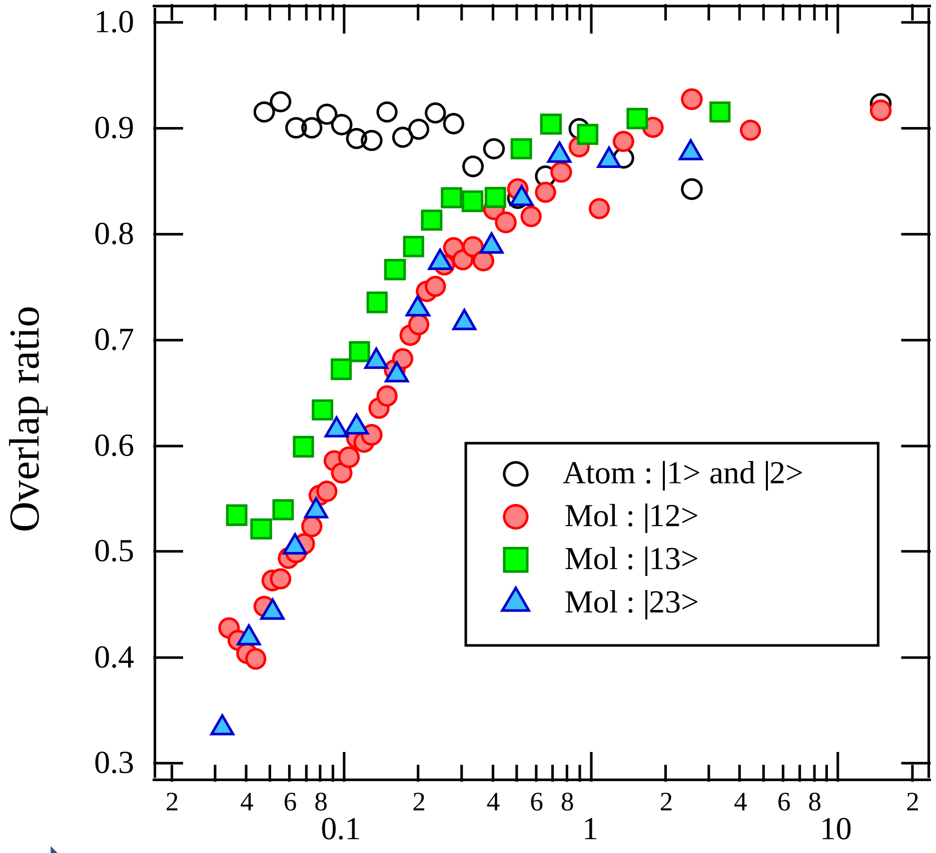
Overlapping ratio between experimental data and the line shape of the free atom





Overlapping ratio between experimental data and the line shape of the free atom





$$\frac{a}{\lambda} = \frac{\text{Size of the Feshbach molecule}}{\text{Optical wavelength}}$$

Overlapping ratio between experimental data and the line shape of the free atom

Simple model

Feshbach molecule has a spherical density distribution :

$$\psi_b(R) = \frac{1}{\sqrt{2\pi a}} \frac{\exp(-R/a)}{R}$$

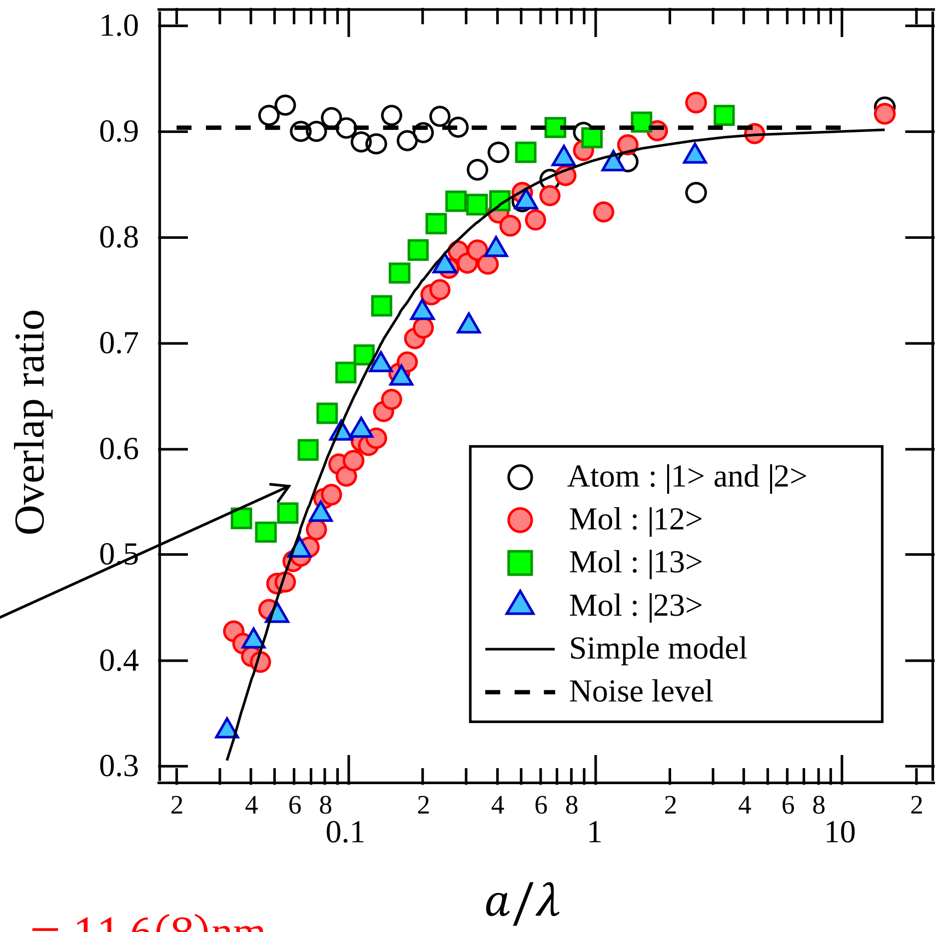
We assume that existence probability outside of $R_c = \lambda/C_\lambda$ contribute to the optical transition as free atoms

$$\int_{R_c}^{+\infty} 4\pi R^2 |\psi_b(R)|^2 dR = \exp\left(-2\frac{R_c}{a}\right) = \exp\left(-2\frac{1}{C_\lambda \cdot \left(\frac{a}{\lambda}\right)}\right)$$

↓

Fitting function : $f\left(\frac{a}{\lambda}\right) = A \exp\left(-2\frac{1}{C_\lambda \cdot \left(\frac{a}{\lambda}\right)}\right)$

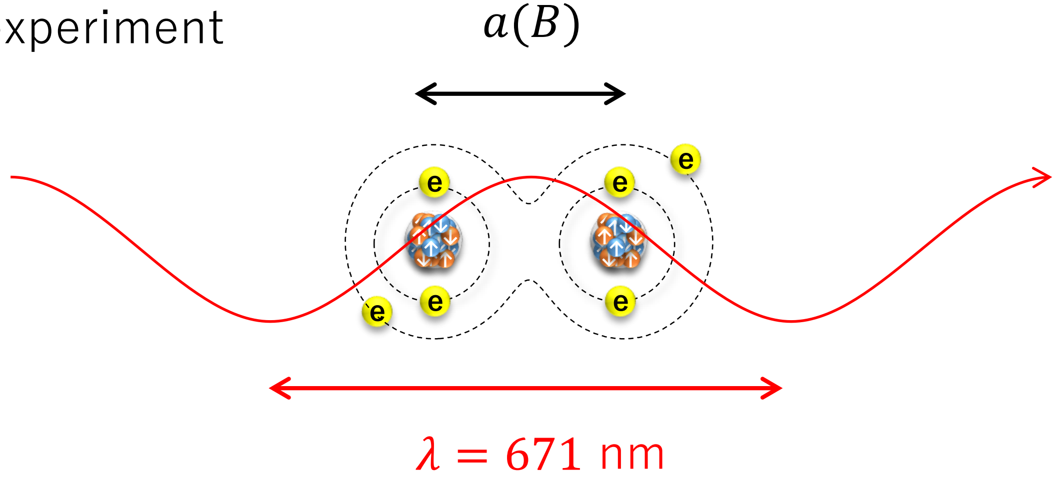
Experimental noise



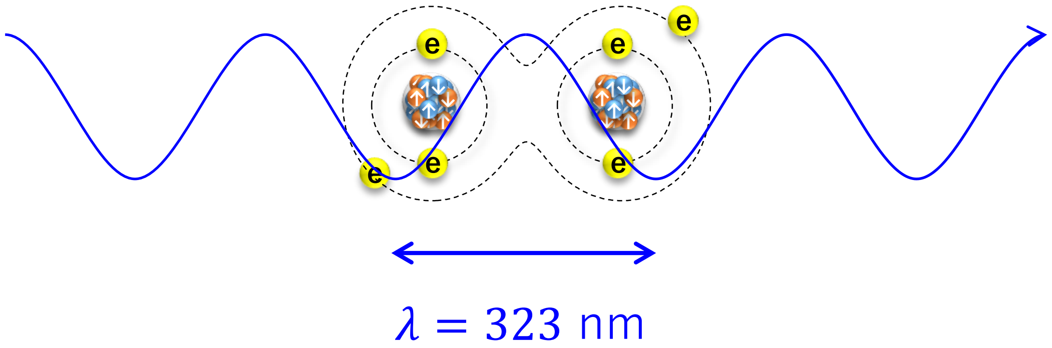
Fitting result : $A = 0.904(4)$
$C_\lambda = 58(4)$, or $R_c = 11.6(8)\text{nm}$

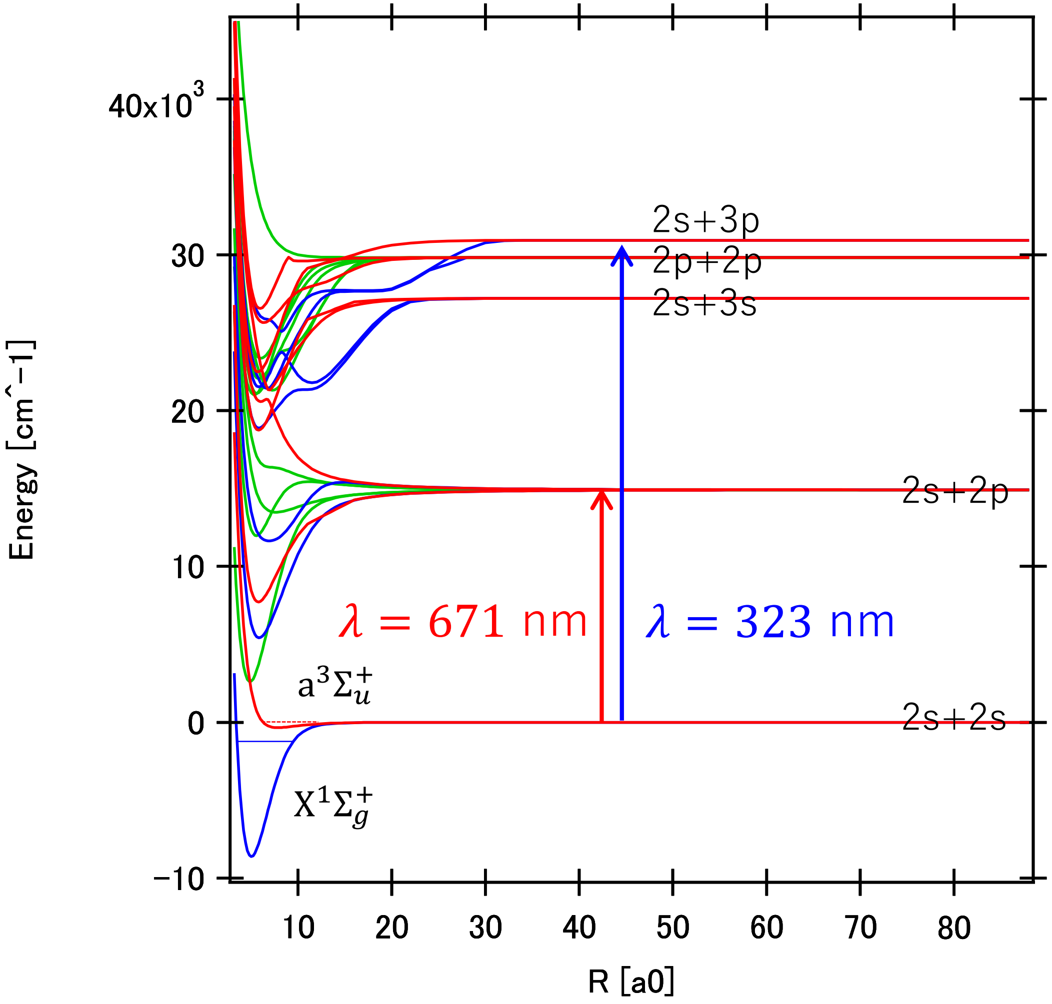
Planning experiment to confirm the universal behavior

This experiment

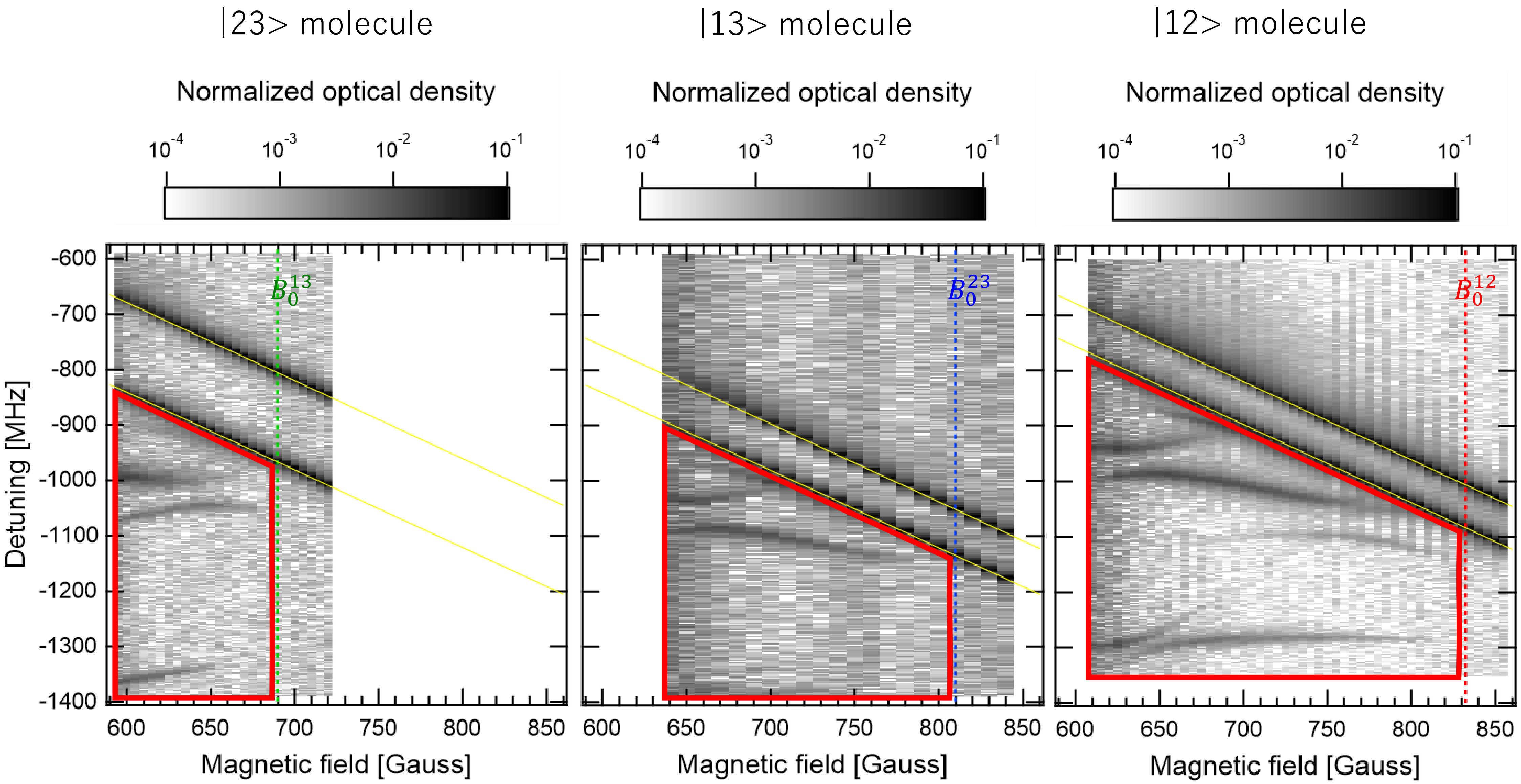


Next experiment



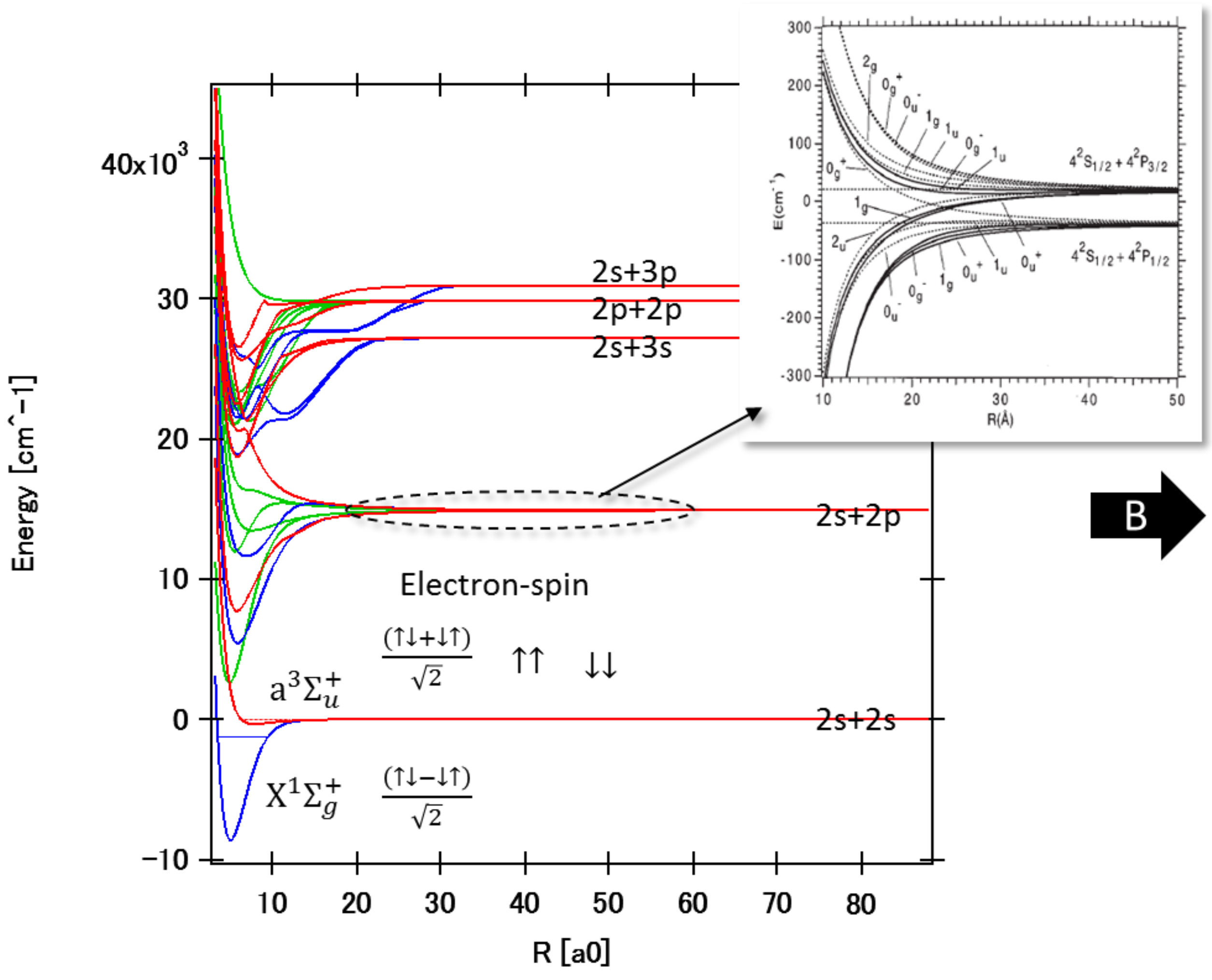


Assignment of the excited molecular states

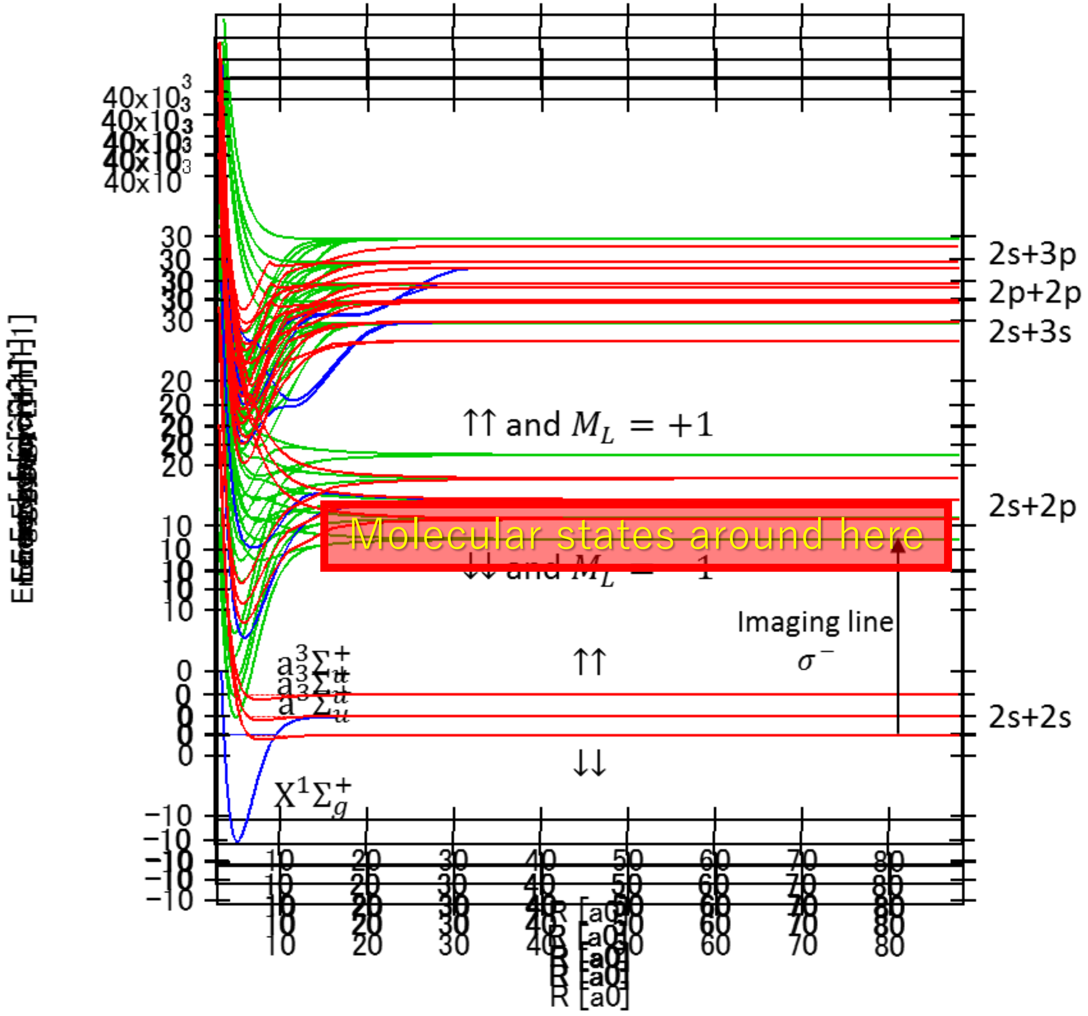


Lithium molecule and Zeeman shift

Li_2 molecular potential



B



P. Jasik and J.E. Sienkiewicz
Chemical Physics 323 (2006) 563–573

How can we assign the excited molecular states

We have not achieved yet, but we have clues

1. Conservation of total angular momentum and the selection rules

Initial state

$$m_{\text{ini}} = m_f^{|1>} + m_f^{|2>} + m_r + m_p = -1$$

Feshbach molecule

$|2\rangle : m_f^{|2>} = -\frac{1}{2} + 0 + 0$

$|1\rangle : m_f^{|1>} = -\frac{1}{2} + 0 + 1$

$(m_f = m_s + m_l + m_i)$

Rotation : $m_r = 0$ (s-wave)

+

Photon

Helicity : $m_p = -1\ (\sigma^{-1})$

Dipole transition

Final state
(Excited molecular state)

$$m_{\text{ini}} = -1$$

Total angular molent:
$\Delta J = 0, \pm 1, J = 0 \nleftrightarrow J = 0$

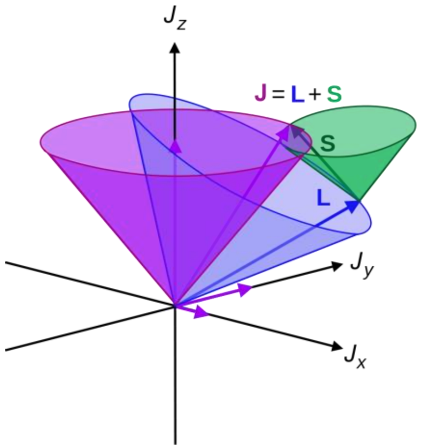
Electron orbital angular momentum along the molecular axis: $\Delta\Lambda = 0, \pm 1$

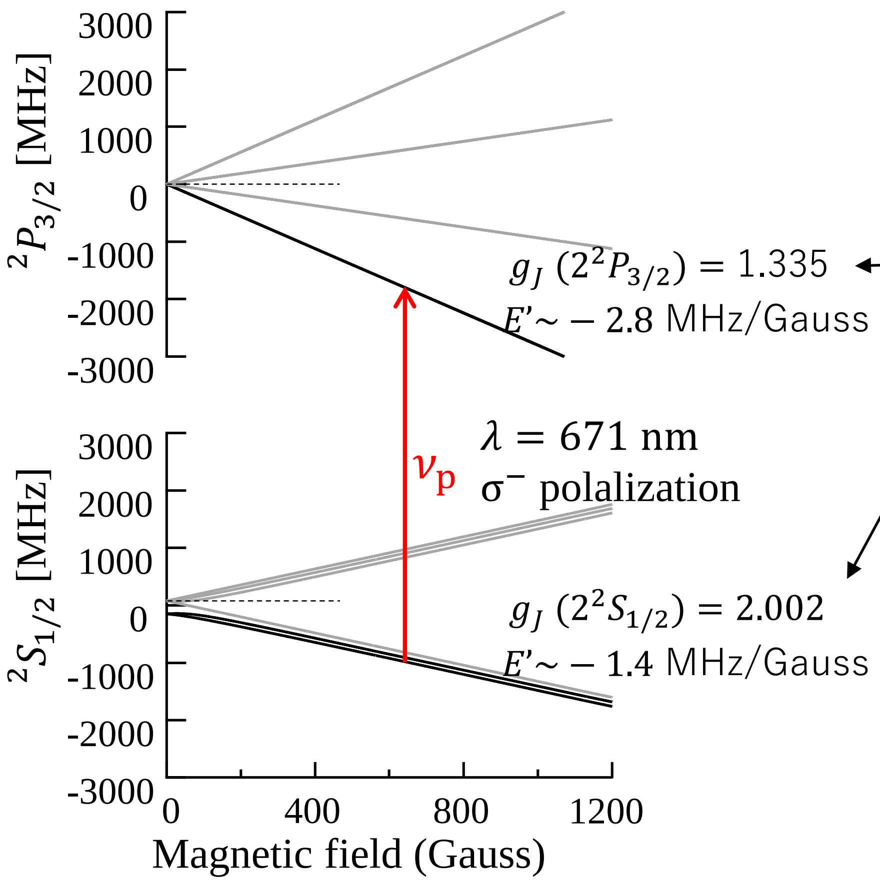
Total electron spin: $\Delta S = 0$

2. Landé g-factor

For atom : $H_B = -\boldsymbol{\mu}_S \cdot \boldsymbol{B} - \boldsymbol{\mu}_L \cdot \boldsymbol{B} - \boldsymbol{\mu}_I \cdot \boldsymbol{B}$
$\sim -\boldsymbol{\mu}_S \cdot \boldsymbol{B} - \boldsymbol{\mu}_L \cdot \boldsymbol{B}$

LS-coupling
$(J = L + S)$





(Without nuclear magnetic moment)

$$H_B \sim -\boldsymbol{\mu}_S \cdot \boldsymbol{B} - \boldsymbol{\mu}_L \cdot \boldsymbol{B}$$

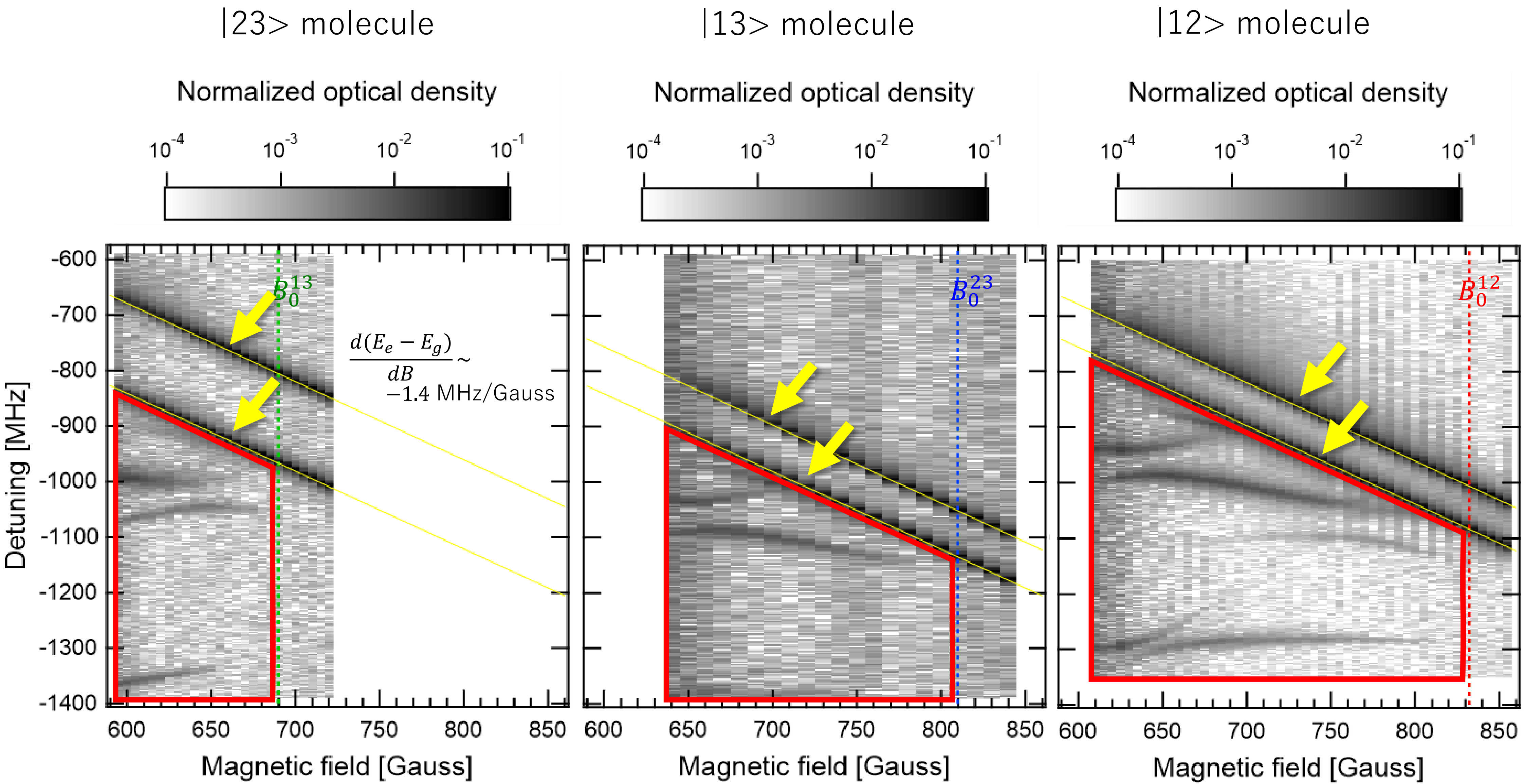
$$= \frac{\mu_B}{\hbar} g_S \frac{(\boldsymbol{S}\cdot\boldsymbol{J})(\boldsymbol{J}\cdot\boldsymbol{B})}{\boldsymbol{J}^2} + \frac{\mu_B}{\hbar} g_L \frac{(\boldsymbol{L}\cdot\boldsymbol{J})(\boldsymbol{J}\cdot\boldsymbol{B})}{\boldsymbol{J}^2}$$

$$= \frac{\mu_B}{\hbar}\left(\frac{\boldsymbol{S}\cdot\boldsymbol{J}}{\boldsymbol{J}^2} + \frac{\boldsymbol{L}\cdot\boldsymbol{J}}{\boldsymbol{J}^2}\right) m_J \mathrm{B}$$

$$= \frac{\mu_B}{\hbar} g_J m_J \mathrm{B}$$

$$g_J = g_S \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} + g_L \frac{J(J+1) - S(S+1) + L(L+1)}{2J(J+1)}$$

$$\begin{pmatrix} g_S = 2.0023193043737 \\ g_L = 0.99999587 \\ g_I = -0.0004476540 \\ \frac{\mu_B}{h} = 1.3996 \text{ MHz/Gauss} \end{pmatrix}$$



|23> molecule
|13> molecule
|12> molecule
Normalized optical density
Normalized optical density
Normalized optical density
10^-4
10^-3
10^-2
10^-1
B_0^{13}
B_0^{23}
B_0^{12}
$\frac{d(E_e - E_g)}{dB} \sim -1.4$ MHz/Gauss
Detuning [MHz]
-600
-700
-800
-900
-1000
-1100
-1200
-1300
-1400
Magnetic field [Gauss]
Magnetic field [Gauss]
Magnetic field [Gauss]
600
650
700
750
800
850

2. Landé g-factor

For diatomic molecule :

$$H_B = -\boldsymbol{\mu}_S \cdot \boldsymbol{B} - \boldsymbol{\mu}_L \cdot \boldsymbol{B} - \boldsymbol{\mu}_I \cdot \boldsymbol{B} - \boldsymbol{\mu}_R \cdot \boldsymbol{B}$$
$$\sim -\boldsymbol{\mu}_S \cdot \boldsymbol{B} - \boldsymbol{\mu}_L \cdot \boldsymbol{B}$$

Unit vector along the molecular axis: $\boldsymbol{k}$ ⟶

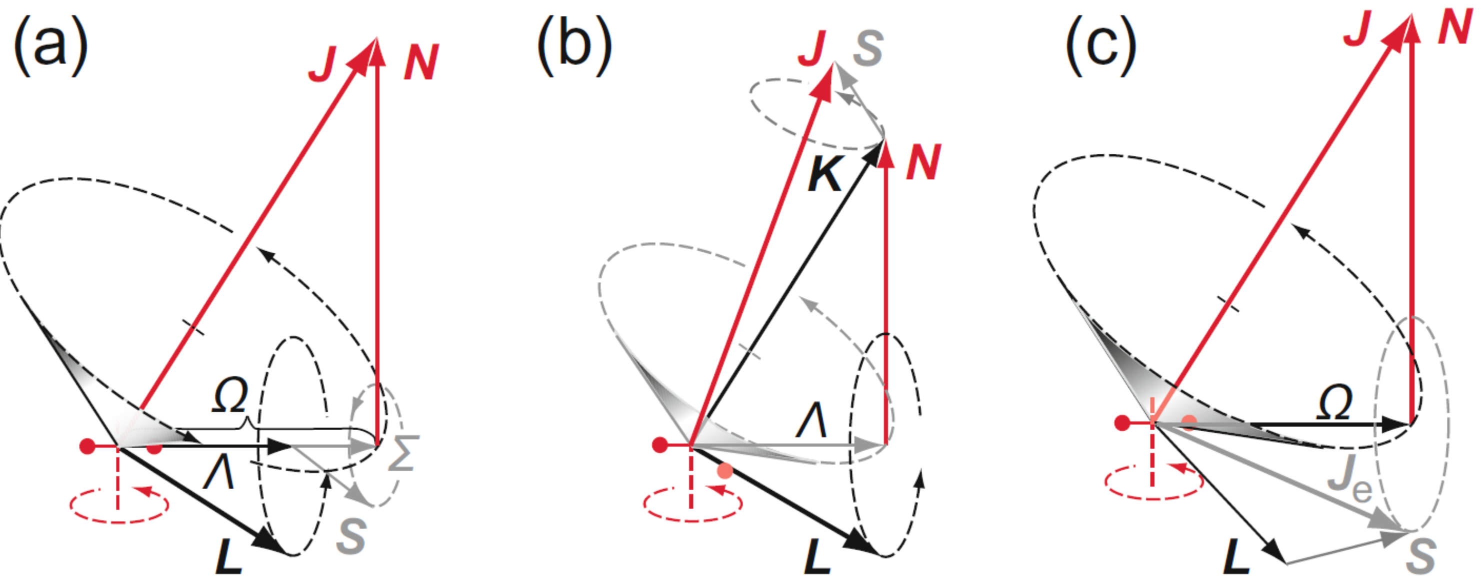
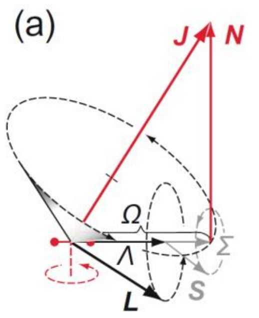


Fig. 3.40 HUND's cases **(a)**, **(b)**, **(c)**

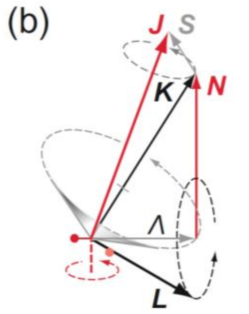
Hertel I.V., Schulz CP. (2015) Diatomic Molecules. In: Atoms, Molecules and Optical Physics 2. Graduate Texts in Physics. Springer, Berlin, Heidelberg

2. Landé g-factor



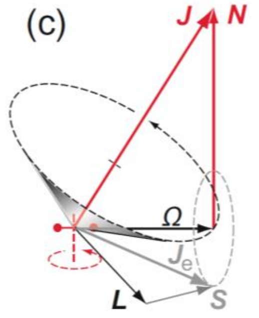
$$H_B \sim \frac{\mu_B}{\hbar} g_s \frac{(\boldsymbol{S}\cdot\boldsymbol{k})(\boldsymbol{k}\cdot\boldsymbol{J})(\boldsymbol{J}\cdot\boldsymbol{B})}{\boldsymbol{J}^2} + \frac{\mu_B}{\hbar} g_L \frac{(\boldsymbol{L}\cdot\boldsymbol{k})(\boldsymbol{k}\cdot\boldsymbol{J})(\boldsymbol{J}\cdot\boldsymbol{B})}{\boldsymbol{J}^2}$$

Strong coupling of L along the molecular axis, and strong LS coupling



$$H_B \sim \frac{\mu_B}{\hbar} g_s \frac{(\boldsymbol{S}\cdot\boldsymbol{J})(\boldsymbol{J}\cdot\boldsymbol{B})}{\boldsymbol{J}^2} + \frac{\mu_B}{\hbar} g_L \frac{(\boldsymbol{L}\cdot\boldsymbol{k})(\boldsymbol{k}\cdot\boldsymbol{K})(\boldsymbol{K}\cdot\boldsymbol{J})(\boldsymbol{J}\cdot\boldsymbol{B})}{\boldsymbol{K}^2\boldsymbol{J}^2}$$

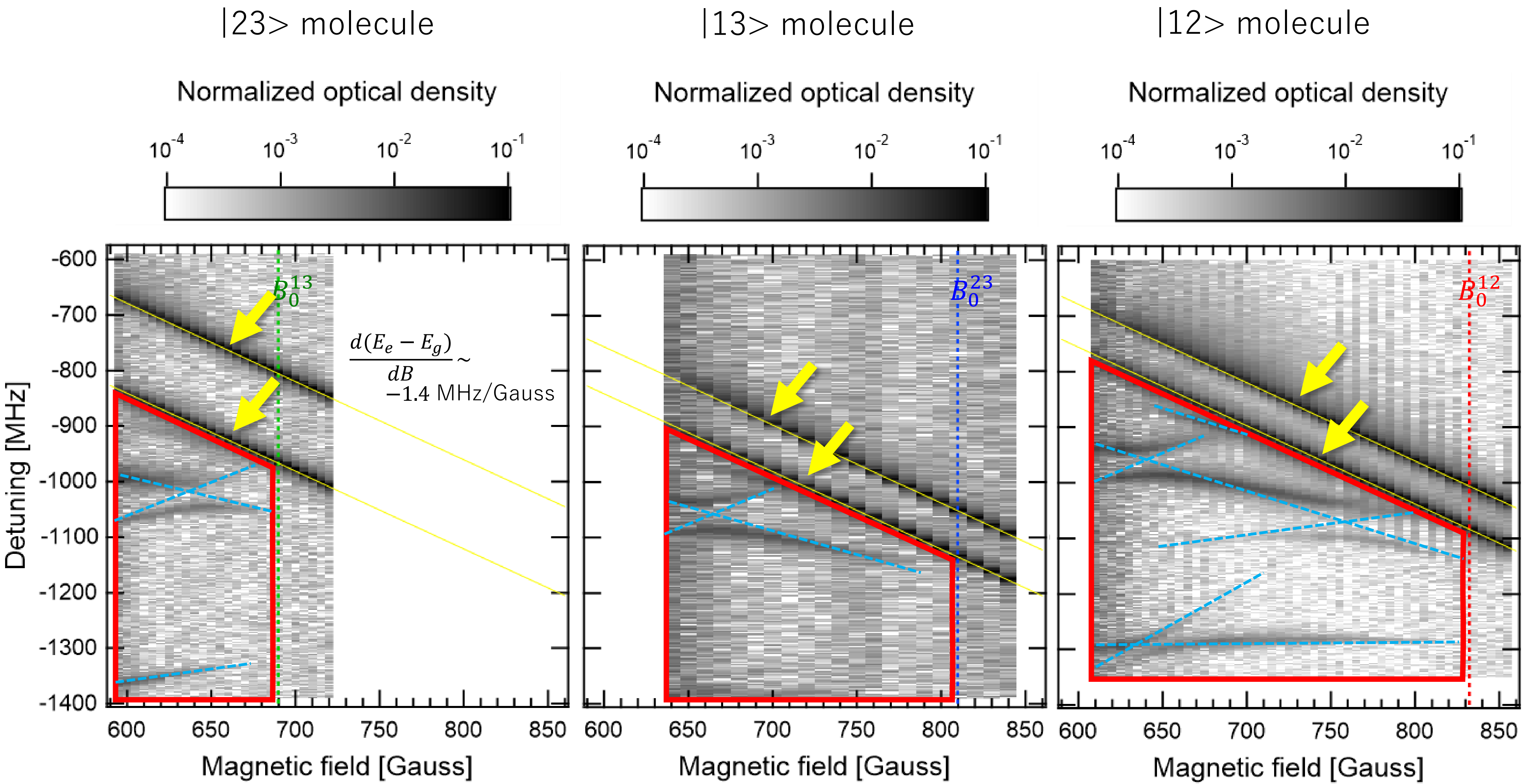
$\Lambda = 0$, or high rotational molecule



$$H_B \sim \frac{\mu_B}{\hbar} g_s \frac{(\boldsymbol{S}\cdot\boldsymbol{J_e})(\boldsymbol{J_e}\cdot\boldsymbol{k})(\boldsymbol{k}\cdot\boldsymbol{J})(\boldsymbol{J}\cdot\boldsymbol{B})}{\boldsymbol{J_e}^2\boldsymbol{J}^2} + \frac{\mu_B}{\hbar} g_L \frac{(\boldsymbol{L}\cdot\boldsymbol{k})(\boldsymbol{k}\cdot\boldsymbol{K})(\boldsymbol{K}\cdot\boldsymbol{J})(\boldsymbol{J}\cdot\boldsymbol{B})}{\boldsymbol{J_e}^2\boldsymbol{J}^2}$$

Dissosiation limit

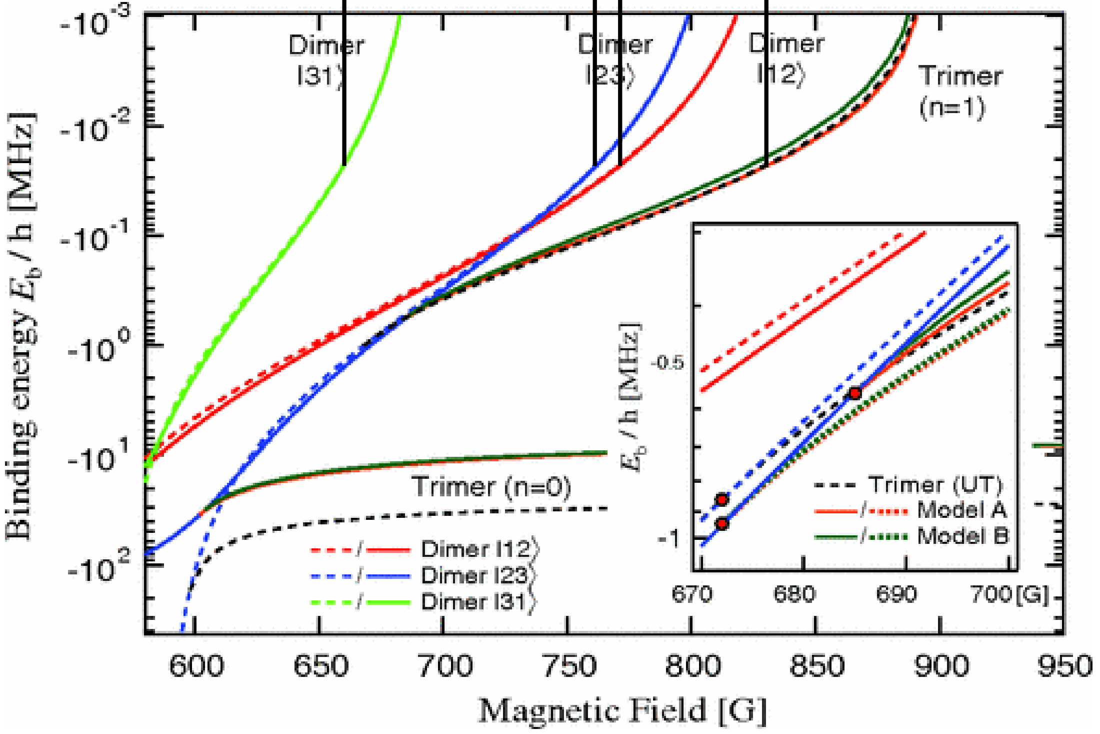
I will evaluate later, and assign them.



Planning experiment to access triatomic molecules

This work

Next challenge



[P. Naidon, Phys. Rev. Lett. 105, 023201 (2010)]

Feshbach molecule and Efimov trimer by 6Li atoms

Calculation of the real Li2 potential is challenging problem

ELSEVIER

Chemical Physics
Volume 323, Issues 2–3, 21 April 2006, Pages 563-573

Calculation of adiabatic potentials of Li_2

P. Jasik, J.E. Sienkiewicz

JCTC Journal of Chemical Theory and Computation

Article

pubs.acs.org/JCTC

J. Chem. Theory Comput. (2014), 10, 1200−1211

First Principle Calculations of the Potential Energy Curves for Electronic States of the Lithium Dimer

Monika Musiał* and Stanisław A. Kucharski

Institute of Chemistry, University of Silesia, Szkolna 9, 40-006 Katowice, Poland

Calculation of the real Li3 potential is more challenging problem

Calculations of long-range three-body interactions for $\mathrm{Li}(2\,^2S) - \mathrm{Li}(2\,^2S) - \mathrm{Li}(2\,^2P)$

Pei-Gen Yan, Li-Yan Tang, Zong-Chao Yan, and James F. Babb
Phys. Rev. A **94**, 022705 – Published 9 August 2016

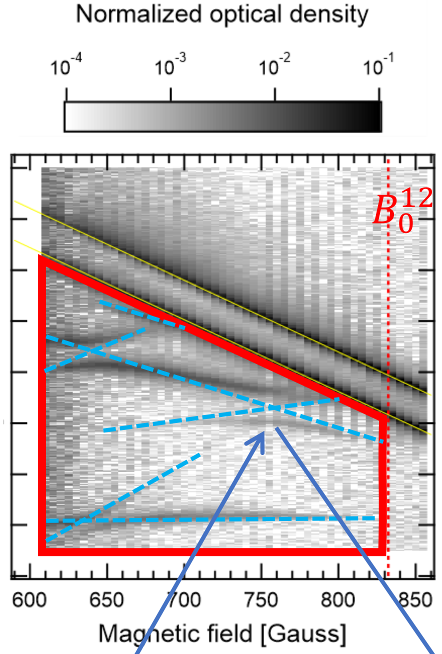
A diabatic representation of the two lowest electronic states of Li_3

J. Chem. Phys. 140, 154304 (2014); https://doi.org/10.1063/1.4871014

Elham Nour Ghassemi[1], Jonas Larson[2,3], and Åsa Larson[2, a)]

Planning experiment to access triatomic molecules

|12> molecule



Coherent transfer by laser light

BEC of Feshbach molecules

BEC of rotating molecules

Summary

Ultracold AMO experiment for quantum few-body and many-body

- Road from complex molecular potentials to Universal Feshbach molecules
  - ✓ Low energy scattering with a short range potential is origin of the universal physics
  - ✓ Two-channel coupling realize Feshbach resonance

- Absorption spectroscopy of Feshbach molecules
  - ✓ We experimentally studied optical response on Feshbach molecules for the precision measurement
  - ✓ The change of the line shapes looks universal behavior as a function of a/λ
  - ✓ Various excited molecular states were found, they will improve molecular calculation

- Next challenge
  - ✓ Taking spectroscopy with shorter wave length
  - ✓ Dipole transition of Efimov trimer to the excited triatomic molecules
  - ✓ Coherent transfer from BEC of the Feshbach molecule to the rotating molecules