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Modeling cold collisions

Atoms ←→ Molecules

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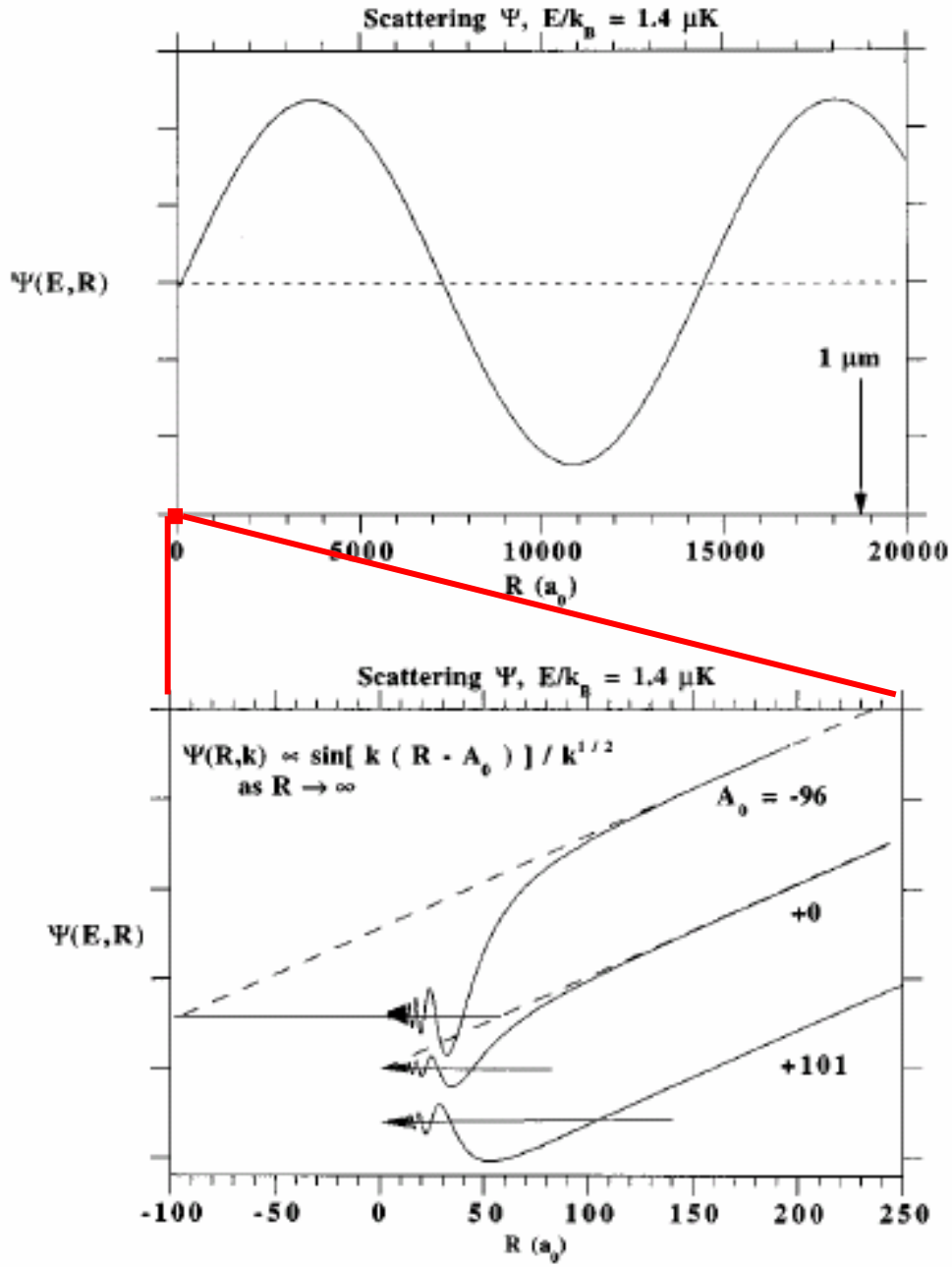
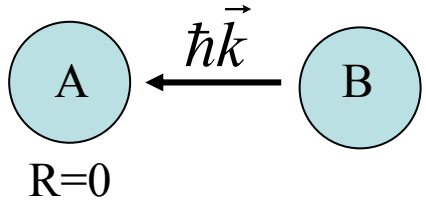
collisional wave function for E ≈ 0





adopted from J. Weiner et al, Rev. Mod. Phys., Vol. 71, 1 (1999)

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Accumulated phase method

Moerdijk, Verhaar, Axelsson,
Phys.Rev.A51,4852 (1995)

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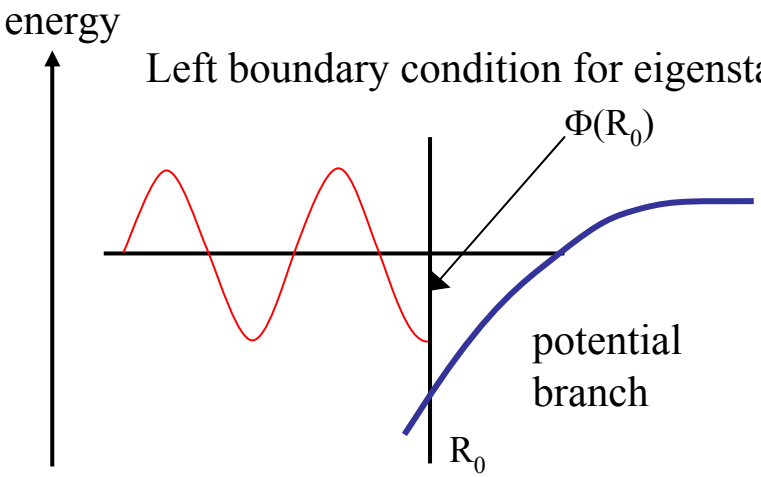

$$\Phi(R_0) = \Phi_0 + \Phi_E(D_e - E) + \Phi_J J(J+1) + \ldots$$

3 phenomenological parameters

eigenstates are described by $\Phi(R_0)$, D_e *and* C_i

phase scattering length

at asymptotic energy

dispersion coefficient

reliable extrapolation by fitting spectroscopic observations

estimation of spectral intensities by the asymptotic wave function,
the inner part keeps its form

Extension to multi channel problem → channel dynamics in the inner region

Collisions of atoms with internal structure

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alkali atom: $|s_A i_A f_A m_A\rangle$

atom pair A + B with rotation l

hamiltonian

basis Hund's case (e) — atomic hfs and mechanical rotation — diagonal

$|(f_A,f_B)f,l,F,M_F\rangle$ — potential energy and spin-spin/spin-orbit — non-diagonal

$^1\Sigma_g^+$ and $^3\Sigma_u^+$

manifold of channels to 3 asymptotes

f_A+1 -- f_B+1

f_A+1 -- f_B or f_A -- f_B+1

f_A -- f_B

How much knowledge of molecular potentials?

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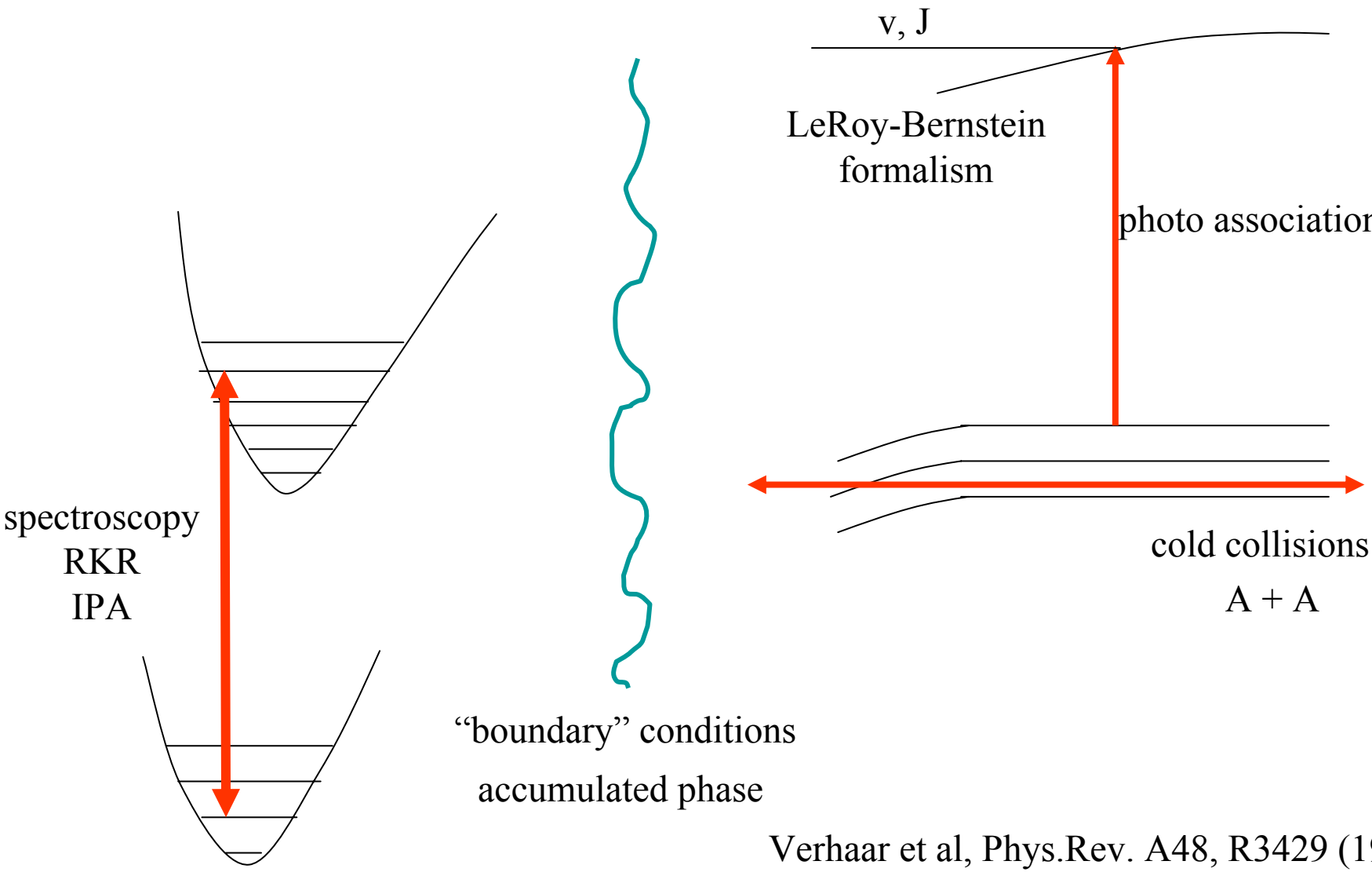

Verhaar et al, Phys.Rev. A48, R3429 (1993)

Vogels et al, Phys.Rev. A61, 043407 (2000)

Test case Rb + Rb

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highly precise measurements and theory:

1. Raman transitions Heinzen et al (2000) and Bloch et al (2003)
2. Feshbach resonances on ^{87}Rb and ^{85}Rb from several authors
3. Theoretical analysis by Verhaar group 2002/03

Observed Levels by D. Heinzen et al 2000

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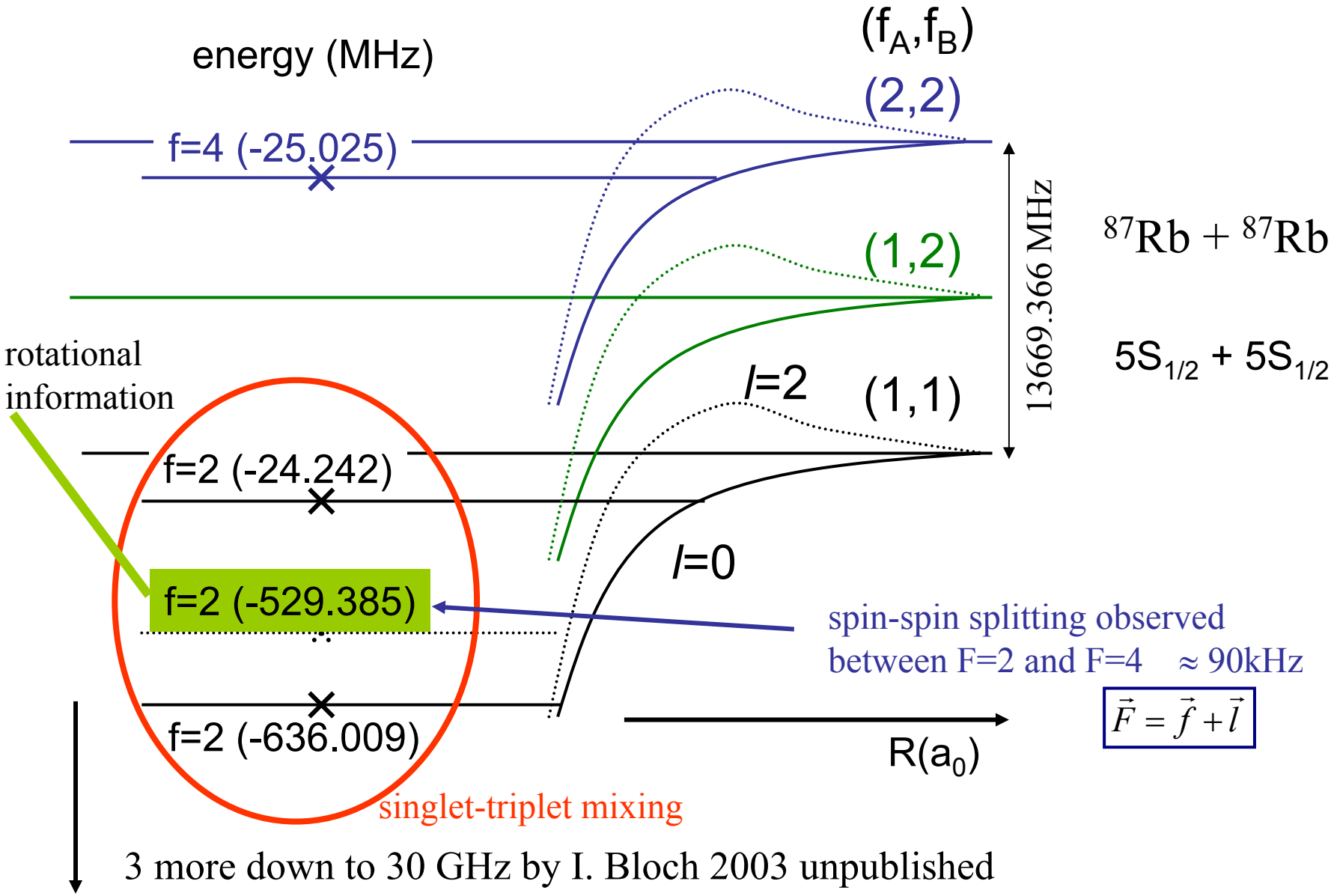

Reconstruction of scattering calculation

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1. Long range behavior: dispersion parameters C_6 C_8 and C_{10} and exchange energy

$$U(R) = D_{asymptote} - \frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} \pm A_{ex} R^{\gamma} \exp(-\alpha R)$$

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2. Add potential branch for $X^1\Sigma^+_g$ and $a^3\Sigma^+_u$ and
adjust it to get scattering lengths as reported from the analysis

3. Set up the hyperfine and rotational Hamiltonian for calculating the observed spectra
and compare with reported ones

2'. Fit the observed spectra while keeping C_i and exchange energy,
but vary "accumulated phase" or "logarithmic derivative"

3'. Calculate the scattering lengths
and compare with reported ones

Comparison of the two cases

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1. Use the spectra fit

$\sigma = 0.89$

property (au)	Verhaar 2002	Rempe 2003	present with V./R.
a_t (87)	98.98(4)	98.96	98.91/98.98
a_s (87)	90.4(2)	90.6	91.9/91.5
a_t (85)	-388(3)		-376/-373
a_s (85)	2795^{+420}_{-290}		8400/5331

2. Use scattering lengths of ^{87}Rb

spectral data of ^{87}Rb gives σ with about ten times bigger value

scattering length of ^{85}Rb a_s=2768 au and a_t=-373au

singlet – triplet coupling not properly described!

Construction of the adiabatic potentials and Hamiltonian

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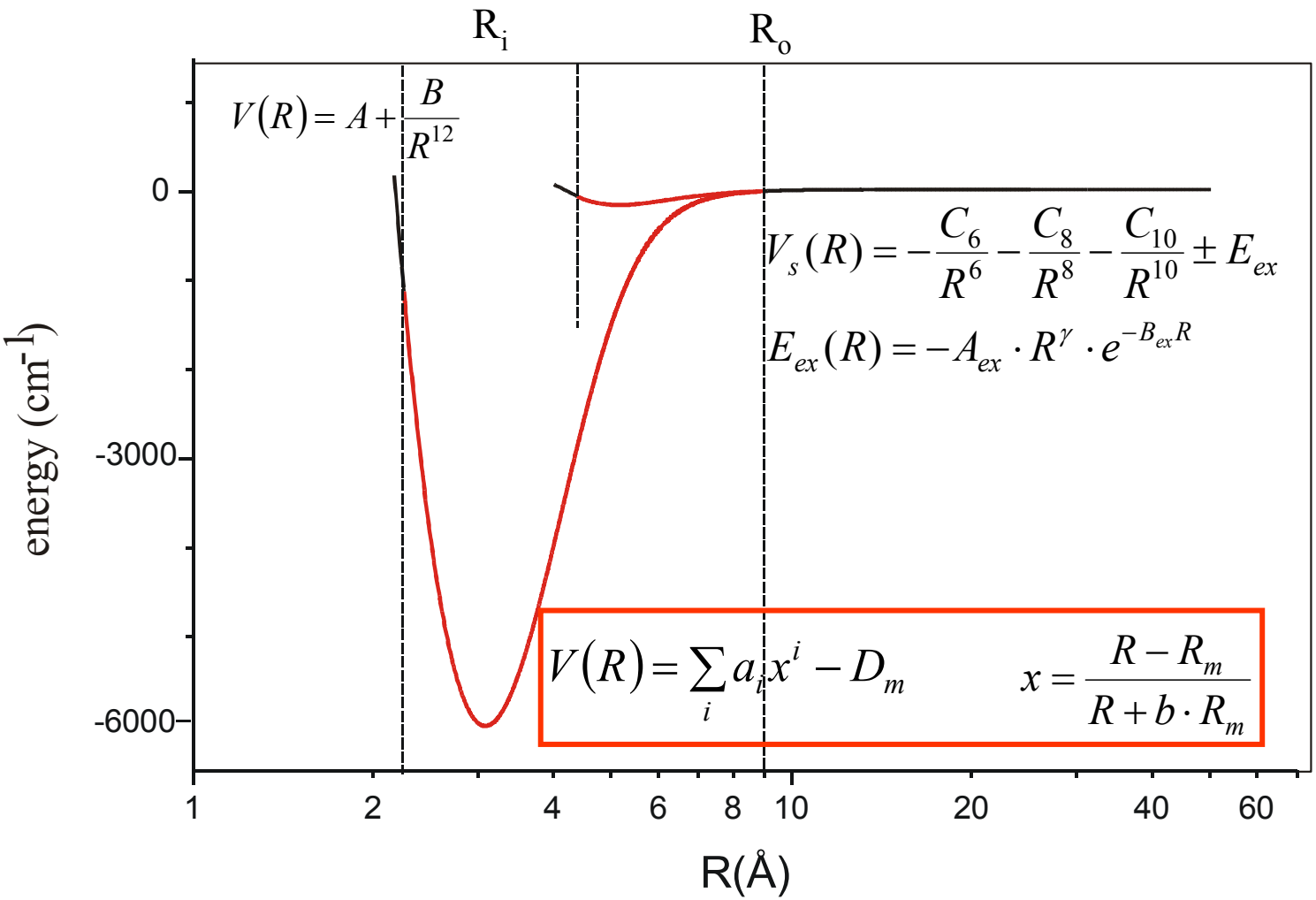

Status of Rb_2

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- Fourier transform spectroscopy of $X^1\Sigma^+_g$ — C. Amiot et al 2000

  accuracy 30 MHz — highest level 6.5 cm^{-1} ≈ 195GHz below the asymptote, outer turning point 12.8Å

- Ab initio calculation of $a^3\Sigma^+_u$ — Krauss/Stevens 1990 and Foucrault et al 1992

- Two-color photo association in ^{85}Rb accuracy 60 MHz — Heinzen et al 1997/2000

- Raman spectroscopy in BEC of ^{87}Rb accuracy 12 kHz — Heinzen et al 2000, Bloch et al 2003

pure triplet and mixed levels

- Feshbach resonance in ^{85}Rb $f_a = 2$ $m_{fa} = -2$ — JILA, revision in 2001

  l=0 f=4 f_a=3 f_b=3 singlet-triplet mixed resonance <S> = 0.749

- Feshbach resonances in ^{87}Rb with high precision — Rempe et al 2003, Sengstock et al 2004

Potentials

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potential for $X^1\Sigma^+_g$ with 30 parameters

construction of a potential for $a^3\Sigma^+_u$ with 9 parameters

common long range behavior of $X^1\Sigma^+_g$ and $a^3\Sigma^+_u$

Results for ^{87}Rb

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spectroscopic data described in the full range of observations

resonance positions modeled by
accumulated phase method $< 0.5\%$
with potentials about 0.1% or $\sigma = 0.37$G

reliable potentials
for future modeling:
cold collisions and
cold molecules

property (au)	Verhaar 2002	Rempe 2003	present with V./R.	present new C_i
a_t (87)	98.98(4)	98.96	98.91/98.89	98.97
a_s (87)	90.4(2)	90.6	91.9/91.4	91.60
a_t (85)	-388(3)		-376/-376	-389
a_s (85)	2795^{+420}_{-290}		8400/4800	5777
C_6	4703	4707	same C_i assumed as by Verhaar and Rempe	4713
C_8	$5.79 \cdot 10^5$	$5.73 \cdot 10^5$		$5.648 \cdot 10^5$

resonances calculated

Scaling to ^{85}Rb ?

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Using the potentials derived from ^{87}Rb:

^{85}Rb : spectra show systematic deviation of 45MHz and large scatter

Feshbach resonance $f_a = 2$ $m_{fa} = -2$ calculated at 155.6 G

observed at 154.9(4) G

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^{85}Rb separate evaluation with C_i and exchange force from theoretical estimates

spectra described within error limits Feshbach resonance at 151.8 G

isotope	a_s(from 85)	a_t(from 85)	a_s(from 87)	a_t(from 87)
^{85}Rb(au)	3781	-453.7	5777	-389
^{87}Rb(au)	91.1	96.87	91.6	98.97

Isotope effect beyond mass scaling? Correction to Born-Oppenheimer approximation?

Advantage by full potentials

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- scientifically complete system within definition of potentials
- systematic analysis of existing data set and internal consistency
- connecting experimental regimes
- check for isotope effects in the cold collision regime
- transformation of atom pairs ←→ molecules

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data available for Na_2, Rb_2, NaRb, NaCs

KRb and LiCs are processed presently

Potential scheme of mixed alkalis

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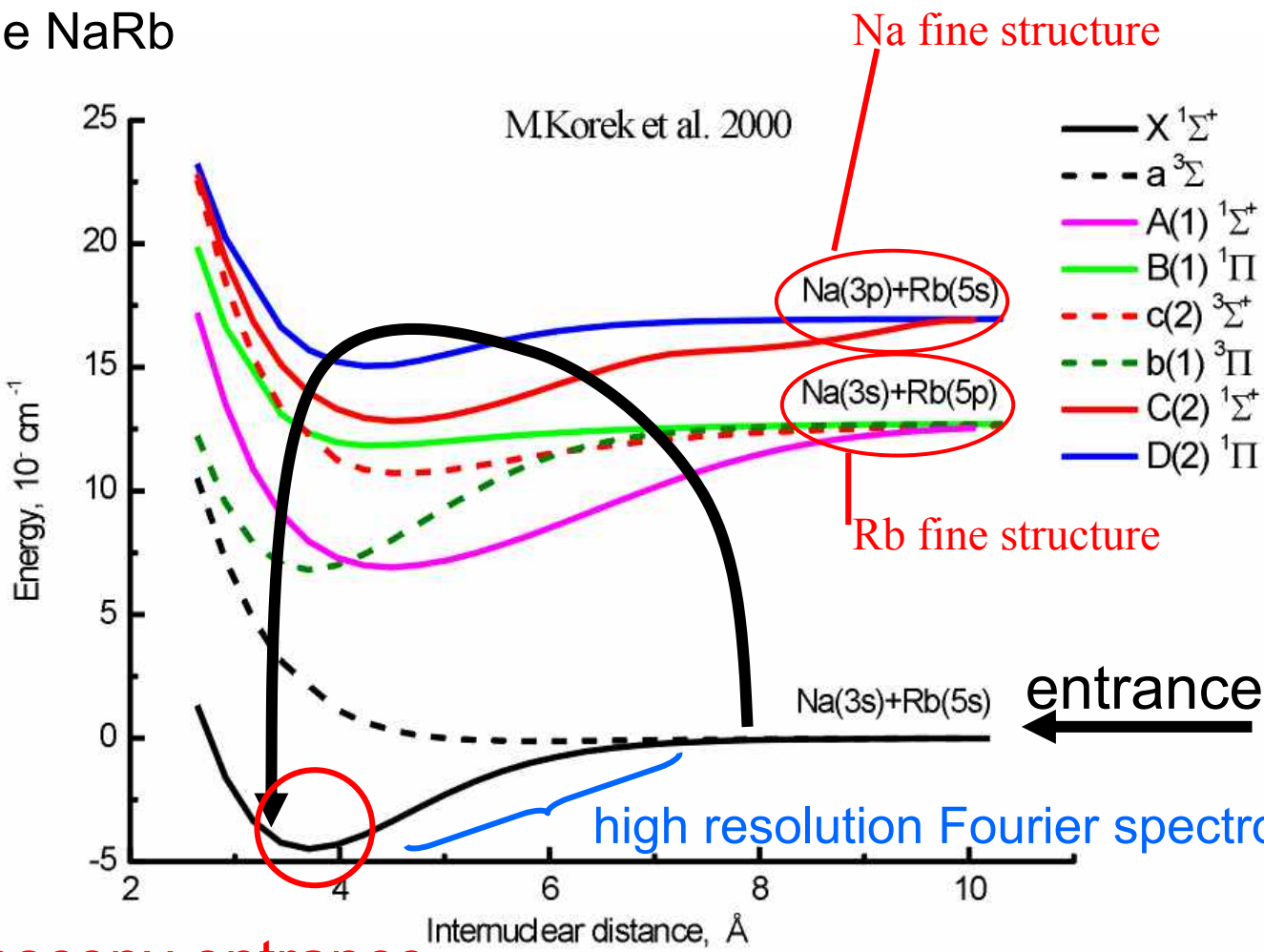
example NaRb



Example NaRb

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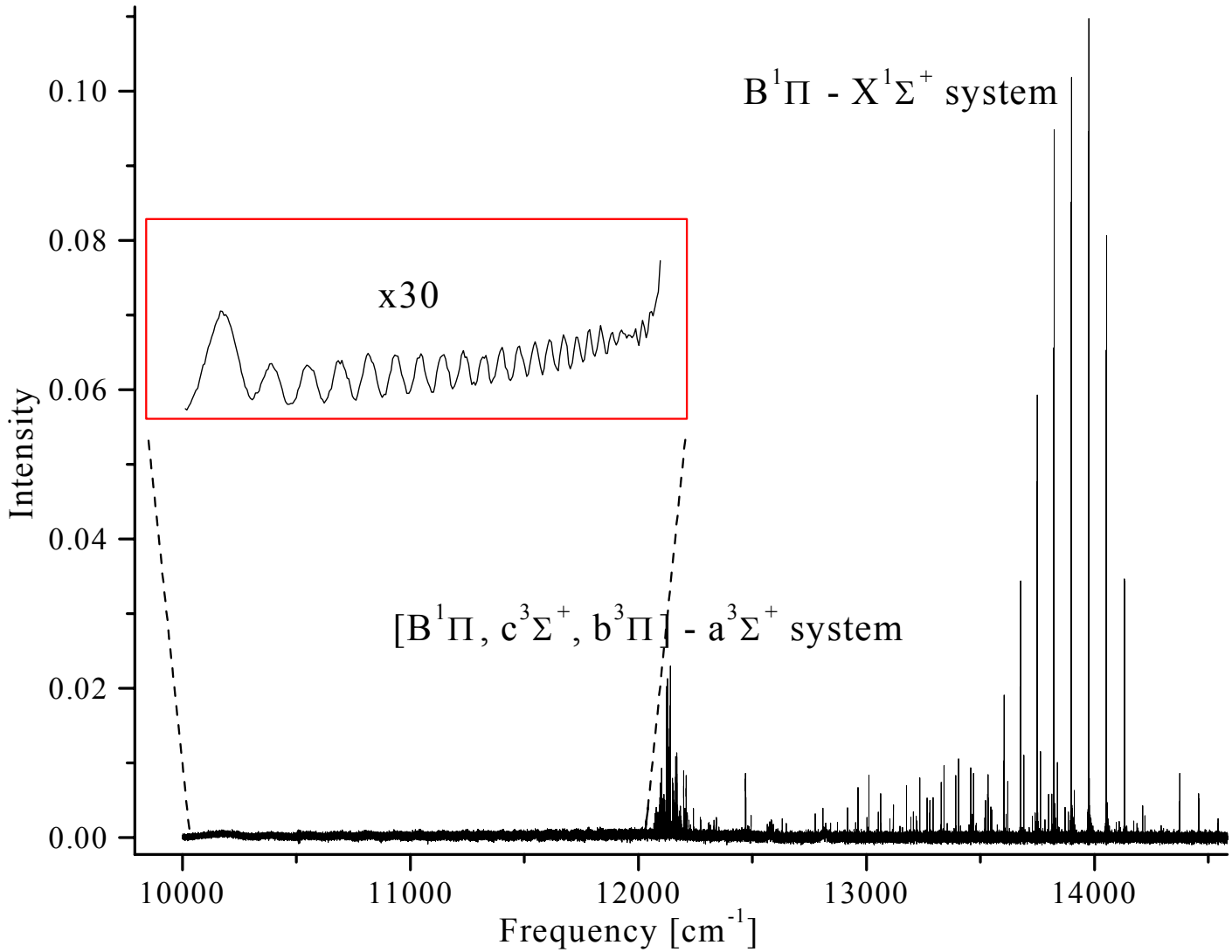
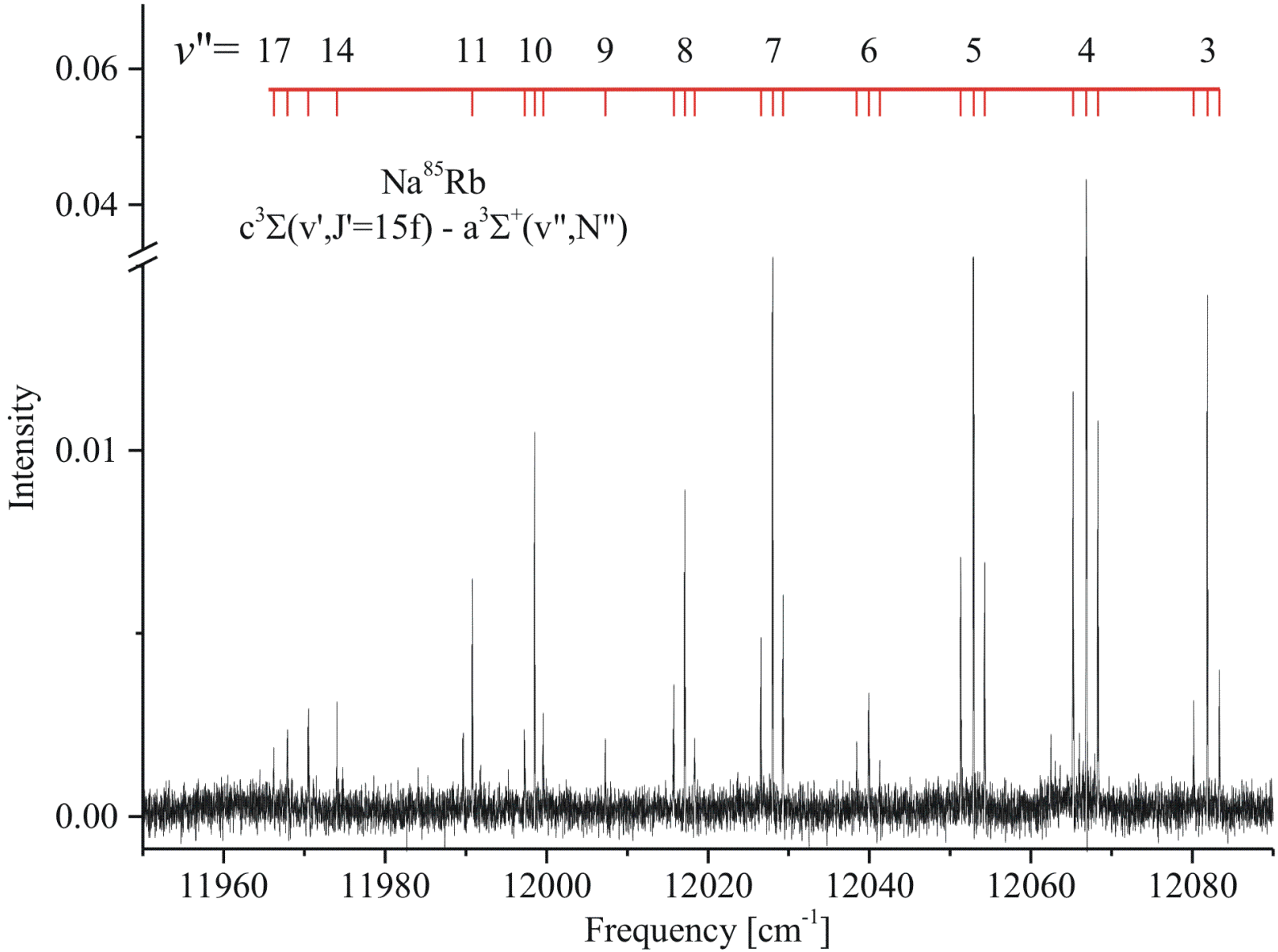


Progression to state $a^3\Sigma^+$



Overlap of $X^1\Sigma^+$ and $a^3\Sigma^+$

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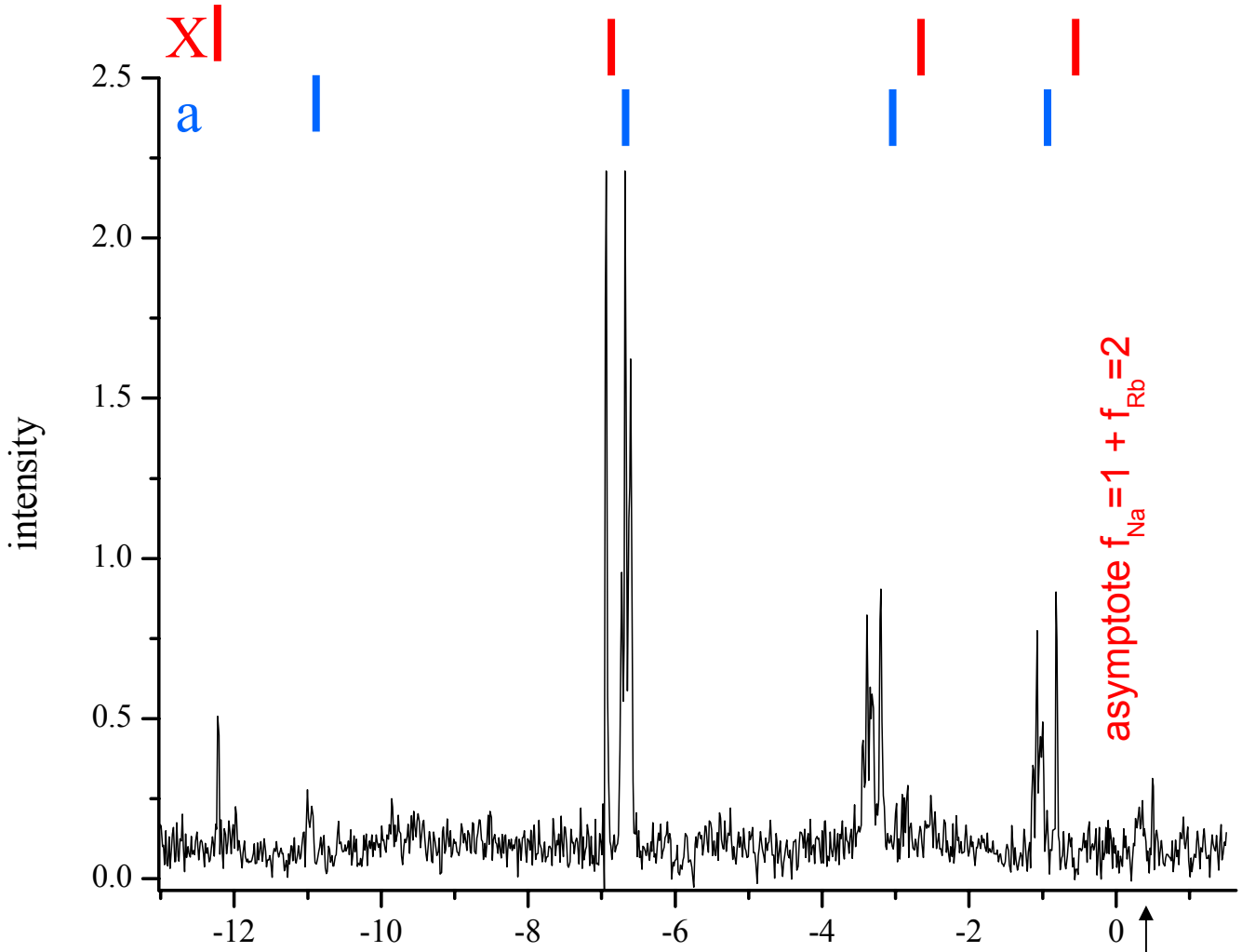

J = 19

compare spacing → exchange energy

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Full potentials for states $X^1\Sigma^+$ and $a^3\Sigma^+$ of NaRb

Prediction of collision properties in the energy range up to 10mK

and Feshbach resonances up to 1000G

approximations: atomic hyperfine interaction

neglected second order spin-orbit interaction

Born-Oppenheimer approximation

Collisions at different asymptotes → Scattering length and resonances

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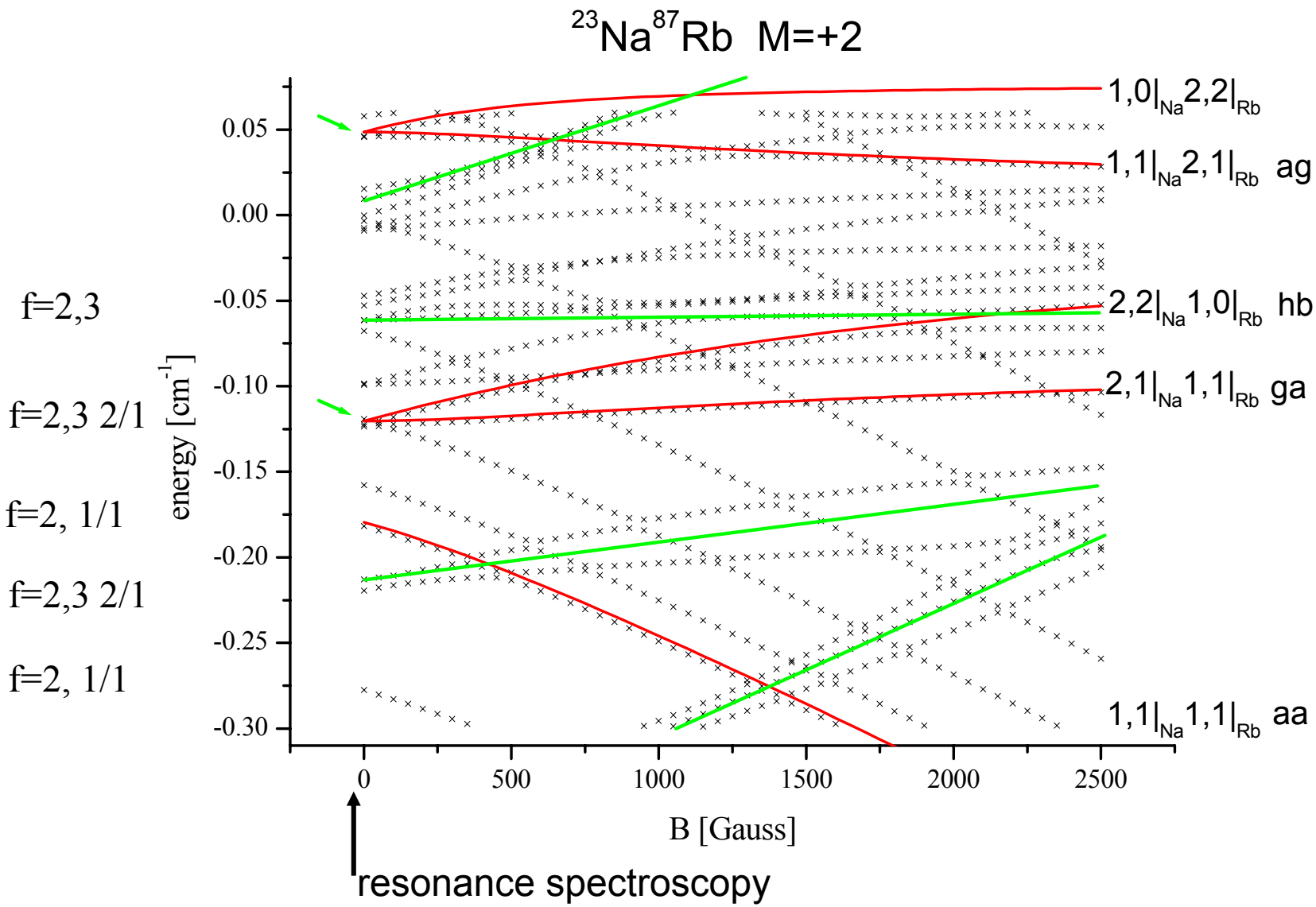

Summary and Conclusions on polar molecules

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Full potentials at ground state asymptote
"available" with sufficient accuracy

NaRb, NaCs, (KRb), LiCs

Description with atomic hyperfine parameters very accurate

Feshbach resonance structure very rich

Electronic structure of excited states very complex

Doorways to cold molecules
with good predictions of transition moments from theory

channel $1,1|_{Na}\ 1,1|_{Rb}$ lowest asymptote

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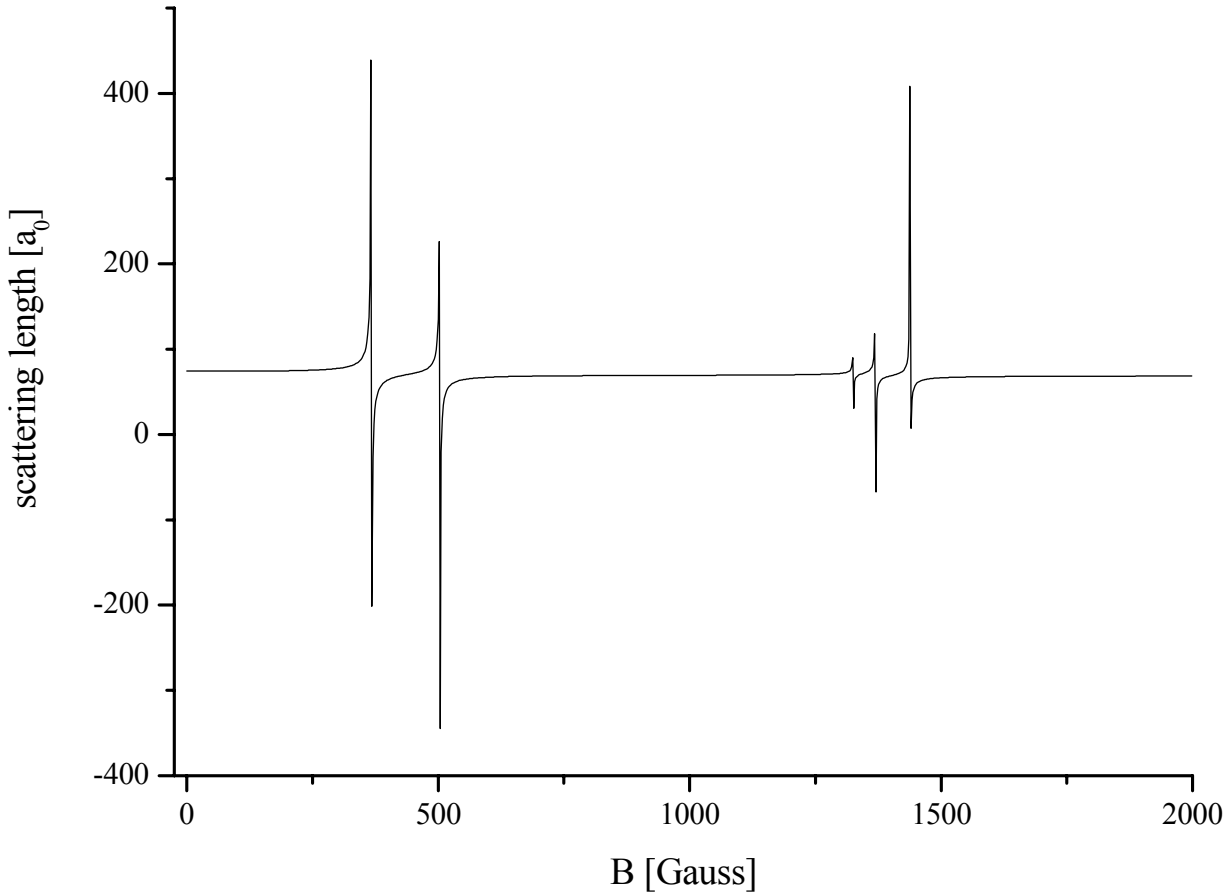

channel $1,1|_{Na}\ 2,1|_{Rb}$

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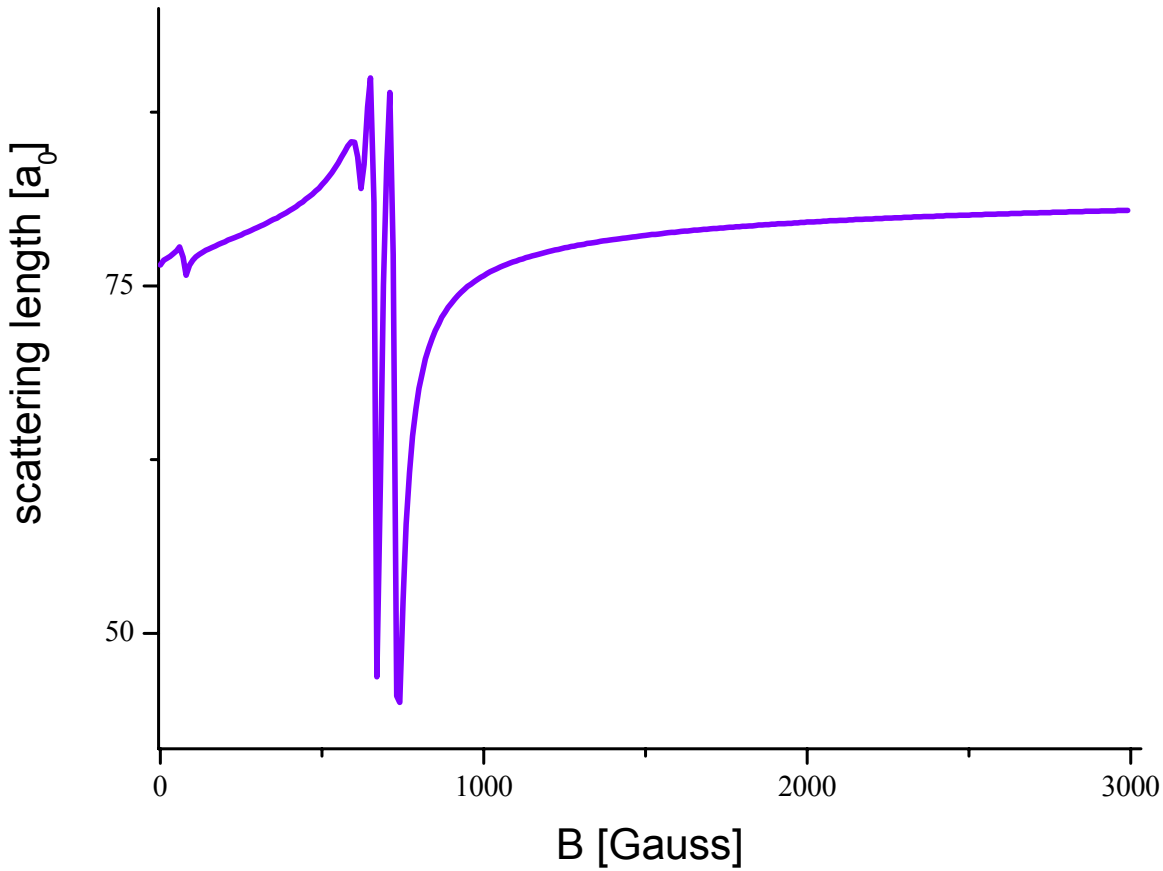

mass scaling of scattering properties

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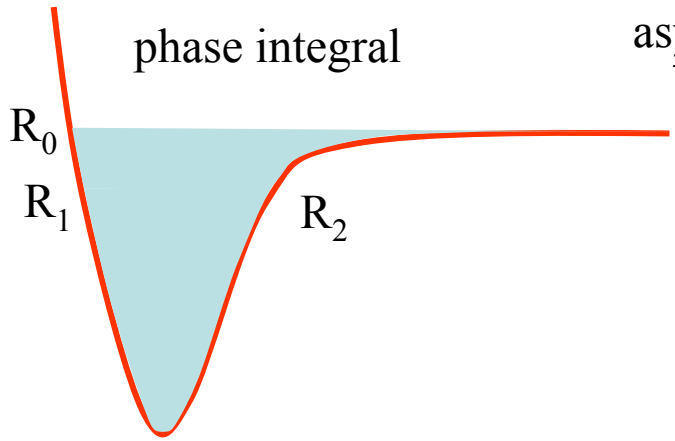

$$\pi\left(v_\infty + \tfrac{1}{2}\right) = \frac{\sqrt{2\mu}}{\hbar}\int_{R_0}^{\infty}\sqrt{0 - U(R)}\,dR$$

$$\pi\left(v + \tfrac{1}{2}\right) = \frac{\sqrt{2\mu}}{\hbar}\int_{R_1}^{R_2}\sqrt{E_v - U(R)}\,dR$$

$v_\infty = v_{max} + v_d$ $\quad$ $v_d \rightarrow$ scattering length

isotope relation

$$\frac{\mathbf{v}_\infty(A) + 1/2}{\sqrt{\mu(A)}} = \frac{\mathbf{v}_\infty(B) + 1/2}{\sqrt{\mu(B)}}$$

scattering length(A) $\rightarrow$ v_d(A)

v_{max}(A) $\quad$ knowledge of "full" potential

v_∞(B) $\rightarrow$ v_{max}(B) and v_d(B) $\rightarrow$ scattering length(B)

Feshbach resonances compared to magnetic resonance spectroscopy (NMR)

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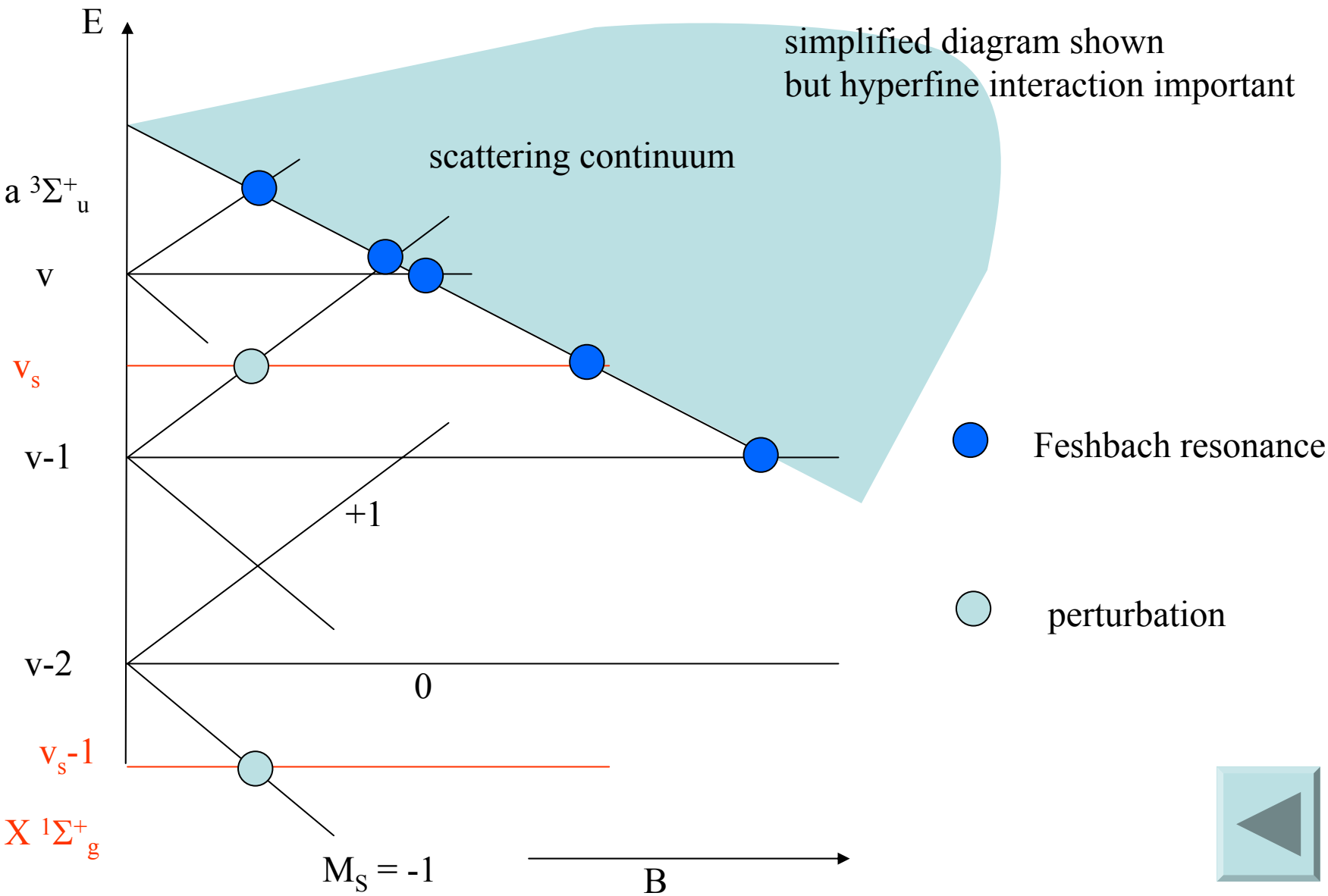

Extrapolating from Feshbach resonances

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typical magnetic resonance spectroscopy