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Potentials and molecular properties

Two-body interaction potentials from spectroscopy

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Different experimental situations!

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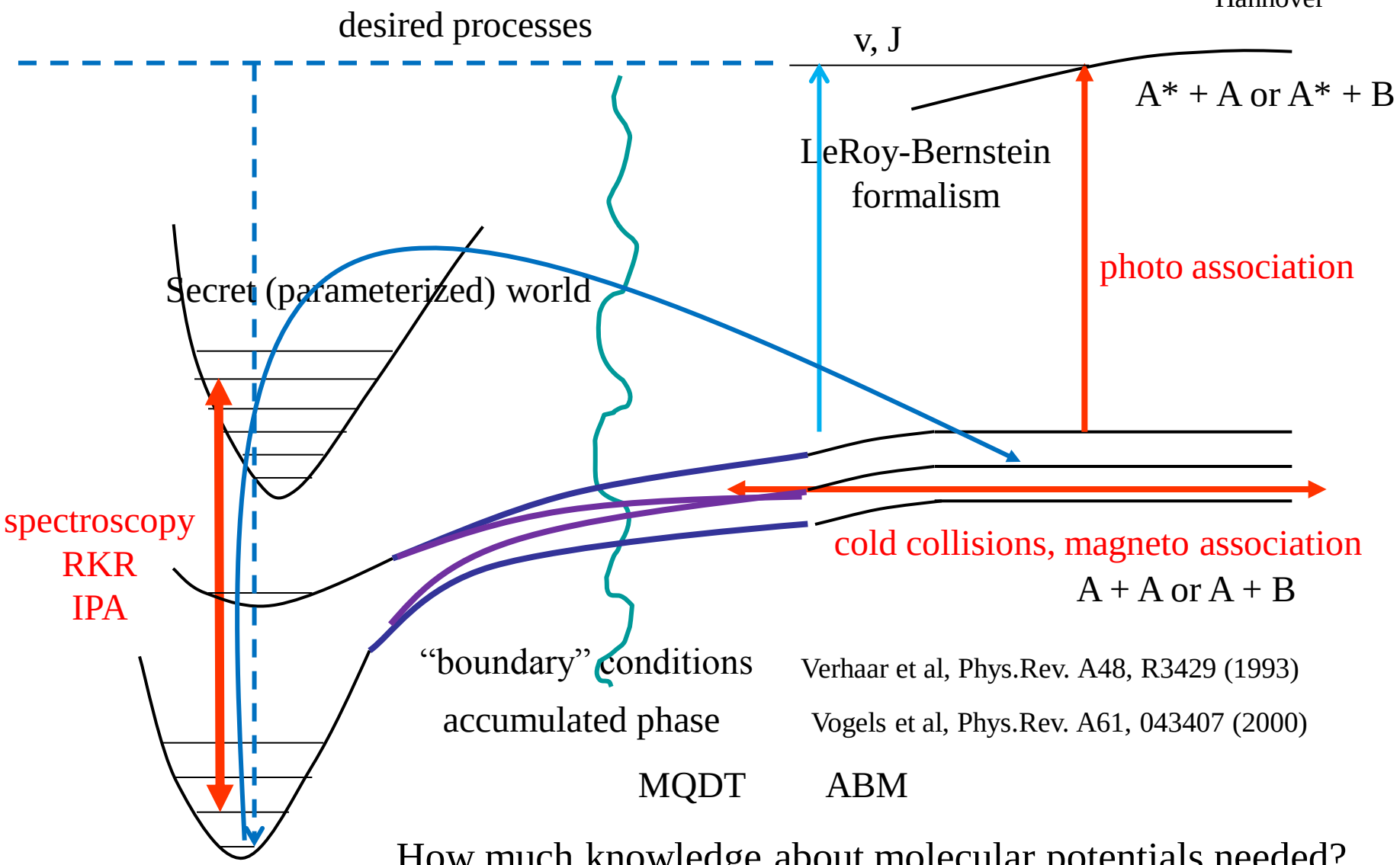

Verhaar et al, Phys.Rev. A48, R3429 (1993)

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

How much knowledge about molecular potentials needed?

Types of representations

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qualitative forms:

no generic analytic form or families of forms

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list of potential points and spline interpolation

power expansion $\sum_{i=1}^{n} a_i \, \xi(R)^i$ $\xi(R) = \frac{R - R_m}{R + b\, R_m}$

modified Morse $D_e[1 - \frac{u_{LR}(R)}{u_{LR}(R_e)} exp[-\beta_p^q(R) \cdot y_p^{eq}(R)]]^2$

R.J. LeRoy, C.C, Haugen, J. Tao, H.Li, Mol. Phys. **109**, 435 (2011)

$y_p^{ref}(R) = \frac{R^p - R_{ref}^p}{R^p + R_{ref}^p}$

Chebychev polynomial $T_{dis} - \frac{\sum_{k=0}^{m} c_k T_k(y_p)}{1 + (R/R_{ref})^n}$

L. Busevica, I. Klincare, O. Nikolayeva, M. Tamanis, R. Ferber, V.V. Meshkov, E.A. Pazyuk, A.V. Stolyarov, J. Chem. Phys. **134**, 104307 (2011)

Construction of the adiabatic ground state potentials

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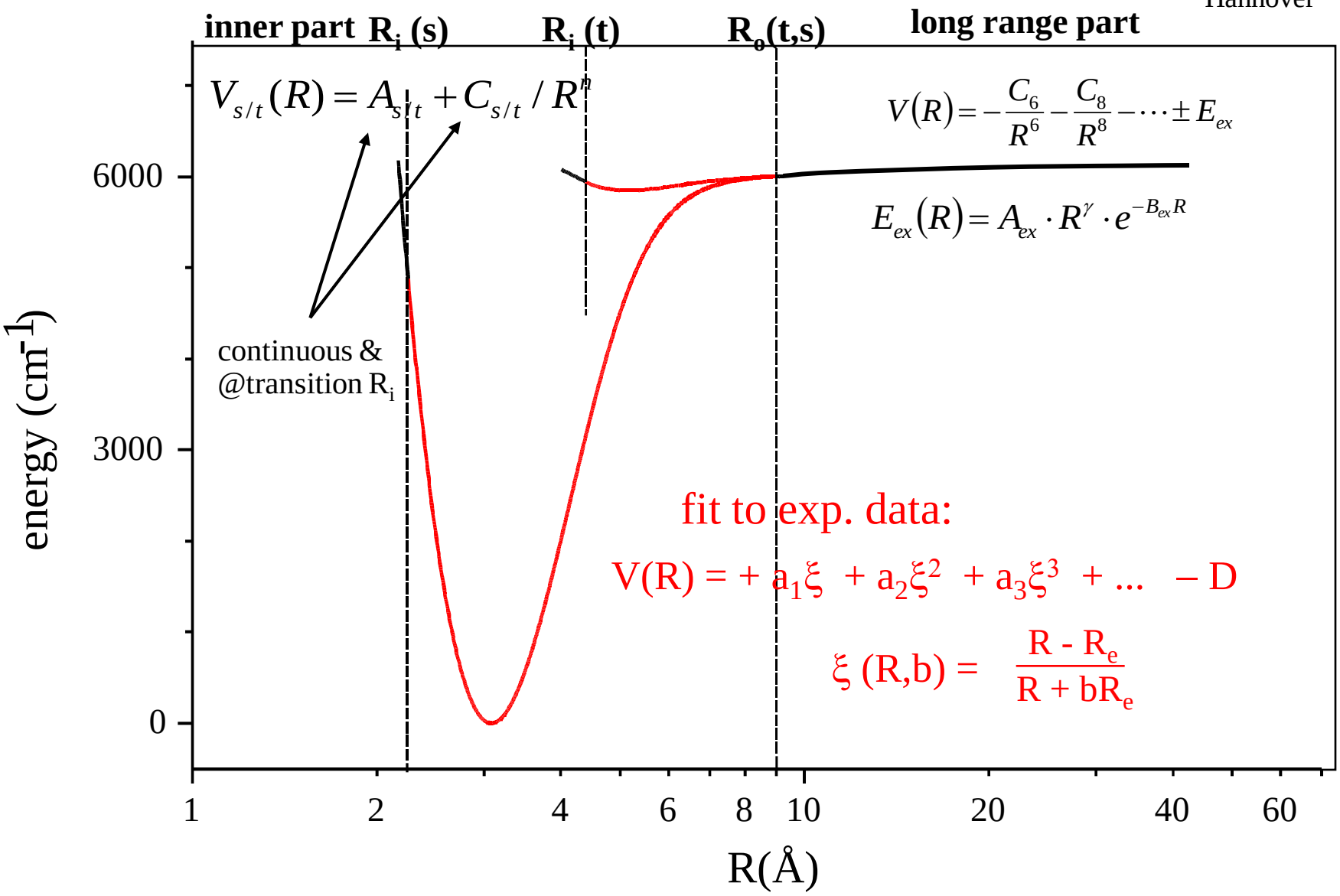

Potential differences from fits: equal data set

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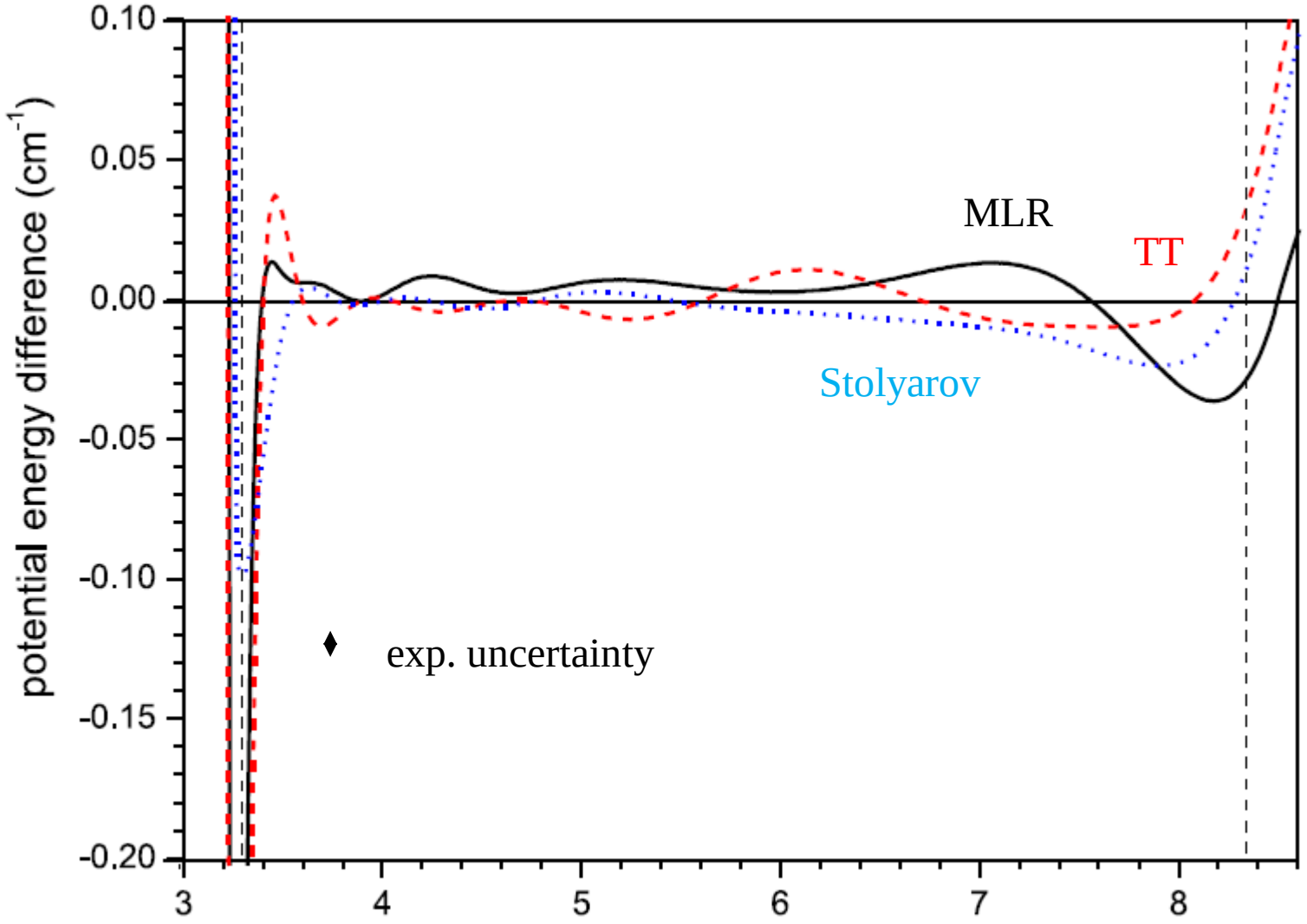

example Mg_2

K.T. Tang, J.P. Toennies, J. Chem. Phys. **80**, 3726 (1984)

Complete set of molecular levels?

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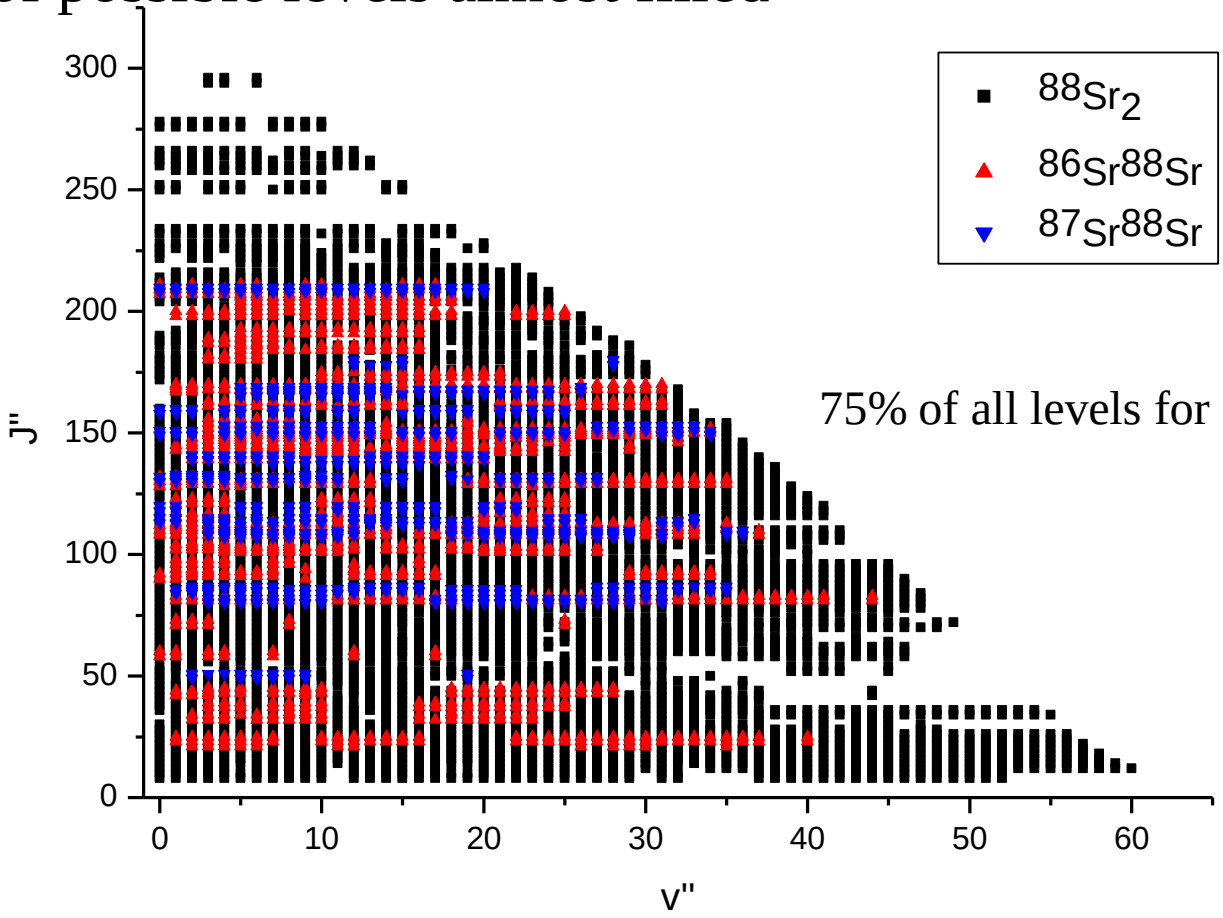
area of possible levels almost filled

example Sr_2



75% of all levels for $^{88}Sr_2$ observed

Derive a continuous function for the potential?!

Separate the long range contributions → C_6 C_8 C_{10} …

Sr_2: Stein et al, Eur. Phys. J. D 57, 171 (2010) Ca_2: Allard et al, Eur. Phys. J. D **26**, 155 (2003)

Monte Carlo simulation

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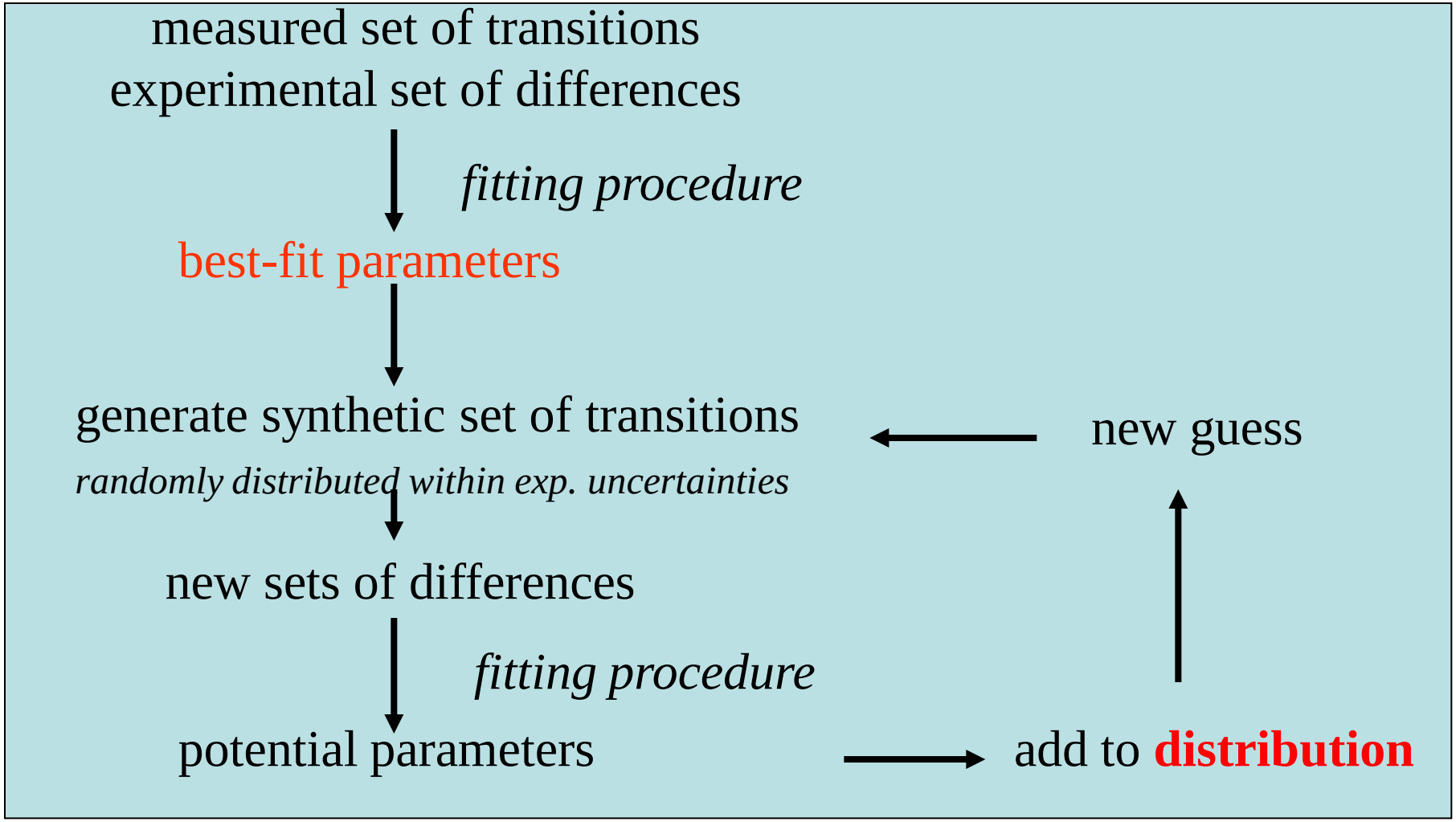
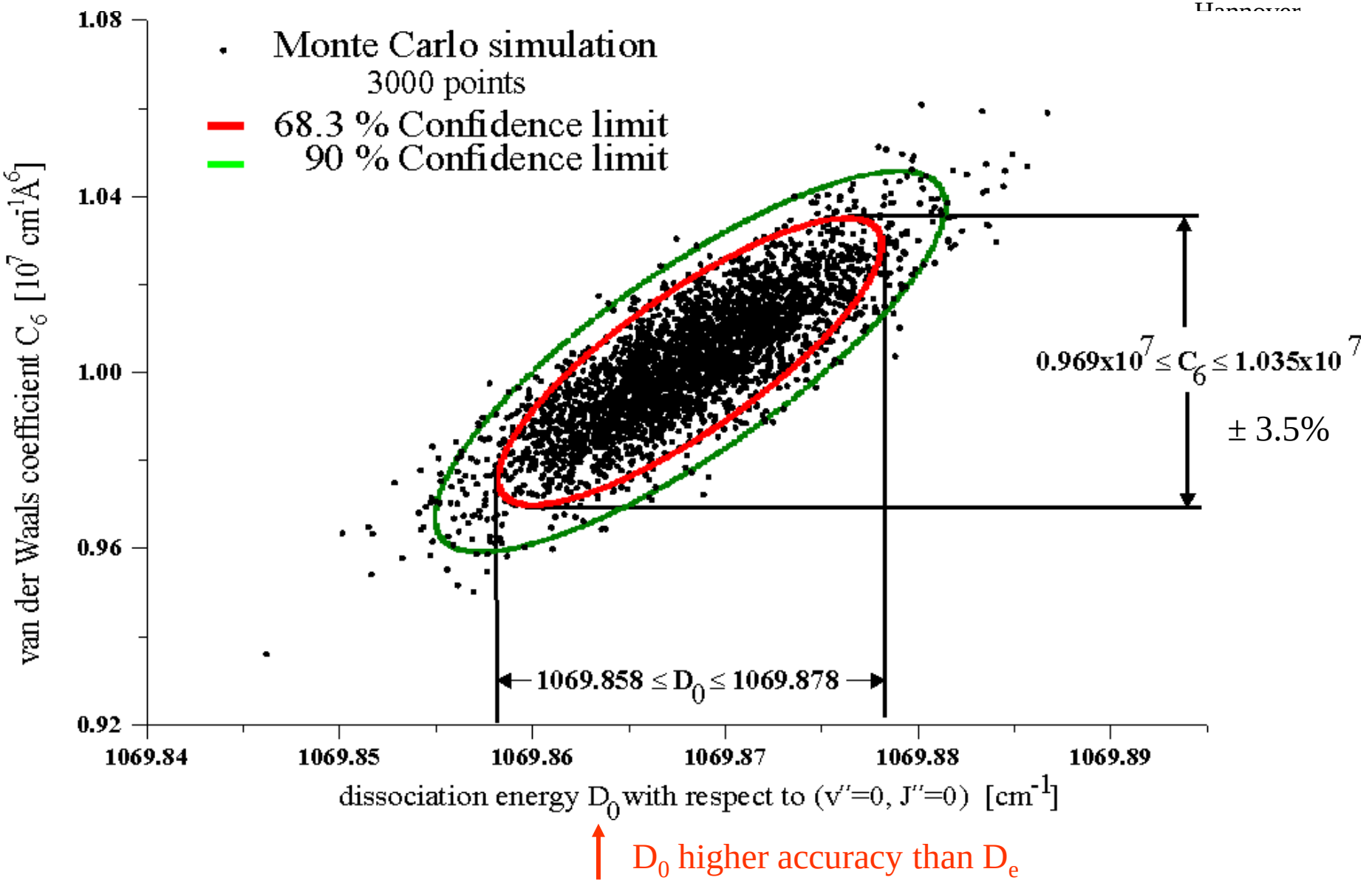
reliability limits of the derived parameters



Correlation: D_0 and C_6

example Ca_2



D_0 higher accuracy than D_e

Correlation: C_6 and C_8

example Ca_2

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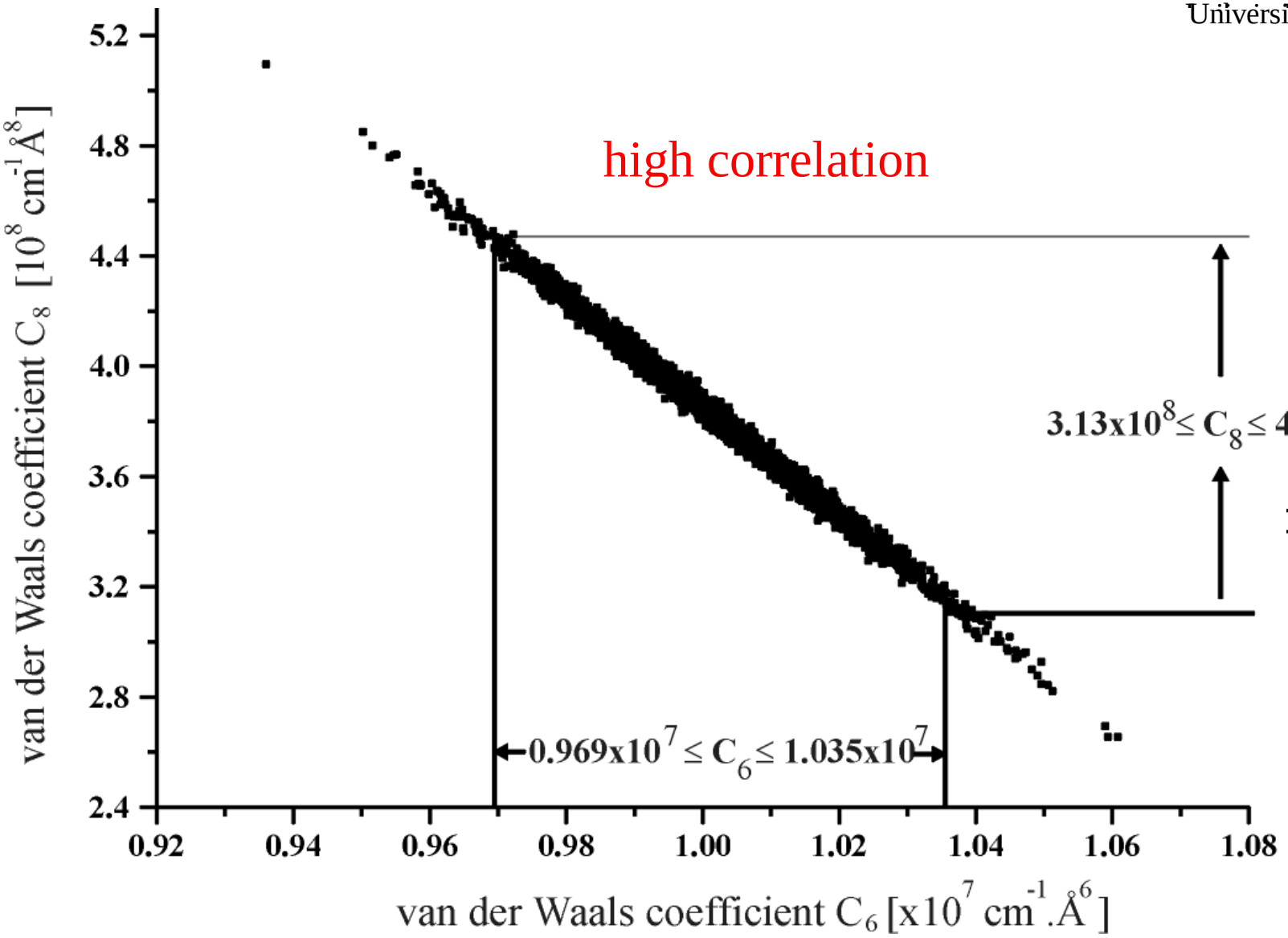

±3.5%

Diagram of evaluation diatomic alkalis

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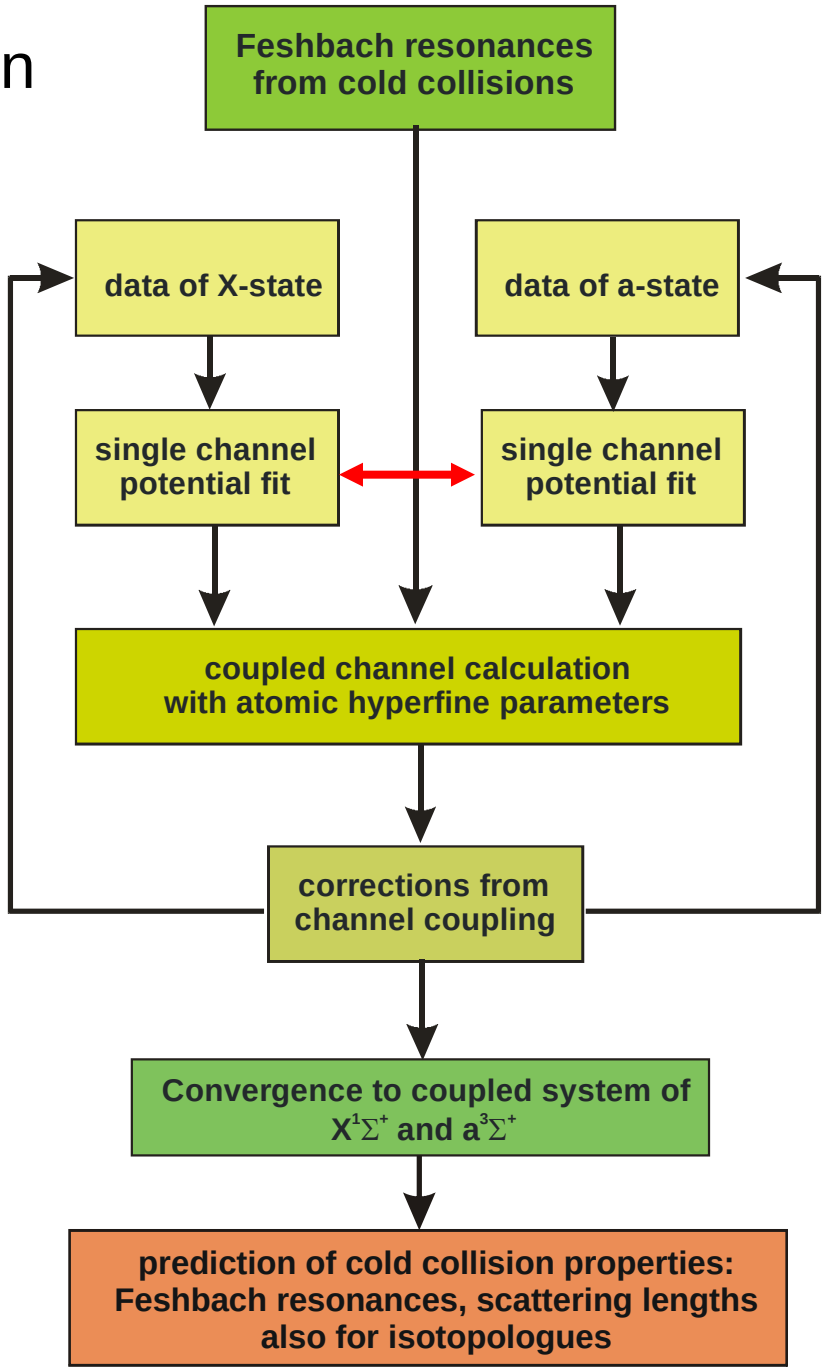

common asymptote simultaneous fit

Overview of results

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FR: Feshbach resonances observed a: potential for $a^3\Sigma^+$ determined

	Li	**Na**	**K**	**Rb**	**Cs**
Li	FR				
Na	FR	FR (a)			
K	FR a	FR a	FR a		
Rb	FR (a)	FR a	FR a	FR a	
Cs	FR (a)	a	a	FR a	FR (a)

For all cases precise ground state potential $X^1\Sigma^+$ known

Alkaline earth ground state $X^1\Sigma^+_g$ Mg_2 Ca_2 Sr_2

Mixed alkali/alkaline earth ground state $X^2\Sigma^+$ LiCa LiSr KCa

Molecular parameters – R-functions of interactions

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- hyperfine interaction
- g-factors for Zeeman energy
- Born-Oppenheimer correction (adiabatic, non-adiabatic)

- spin-orbit interaction
- spin-spin interaction

correlation between potentials and other interactions

Coupling Π+Σ in LiRb

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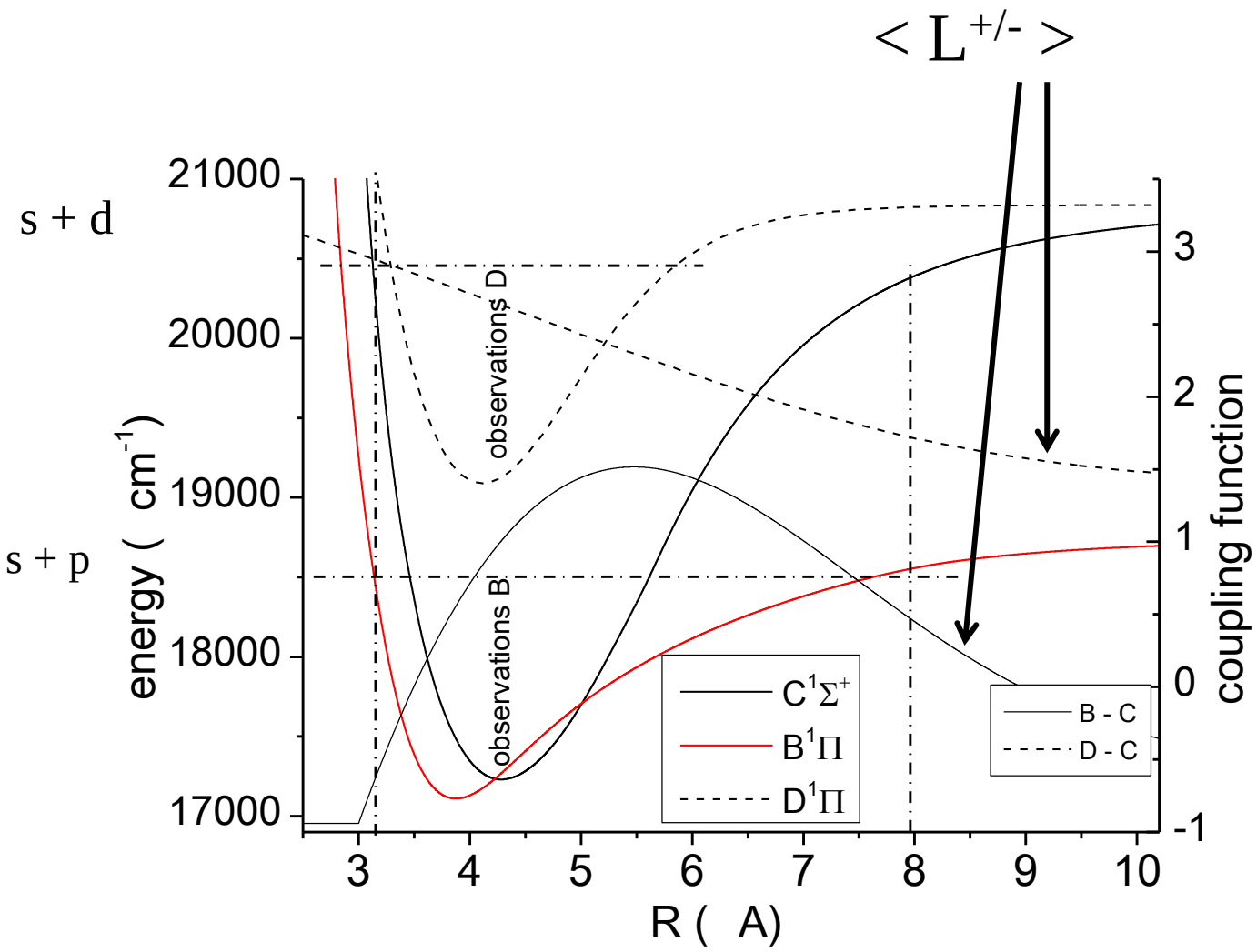

Spin-rotation interaction in LiCa $X^2\Sigma^+$

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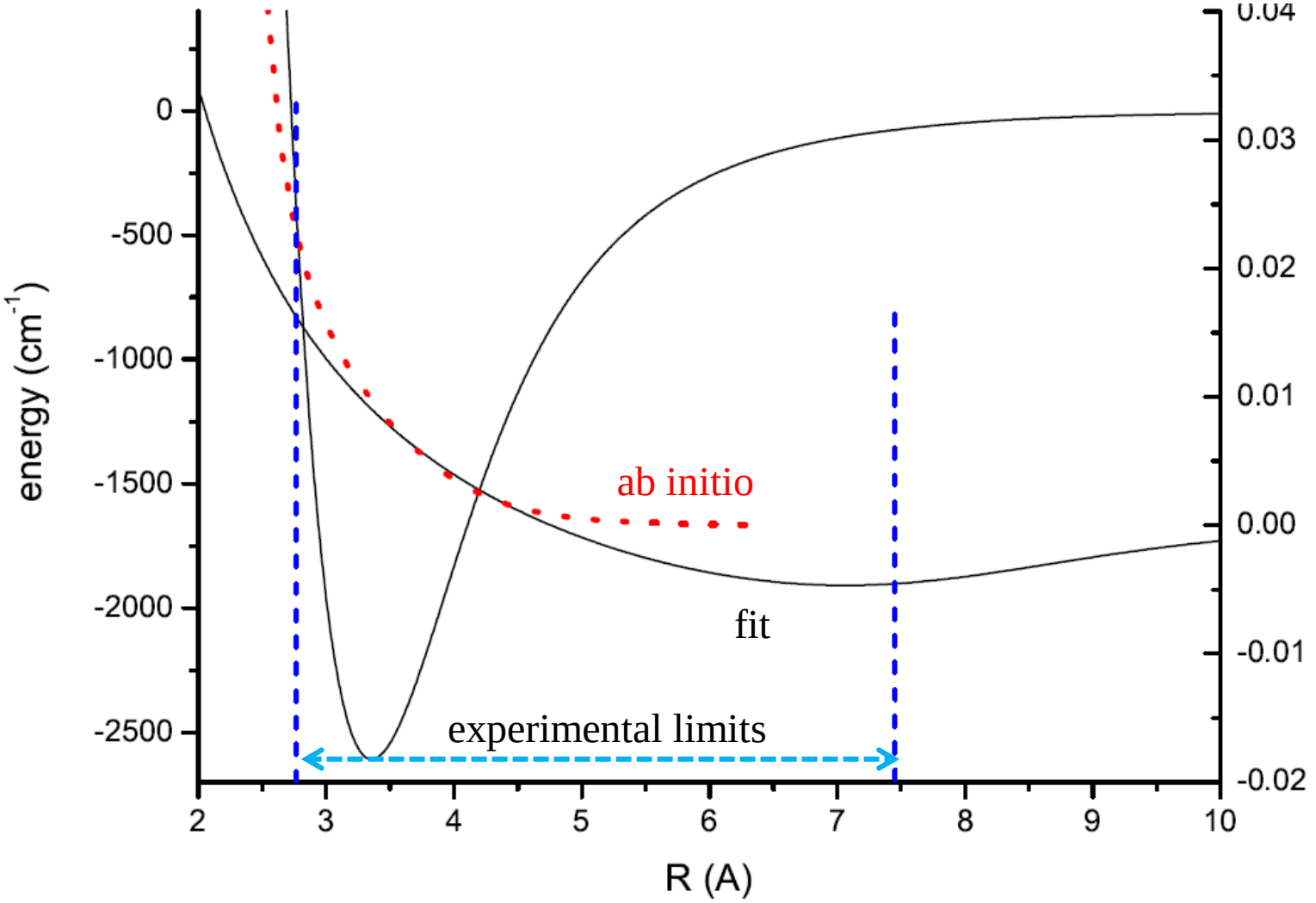
contributions: direct spin-rotation, spin-orbit or L-uncoupling



Conclusion and outlook

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- all alkali dimers studied, but not yet fully evaluated
- enough data on excited states for work on coupled systems
- connection theory-experiment for consistent molecular properties → breaking correlations
- good examples LiCa shown or KCs and RbCs by Riga/Moscow
- desired new molecular groups? YbRb etc.?
- experimental difficulties with samples containing alkali atoms → overlapping strong signals from such dimers