

COUPLED-CLUSTER DEVELOPMENTS IN ELECTROMAGNETIC FIELDS

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UNIVERSITÄT
DES
SAARLANDES

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UiO
University of Oslo

 Hylleraas

TRR 306

QuCoLiMa

Quantum Cooperativity of Light and Matter



ECm²

**TRR
146**

PCT
CRC 1633

DFG

Deutsche
Forschungsgemeinschaft

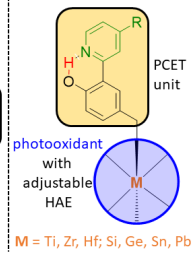
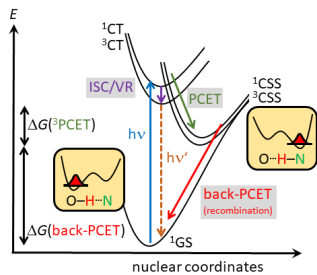
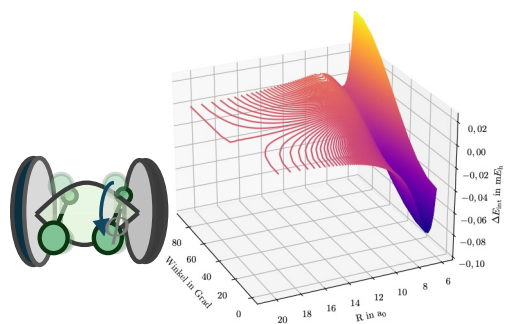
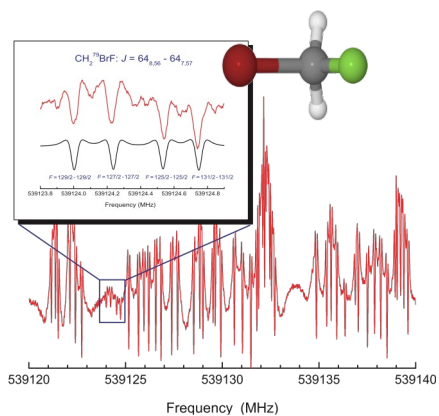
Saarland University



Saarland U



Research profile



NMR & magnetic properties

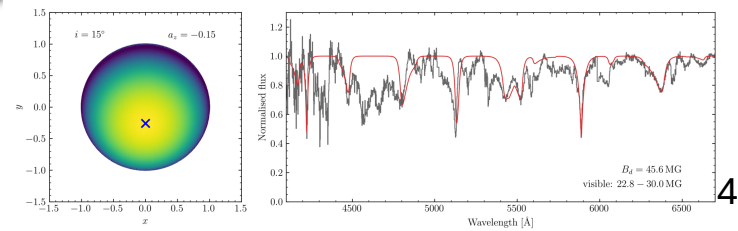
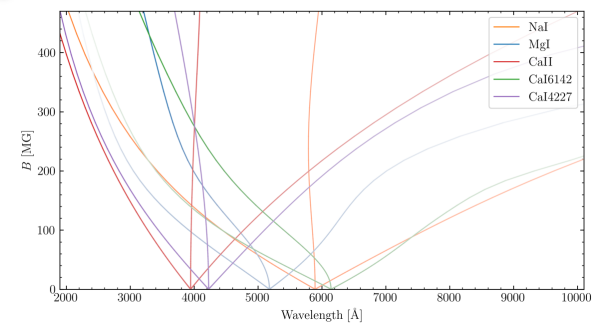
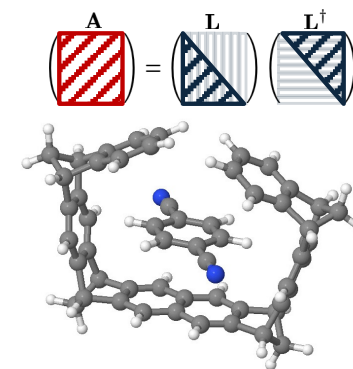
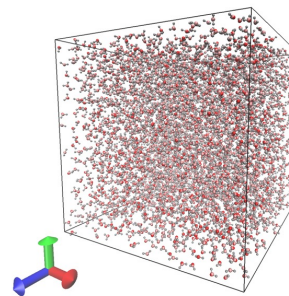
Relativistic effects

Predictive Quantum Chemistry

Light-matter
& Photochemistry

Strong magnetic fields

Cholesky
decomposition
& multiscale
methods



4

INTRO: MOLECULES IN STRONG MAGNETIC FIELDS

Molecules in magnetic fields



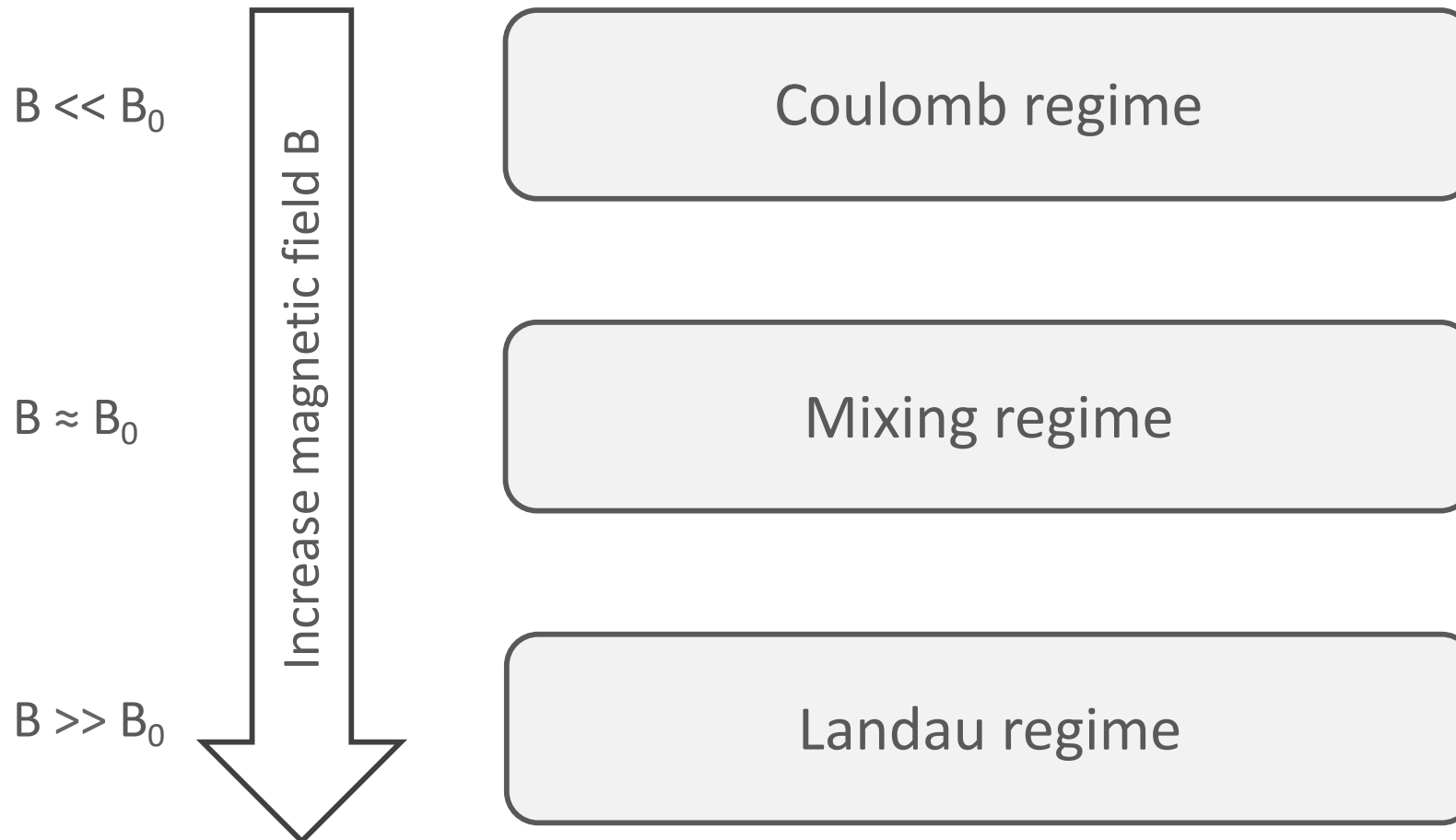
“weak fields”

“strong fields”

Cranking up the magnetic field

Atomic unit of the magnetic field B: **$1B_0 = 235000 \text{ T}$**

Distinguish 3 regimes:

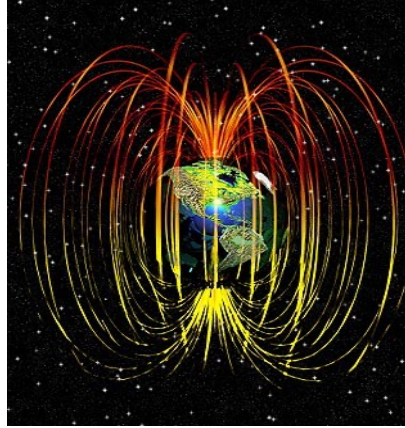


Magnetic fields on Earth

Human brain
 $1\text{pT} = 4.35 \text{ aB}_0$



Earth magnetic field
 $60\mu\text{T} = 260 \text{ pB}_0$



Refrigerator magnet
 $4\text{mT} = 17 \text{ nB}_0$



NMR
 $51 \mu\text{B}_0$



Levitate a frog
 $16\text{T} = 68 \mu\text{B}_0$



Strongest non-destructive magnet
 $100 \text{ T} = 0.4 \text{ mB}_0$



Z-machine
 $\sim 10.000 \text{ T} = 0.04 \text{ B}_0$



Magnetic fields in space

Compact stars

Mixing regime

Magnetic White Dwarf stars $\sim 3\text{T} - 100\text{ kT} \rightarrow$ up to $\sim 0.4 B_0$

Neutron stars $\sim 1\text{-}100\text{ MT}$

$\rightarrow$ up to $\sim 400 B_0$

Magnetars $\sim 100\text{MT-}100\text{ GT}$

$\rightarrow$ up to $\sim 400\text{ k}B_0$

Landau regime

Magnetic fields in space

Compact stars

Mixing regime

Magnetic White Dwarfs $\sim 3 \text{ T} - 100 \text{ kT}$

$\rightarrow$ up to $\sim 0.4 B_0$

- Which atoms/molecules exist in strong fields?
 $\rightarrow$ Astrophysics, observational spectra
- Chemistry in strong magnetic fields?

Theory/Quantum chemistry

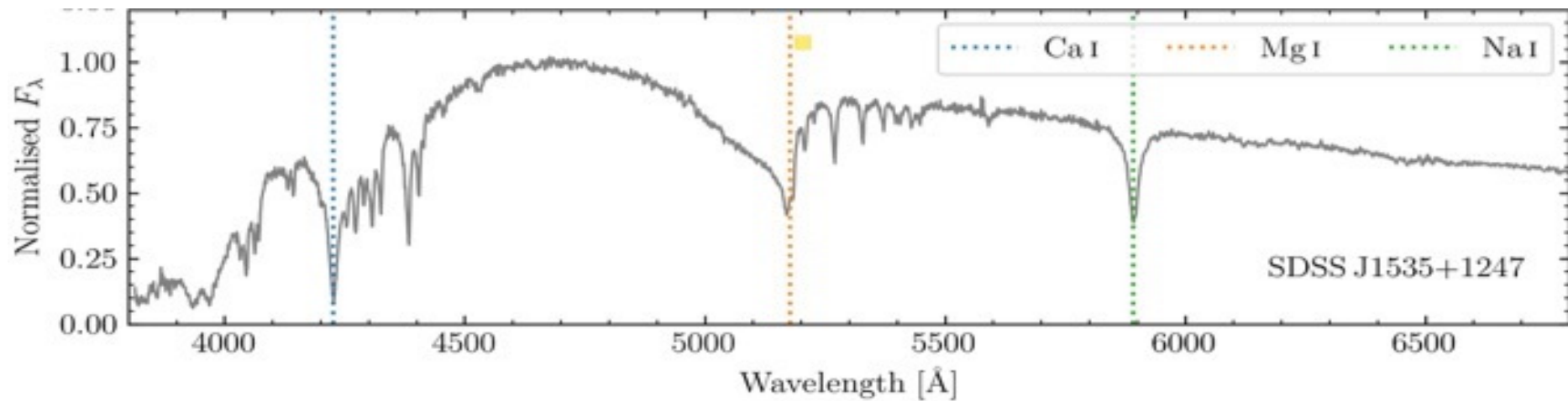
Coulomb and magnetic forces of same order of magnitude! $\rightarrow$ ab-initio finite-field methods (seamless transition from field-free to in principle any field-strength)

White Dwarfs

- Endpoints of stellar evolution (very common!): 97 % of all stars become WDs!
- Very dense!
- Atmospheres: H, He, “Metals” (C, Si, Na, Mg, ...), molecules (H₂, CH-bands, C₂,...)
- The older, the cooler! Effective surface temps: ~4000 K - ~150.000 K (usually 8000-40.000 K)
- Magnetic WDs: 25% → assignment of spectra difficult!

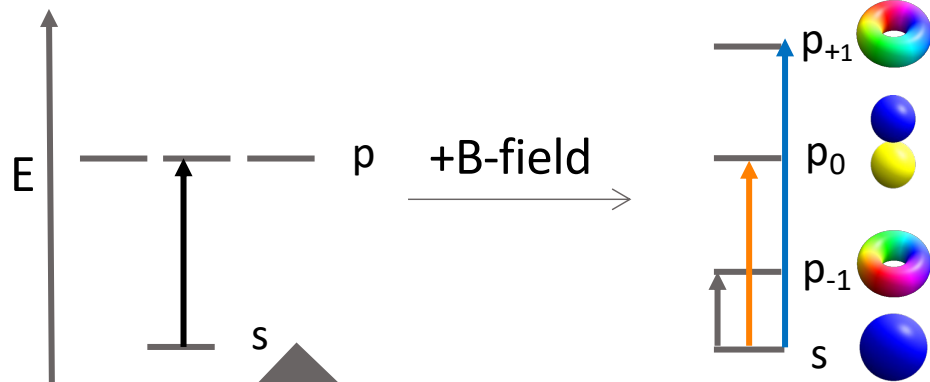
Non-magnetic DZ spectrum

(White Dwarf stars containing metals are called „DZ“)

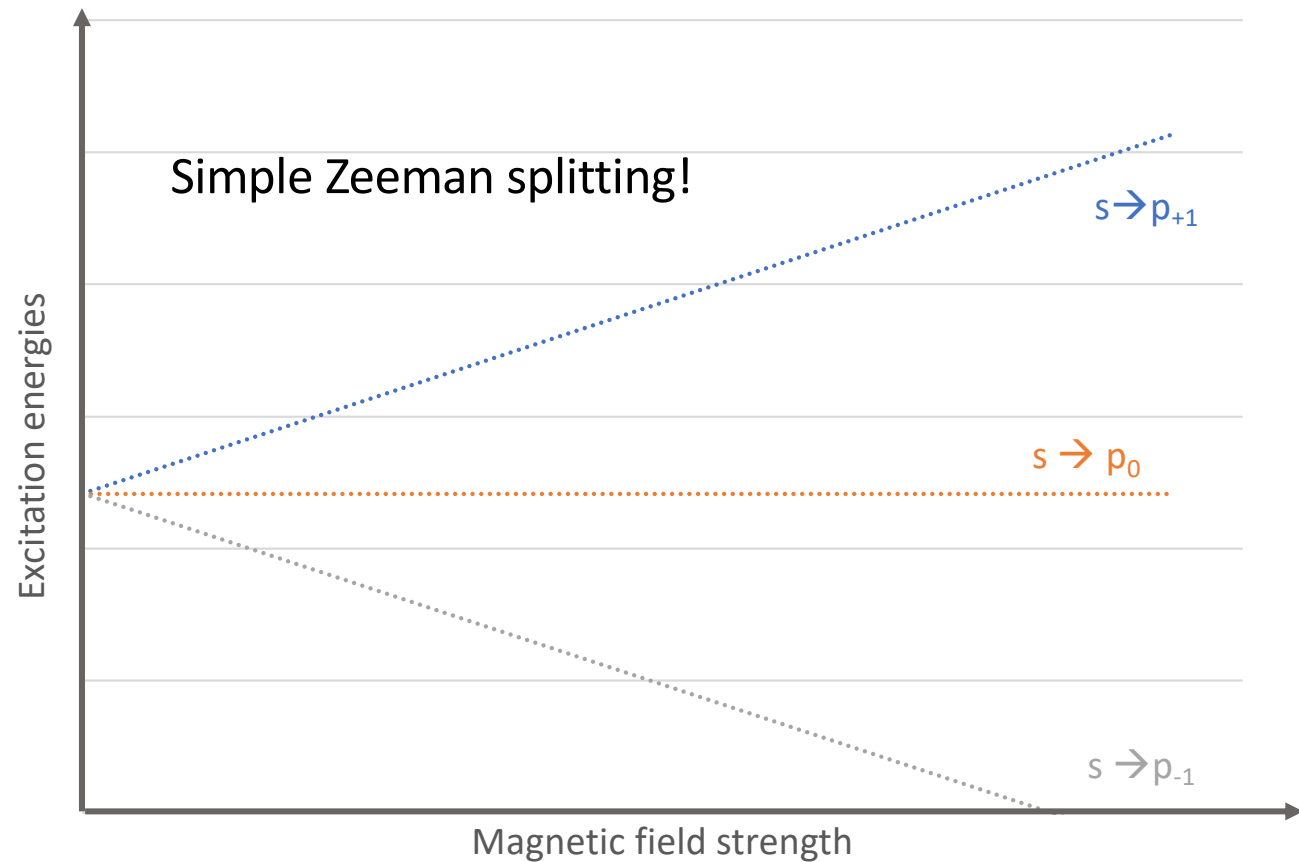


Excitation energies in (weak) magnetic field

Excitation energies $s \rightarrow p$ transitions

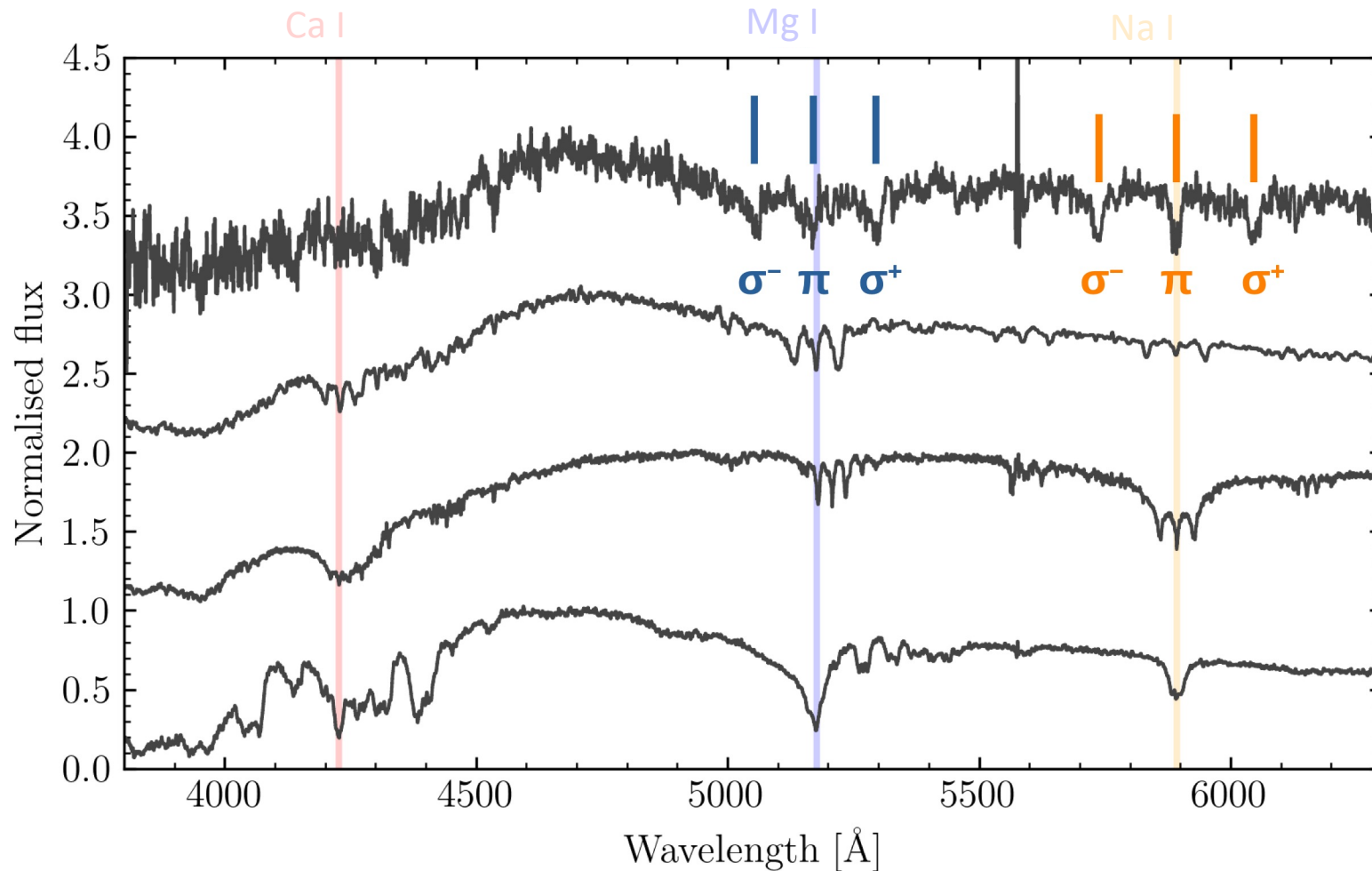


weak field:
 $E \sim 1/2 BL$



(Weakly) magnetic-field DZ spectra

Simple linear slitting



SDSSJ1536+4205
B= 959 T
Hollands et al (2015)

SDSSJ0157+4205
B= 349 T
Schmidt et al (2003)

LHS2534
– B= 210 T –
Reid et al (2001)

G165-7
B= 58 T
Dufour et al (2006)

Hamiltonian: molecule in magnetic field

Electronic Hamiltonian for molecule in a homogeneous magnetic field in z-direction (in a.u.)

$$\hat{H} = \hat{H}_0 + \frac{1}{2}B\hat{L}_z^O + B\hat{S}_z + \frac{1}{8}B^2 \sum_k^N \left(x_k^O{}^2 + y_k^O{}^2 \right)$$

Orbital-Zeeman term

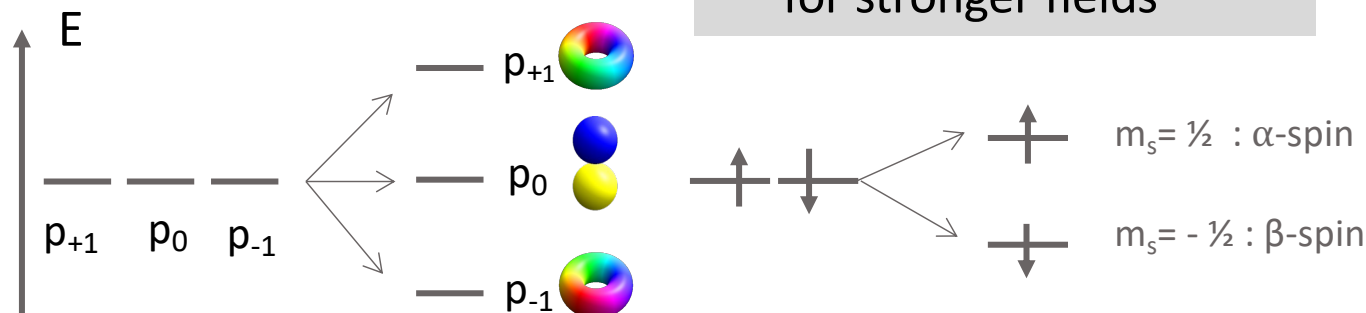
- splitting of orbitals
- favors high negative M_L values

Spin-Zeeman term

- lifts degeneracy of alpha and beta spin
- favorisation of high-spin states open-shell states for stronger fields

diamagnetic term

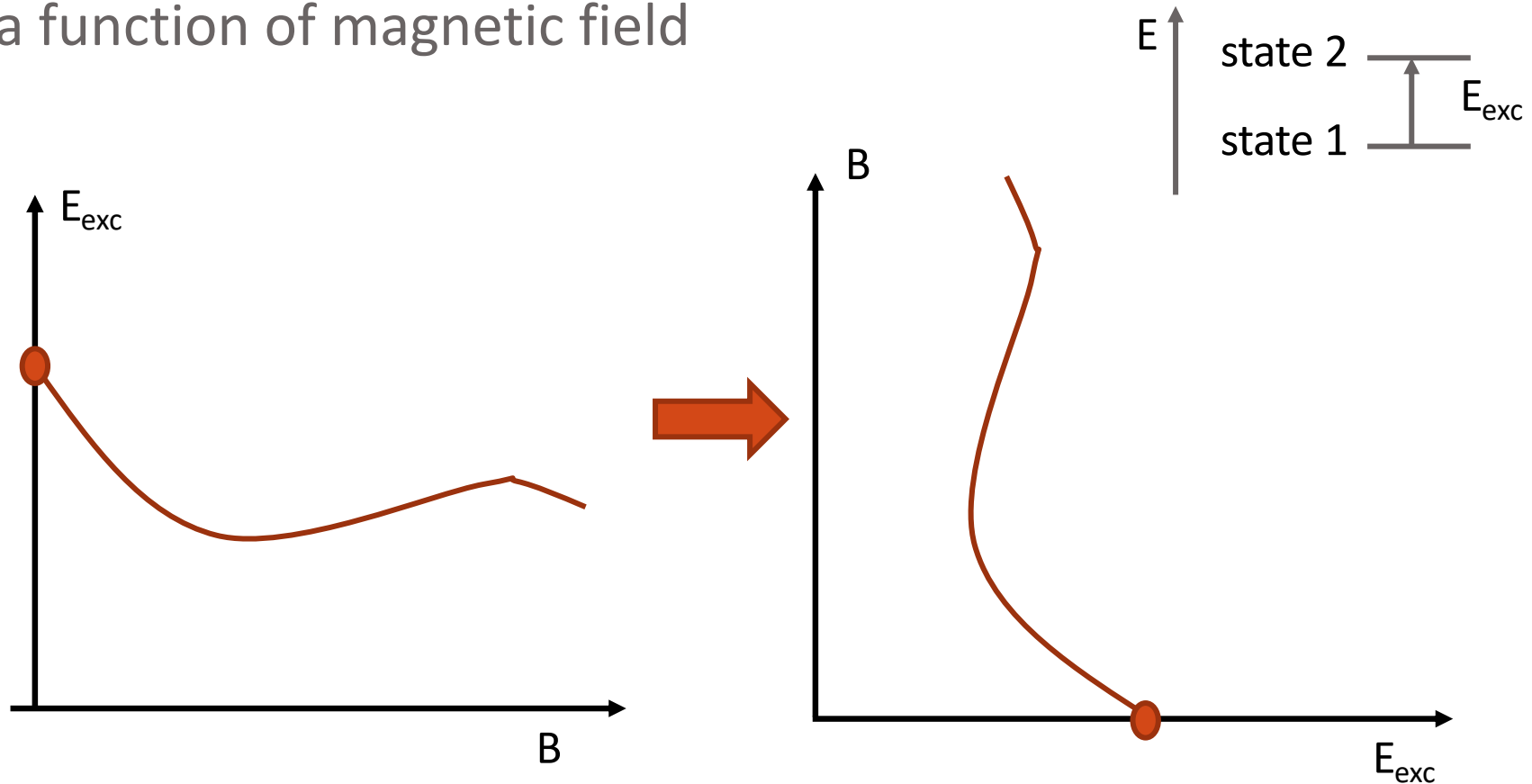
- always positive
- confinement



$$p_{+1} = -\frac{1}{\sqrt{2}}(p_x + ip_y), \quad p_{-1} = \frac{1}{\sqrt{2}}(p_x - ip_y)$$

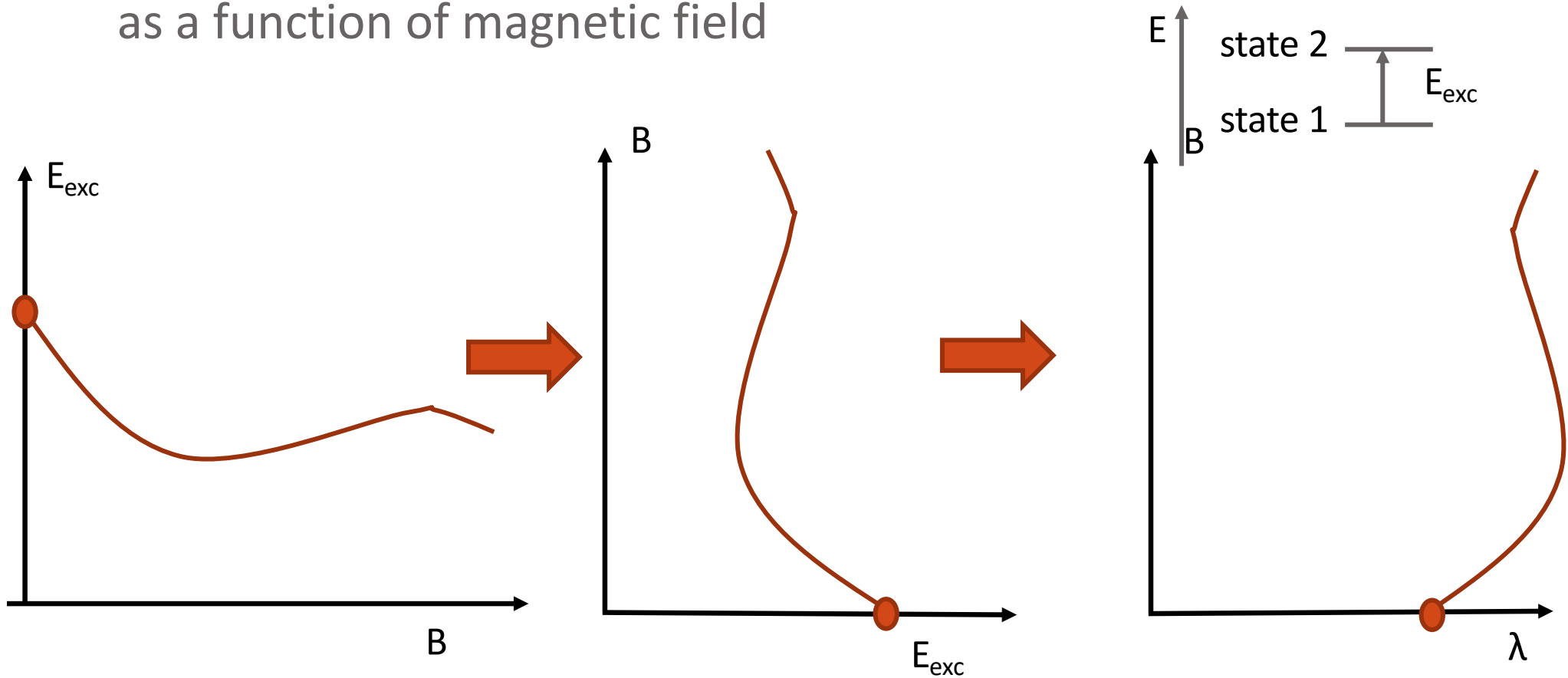
Strong fields: B- λ curve

- Info: essentially the excitation energy between two energy levels as a function of magnetic field



Strong fields: B- λ curve

- Info: essentially the excitation energy between two energy levels as a function of magnetic field



B- λ curves: Hydrogen

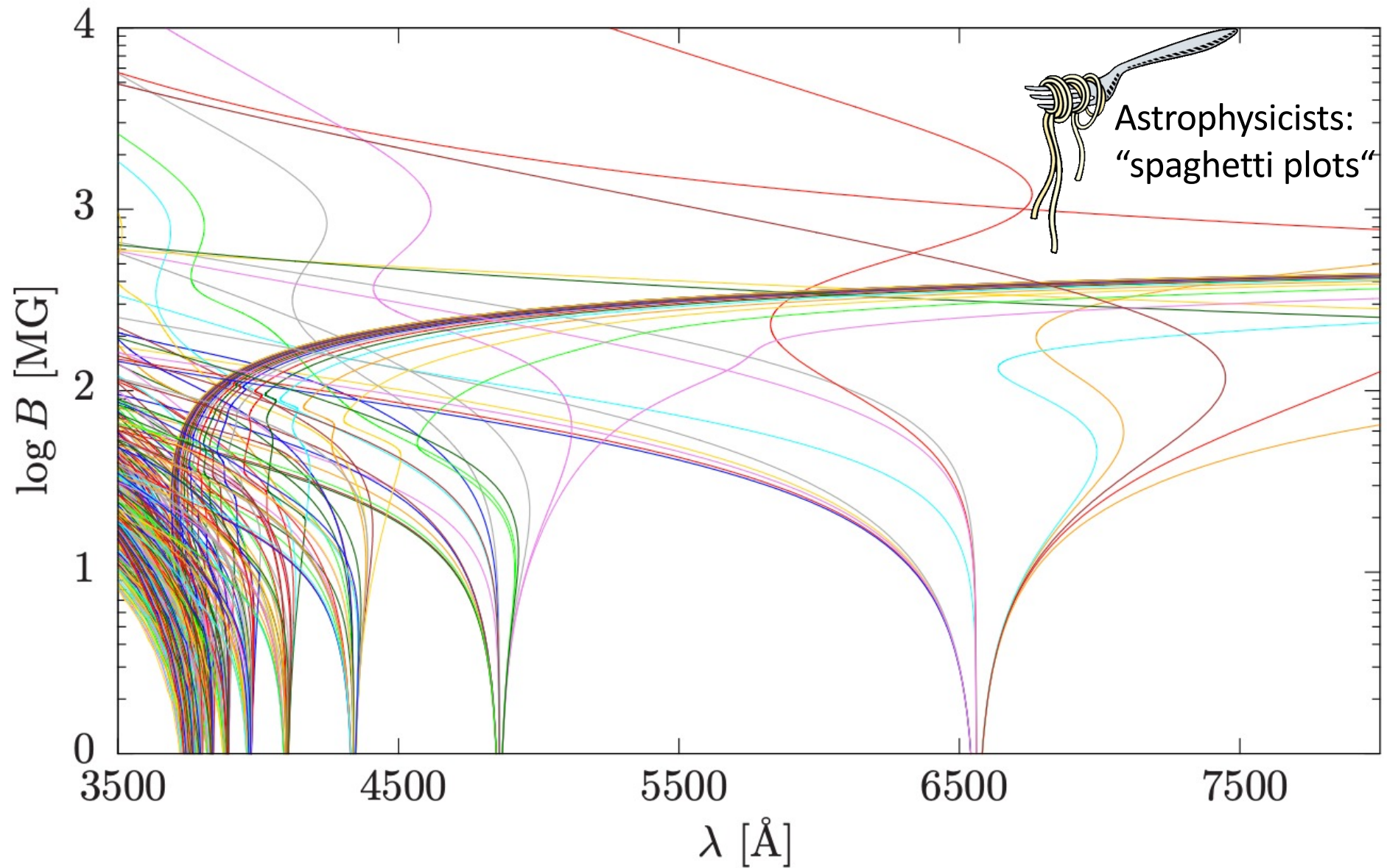
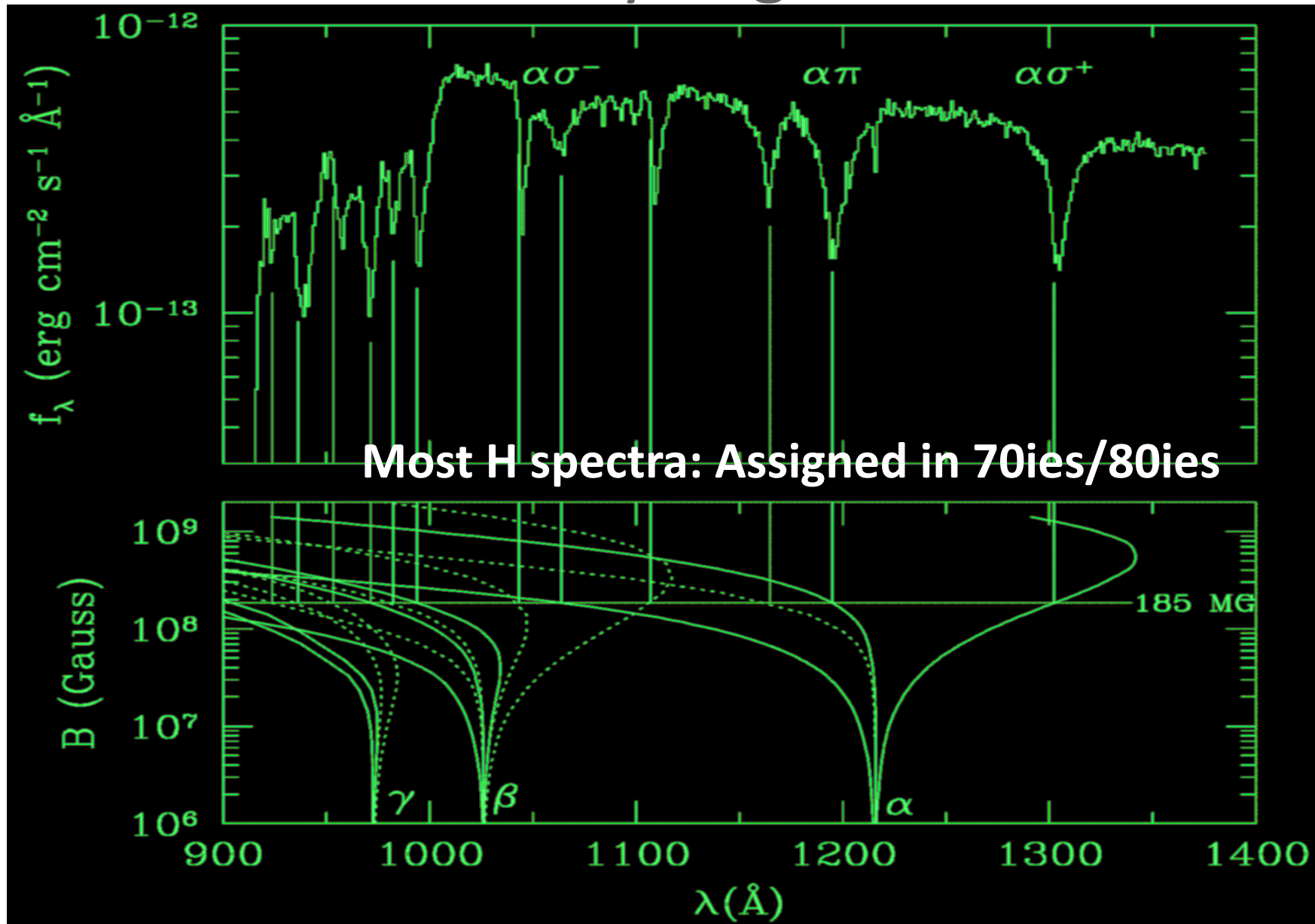


Figure: Schimeczek, Wunner, ApJS 212, 26 (2014)

Strong magnetic fields in WD spectra: Hydrogen



Strong magnetic fields in WD spectra: Hydrogen

GD 229
helium
atmosphere

finite-field FCI
calculations on
Helium

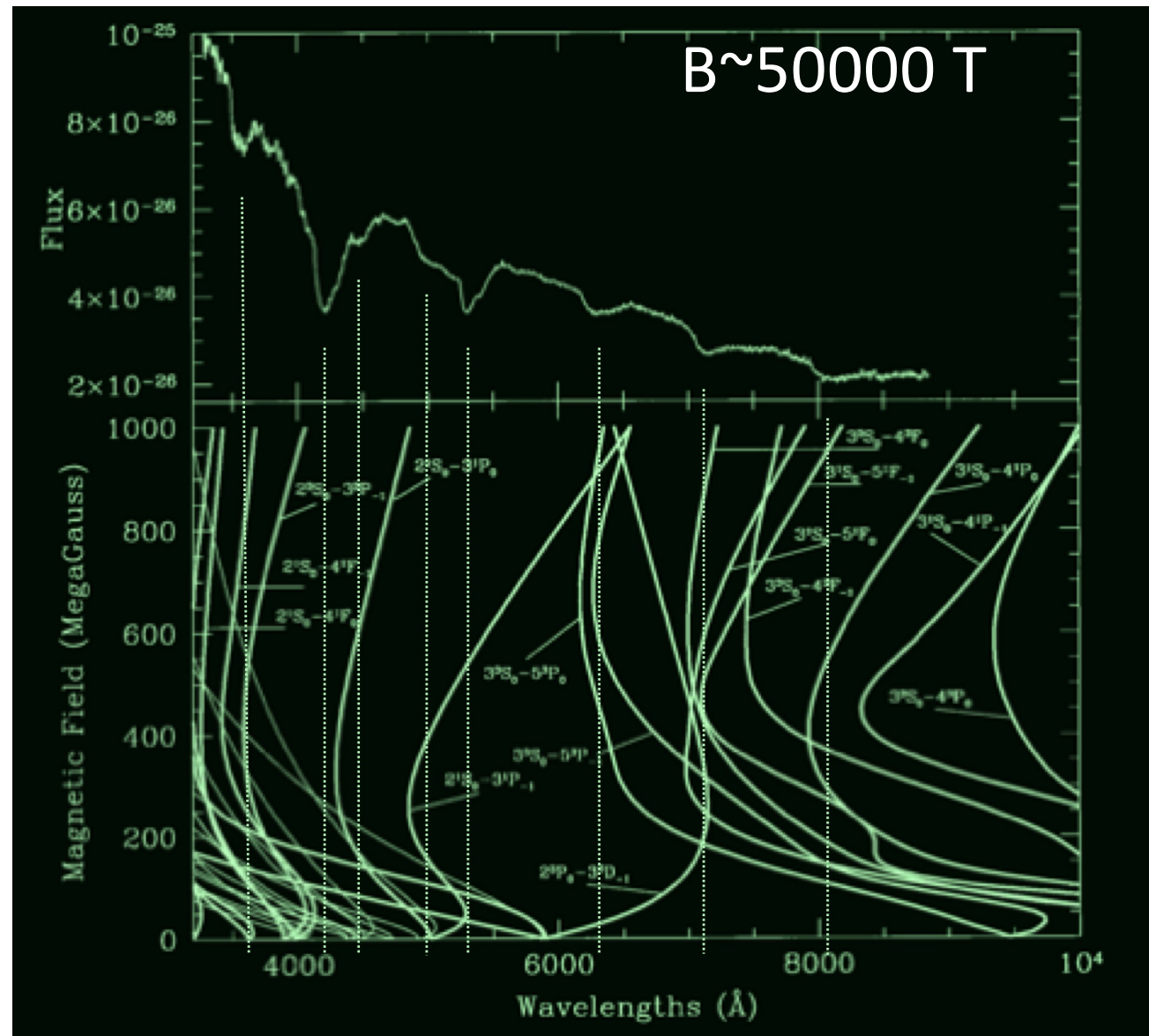


Figure: Wickramasinghe and Ferrario (2000),
Assignment/calculations: Jordan et al. (1998), Becken et al. (1999)

Assignment of spectra from magnetic WDs: „Metals“

ff-FCI unfeasible
→ ff-CC methods

Hamiltonian: molecule in magnetic field

Electronic Hamiltonian for molecule in a homogeneous magnetic field in z-direction (in a.u.)

$$\hat{H} = \hat{H}_0 + \frac{1}{2} B \hat{L}_z^O + B \hat{S}_z + \frac{1}{8} B^2 \sum_k^N \left(x_k^O{}^2 + y_k^O{}^2 \right)$$


$$\hat{L}_z^O = -i \sum_k^N \left(x_k^O \frac{\partial}{\partial y_k} - y_k^O \frac{\partial}{\partial x_k} \right)$$

- for molecules: no eigenfunction (except lin. mol. in parallel field)
- complex wave function! → new software implementations required
- reduced symmetry
- origin dependence in Hamiltonian → use of GIAOs essential

Gauge-origin dependence

- Hamiltonian depends on gauge origin
- Physical properties should not depend on choice of gauge origin

→ ensured by according trafo of wave function

$$\Psi_{\text{trans}} = \exp \left(\frac{i}{2} \underline{B} \times (\underline{R}_{\text{trans}} - \underline{R}_{\text{orig}}) \cdot \underline{r} \right) \Psi_{\text{orig}}$$

- Problem: **approximate** wave function does not reproduce phase oscillation seen before

Gauge-Including Atomic Orbitals

- How to solve this problem? $\Psi_{\text{trans}} = \exp\left(\frac{i}{2}\underline{B} \times (\underline{R}_{\text{trans}} - \underline{R}_{\text{orig}}) \cdot \underline{r}\right) \Psi_{\text{orig}}$
- build transformation behavior into the basis functions!

Gauge-Including Atomic Orbitals
(GIAOs, also known as London orbitals)

$$\chi_{\mu}(\underline{r}, \underline{B}) = \exp\left(-\frac{i}{2}\underline{B} \times ((\underline{R}_{\mu} - \underline{R}_{\text{O}}) \cdot \underline{r})\right) \chi_{\mu}(\underline{r})$$

(London, 1937)

- equivalent to local gauge-origins $\underline{R}_{\mu}$ for AOs
- unique results
- fast basis-set convergence

nowadays standard for calculations of molecules in mag. fields

Finite-field CC and EOM-CC developments

New implementation needed!

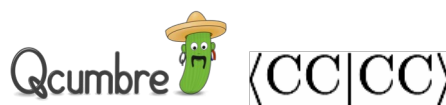
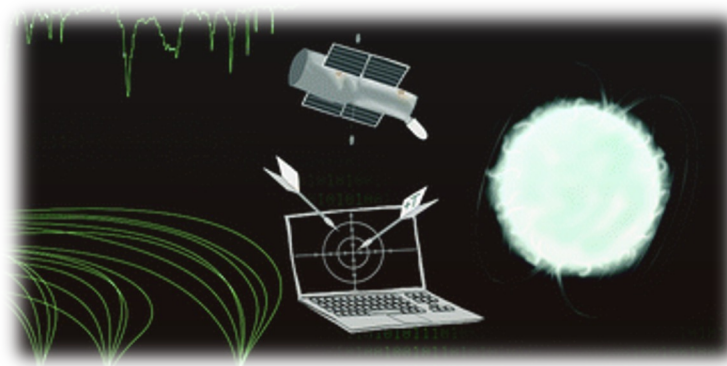
GROUND STATE

Energies:

- CCSD
- CCSD(T)
- CCSD(T)(a)
- CCSDT
- CC2, CC3
- UCC3
- QED-CCSD, QED-UCC2, QED-CCSDT

transition dipole moments:

- CCSD
- CC2
- UCC2, UCC3
- LR-CCSD



target states from different
starting points and different levels
of accuracy

EXCITED STATE



- EOM-EE: CCSD, CCSDT, CC2, CC3, CCSD(T)(a)*, UCC3, QED-CCSD
- EOM-EA: CCSD, CCSD(T)(a)*
- EOM-SF: CCSD, CCSD(T)(a)*, QED-CCSD
- EOM-IP: CCSD, CCSD(T)(a)*
- EOM-DIP: CCSD
- EOM-DEA: CCSD

- EOM-EE-CCSD, CCSD(T)(a)*
- EOM-SF-CCSD
- EOM-EA-CCSD, CCSD(T)(a)*
- EOM-IP-CCSD, CCSD(T)(a)*
- LR-CCSD

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ASSIGNMENT OF A MAGNETIC WD SPECTRUM WITH METALS

with Mark Hollands (U Warwick, Astrophysics)

Marios-Petros Kitsaras

Florian Hampe

Simon Blaschke

This is a detailed star map of the northern sky, showing several constellations and their associated stars and objects. The constellations visible include Ursa Minor, Ursa Major, Camelopardalis, Lynx, Canes Venatici, and Draco. The map features numerous star names, coordinates, and celestial objects like galaxies and clusters. A red circle highlights a specific star in Ursa Major. The Google Earth logo is in the bottom right corner.

Constellations and Stars:

- Ursa Minor:** HD 151613, HD 150449, HD 147232, HD 143466, HD 134190, HD 123657.
- Ursa Major:** HD 61931, HD 61932, HD 61933, HD 61934, HD 61935, HD 61936, HD 61937, HD 61938, HD 61939, HD 61940, HD 61941, HD 61942, HD 61943, HD 61944, HD 61945, HD 61946, HD 61947, HD 61948, HD 61949, HD 61950, HD 61951, HD 61952, HD 61953, HD 61954, HD 61955, HD 61956, HD 61957, HD 61958, HD 61959, HD 61960, HD 61961, HD 61962, HD 61963, HD 61964, HD 61965, HD 61966, HD 61967, HD 61968, HD 61969, HD 61970, HD 61971, HD 61972, HD 61973, HD 61974, HD 61975, HD 61976, HD 61977, HD 61978, HD 61979, HD 61980, HD 61981, HD 61982, HD 61983, HD 61984, HD 61985, HD 61986, HD 61987, HD 61988, HD 61989, HD 61990, HD 61991, HD 61992, HD 61993, HD 61994, HD 61995, HD 61996, HD 61997, HD 61998, HD 61999, HD 62000.
- Camelopardalis:** HD 42818, HD 42819, HD 42820, HD 42821, HD 42822, HD 42823, HD 42824, HD 42825, HD 42826, HD 42827, HD 42828, HD 42829, HD 42830, HD 42831, HD 42832, HD 42833, HD 42834, HD 42835, HD 42836, HD 42837, HD 42838, HD 42839, HD 42840, HD 42841, HD 42842, HD 42843, HD 42844, HD 42845, HD 42846, HD 42847, HD 42848, HD 42849, HD 42850, HD 42851, HD 42852, HD 42853, HD 42854, HD 42855, HD 42856, HD 42857, HD 42858, HD 42859, HD 42860, HD 42861, HD 42862, HD 42863, HD 42864, HD 42865, HD 42866, HD 42867, HD 42868, HD 42869, HD 42870, HD 42871, HD 42872, HD 42873, HD 42874, HD 42875, HD 42876, HD 42877, HD 42878, HD 42879, HD 42880, HD 42881, HD 42882, HD 42883, HD 42884, HD 42885, HD 42886, HD 42887, HD 42888, HD 42889, HD 42890, HD 42891, HD 42892, HD 42893, HD 42894, HD 42895, HD 42896, HD 42897, HD 42898, HD 42899, HD 42900.
- Lynx:** HD 61931, HD 61932, HD 61933, HD 61934, HD 61935, HD 61936, HD 61937, HD 61938, HD 61939, HD 61940, HD 61941, HD 61942, HD 61943, HD 61944, HD 61945, HD 61946, HD 61947, HD 61948, HD 61949, HD 61950, HD 61951, HD 61952, HD 61953, HD 61954, HD 61955, HD 61956, HD 61957, HD 61958, HD 61959, HD 61960, HD 61961, HD 61962, HD 61963, HD 61964, HD 61965, HD 61966, HD 61967, HD 61968, HD 61969, HD 61970, HD 61971, HD 61972, HD 61973, HD 61974, HD 61975, HD 61976, HD 61977, HD 61978, HD 61979, HD 61980, HD 61981, HD 61982, HD 61983, HD 61984, HD 61985, HD 61986, HD 61987, HD 61988, HD 61989, HD 61990, HD 61991, HD 61992, HD 61993, HD 61994, HD 61995, HD 61996, HD 61997, HD 61998, HD 61999, HD 62000.
- Canes Venatici:** HD 123657, HD 123658, HD 123659, HD 123660, HD 123661, HD 123662, HD 123663, HD 123664, HD 123665, HD 123666, HD 123667, HD 123668, HD 123669, HD 123670, HD 123671, HD 123672, HD 123673, HD 123674, HD 123675, HD 123676, HD 123677, HD 123678, HD 123679, HD 123680, HD 123681, HD 123682, HD 123683, HD 123684, HD 123685, HD 123686, HD 123687, HD 123688, HD 123689, HD 123690, HD 123691, HD 123692, HD 123693, HD 123694, HD 123695, HD 123696, HD 123697, HD 123698, HD 123699, HD 123700.
- Draco:** HD 151613, HD 150449, HD 147232, HD 143466, HD 134190, HD 123657.

Other Objects:

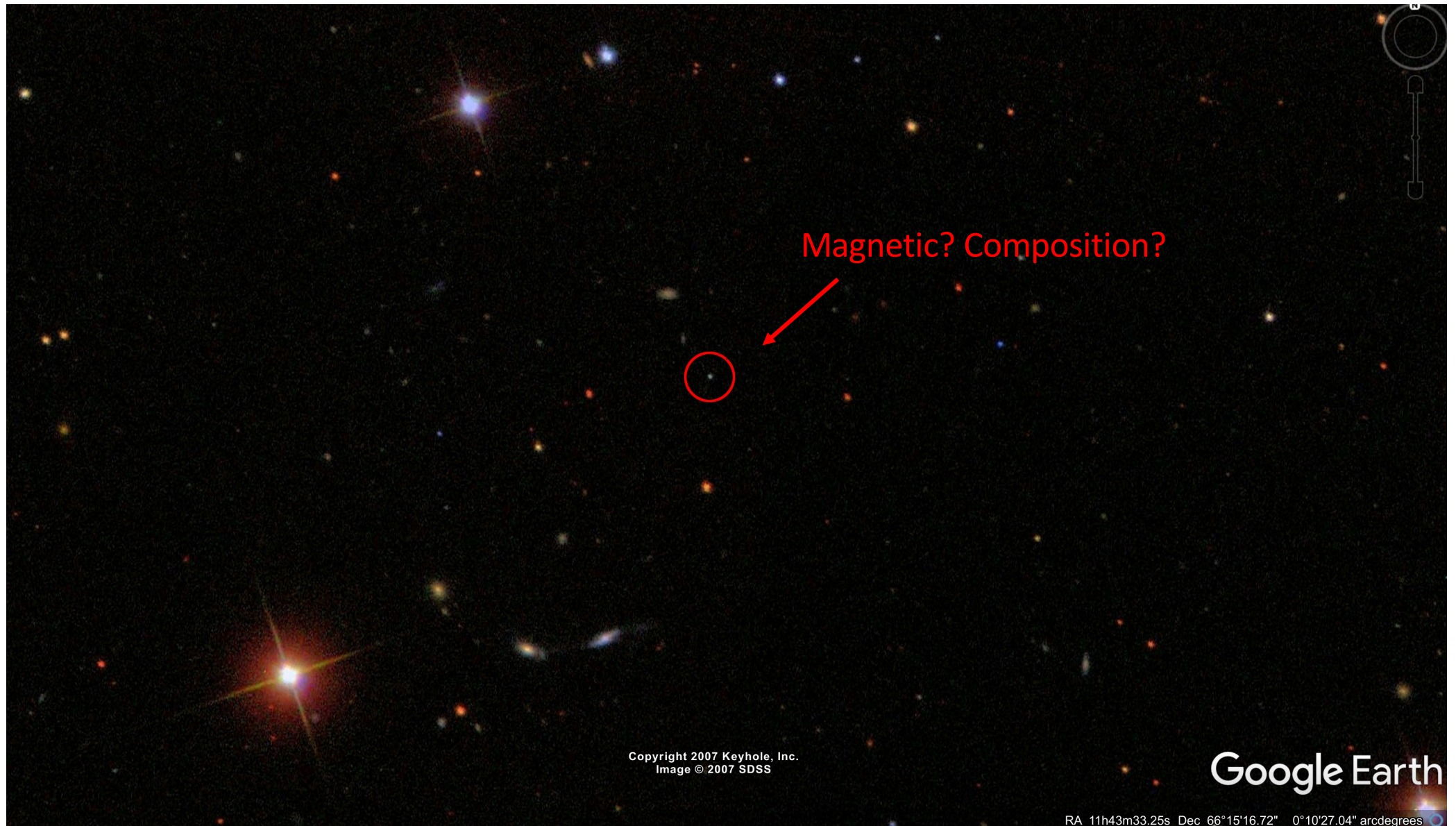
- Galaxies:** Galaxy Seen on Edge, Spindle Galaxy, Galaxy Cluster M68.
- Clusters:** 43 Cam, 42 Cam, 40 Cam, 37 Cam, 36 Cam, 35 Cam, 34 Cam, 33 Cam, 32 Cam, 31 Cam, 30 Cam, 29 Cam, 28 Cam, 27 Cam, 26 Cam, 25 Cam, 24 Cam, 23 Cam, 22 Cam, 21 Cam, 20 Cam, 19 Cam, 18 Cam, 17 Cam, 16 Cam, 15 Cam, 14 Cam, 13 Cam, 12 Cam, 11 Cam, 10 Cam, 9 Cam, 8 Cam, 7 Cam, 6 Cam, 5 Cam, 4 Cam, 3 Cam, 2 Cam, 1 Cam.
- Other:** Rich Background near Tadpole, Stellar Outburst, Five-Star Rated Gravitational Lens.

Coordinates: RA 9h08m07.12s Dec 67°52'29.28" IC 2451

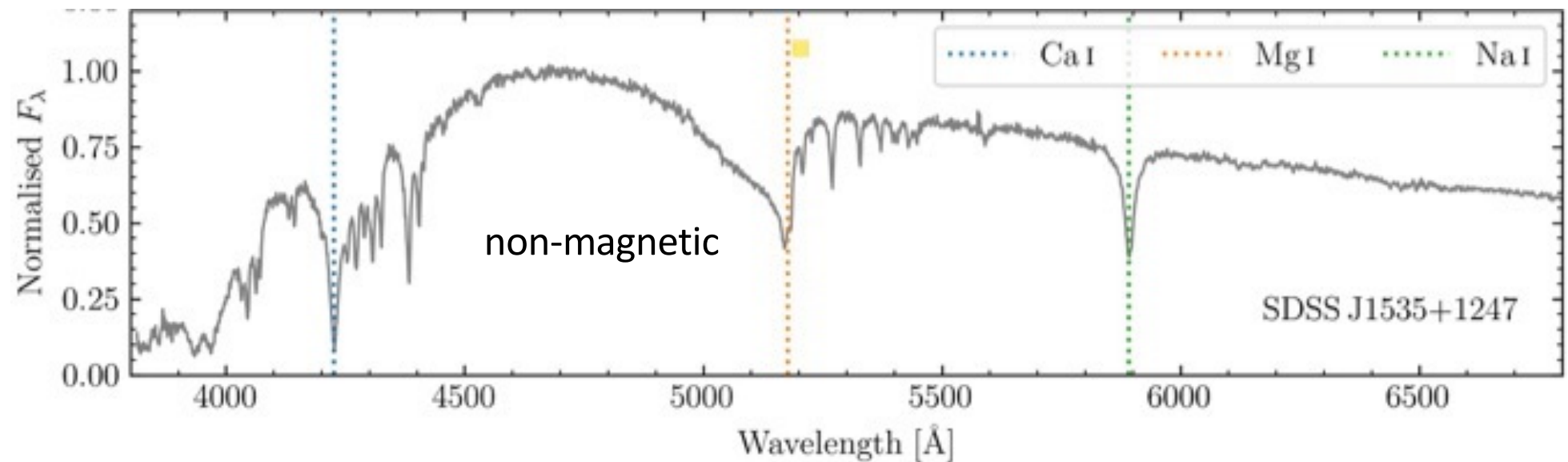
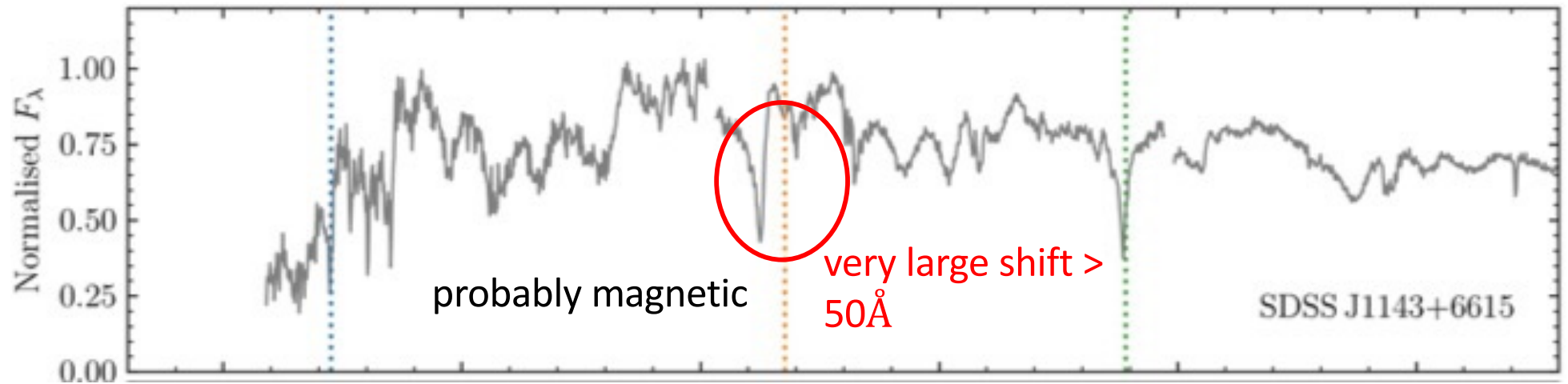
Copyright 2007 Keyhole, Inc. Image © 2007 SDSS Image © 2007 DSS Consortium Tycho Catalog (ESA)

Google Earth

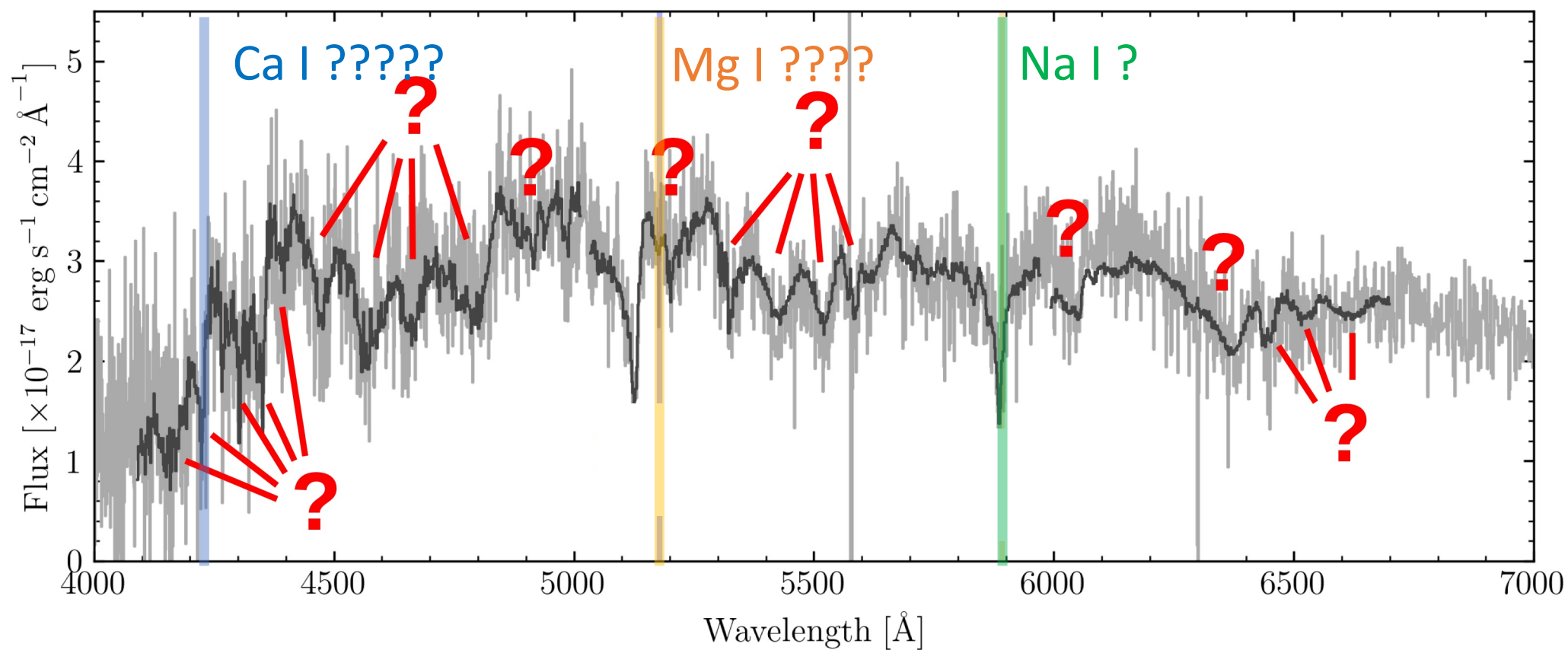
SDSS J1143+6615 – a magnetic WD?



Assignment of spectra

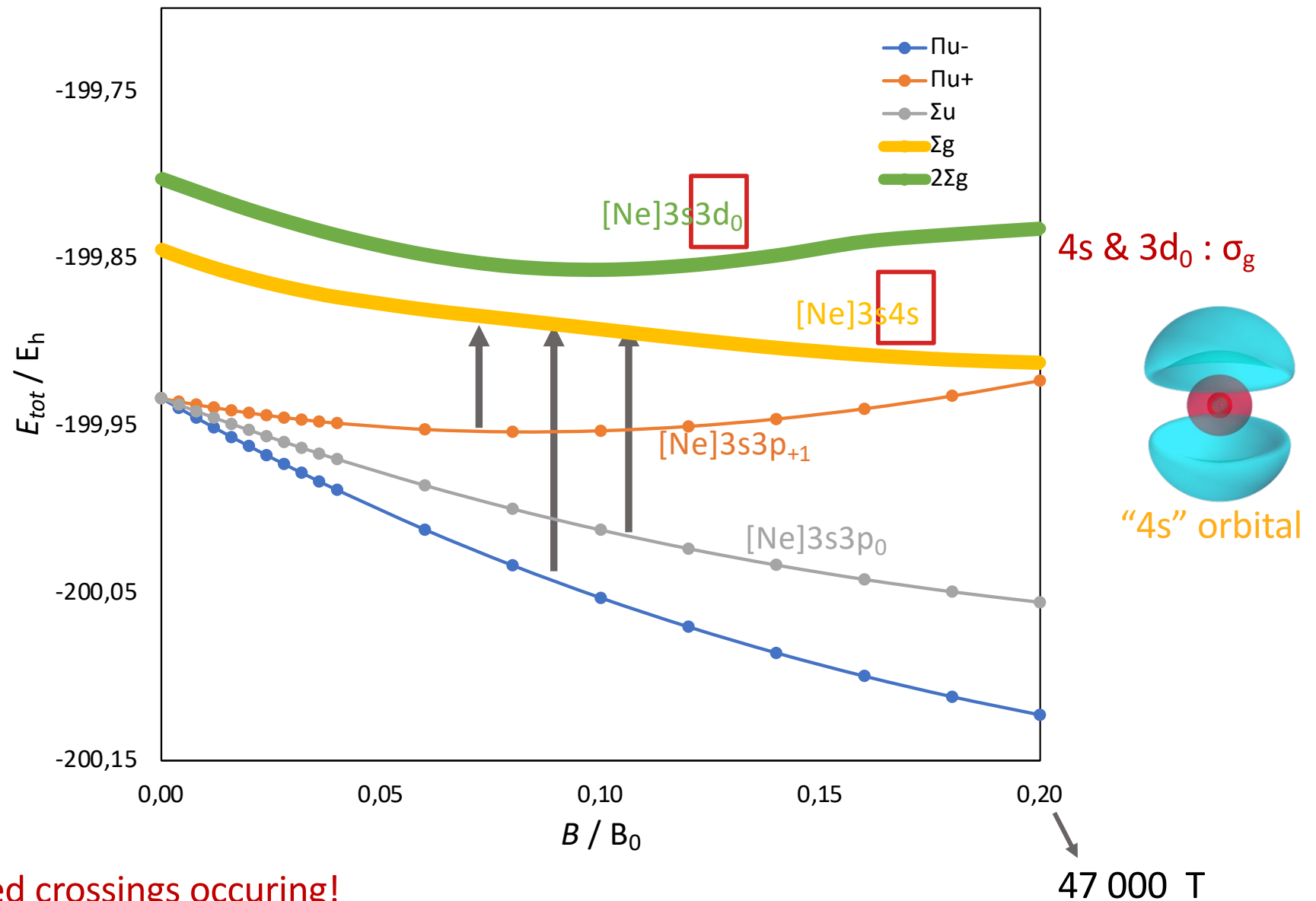


Assignment of spectra

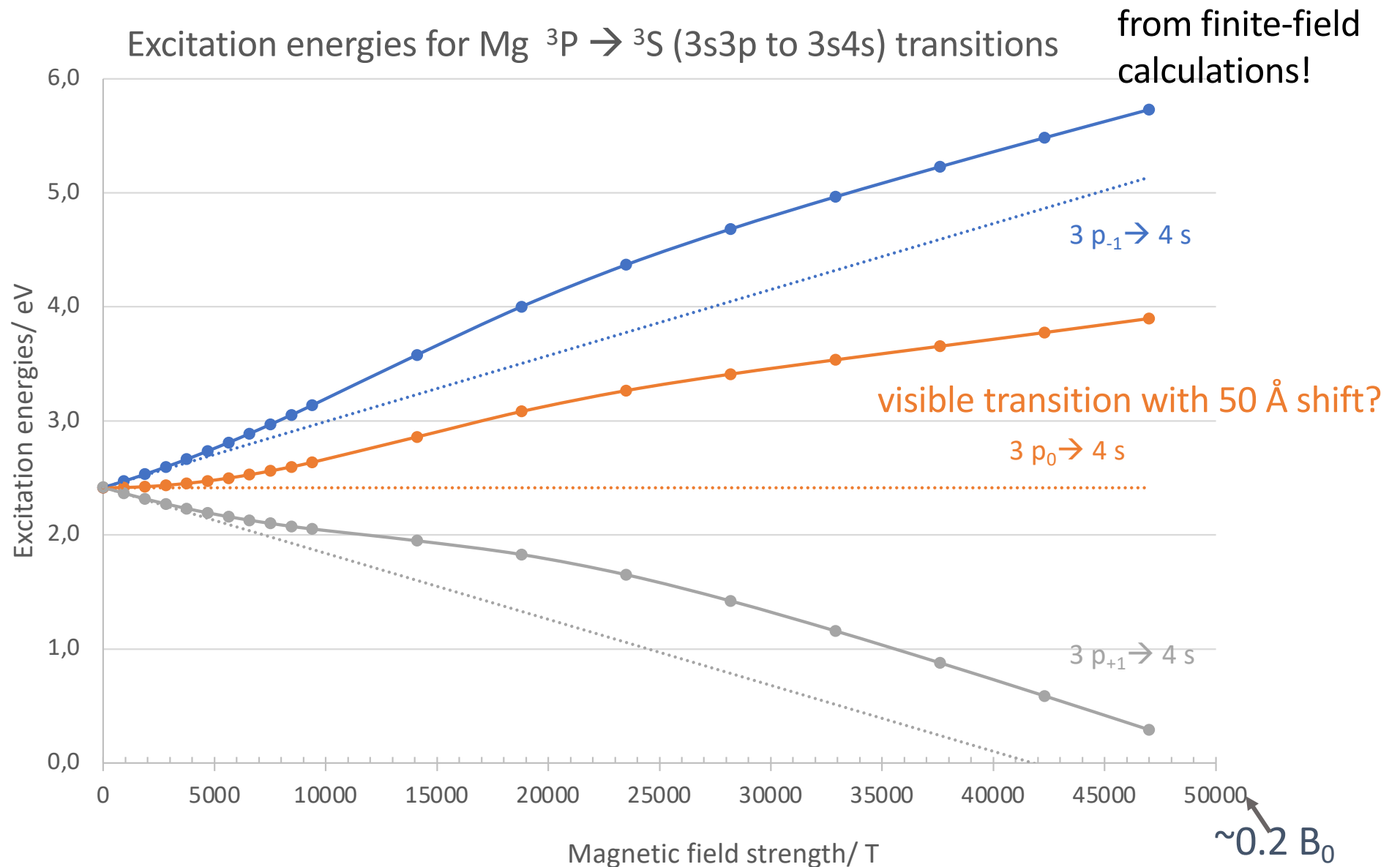


SDSS J1143+6615

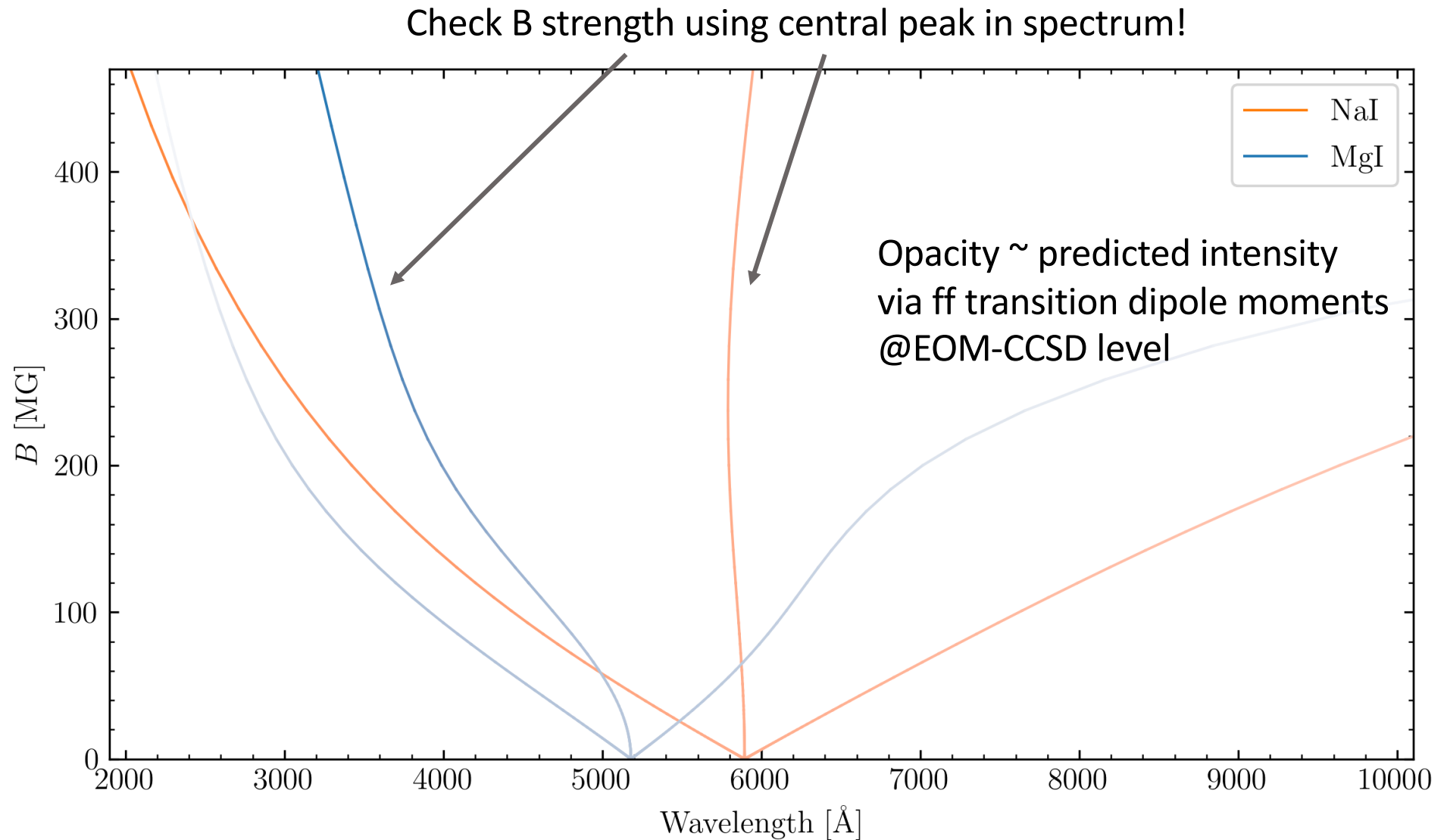
Total energies for Mg in a magnetic field



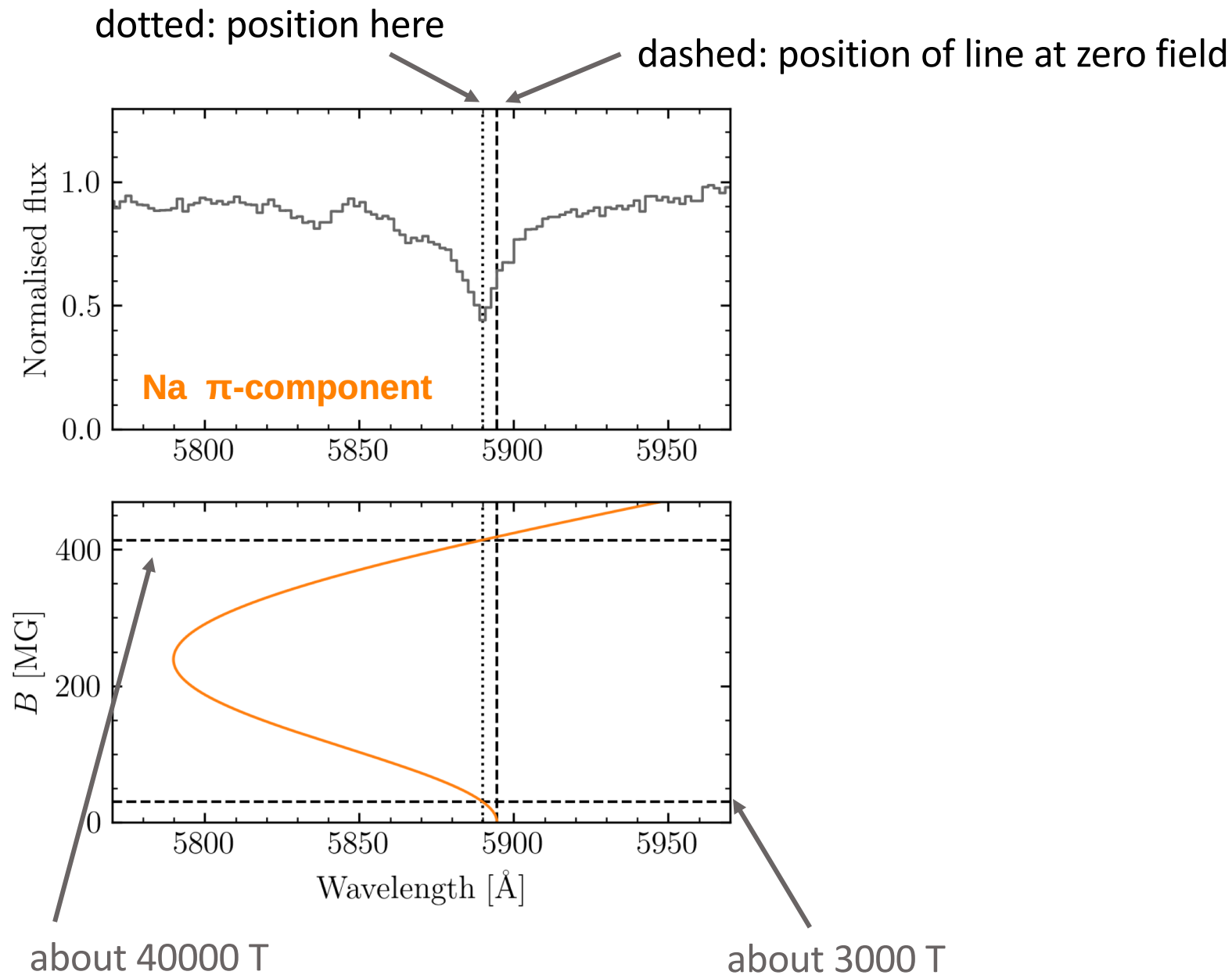
Excitation energies for Mg in magnetic field



B- λ curve for Na and Mg transitions



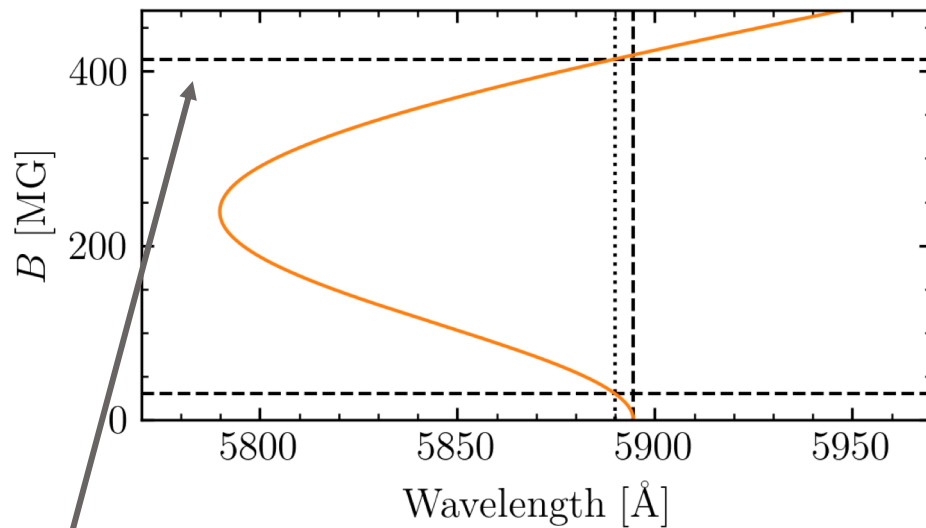
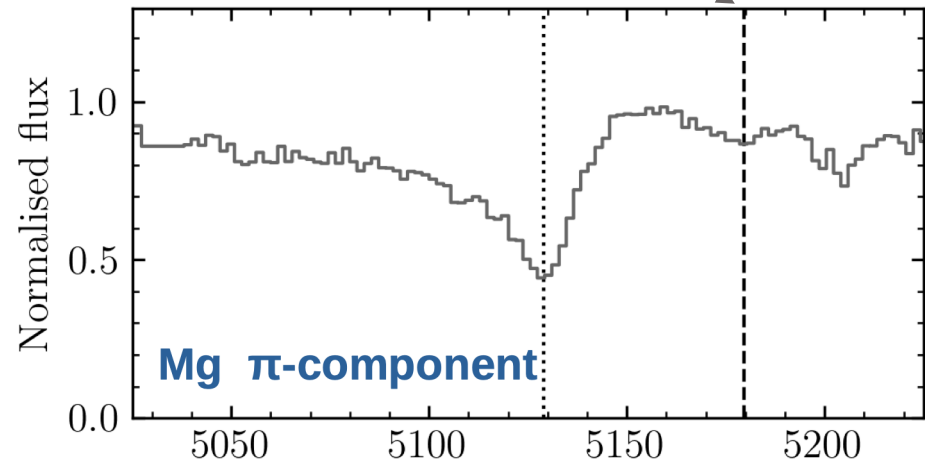
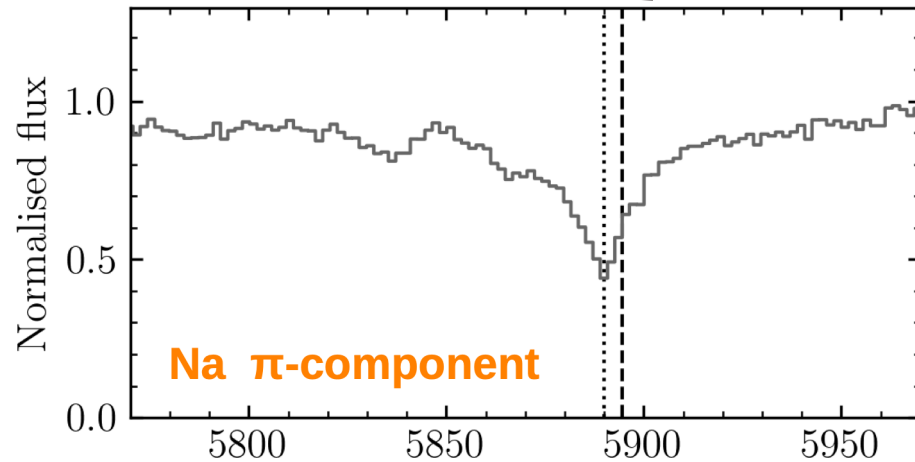
Determining the field strength



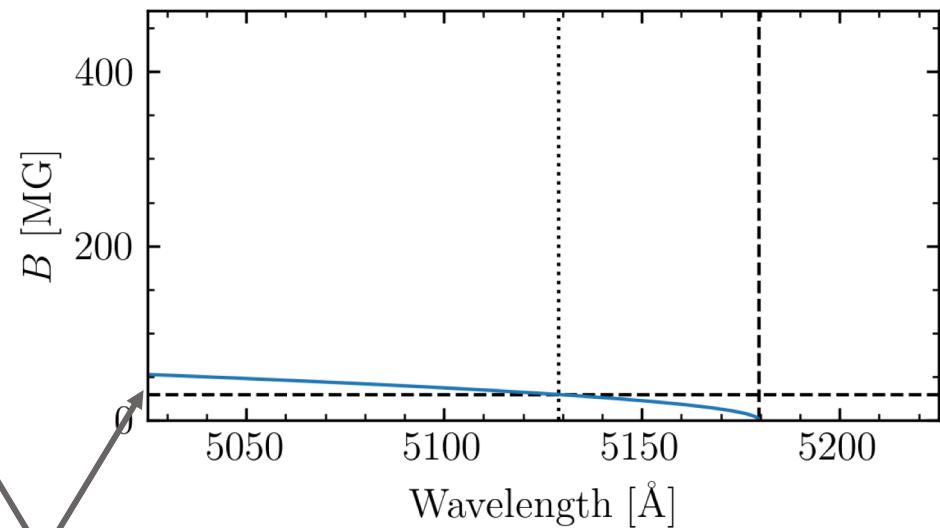
Determining the field strength

dotted: position here

dashed: position of line at zero field

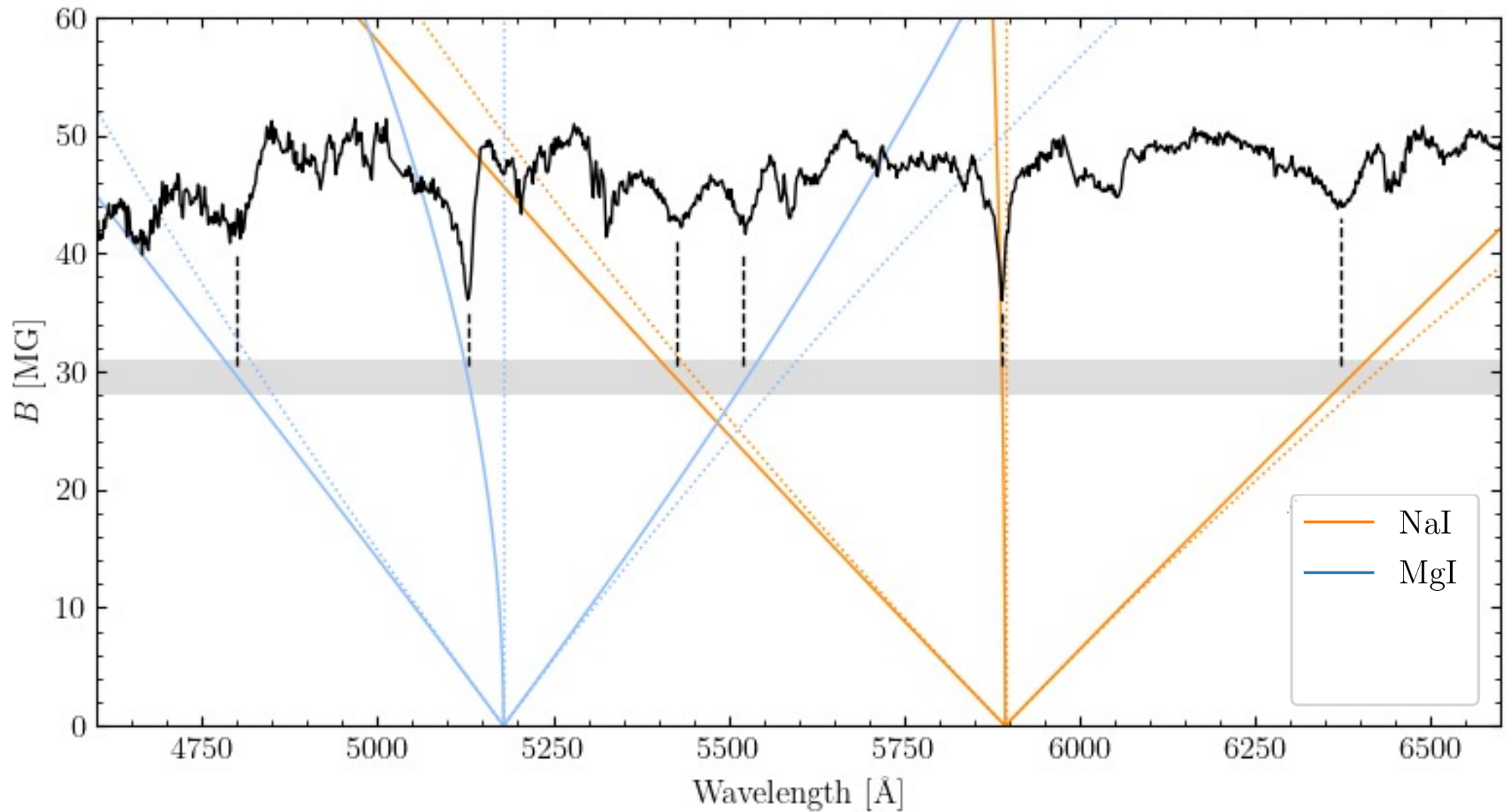


about 40000 T



about 3000 T

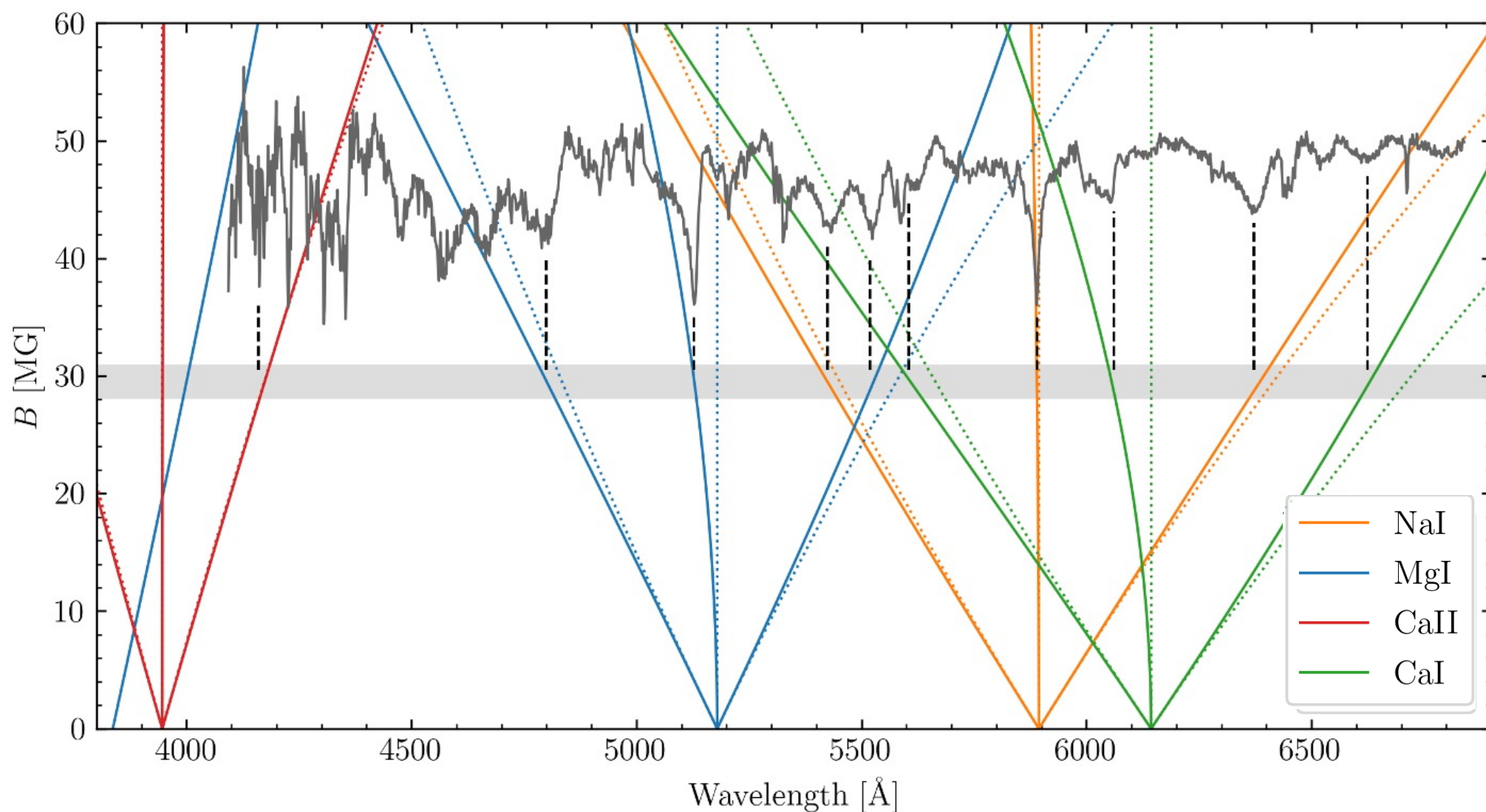
Partial assignment of the spectrum



Full lines : Actual finite-field calculations

Dotted lines: simple linear Zeeman splitting

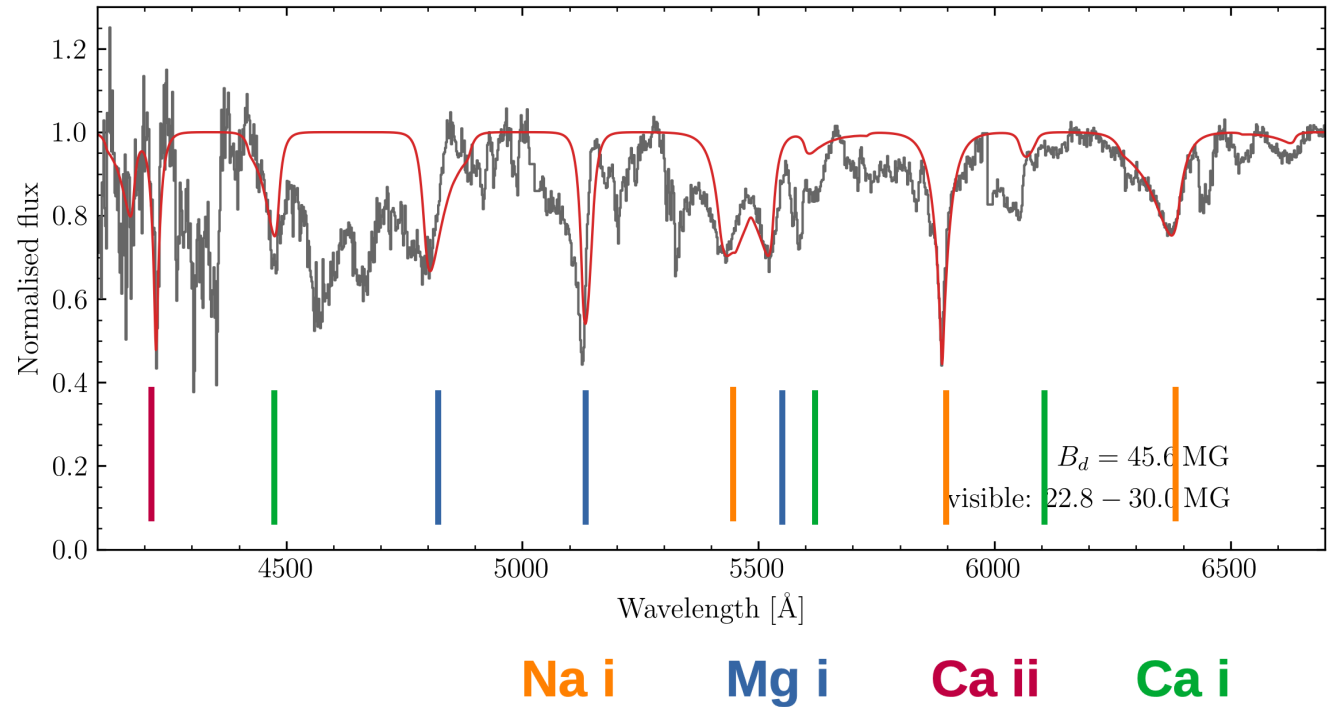
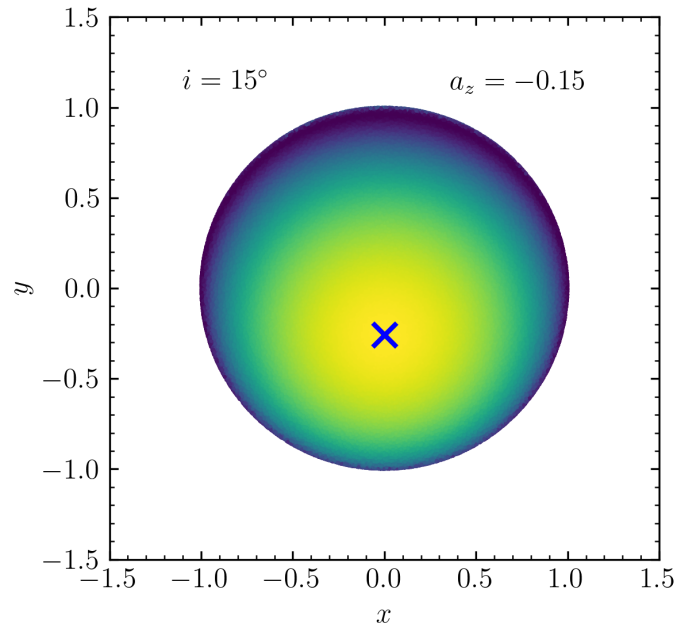
Partial assignment of the spectrum



Dotted: simple linear Zeeman splitting

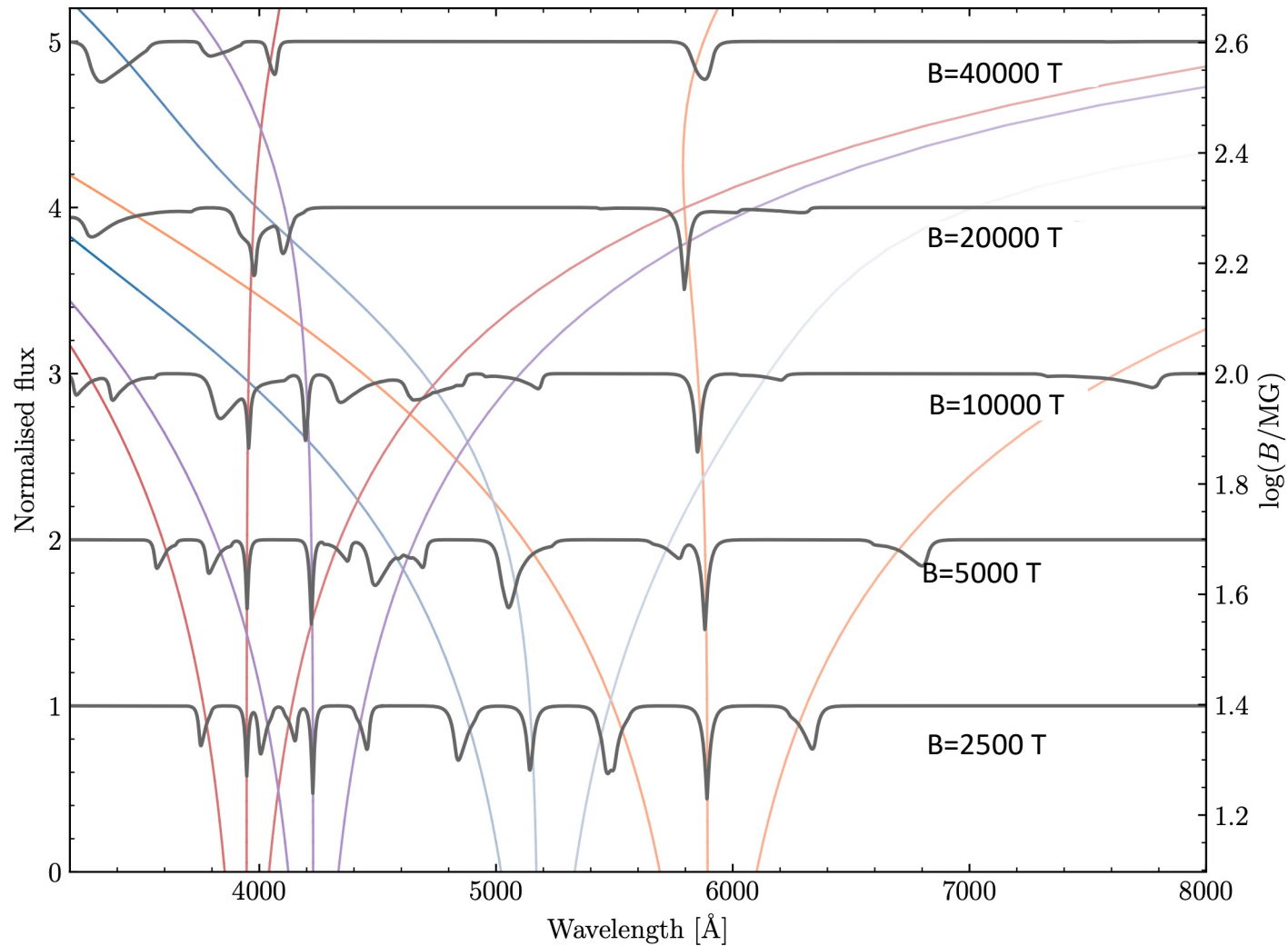
Full: Actual finite-field calculations

Toy model spectrum



- First assignment of metals in the spectrum of a strongly magnetic WD ($\sim 3000 \text{ T}$)
- Further elements/transitions present – possibly iron ...

Simulated spectra for various field strengths



PRESSURE BROADENING OF MG BY HE ATMOSPHERE (USING FF-CD-CC METHODS)

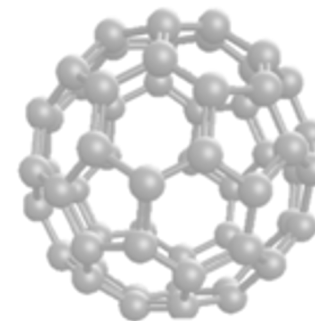
with Mark Hollands (U Warwick, Astrophysics)

Simon Blaschke

Marios-Petros Kitsaras

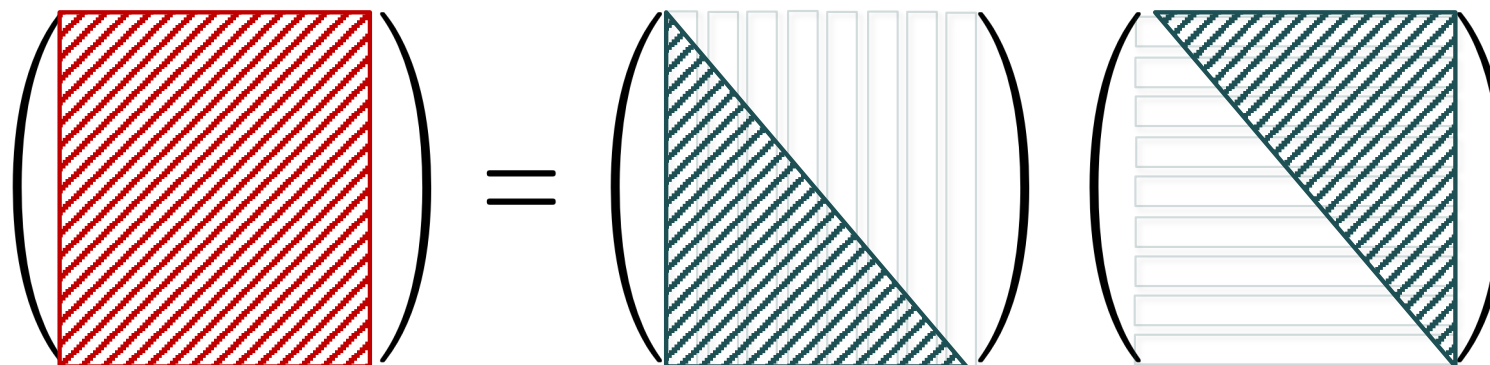
Towards larger systems

- Currently: severe limitation w.r.t. system size
- Predictive power and controlled accuracy wanted



Cholesky-decomposition techniques

$$\mathbf{A} = \mathbf{L}\mathbf{L}^\dagger$$



For 2el-integrals^{1,2}:

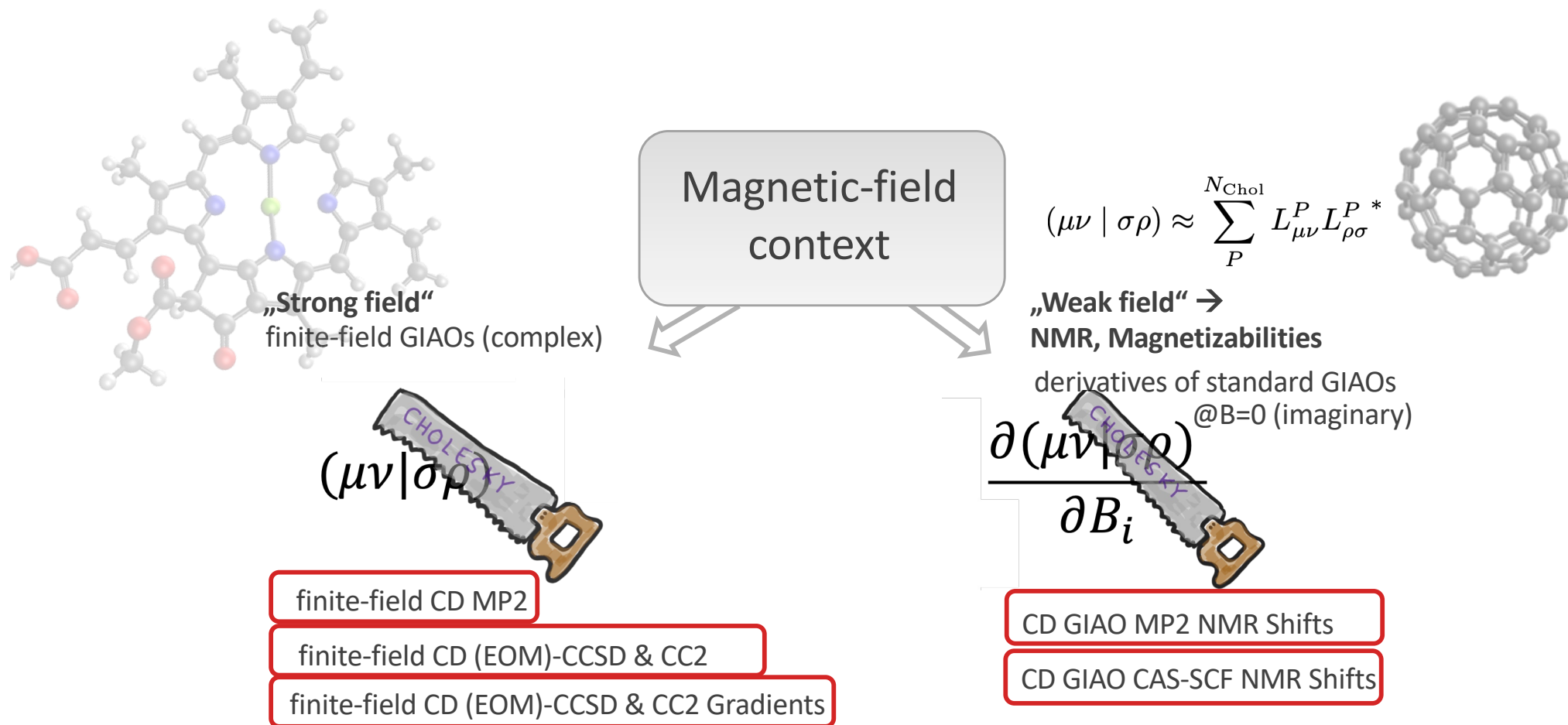
$$(\mu\nu|\sigma\rho)_{\text{CD}} = \sum_{J=1}^{N_{\text{CH}}} L_{\mu\nu}^J L_{\rho\sigma}^{J*}$$

Numerical rank,
number of
Cholesky-vectors

¹ Beebe, Linderberg, *Int. J. Quantum Chem.* 12, 683 (1977)

² Koch, Sánchez De Merás, Bondo Pedersen, *J. Chem. Phys.*, 118, 0481 (2003)

Cholesky Decomposition methods



Blaschke, [Stopkowicz](#), J. Chem. Phys. 156, 044115 (2022)

Blaschke, Kitsaras, [Stopkowicz](#), Phys. Chem. Chem. Phys., 26, 28828 (2024)

Kitsaras, Blaschke, Oswald, [Stopkowicz](#) (ff-EOM Gradients), in prep (2026)

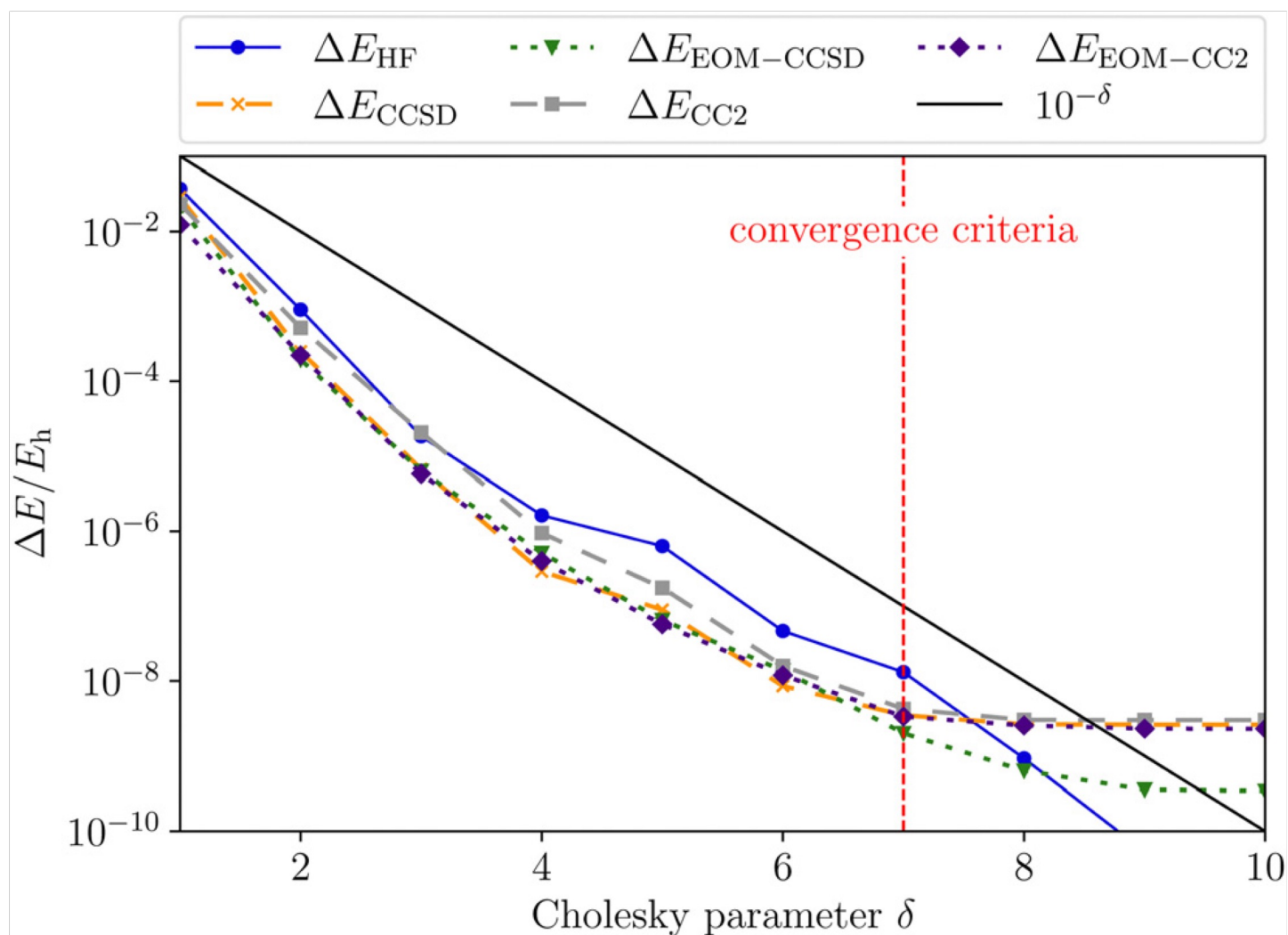
Burger, Lipparini, Gauss, [Stopkowicz](#), J. Chem. Phys., 155, 074105 (2021)

Gauss, Blaschke, Burger, Nottoli, Lipparini, [Stopkowicz](#), Mol. Phys. 120, e2101562 (2022)

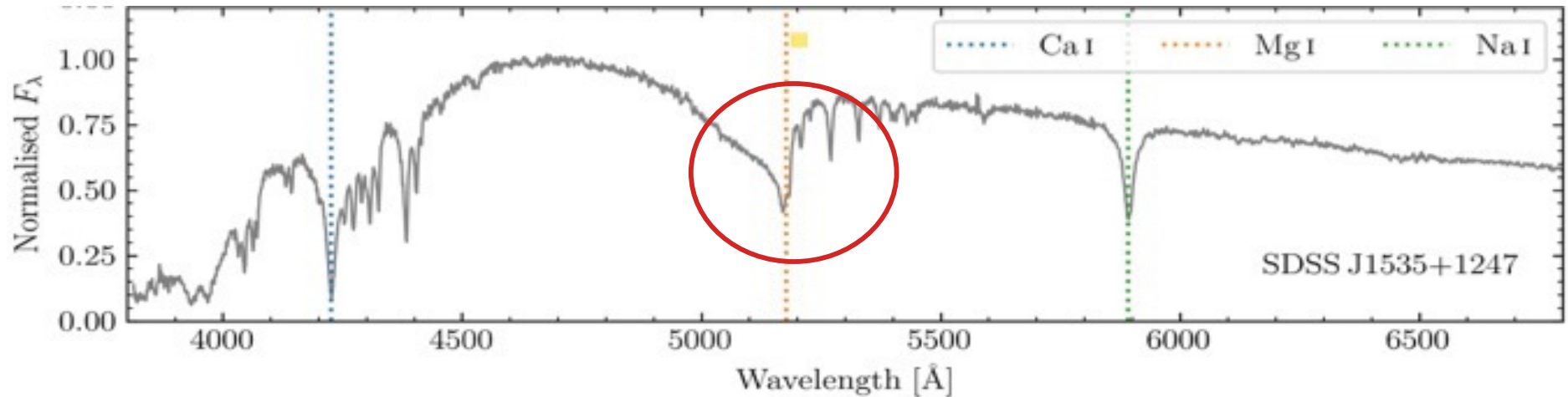
Nottoli, Burger, [Stopkowicz](#), Gauss, Lipparini, J. Chem. Phys., 157, 084122 (2022)

Burger, [Stopkowicz](#), Gauss, J. Phys. Chem. A 129, 2, 623 (2025)

Finite-field Cholesky Decomposition for (EOM)-CCSD



Mg pressure broadening



- Asymmetric line shapes and broadening due to interaction with surrounding Helium atoms in the atmosphere of DZ WDs
- Light escapes from various layers of the atmosphere where densities vary considerably

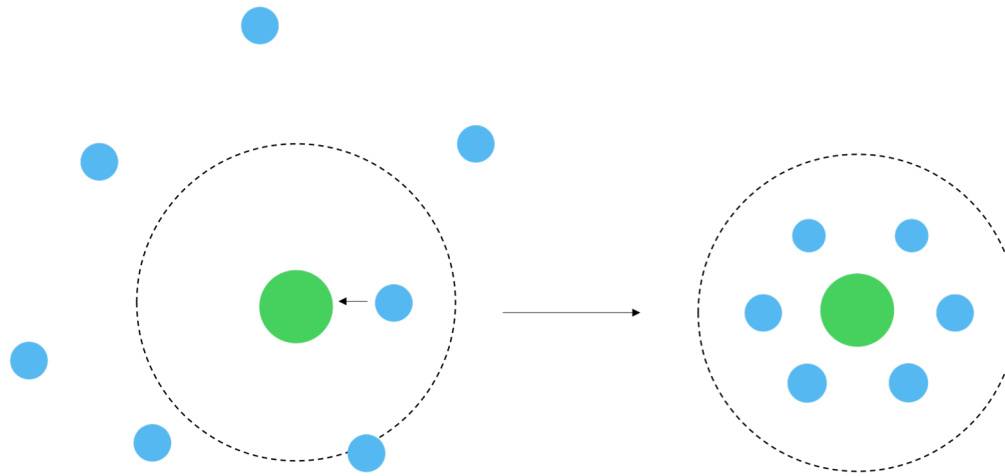
1 Hollands, Koester, Alekseev, Herbert, Gänsecke, Mon. Not. R. Astron. Soc (2017)

2 Allard, Leininger, Gadéa, Brousseau-Couture, Dufour, Astron. Astrophys. 588, A412 (2016)

Mg line broadening

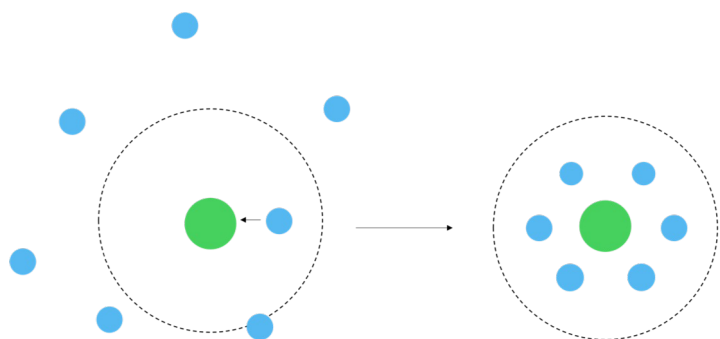
Lower densities

Higher densities

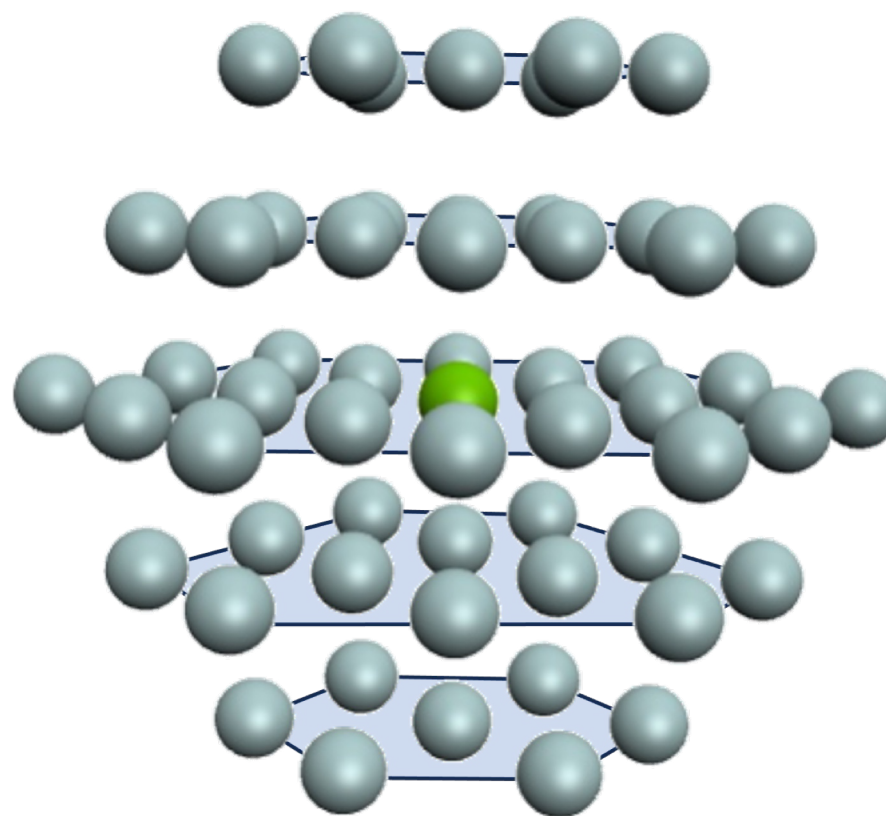


interperturber
interactions?

Mg line broadening



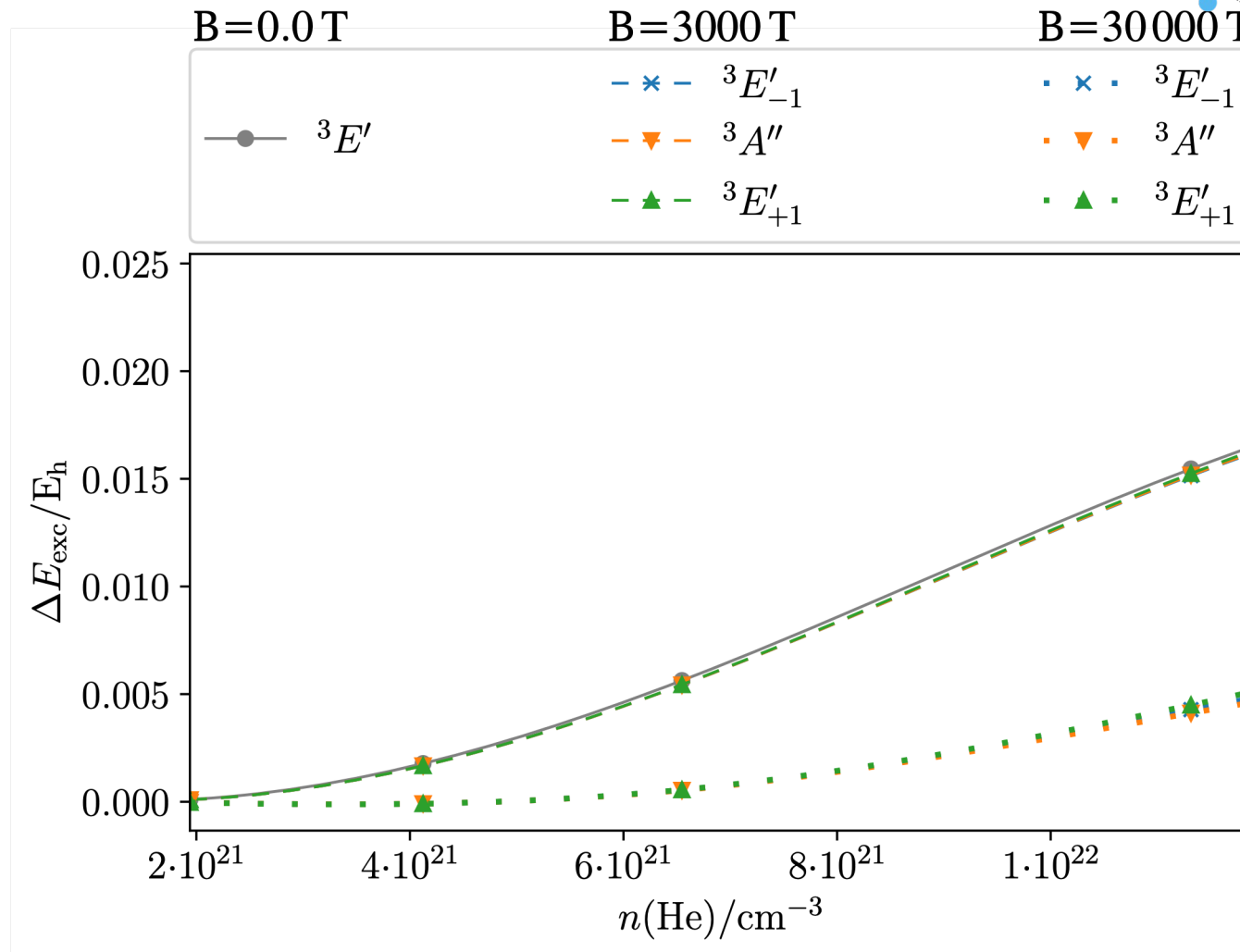
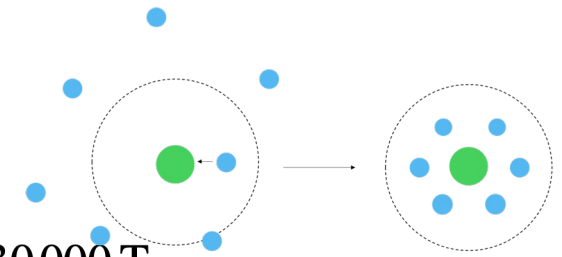
MgHe₅₆
(two shells)
hcp lattice



significant reduction of
memory

Calculated using Cholesky-decomposition
methods together with ff-EOM-CC2 & ff-EOM-
CCSD theory

Mg line broadening



field-free & 3000 T

30000 T

Large effects for high densities (but also less light coming out)

3000 T: field-free model ok

30000 T: broadening should be much less pronounced → close to atomistic case!

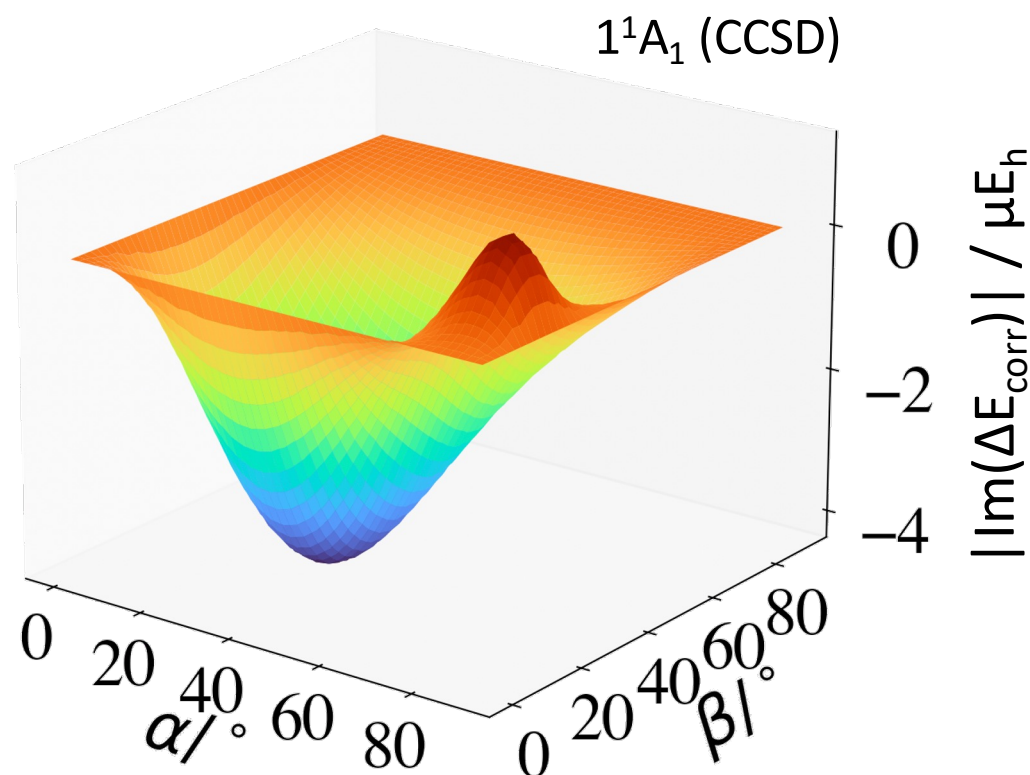
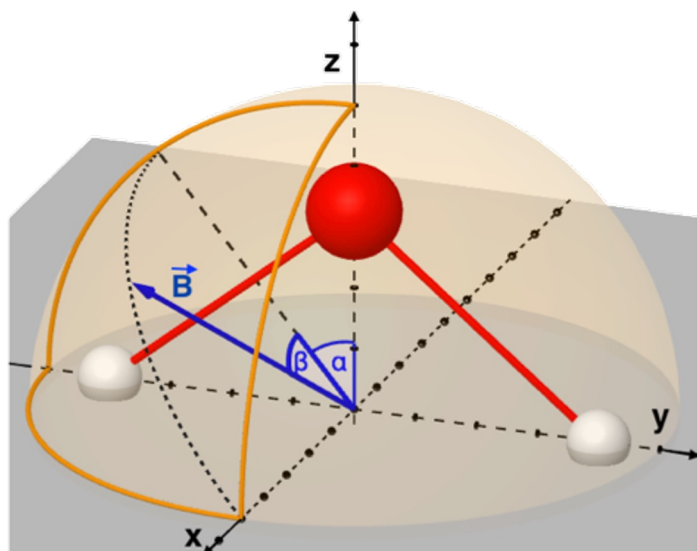
FINITE-FIELD UNITARY CC

Laura Grazioli

Marios-Petros Kitsaras

Complex energies in finite-field CC

H₂O: CCSD/unc-aug-cc-pVTZ, B=0.5 B₀



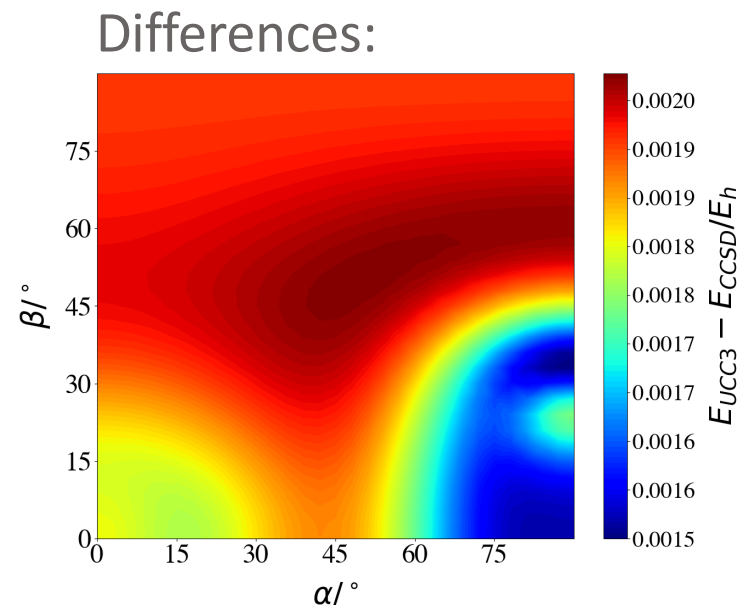
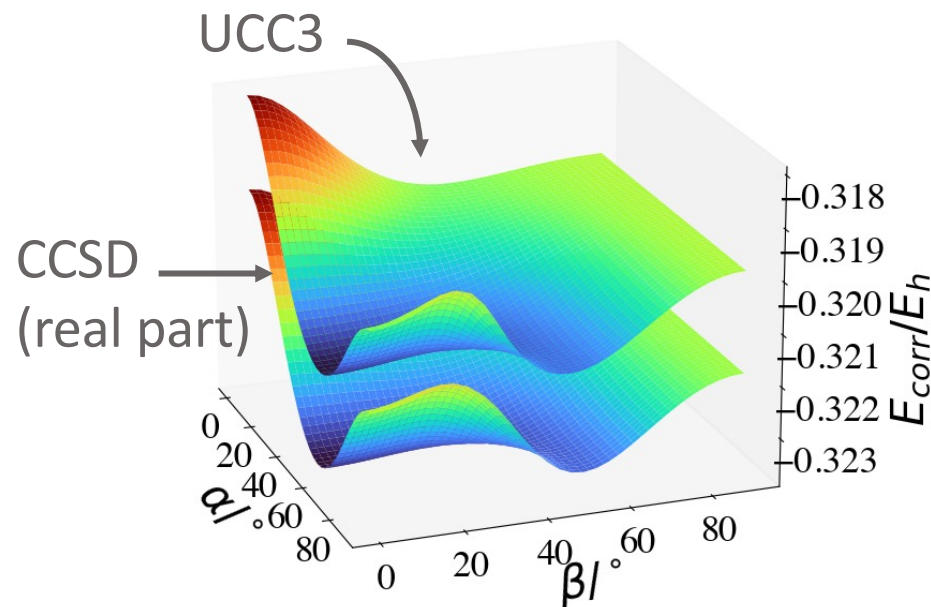
- Consequence of non-Hermiticity
- Real energies when one component of B vanishes. (Atoms, diatomics, special symmetries)
→ Ignore? Use as diagnostic? Hermitian theory?

→ UCC theory

Finite-field Unitary CC

Unitary CC Theory $|\Psi_{\text{UCC}}\rangle = e^{\hat{\sigma}} |\Phi_0\rangle = e^{\hat{\sigma} - \hat{\sigma}^\dagger} |\Phi_0\rangle$

- Non-terminating series
- Restriction to S+D & 2nd or 3rd -order truncation in amplitude eqs.¹ → UCC2 & UCC3
- Useful in finite-field context? Water example



¹ Liu, Asthana, Cheng, Mukherjee, J. Chem. Phys, 148, 244110 (2018)
Grazioli, Kitsaras, Stopkowicz, J. Chem. Theory Comput., 21, 12634 (2025)

QED-CC

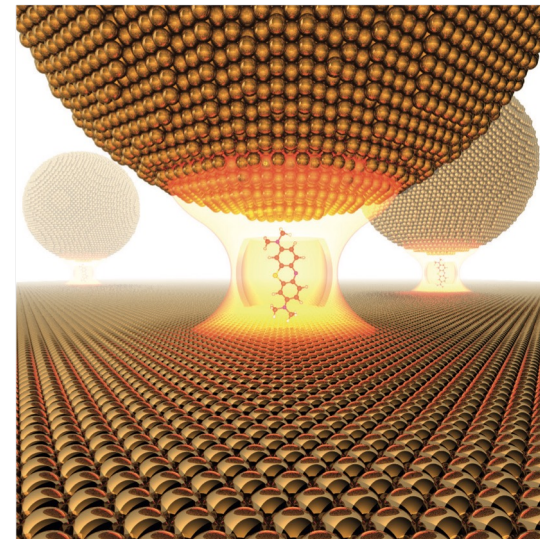
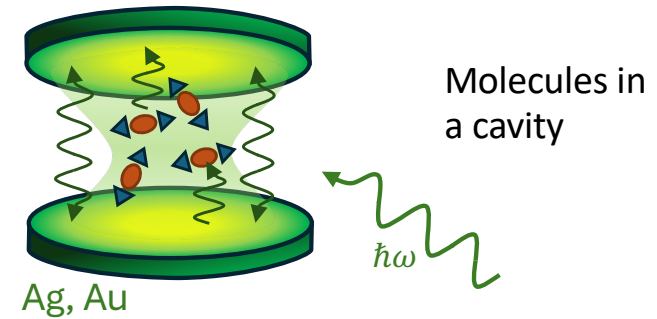
Laurenz Monzel

Christoph Harrer

Polaritonic Chemistry and QED-CC theory

Currently large interest in chemistry as so-called **strong coupling** can **modify**:

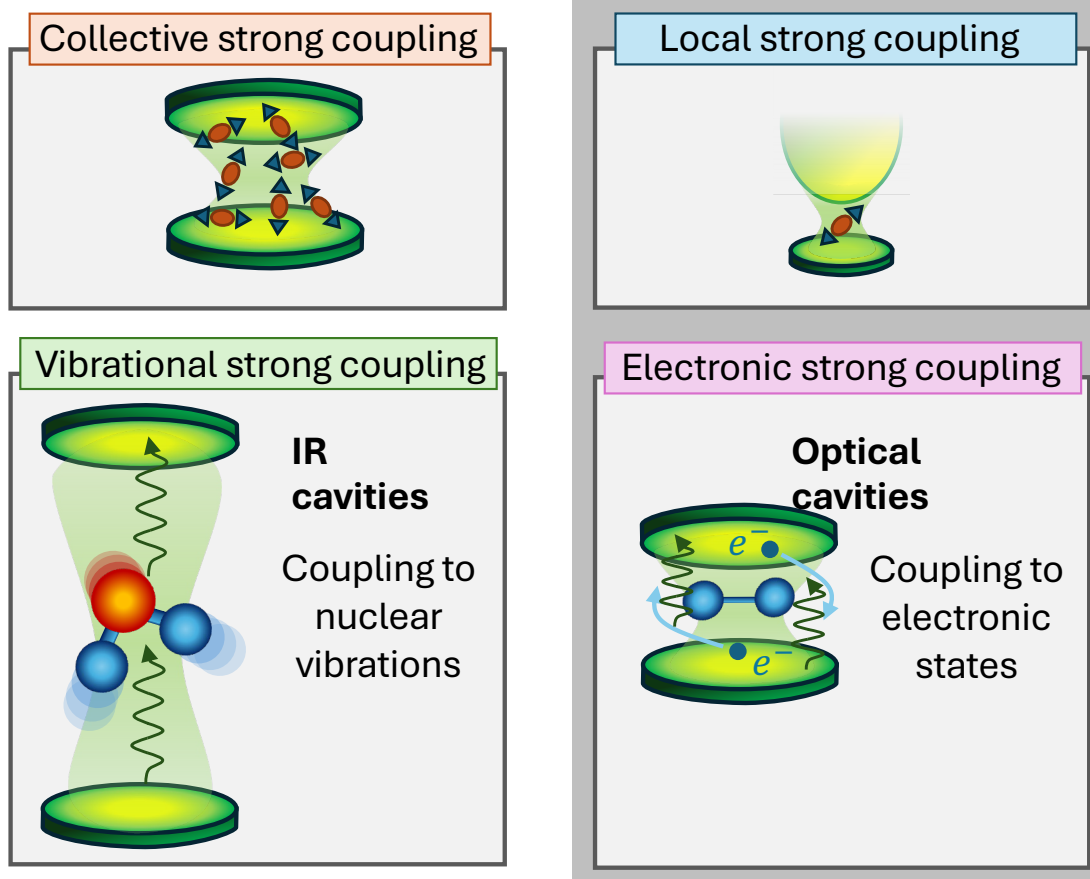
- reaction rates
- reaction selectivity
- reaction pathways
- catalytic activity
- charge transfer
- energy transfer
- photochemistry
- excited-state dynamics
- spin dynamics
- molecular spectroscopy
- potential energy surfaces
- conical intersections



Taken from Chikkaraddy, et al. (2016)

Not yet well understood! Theory developments needed

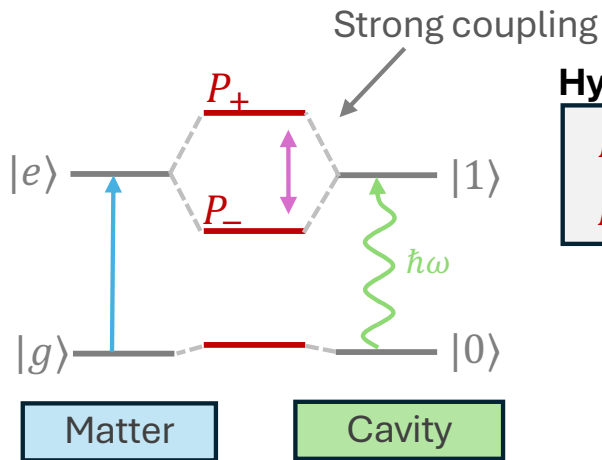
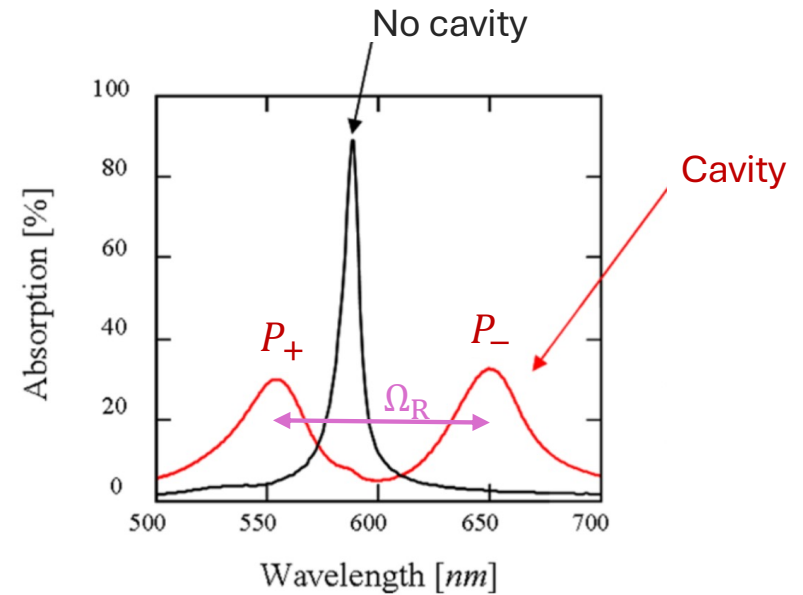
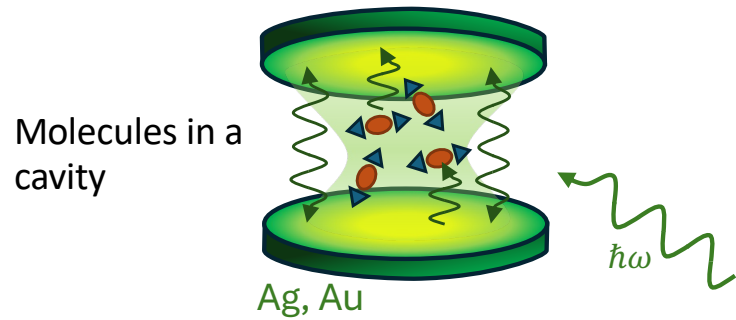
Strong coupling



Highly accurate
description via
Quantum-
electrodynamics
Coupled-Cluster
Theory
(QED-CC)

Monzel, Stopkowicz, J. Phys. Chem. A **128**, 44, 9572–9586 (2024)
 Monzel, Stopkowicz, J. Chem. Theory Comput. **22**, 5991–6007 (2026)
 Monzel, Stopkowicz, (finite field developments) in prep (2026)

Polaritonic Chemistry and QED-CC theory



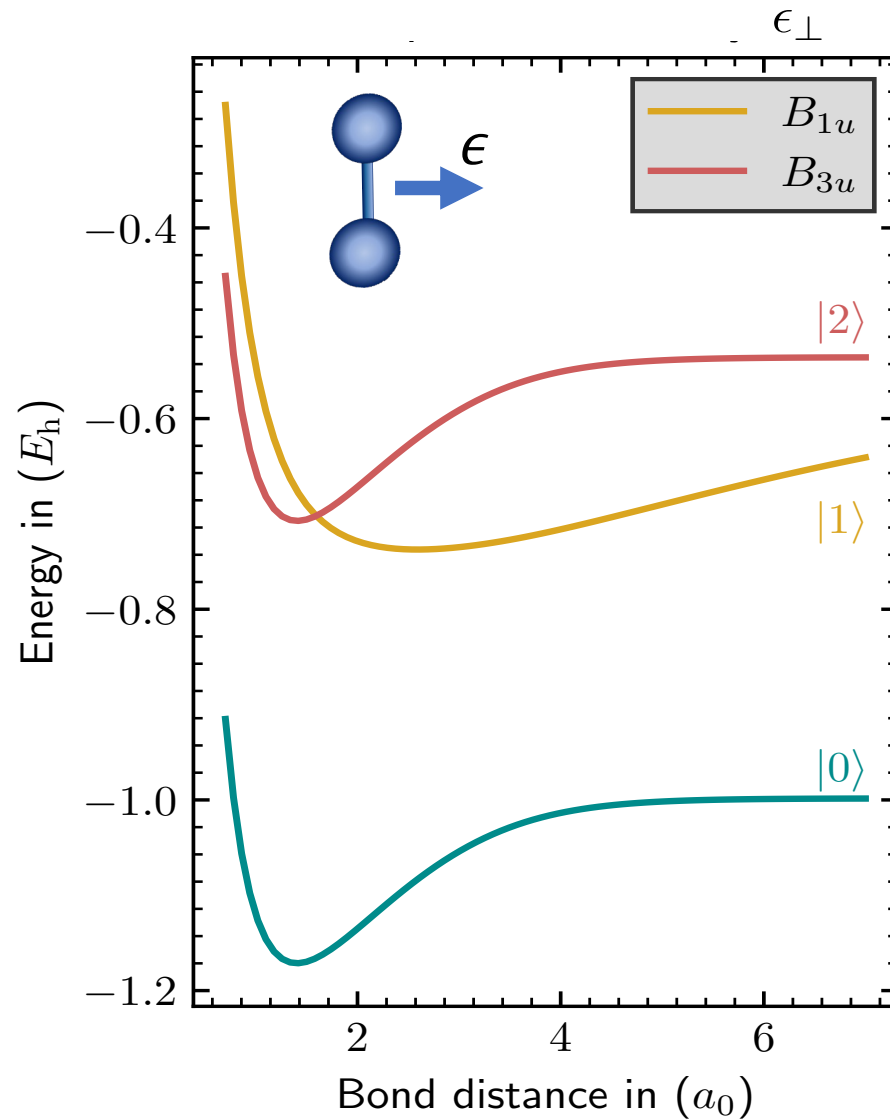
Hybrid light-matter states

P_+ : Upper polariton

P_- : Lower polariton

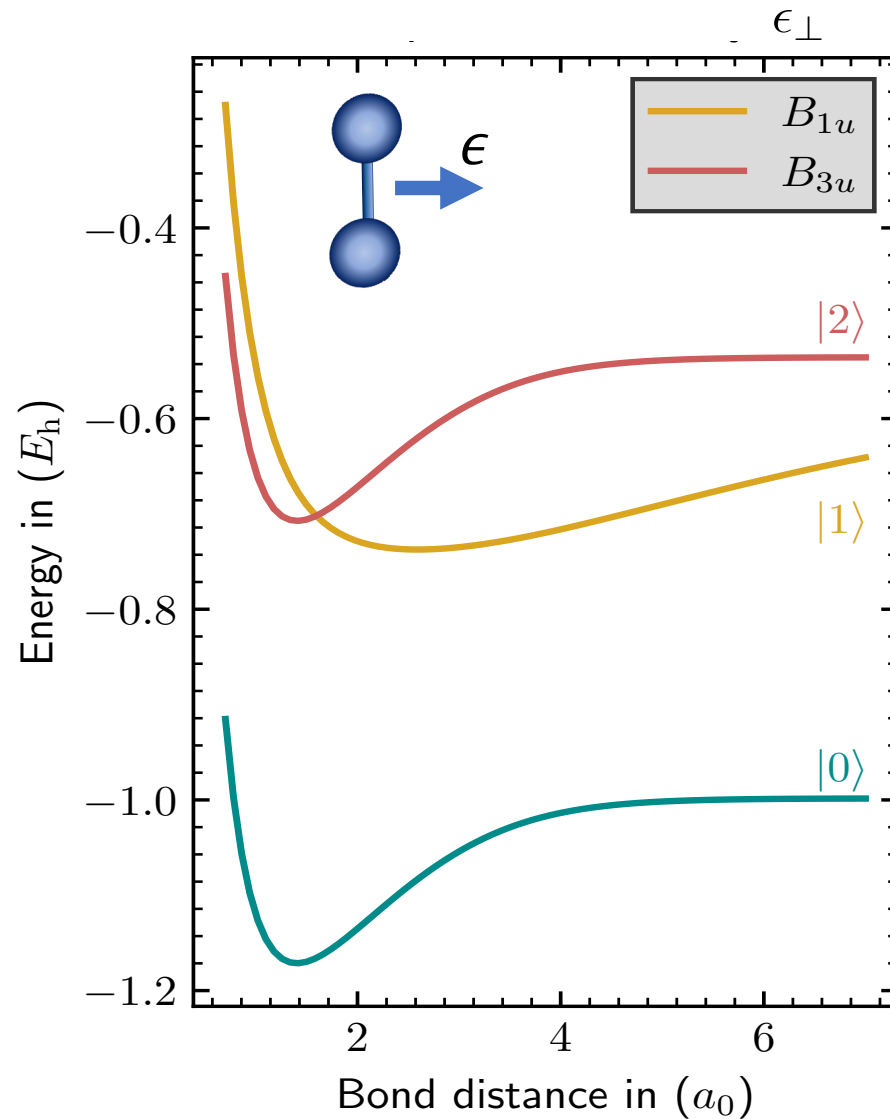
Ω_R : Rabi frequency

H₂ in linearly polarized cavity in two orientations

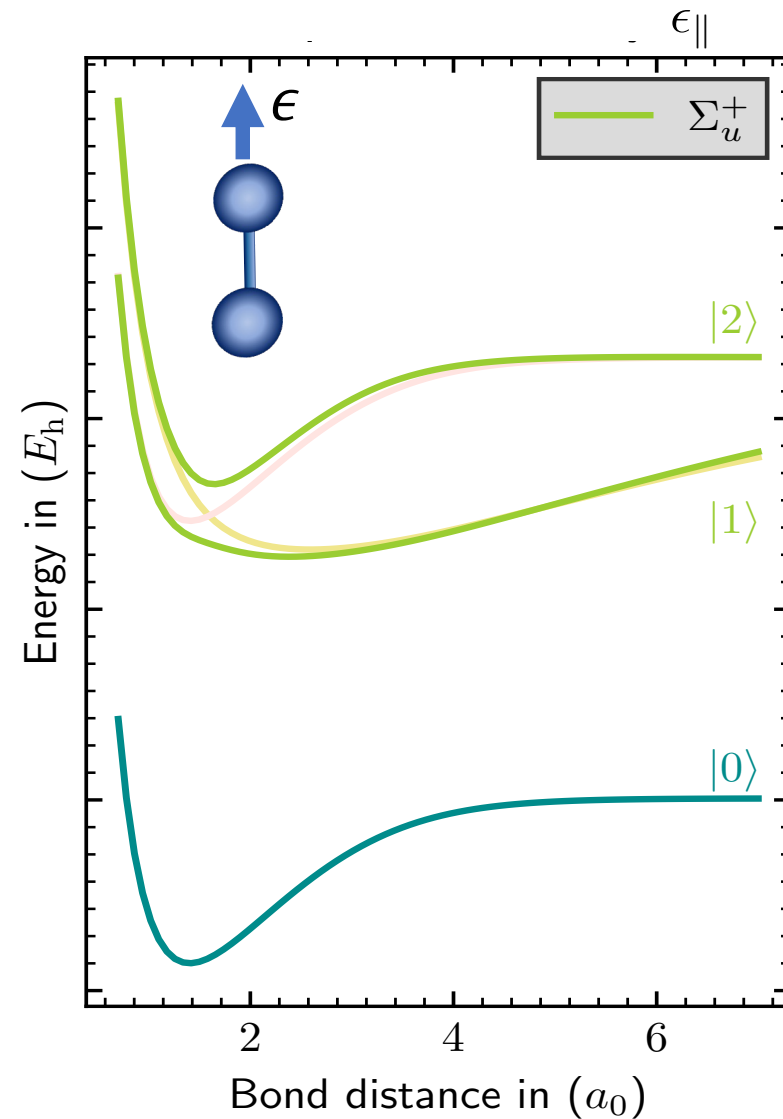


No coupling (states of different symmetries)

H₂ in linearly polarized cavity in two orientations



No coupling (states of different symmetries)



Hybrid light-matter states

Polaritonic partitioning

$$\hat{H}\Psi = E\Psi$$

Wave function: $\Psi(r, R, q)$



Born-Oppenheimer approximation

Polaritonic partitioning

$$\varphi(r, q; \{R\})\Phi(R)$$

Polaritonic wave function: Photons and electrons treated at same level, nuclear coordinates as parameters,

Nuclear wave function: depends on nuclei only

Pauli-Fierz Hamiltonian

$$\hat{H} = \hat{H}_{\text{el}} + \hat{H}_{\text{int}} + \hat{H}_{\text{cav}}$$

Molecular non-relativistic Hamiltonian

Interaction part, contains bilinear coupling and dipole self energy

$$\hat{H}_{\text{int}} = \sum_{\alpha} \hat{\mathbf{E}}_{\alpha} \cdot \hat{\mathbf{d}} + \frac{1}{2} \sum_{\alpha} (\boldsymbol{\lambda}_{\alpha} \cdot \hat{\mathbf{d}})(\boldsymbol{\lambda}_{\alpha} \cdot \hat{\mathbf{d}})$$

Sum over modes

$$\hat{\mathbf{E}} = i \sqrt{\frac{\lambda^2 \omega}{2}} [\boldsymbol{\epsilon}(\hat{\alpha}^{\dagger} - \hat{\alpha})]$$

For linear polarization

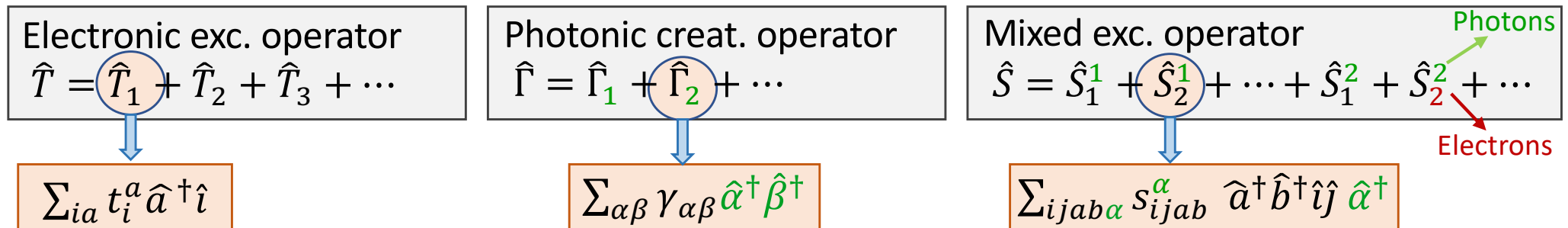
Pure cavity part

$$\hat{H}_{\text{ph}} = \sum_{\alpha} \omega_{\alpha} \hat{\alpha}^{\dagger} \hat{\alpha}$$

Here: 1 mode

Polaritonic coupled-cluster theory

- CC wave function: $e^{\hat{Q}} |\Psi_{\text{ref}}\rangle$
- QED-CC ansatz¹: $e^{\hat{Q}} \Psi_{\text{ref}} = e^{\hat{T} + \hat{S} + \hat{\Gamma}} \Psi_{\text{ref}}$



- Solved via projection techniques

$$\langle \Phi_I | e^{-\hat{Q}} \hat{H} e^{\hat{Q}} | \Psi_{\text{ref}} \rangle = 0 \quad \rightarrow \text{Get amplitudes}$$

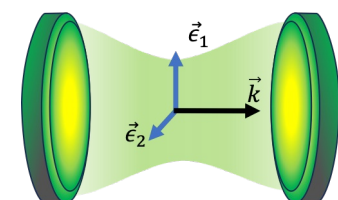
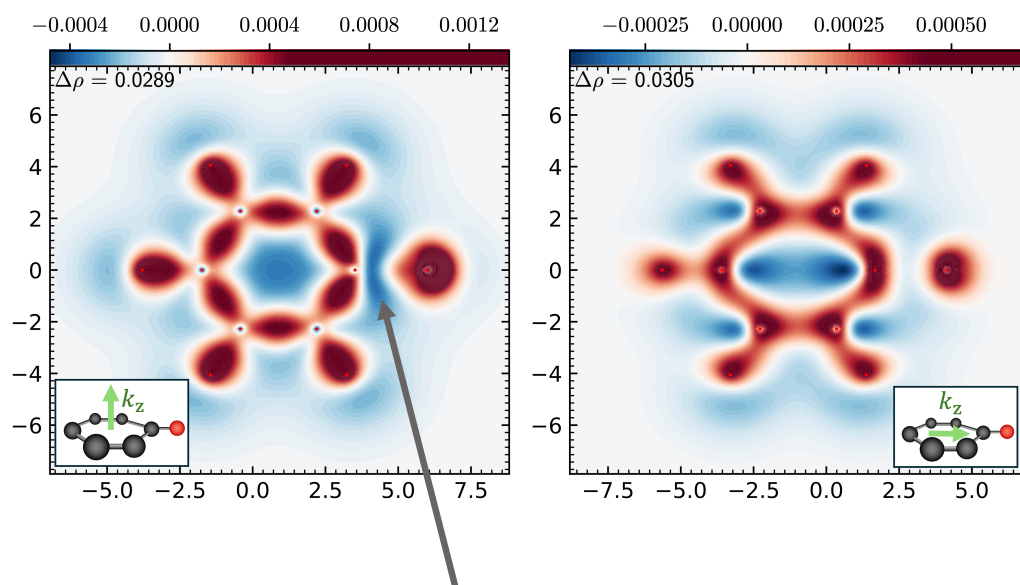
$$\langle \Psi_{\text{ref}} | e^{-\hat{Q}} \hat{H} e^{\hat{Q}} | \Psi_{\text{ref}} \rangle = E_{\text{CC}}$$

- Implemented for truncation QED-CCSD-12-SD

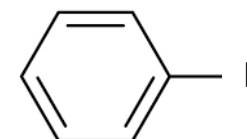
$$\hat{Q} = \hat{T}_1 + \hat{T}_2 + \hat{S}_1^1 + \hat{S}_2^1 + \Gamma_1 + \Gamma_2$$

Can treat open-shell systems and use point-group symmetry

Fluorobenzene density differences



Two polarization vectors, resulting k -vector along mirror axis



Density difference *with and without* cavity (red: increase of density, blue: decrease)
 Electron density removed from the F-C bond if k -vector is perpendicular to molecular plane!
 Similar: polarization vector along the bond (linear pol.)

Summary

- CC developments for molecules in **electromagnetic fields**:
- **Finite magnetic field CC** developments for molecules in strong magnetic fields → Assignments of white dwarf spectra
- **QED-CC** developments for the investigation of polaritonic chemistry

Acknowledgement

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Burger, Dr. Simon Blaschke**



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Dr. Laurenz Monzel, Lukas Schank, Christoph Harrer,
Jolanda Colbus, Dunbo Xiao

