

Prediction of Accurate Vibronic Spectra of Molecules in Strong Magnetic Field

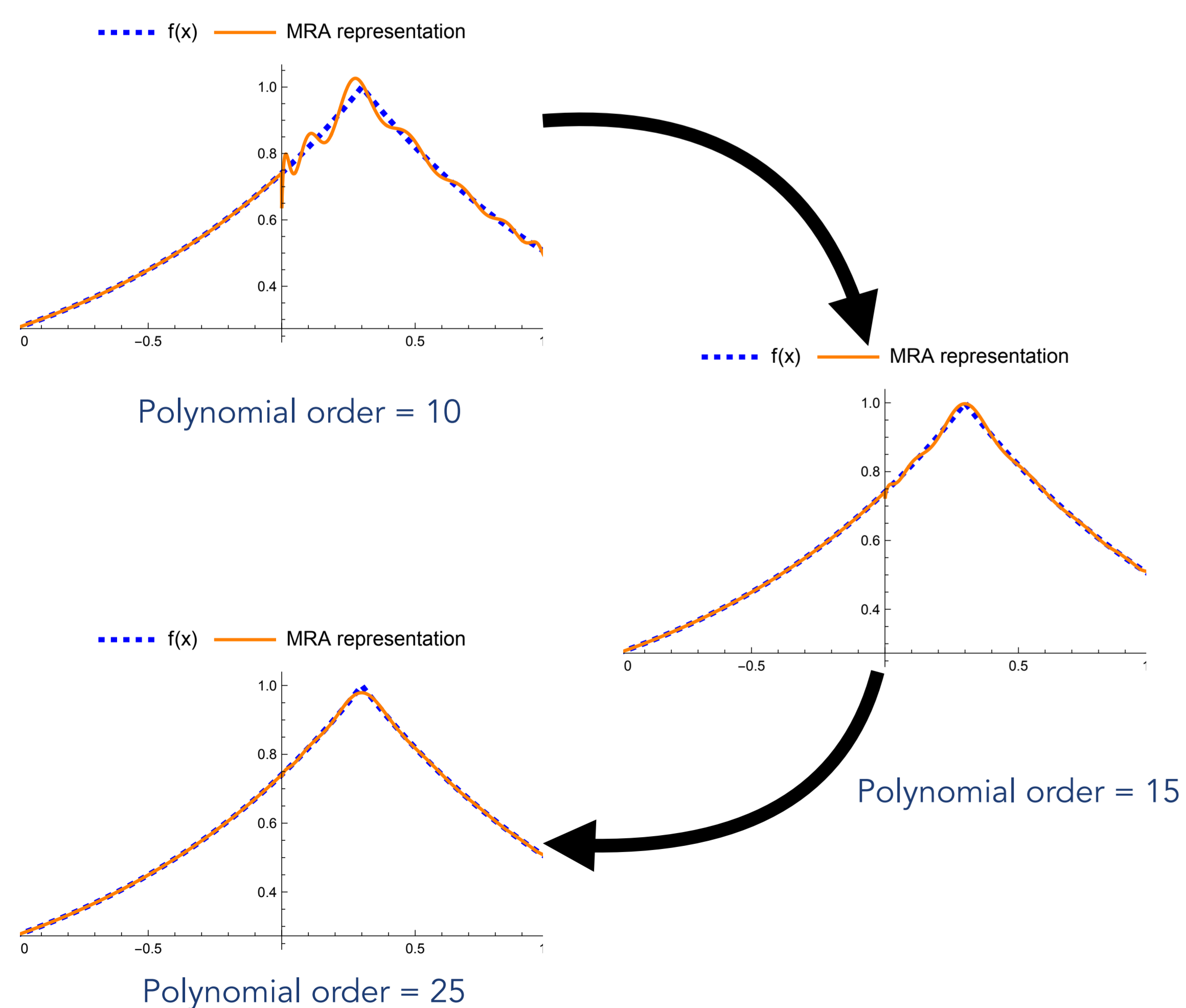
Motivation & Background

- > Chemical bonds in very strong magnetic field (\vec{B}), 10^5 to 10^8 T behave non-conventionally (**0.5 a.u. = 10^5 T**)
- > Linear Combination of Atomic Orbital (LCAO) approach in computational chemistry in strong \vec{B} faces numerical difficulties
- > Multiresolution Analysis (MRA) comes to rescue

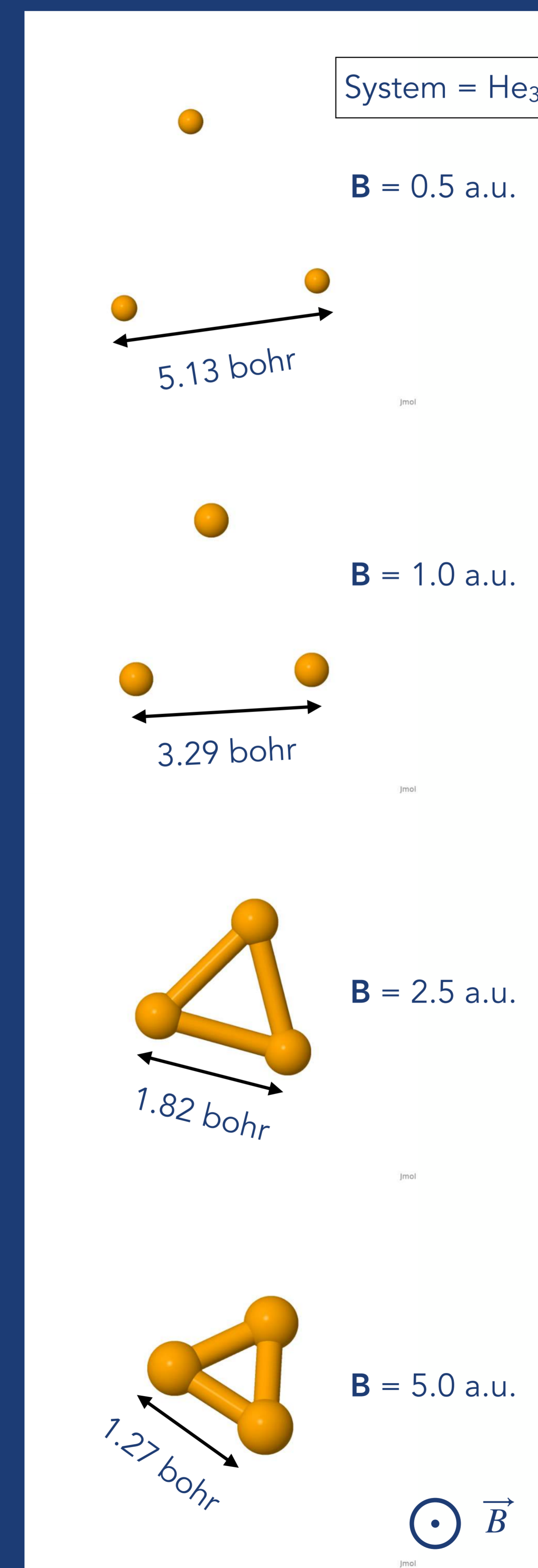
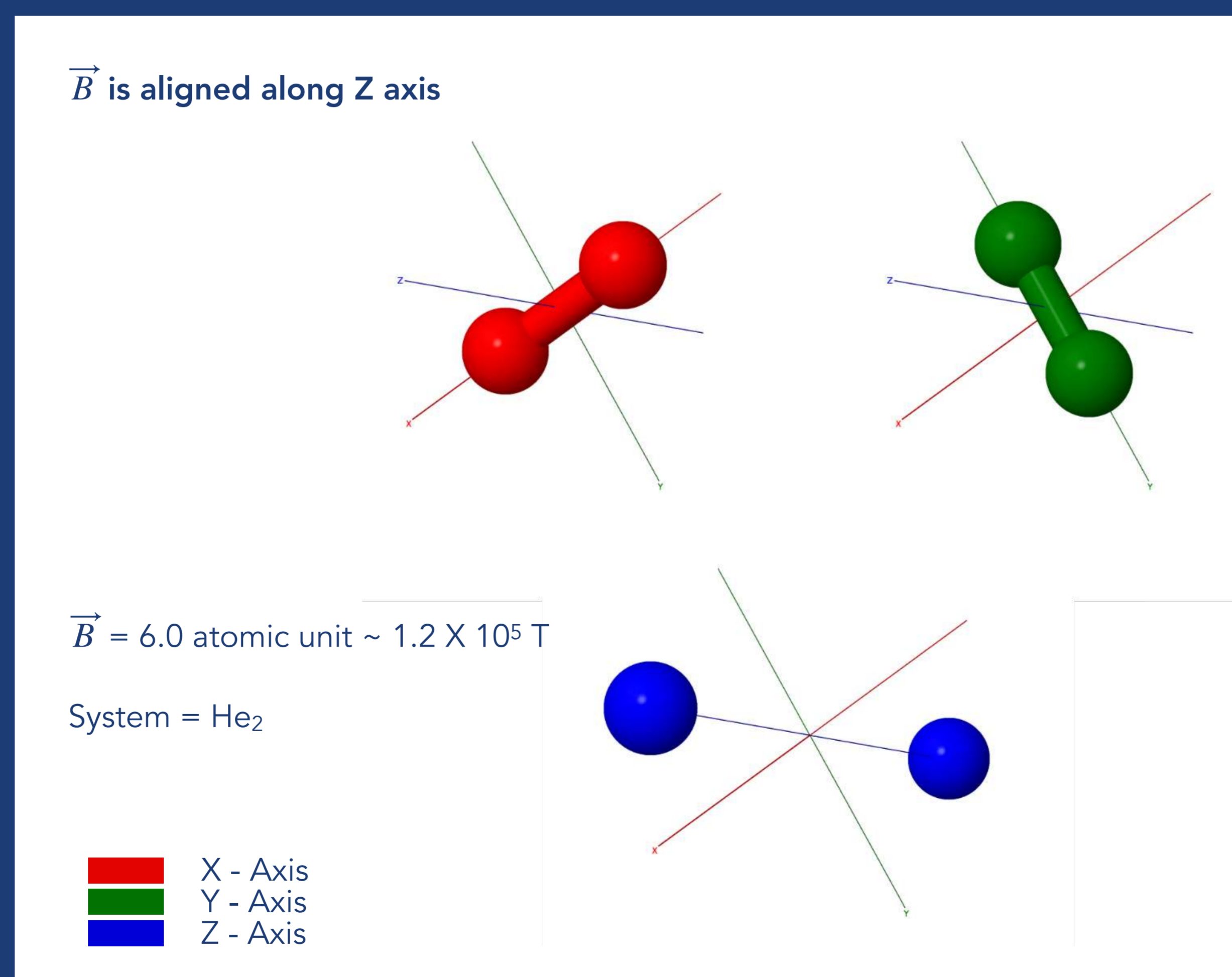
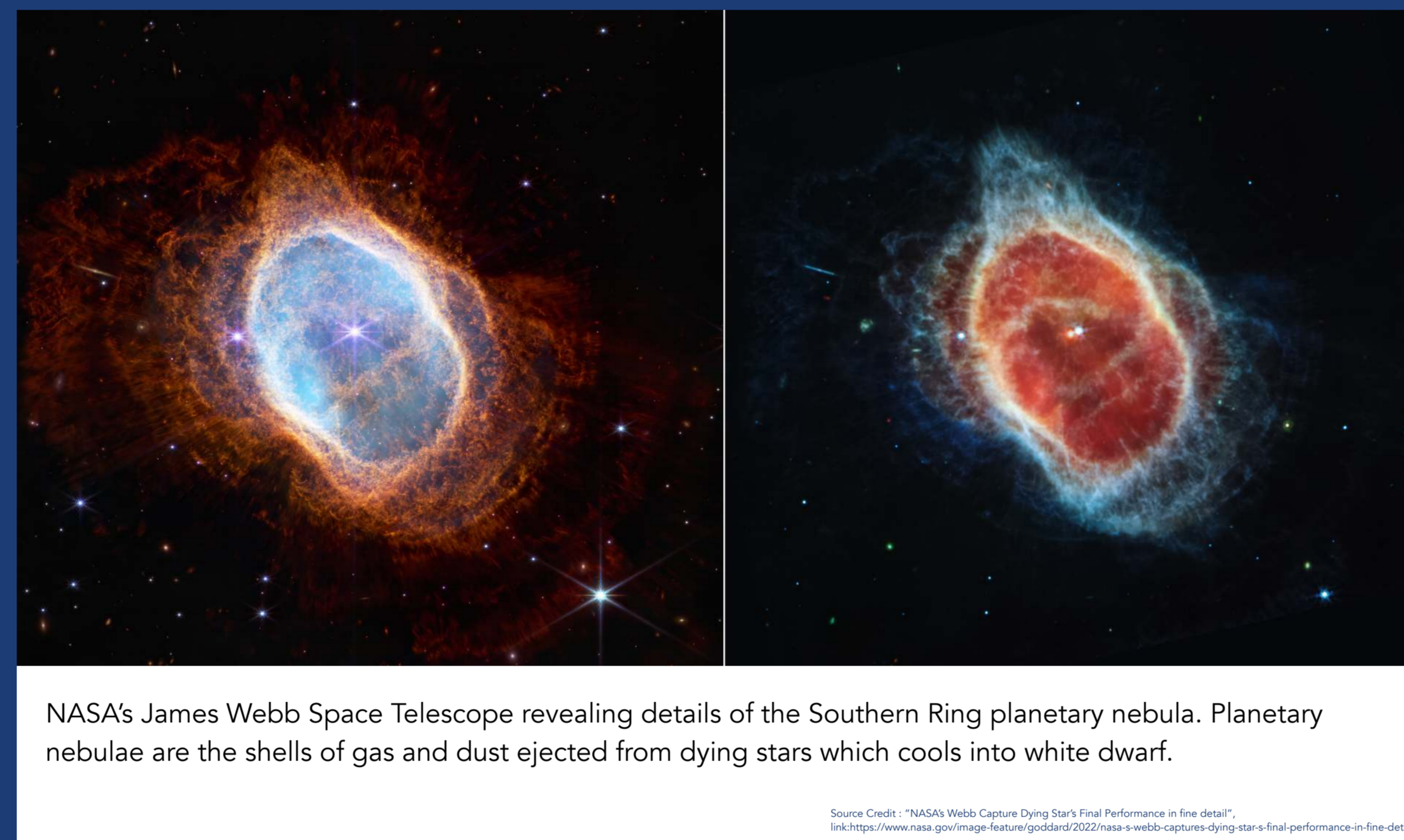
Multiresolution Analysis

- > Quantum State of a chemical system is described by a **wavefunction** (ψ)
- > MRA is an excellent way to represent ψ , which is basis set independent
- > M-A-D-N-E-S-S is a numerical environment for scientific simulation based on MRA

Illustration : $f(x) = e^{-|x-0.3|}$



Computational Chemists have a good alternative for calculating chemical systems in strong magnetic field : **Multiresolution Analysis**



My Contribution

- > Hartree Fock (HF) using M-A-D-N-E-S-S in strong \vec{B} was already developed
- > Geometry optimisation code based on Monte-Carlo algorithm is developed that uses HF code
- > Current interest is geometry of Helium clusters: He_n (n = 3, 4, 5, 6, ...)

Future Works

- > The impact of Electron Correlation in molecular geometry is of interest
- > Development of - - -
 - Configuration Interaction
 - Coupled-Cluster
 - Møller-Plesset
- - - codes in M-A-D-N-E-S-S
- > Development of tool for easy determination of molecular signatures in stellar objects

Conclusions

- > exact results within user defined precision
- > no Basis Set Incompleteness Error
- > can access any magnitude of \vec{B}
- > quick and straightforward implementation



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