Magnetic metals modelling eSSENCE 2023

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Team

Mathematical Physics Division, Physics Department, Lund University

- PhD student (currently open position, will work on this project)
- Ayan Pal, PhD student shared with Prof. Aryasetiawan

Partners

- Hugo Strand (Örebro University)
- Olle Eriksson (Uppsala University)

Magnetic metals

- Iron, nickel, cobalt, …
- Earth's core
- Hard to go there
- Hard to mimic in a lab
- Better to model on a computer

  Hausoel et al., Nature Communications **8**, 16062 (2017)

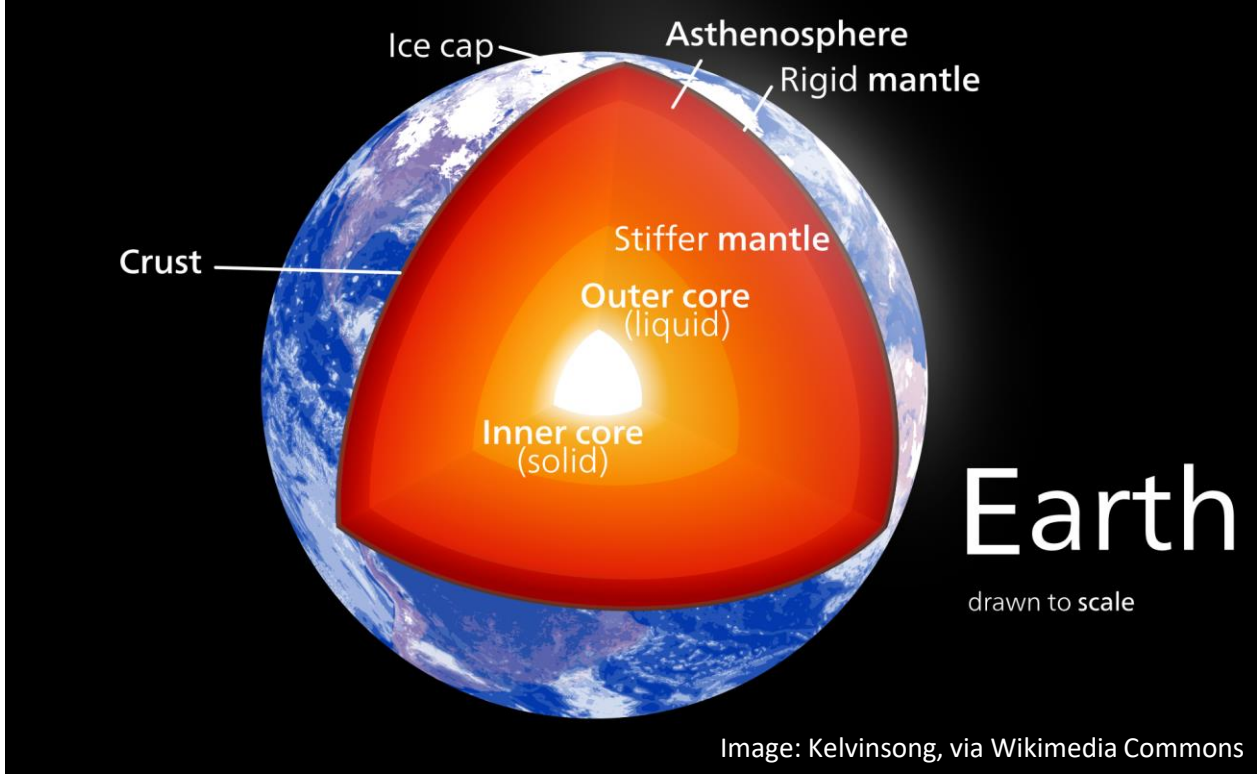
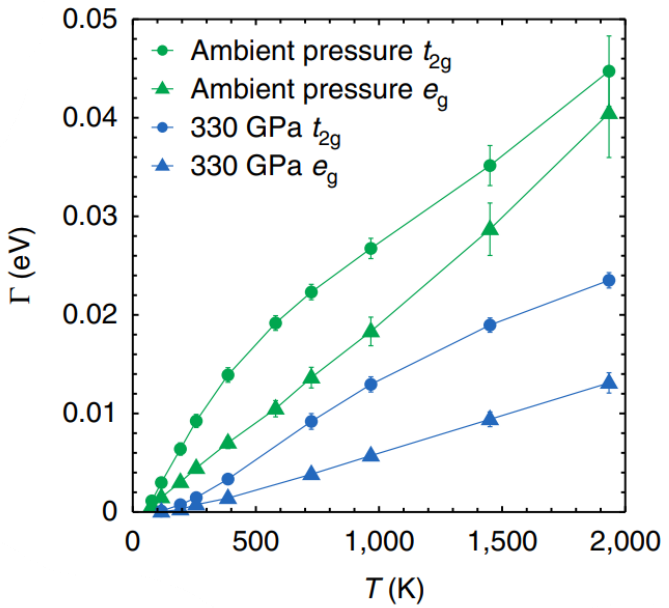


Image: Kelvinsong, via Wikimedia Commons



Technological applications

- Industrial and technological applications (data storage)
  - Data capacity
  - Speed
  - Energy efficiency
  - Cost
  - Sustainability
- Computational studies important
  - Choice of materials
  - Design of device
  - Very different scales!

Photo: Evan-Amos, via Wikimedia Commons

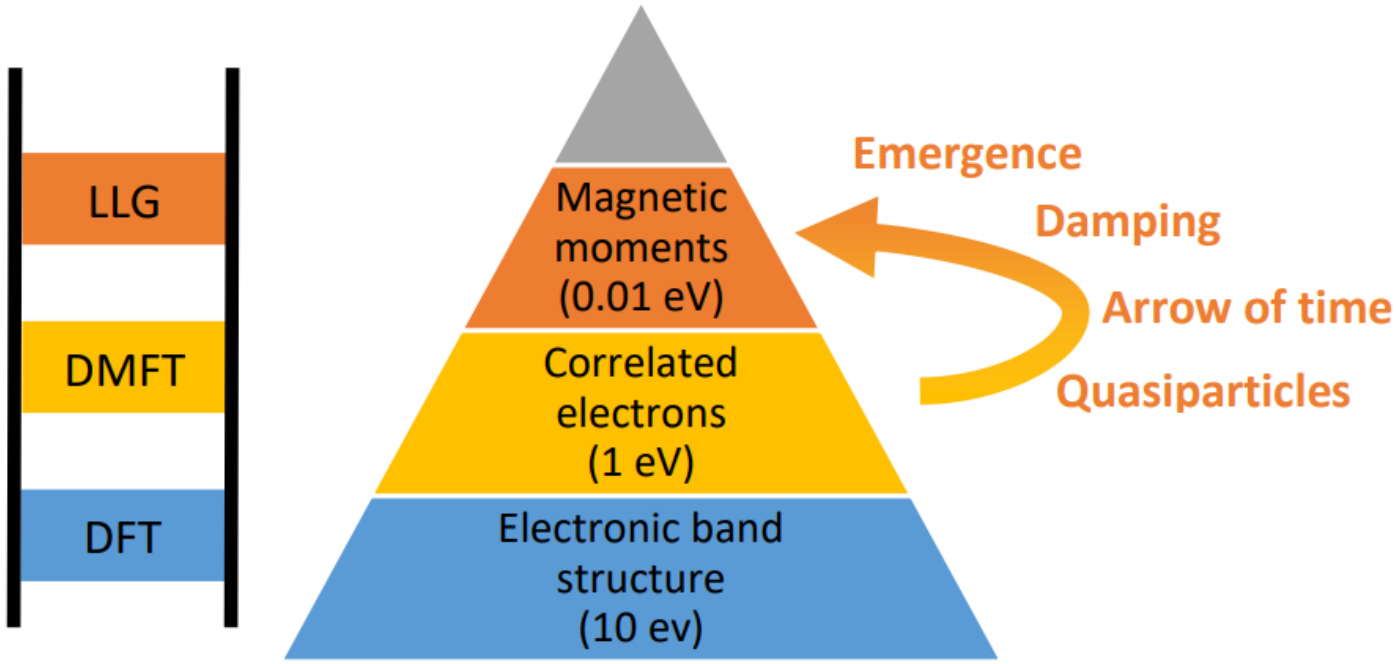
ESS

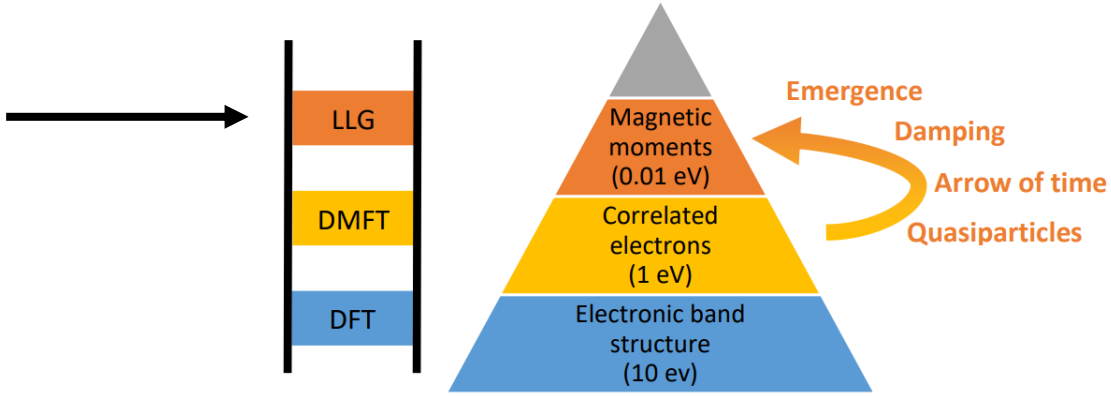
ESS will provide new experimental tools to study magnetism and magnetic materials

This makes computational studies very timely!

Models

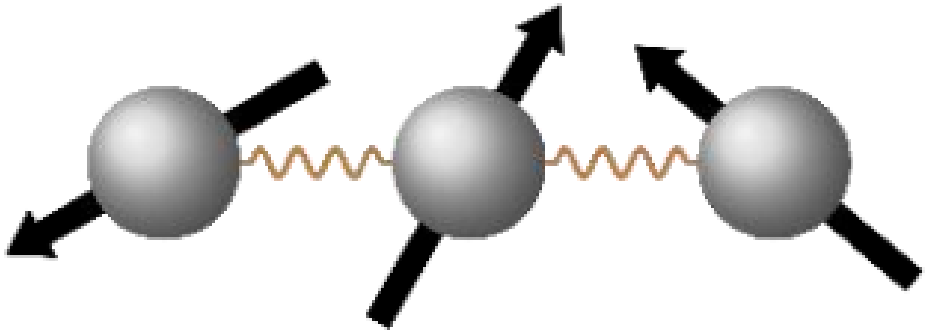
- Different length scales, different time/energy scales
- Computational challenge

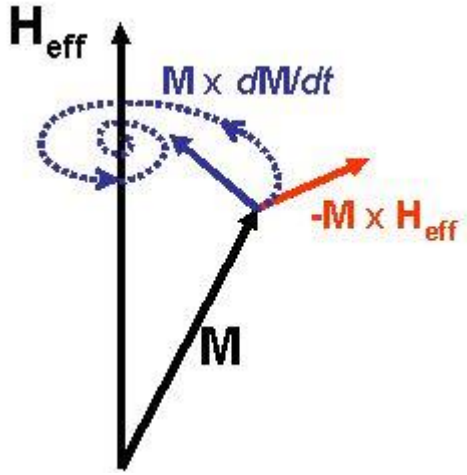




Magnetization

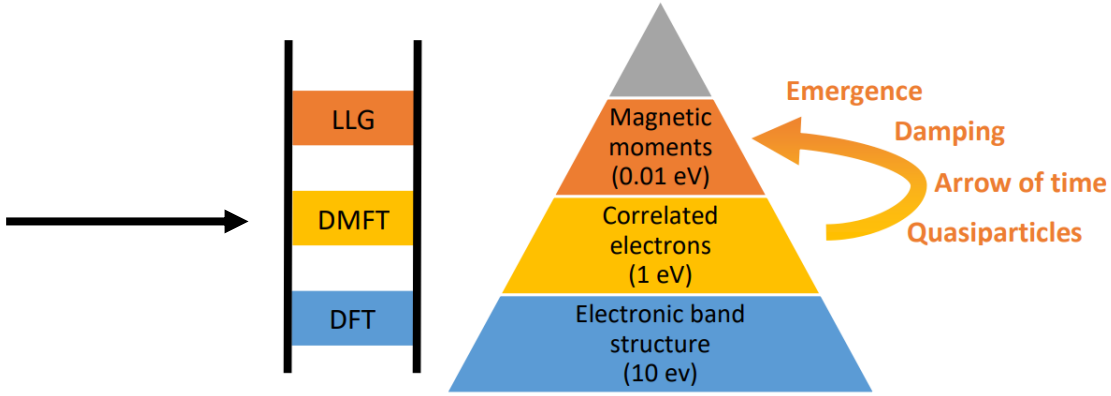
- Large length scale
- Assumes presence of **magnetic moments** or magnetization density
- Time evolution: **LLG equation**
- Includes damping of spin waves as a parameter



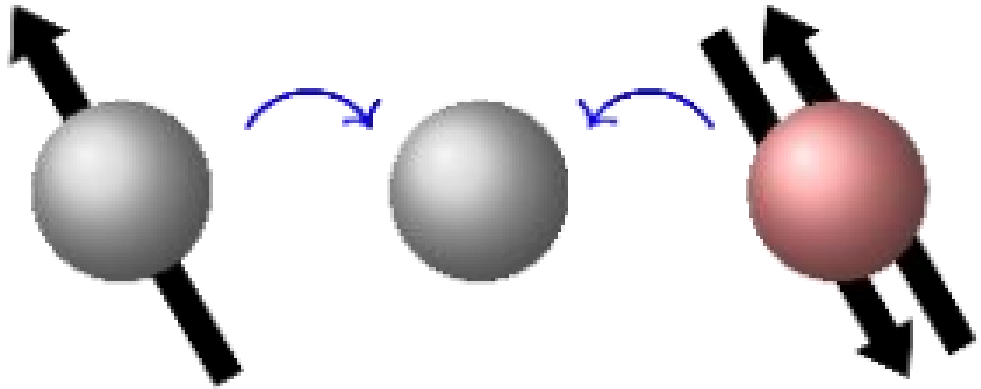


Wikipedia: Landau-Lifshitz-Gilbert equation

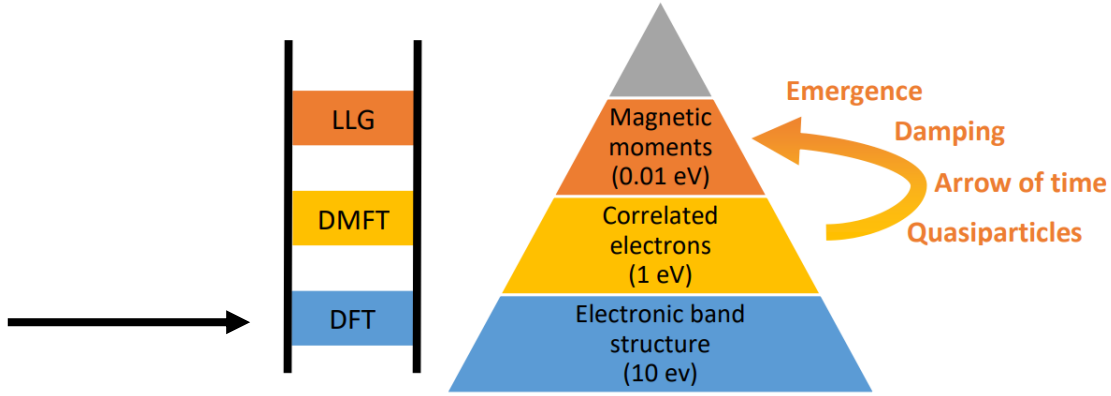
Itinerant electrons



- Electrons provide the magnetic moments (spin)
- The electrons can move, especially in **metals**
- **Correlated motion** since electron avoid each other, like a liquid
- Atomic scale model
- Undamped!

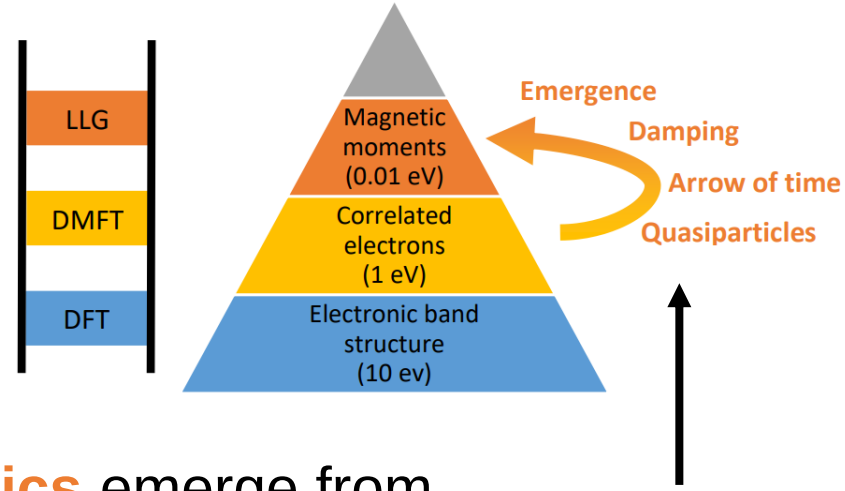


Electronic structure

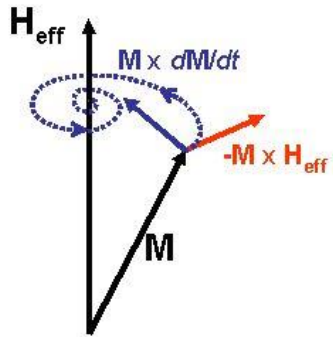


- Electrons/atom: Iron 26, Cobalt 27, Nickel 28
- Our **model**: handful of electrons/atom, only those that can move
- **Electronic structure** → **model**
- Collaboration with Olle Eriksson group (Uppsala)
- Mostly Density Functional Theory (**DFT**)

This project's goal

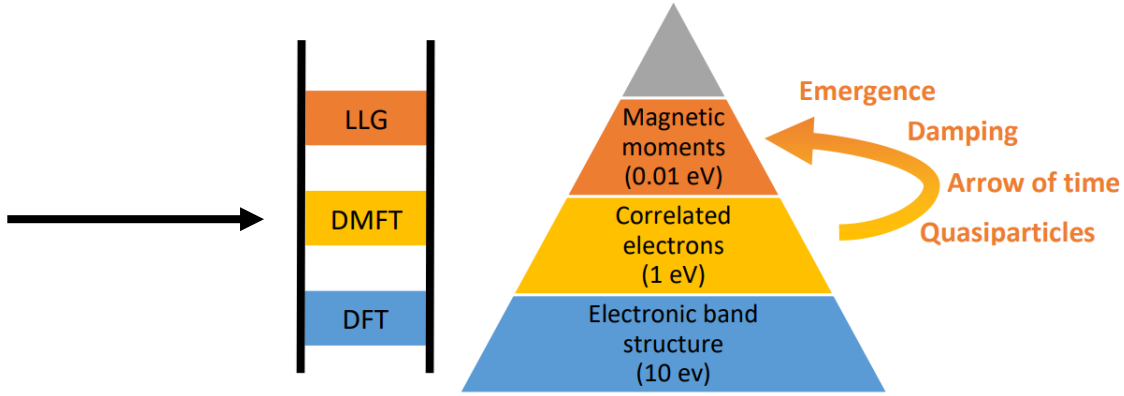


- How does the **large-scale magnetization dynamics** emerge from the **dynamics of correlated electrons**
- Predict the possible magnetization waves and their energy
- How does macroscopic **damping of spin waves** emerge from **undamped electronic dynamics**?
- Which mechanisms are responsible for damping?



- Correlated electrons are difficult to study…

Methods



- Correlated many-particle physics is
- Spatial correlations and temporal/dynamical correlations
- Reasonable approximation: decouple space and time
  - Can treat large correlated systems
  - Dynamical Mean-Field Theory (**DMFT**)
    Georges, A. et al. Rev. Mod. Phys. **68**, 13–125 (1996)
- Calculation of magnetic correlation function $\chi(t, \boldsymbol{R})$ in DMFT
  - This is what will be measurable at ESS

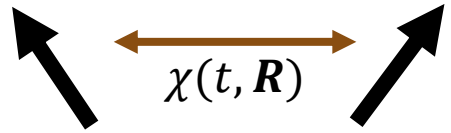
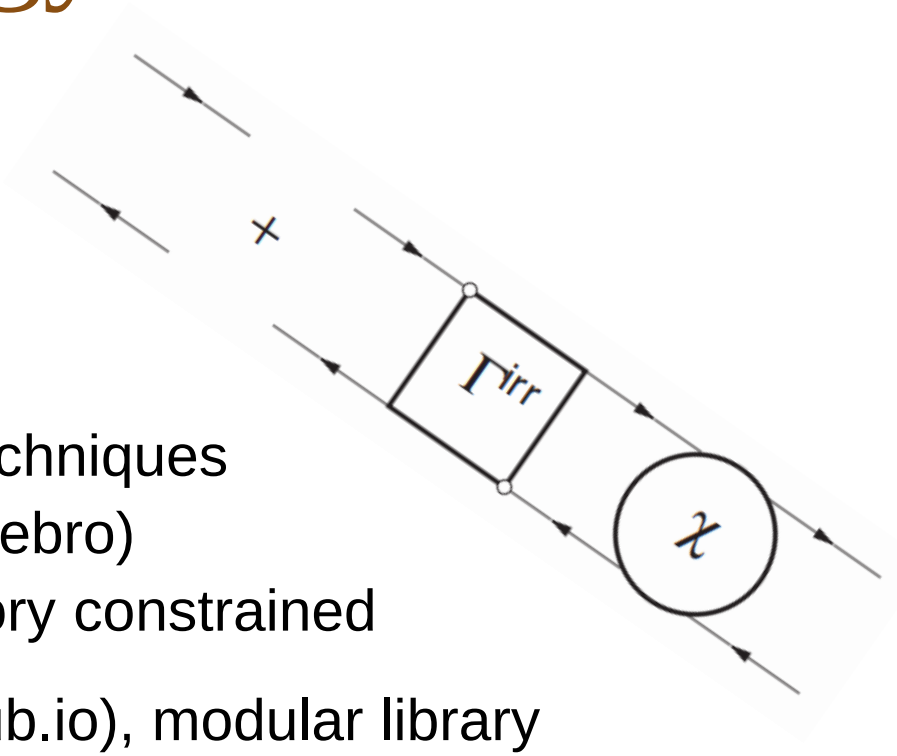


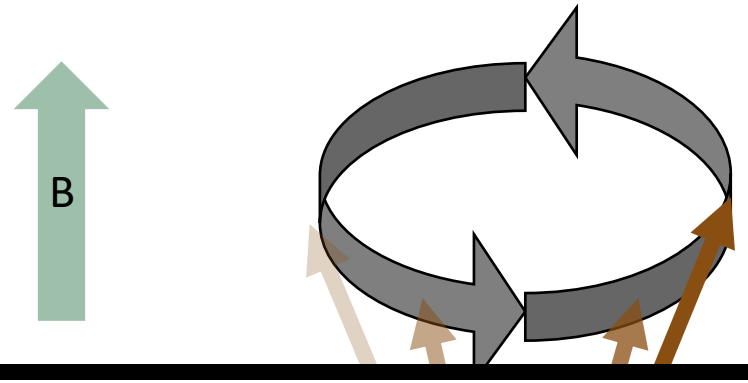
Photo: lunarc.lu.se

Computational technology

- Dynamical correlations: Quantum Monte Carlo
  - Highly parallelizable
  - Open-source solvers available
  - Substantial recent progress
- Spatial correlations: Feynman diagrammatic techniques
  - Our main contributions here (together with Örebro)
  - Not the CPU bottleneck, but eventually memory constrained
- This project based on TRIQS (https://triqs.github.io), modular library



Ongoing work



Intermezzo: (see also Filip Szczepankiewicz's talk last week)

MRI through the eyes of a non-medical physicist:
In a magnetic field, precession of nuclear spin in H atom.
Resonance frequency depends (linearly) on magnetic field,
This shows where the hydrogen atoms are.

In fact, there is more!
Hydrogen nuclei and their spin are not perfectly isolated.
Precession is slightly different based on environment.
This helps medical imaging to distinguish things,
H in water looks different from H in fat, or in a brain

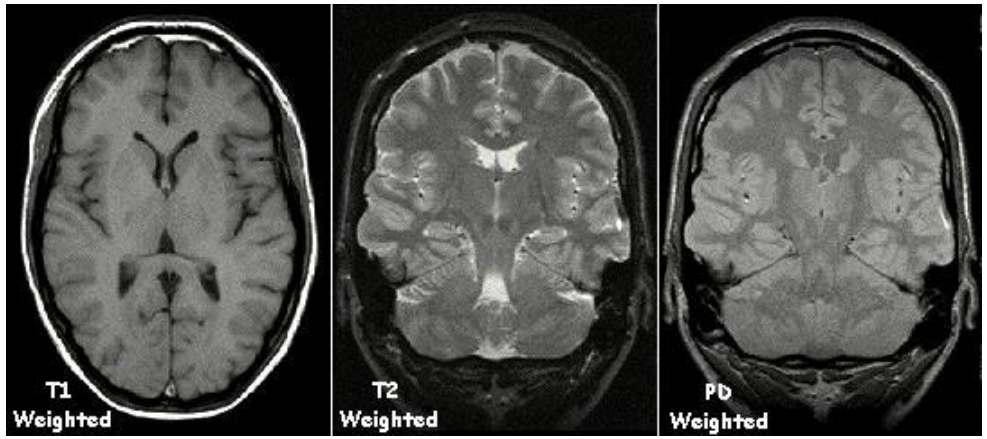
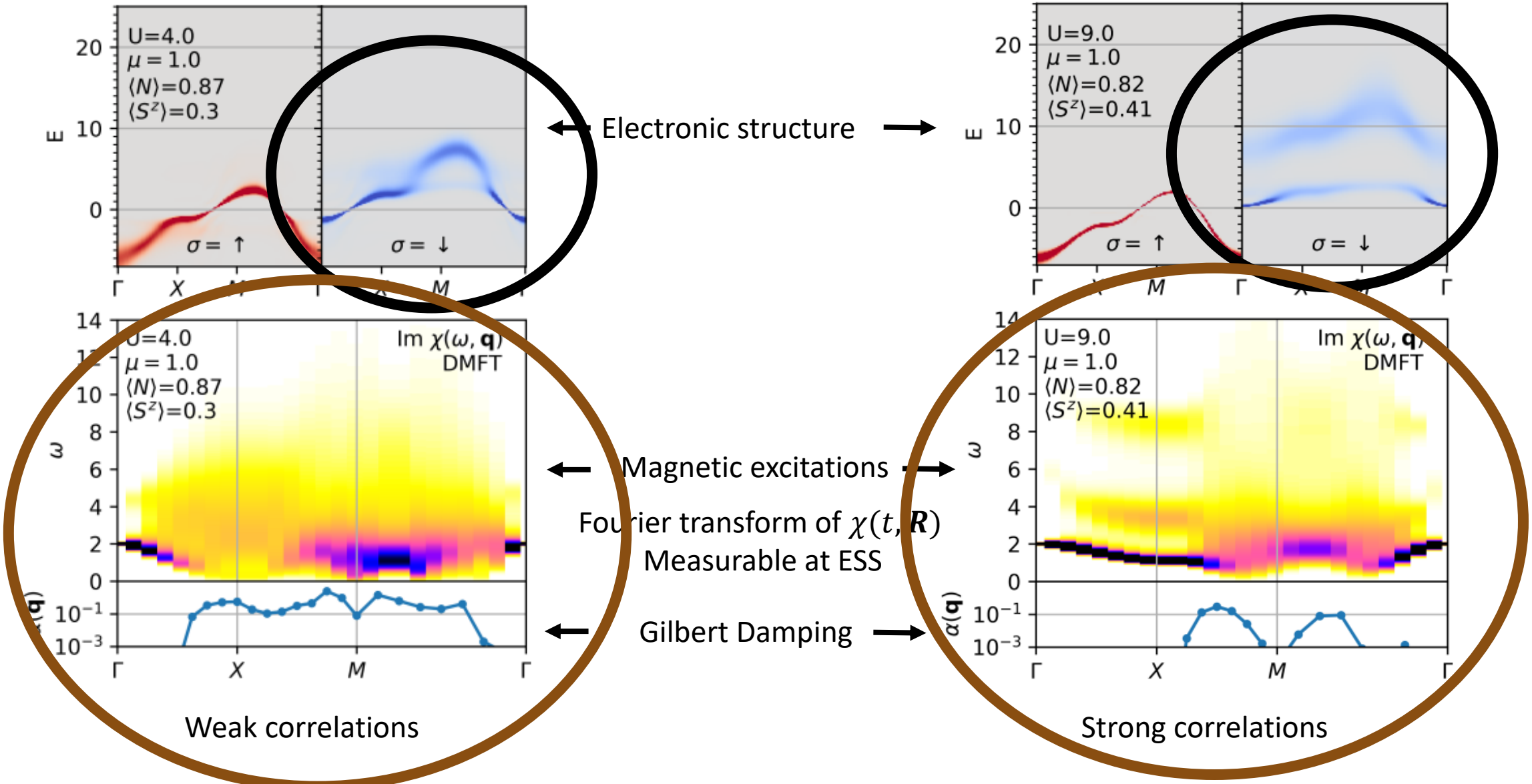


Photo: KieranMaher via Wikipedia

Results [arXiv:2303.03468]



Summary

- Bridge the gap between electronic models and magnetic models
- Spatio-temporal structure
- Understanding of damping mechanisms
- “MRI for many-electron systems”
- Material-specific predictions possible, across wide temperature/pressure range