Observance of Hund's Rules in the Same Setting: Coexistence of Intra-Atomic and Inter-Atomic Exchanges in Cellular Automata

Rule 1: Maximization of total spin S
Reduces Coulomb repulsion
Weak Ferromagnetic coupling
Long-range dipolar interactions

Rule 2: Maximization of total orbital angular momentum L
Reduces Coulomb repulsion

Rule 3: Minimization of spin-orbit energy
Save kinetic energy
Antiferromagnetic coupling[1]

Goktug Islamoglu
Independent Researcher, M.Sc
goktu.github.io/ADama/

1. Paolasini, Luigi. Lectures on Magnetism, Lecture 4 «Magnetic Interactions». ESRF

Significance of Hund's Rule
Determination of the ground states

Aim: To bridge between ferromagnetism and antiferromagnetism, through paramagnetic and ferrimagnetic spin magnetic moments

Antiferromagnetic materials is one of the most popular areas of memory research.

Finding materials generating a 0/1 switch is the current challenge for antiferromagnets.

In this research, the author proposes a framework by a cellular automaton model. A switch between **strained ferromagnetic** state and **antiferromagnetic ground state** is hypothesized as **ferrimagnetic polarization**.

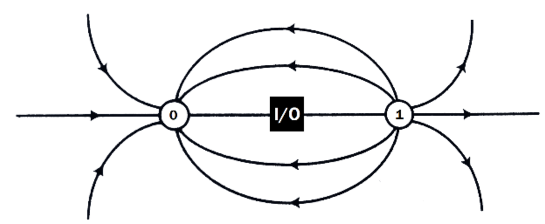
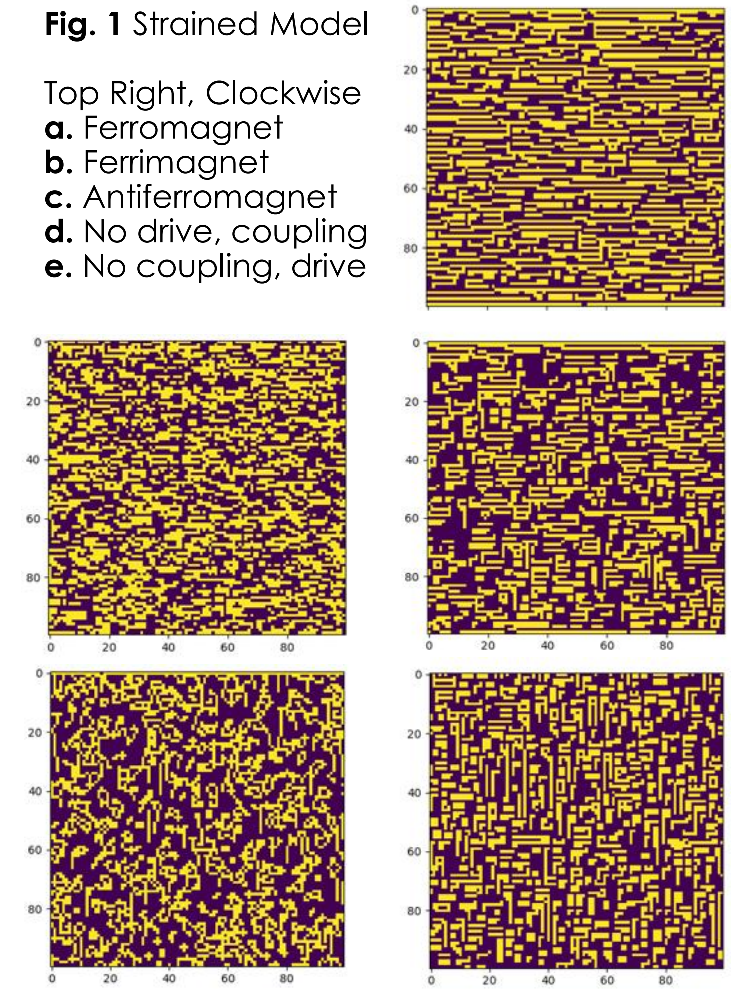


Fig. 1 Strained Model

Top Right, Clockwise
a. Ferromagnet
b. Ferrimagnet
c. Antiferromagnet
d. No drive, coupling
e. No coupling, drive



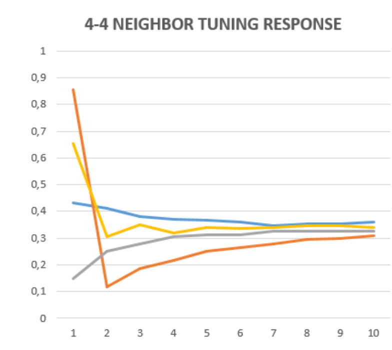
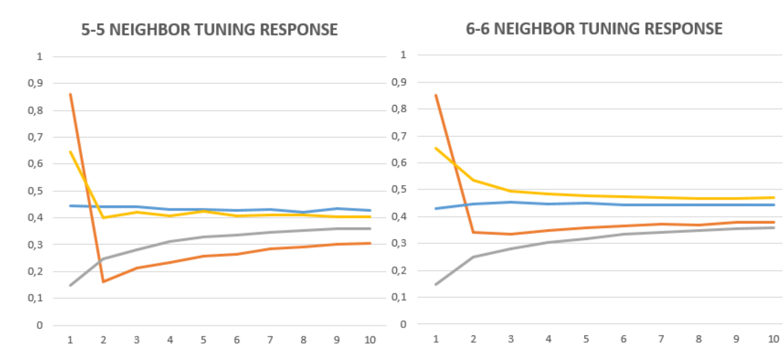


Fig. 2 Neighbor Tuning

Top-Middle Left: State 1 cell counts of 4/9 or 5/9, inverse Ising critical temp. local max, paramagnetic

Middle Right: Count 6/9, global max, spontaneous ferromagnetic transition.

Bottom: Transition model



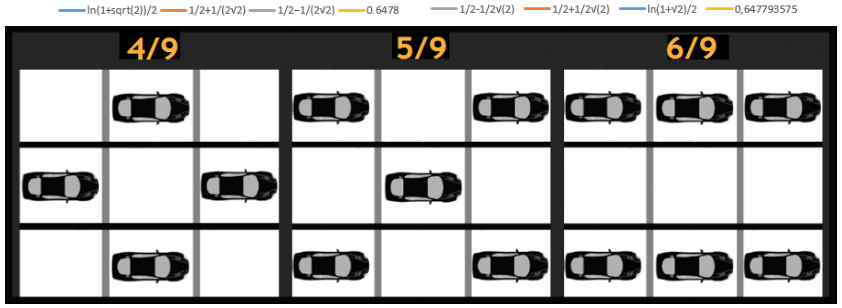
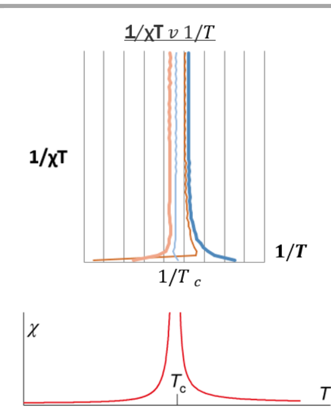


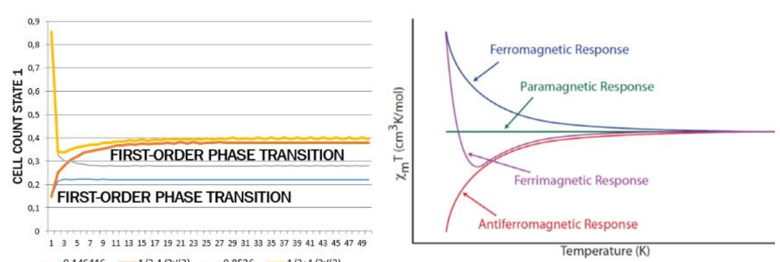
Fig. 3 Types of Transitions

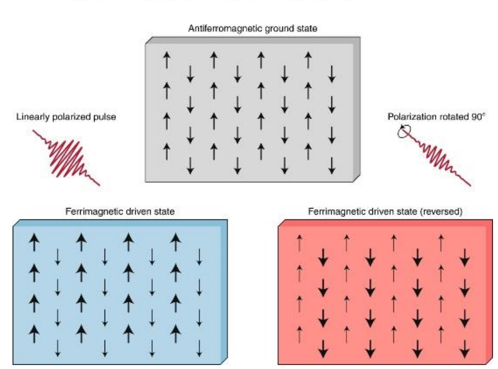
Top: Second-order phase transition at Ising critical temp. is ferromagnetic.

Middle: First-order phase transition at the reversed ferrimagnetic polarization to the AFM ground state.

Bottom: Commentary







Strain Polarized Antiferromagnet
Nature Physics
Shaken not strained

Antiferromagnetic ground state is driven to a **ferrimagnetic** state by laser pulse induced polarization.

https://doi.org/10.1038/s41567-020-0937-2

Results

Exact analytical solutions of transition geometries: First-order (Hund's Rule 3) & second-order (H's R 1)

Presented:
NECSI ICCS 2020
NERCCS 2021

2D Ising model map onto 1D quantum spin chain[1]

Step 1

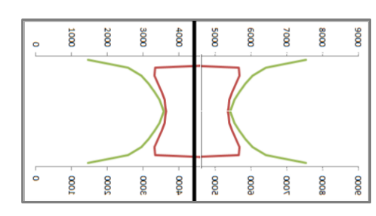
1	1	1
0	1	1
1	1	1

Step 2

1	1	1
0	0	1
1	1	1

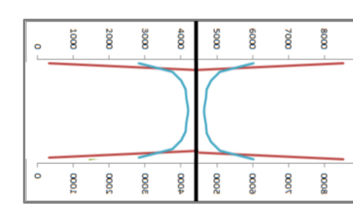
Step 3

1	1	1
0	0	0
1	1	1



Polarization: Catenoid around p = 1/2

FIRST-ORDER PHASE TRANSITION



Ising criticality: Pseudosphere around p = ln(1+√2)/2

SECOND-ORDER PHASE TRANSITION

Underlying evolution function suggests a mode of switching between two types of phase transitions. An I/O (1st rule) that is also a data storage (3rd rule).

This feedback loop is a **dipole state machine.**

1. Wei, BB., Chen, SW., Po, HC. et al. Phase transitions in the complex plane of physical parameters. Sci Rep 4, 5202 (2014). https://doi.org/10.1038/srep05202