THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 07: Symbolic Regression and Physics Discovery

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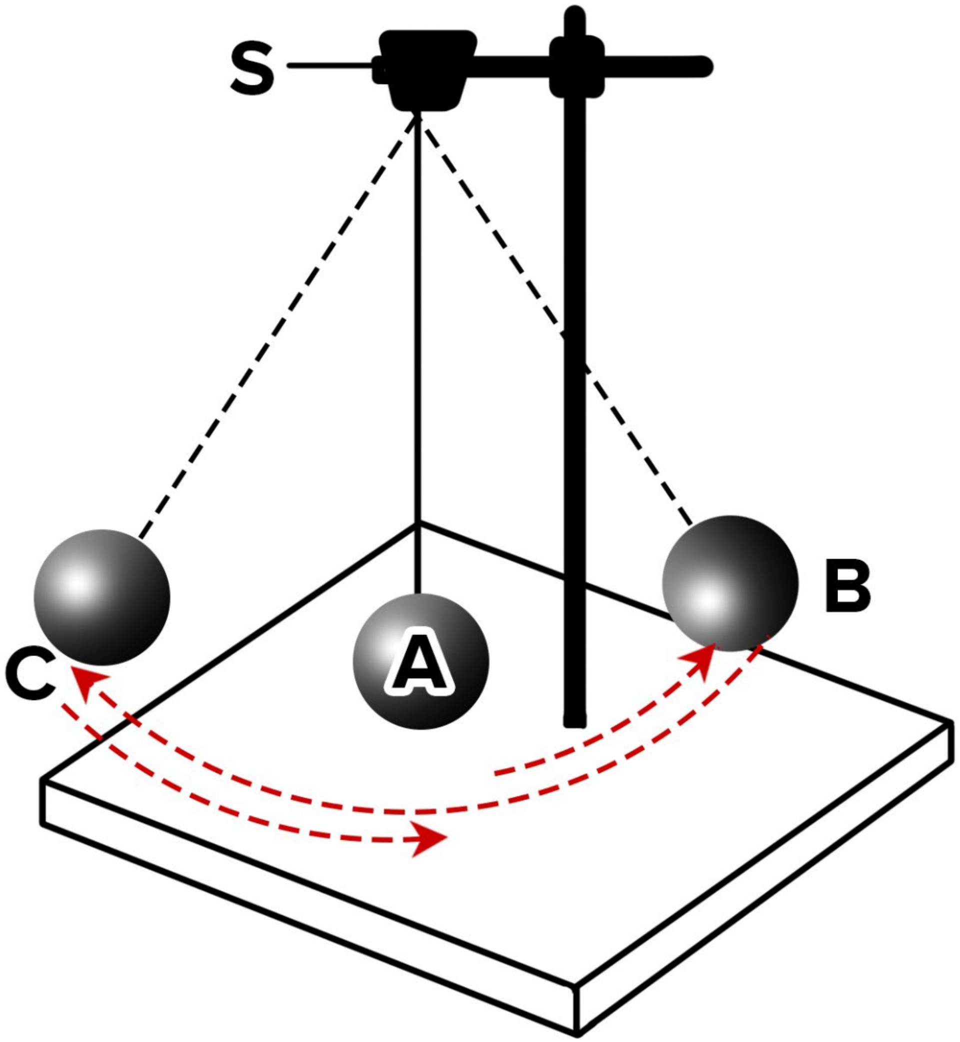
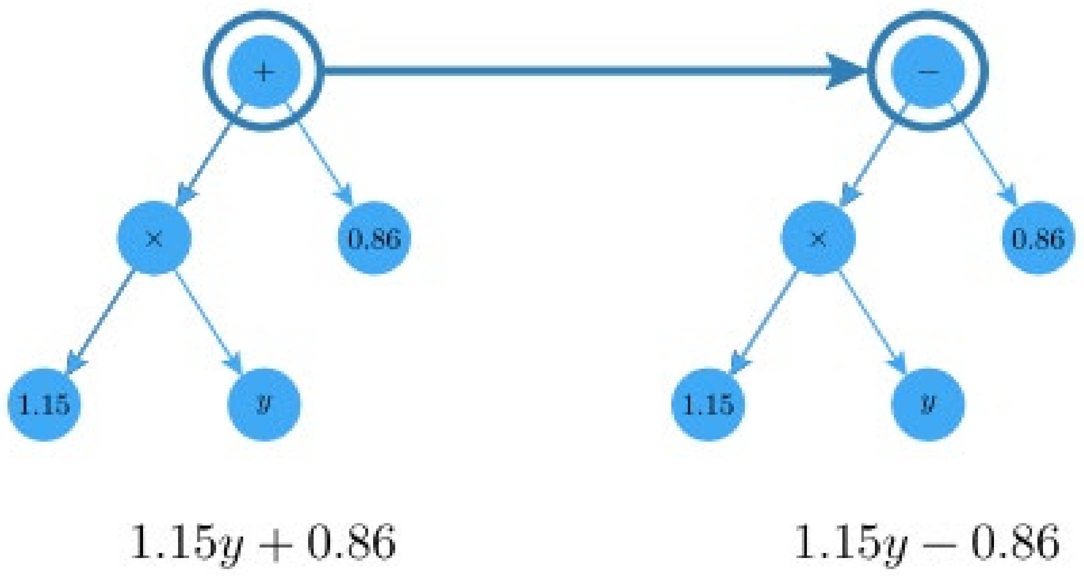
Back to functions from data

- If the function is known, we can fit it to data
- If we have several possible functions, we can fit all of them and compare the quality of fits
- We can also make some judgements based on the parameter values
- But what if we do not know the functions?



Back to functions from data

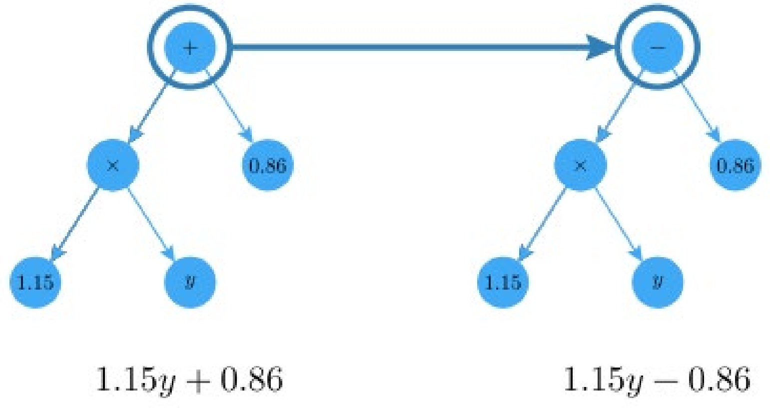
Functions (and programs in general) can be represented as trees of operations!



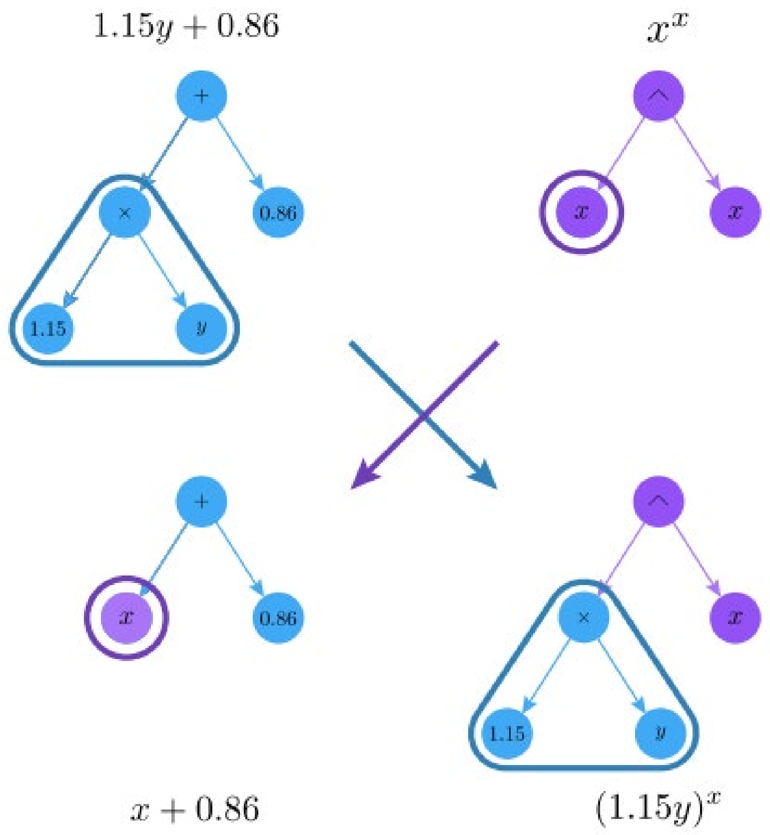
https://arxiv.org/pdf/2305.01582.pdf

PySR

Mutation



Crossover



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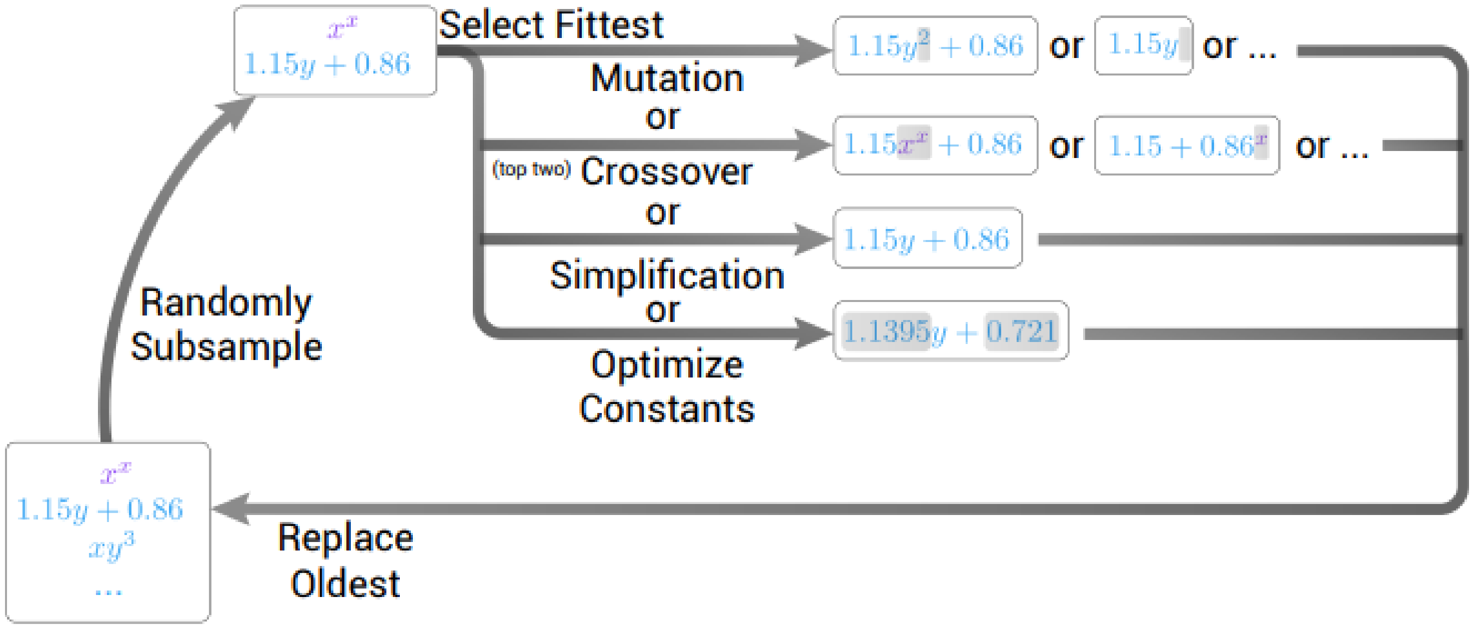
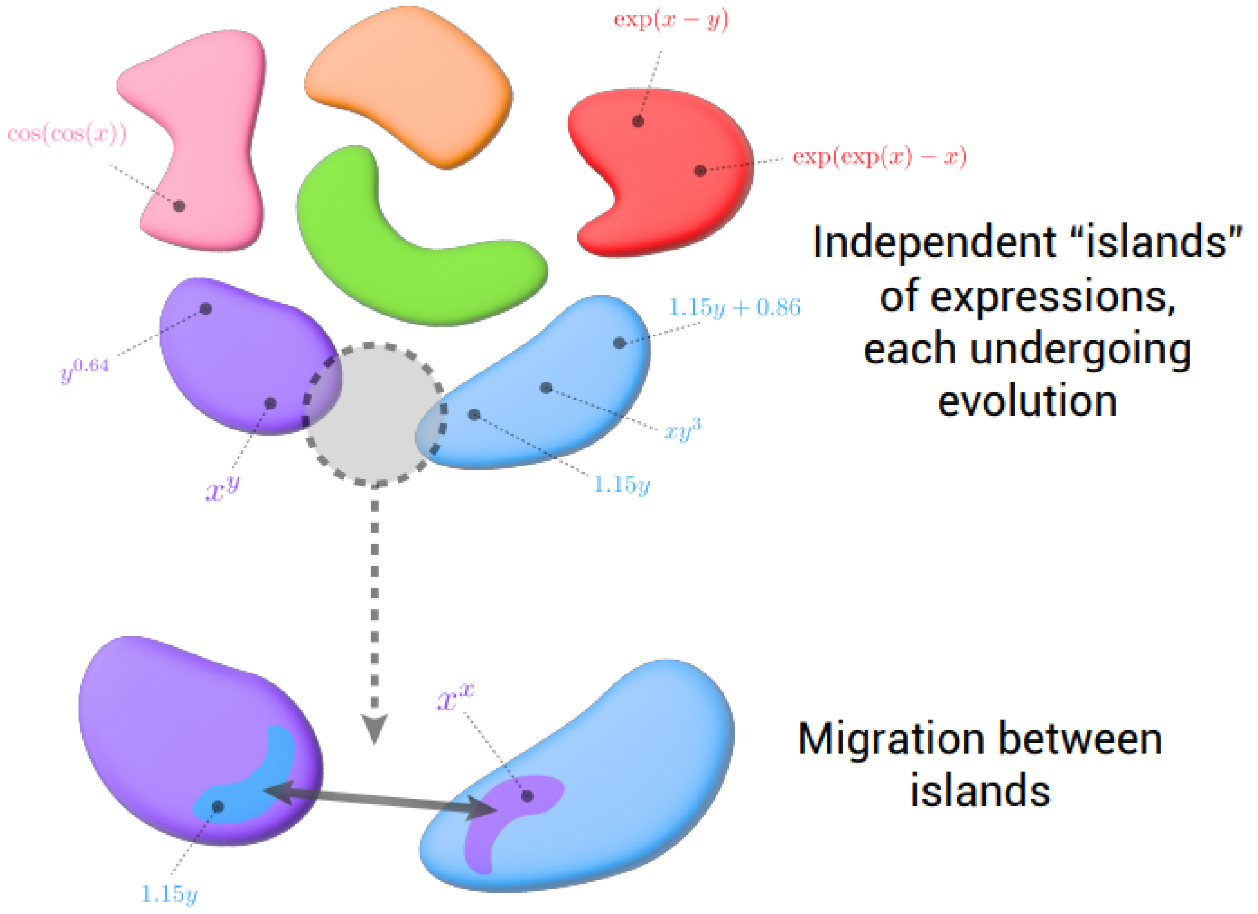
PySR



The inner loop of PySR. A population of expressions is randomly subsampled. Among this subsample, a tournament is performed, and the winner is selected for breeding: either by mutation, crossover, simplification, or explicit optimization. Examples of mutation and crossover operations are visualized in figs. 1 and 2.

https://arxiv.org/pdf/2305.01582.pdf

PySR



The outer loop of PySR. Several populations evolve independently according to the algorithm described in fig. 3. At the end of a specified number of rounds of evolution, migration between islands is performed.

https://arxiv.org/pdf/2305.01582.pdf

PySR Benchmarking

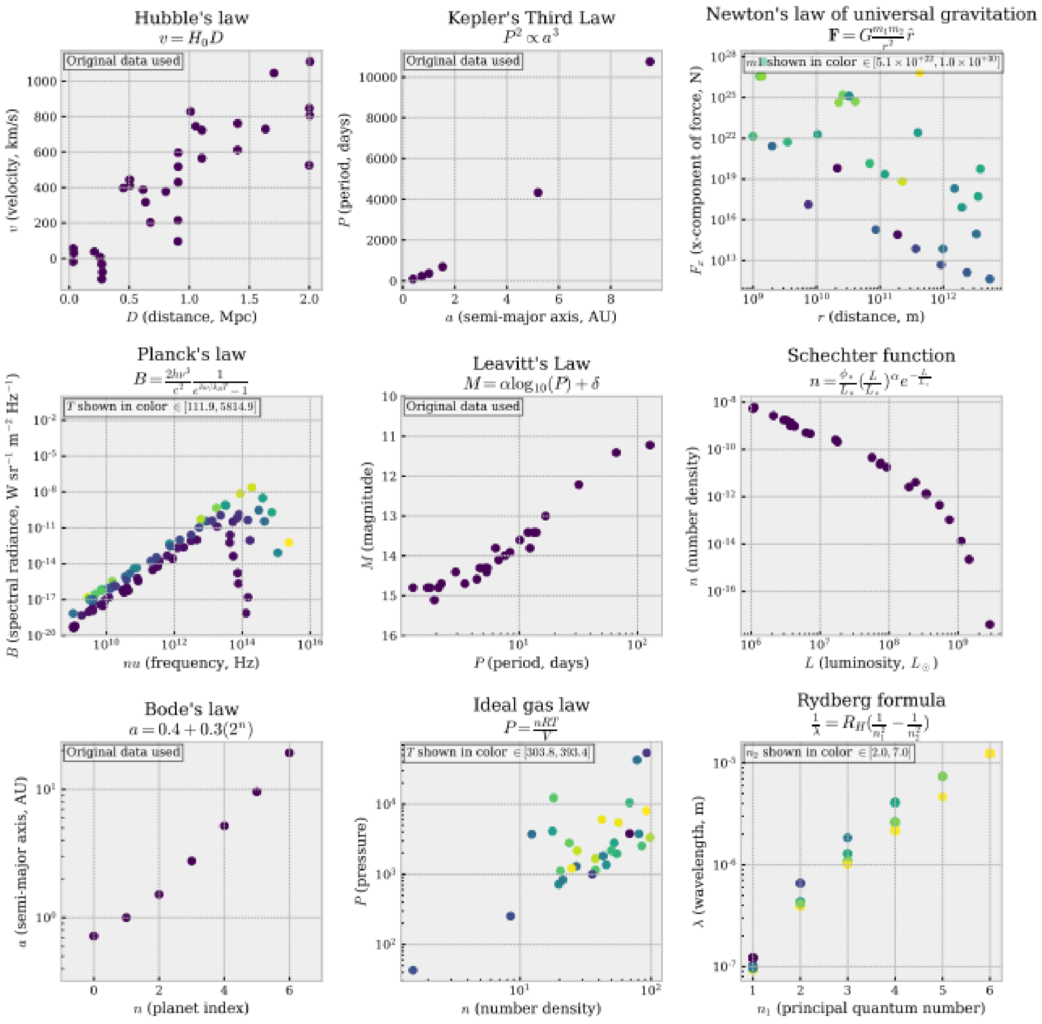


Figure 5: Visualization of all the data in EmpiricalBench, an SR benchmark for science. Color is used to denote additional variables in the cases of relations which depend on more than two inputs. Original data in the discovery of each law is used where easily available. Otherwise, data is generated from the formula with realistic ranges of variables, with a level of noise applied.

Name	Law
Hubble's law	$v = H_0 D$
Kepler's Third Law	$P^2 \propto a^3$
Newton's law of universal gravitation	$\mathbf{F} = G\frac{m_1 m_2}{r^2}\hat{r}$
Planck's law	$B = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/k_B T}-1}$
Leavitt's Law	$M = \alpha \log_{10}(P) + \delta$
Schechter function	$n = \frac{\phi_*}{L_*}(\frac{L}{L_*})^\alpha e^{-\frac{L}{L_*}}$
Bode's law	$a = 0.4 + 0.3(2^n)$
Ideal gas law	$P = \frac{nRT}{V}$
Rydberg formula	$\frac{1}{\lambda} = R_H(\frac{1}{n_1^2} - \frac{1}{n_2^2})$

https://arxiv.org/pdf/2305.01582.pdf

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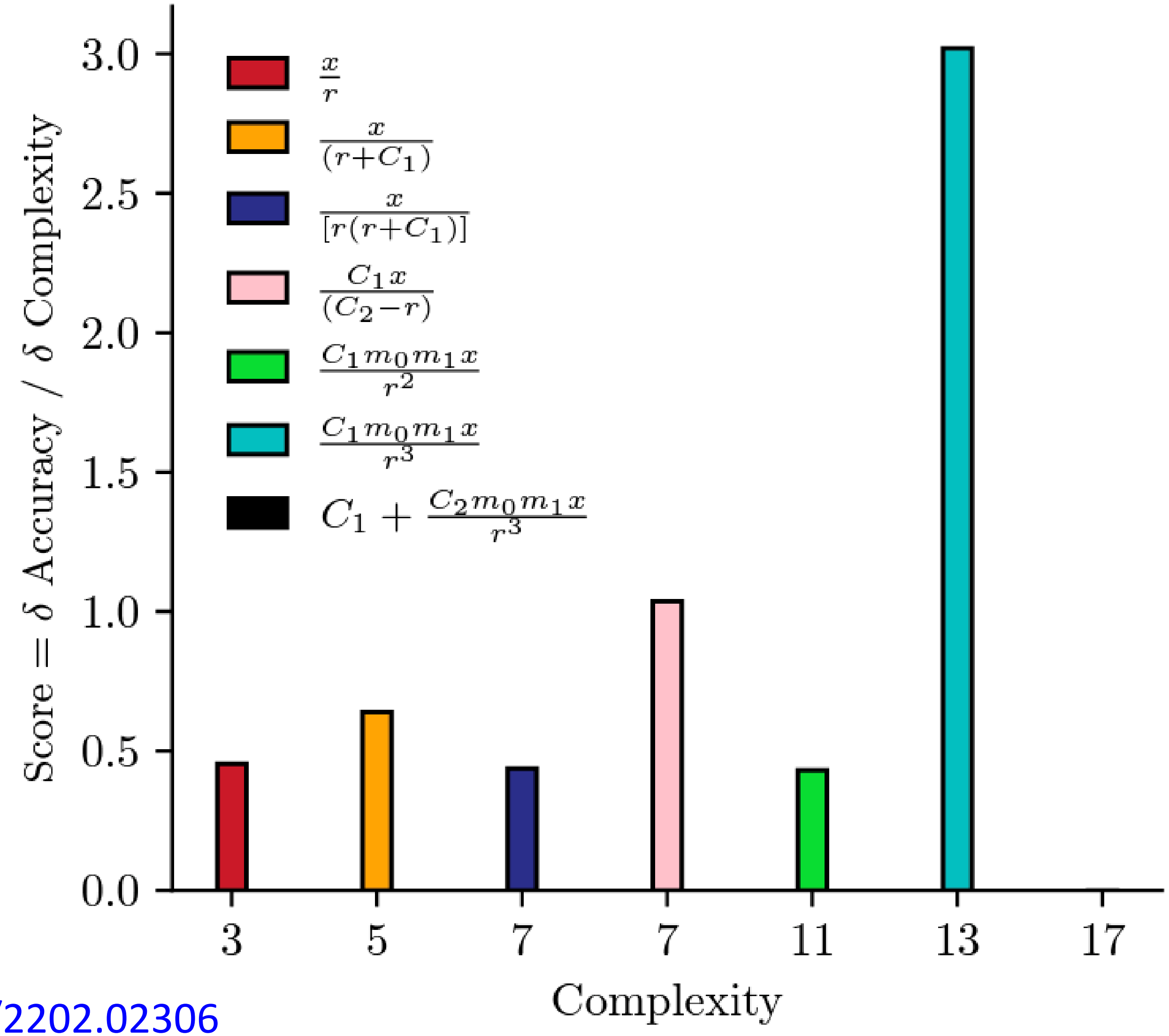
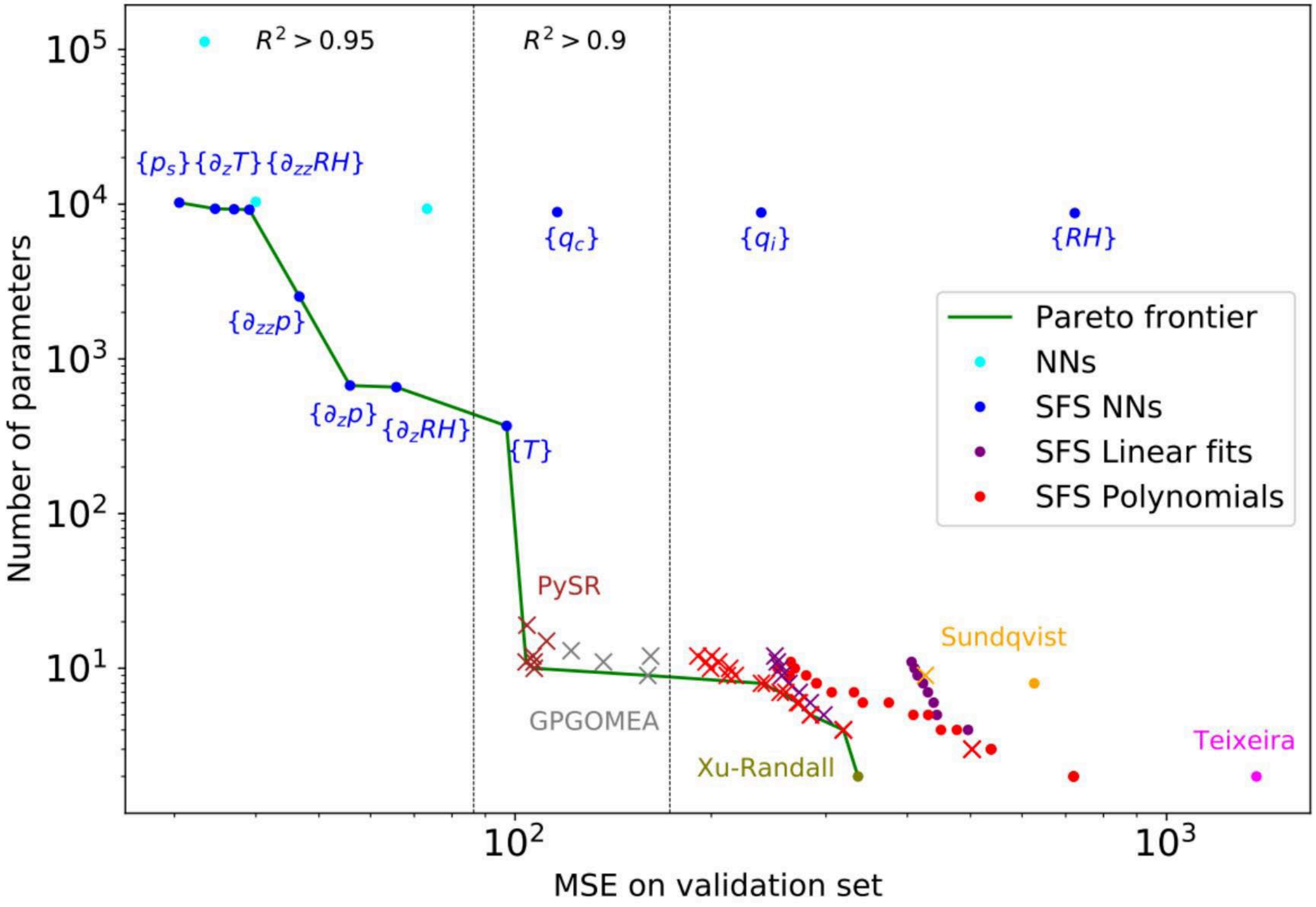
Colab!

Finding the right expression



https://arxiv.org/abs/2202.02306

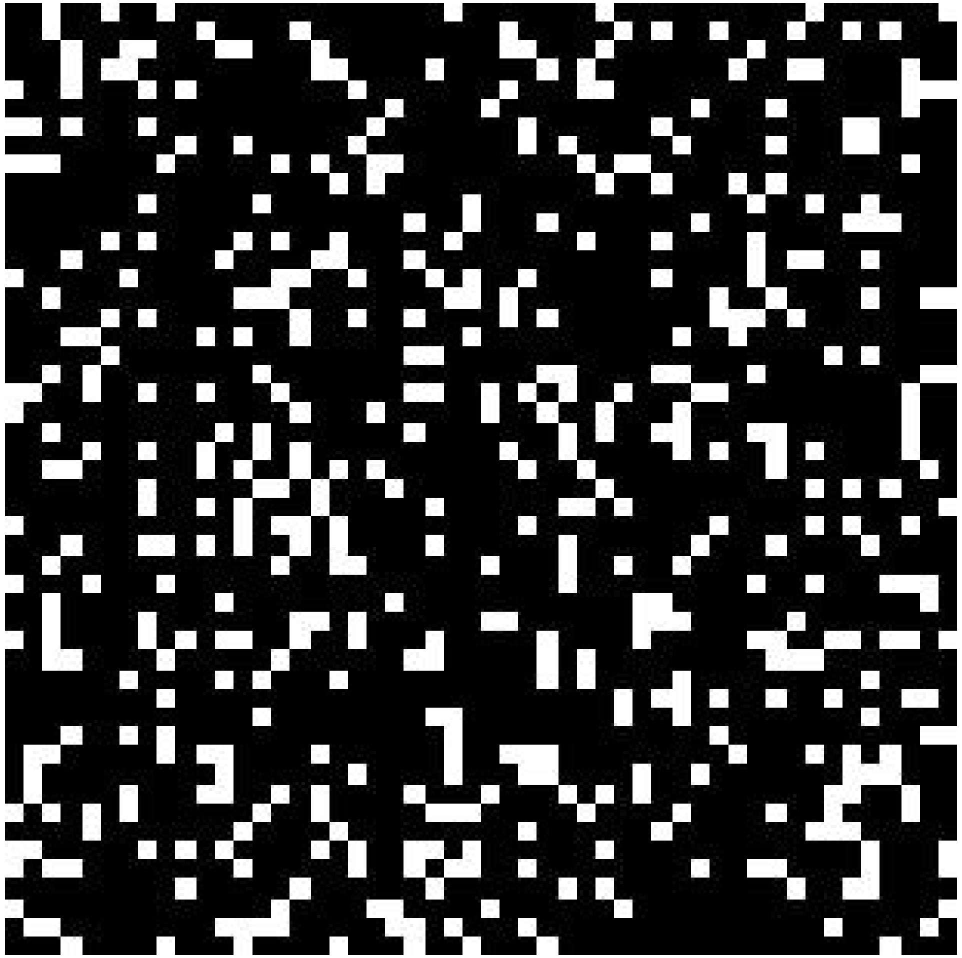
Finding the right expression

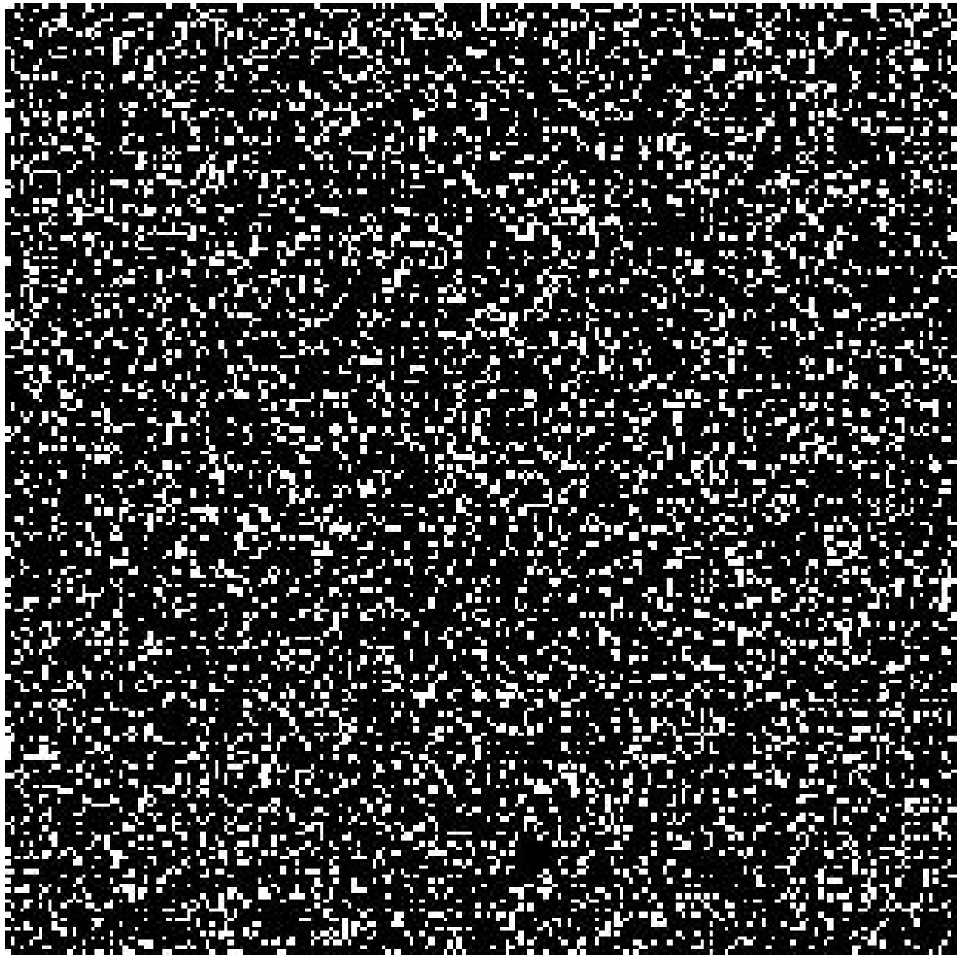


https://arxiv.org/abs/2304.08063

GitHub

Do we always have an expression?



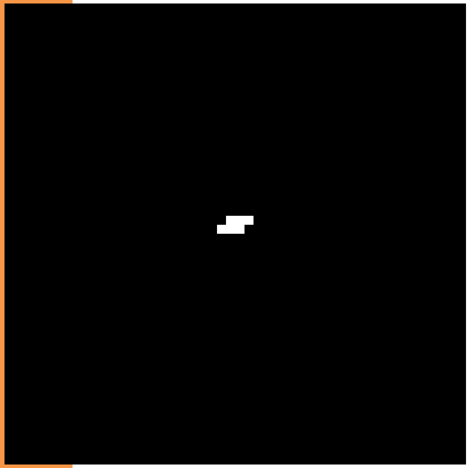


Conway's Game of Life:

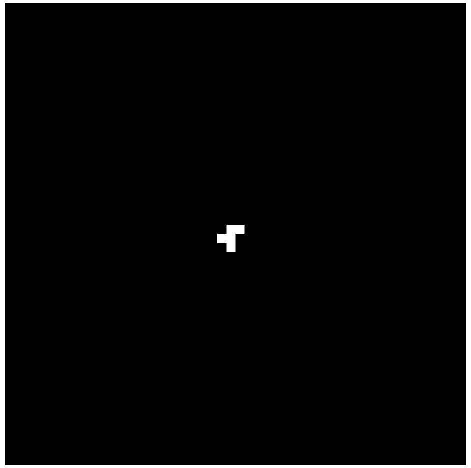
1. Any live cell with 2 or 3 live neighbors stays alive to the next generation.
2. Any live cell with fewer than 2 live neighbors dies
3. Any live cell with more than 3 live neighbors dies

Simple rules can yield complex dynamics!

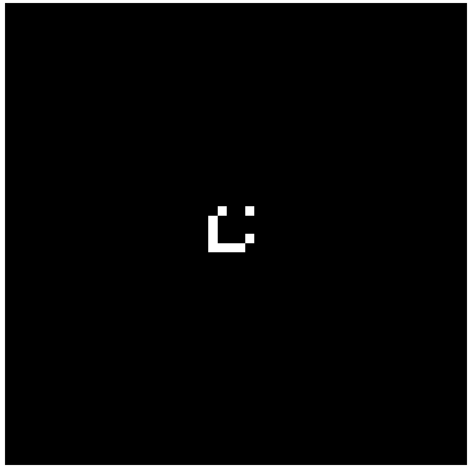
Toad



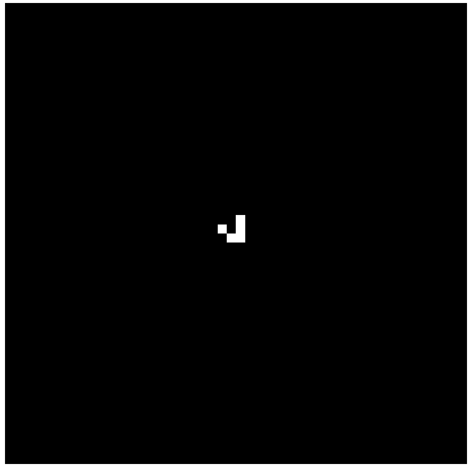
R-Pentomino



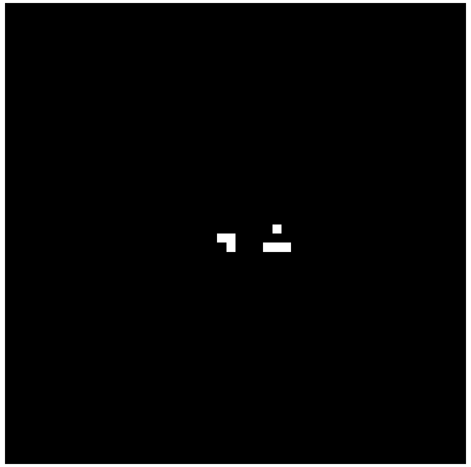
LWSS



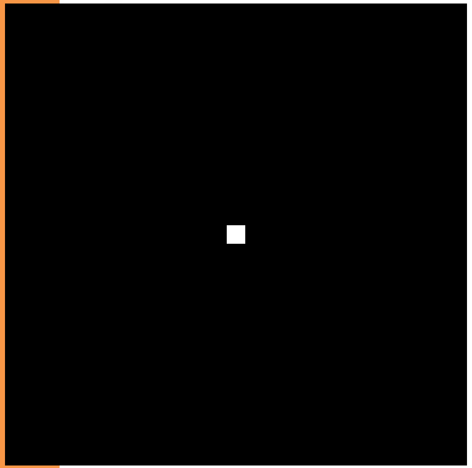
Glider



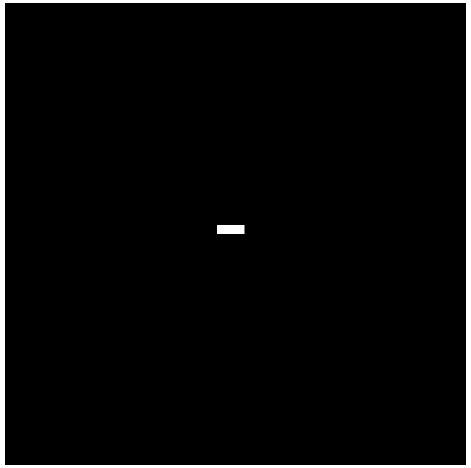
Diehard



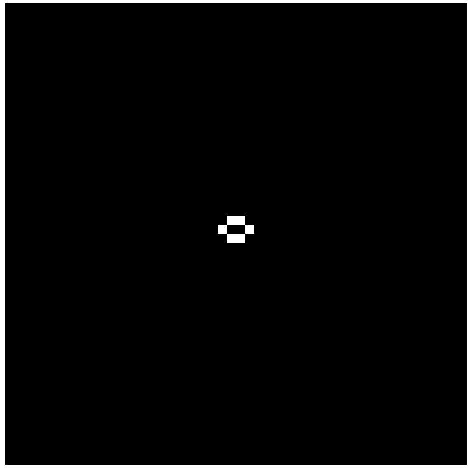
Block



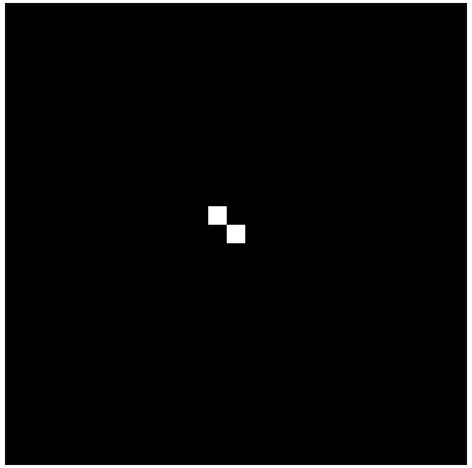
Blinker



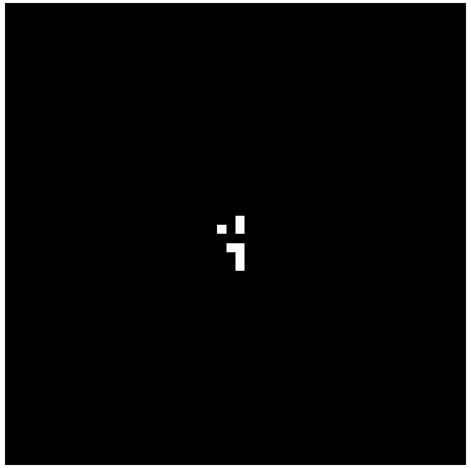
Beehive



Beacon

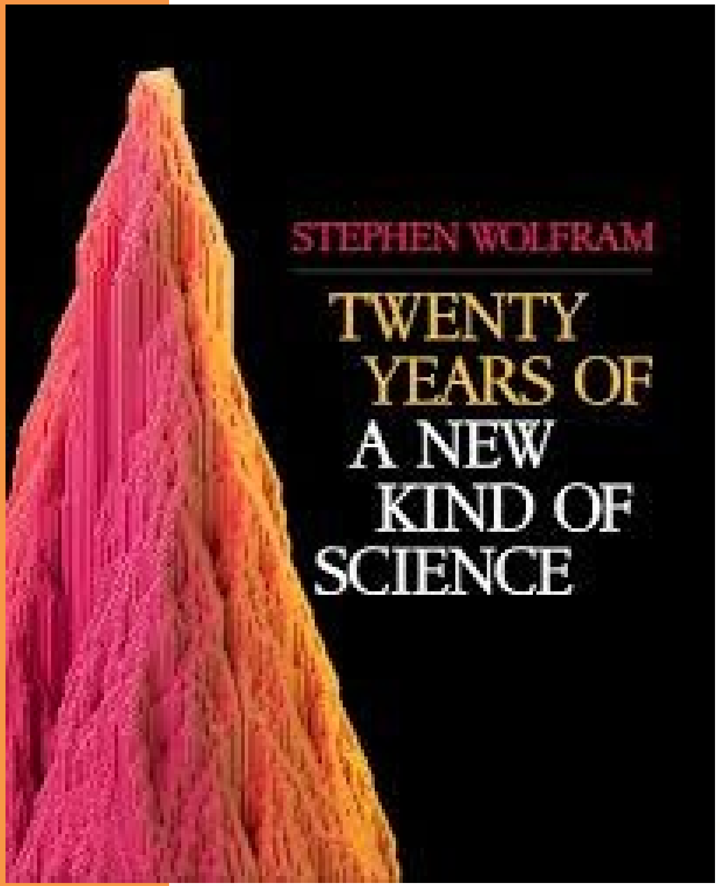


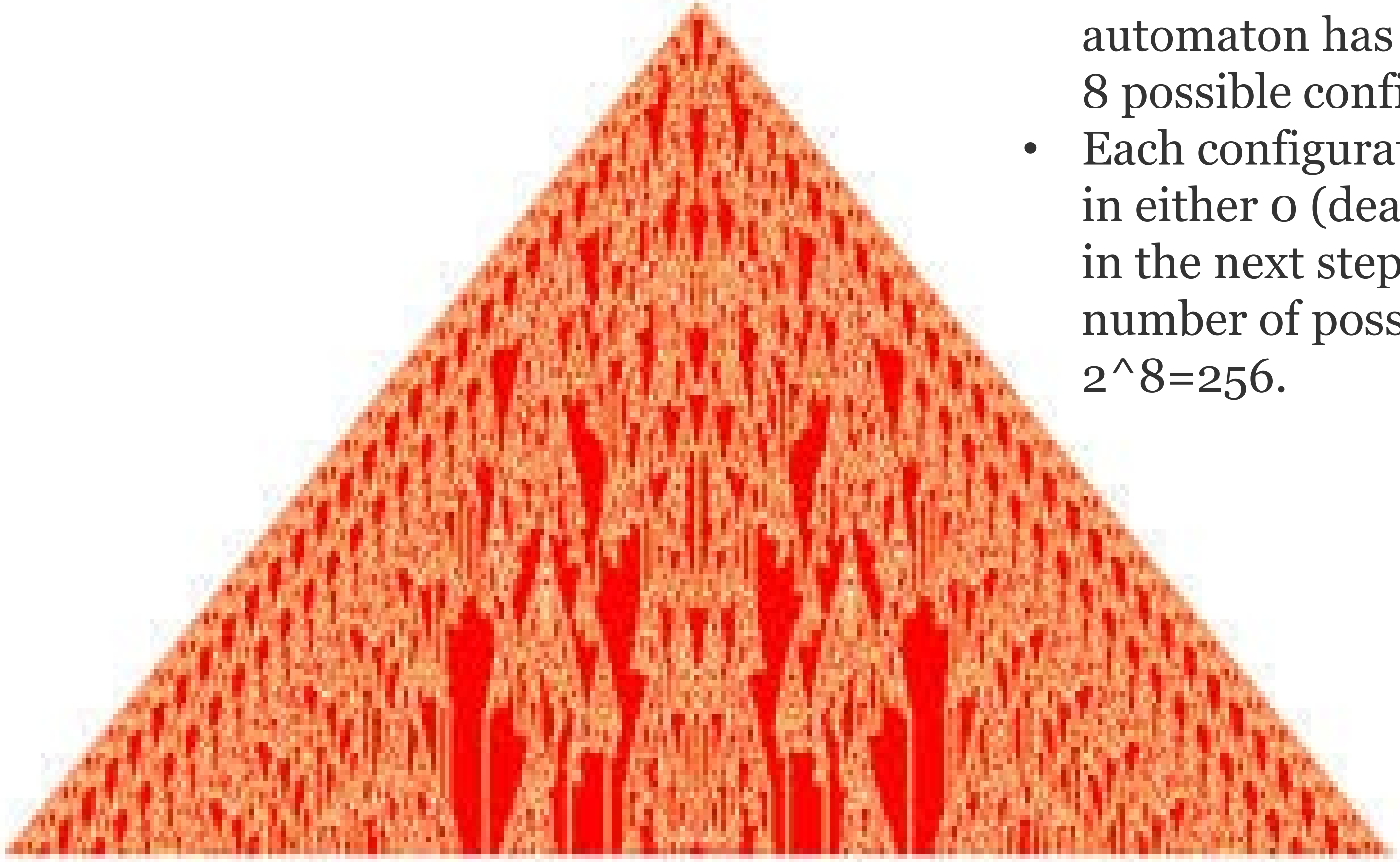
Acorn



1. Static, dynamic, periodic, and chaotic objects
2. Possible long-term dynamics

Complexity emerges even in 1D!



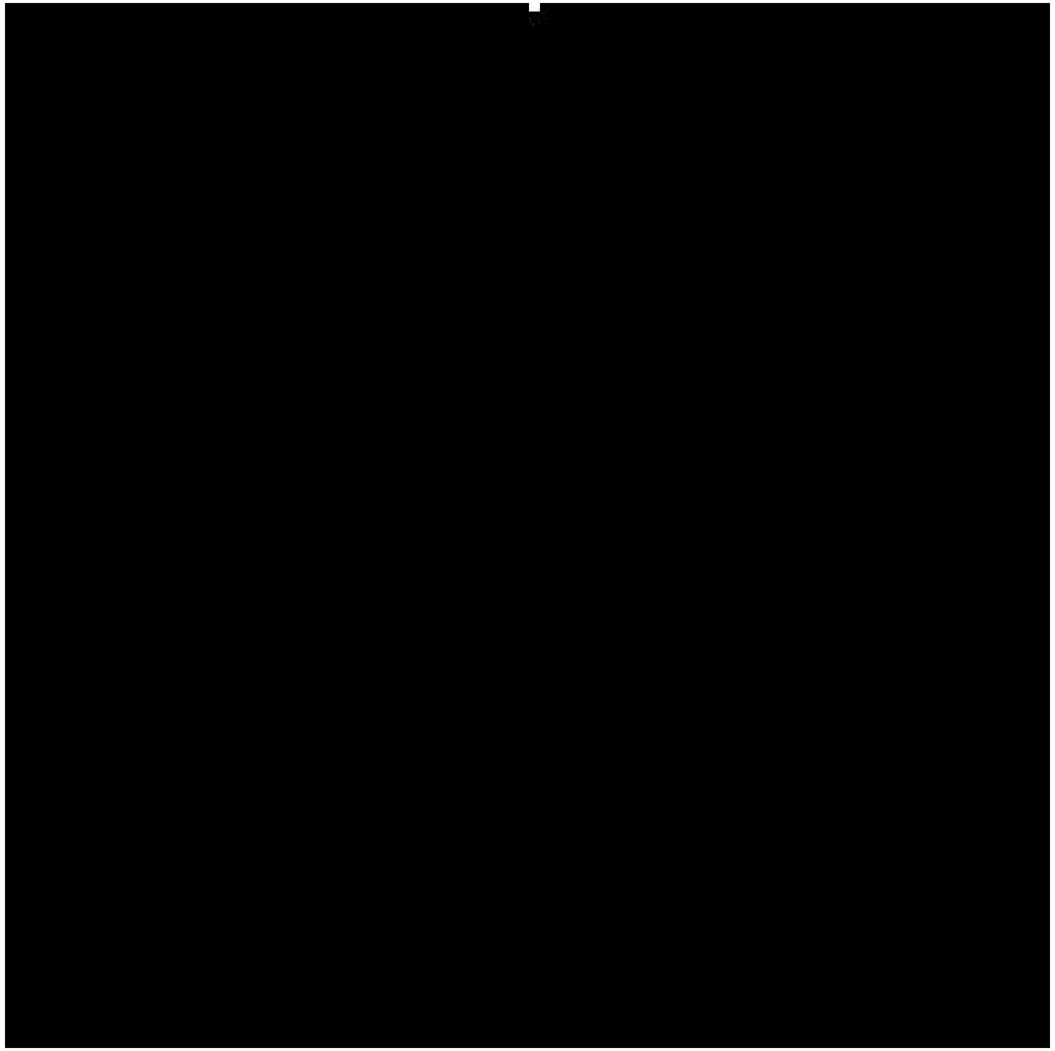


- Each cell in a 1D cellular automaton has 3 input bits: 8 possible configurations.
- Each configuration can result in either 0 (dead) or 1 (alive) in the next step, the total number of possible rule sets is 2^8=256.

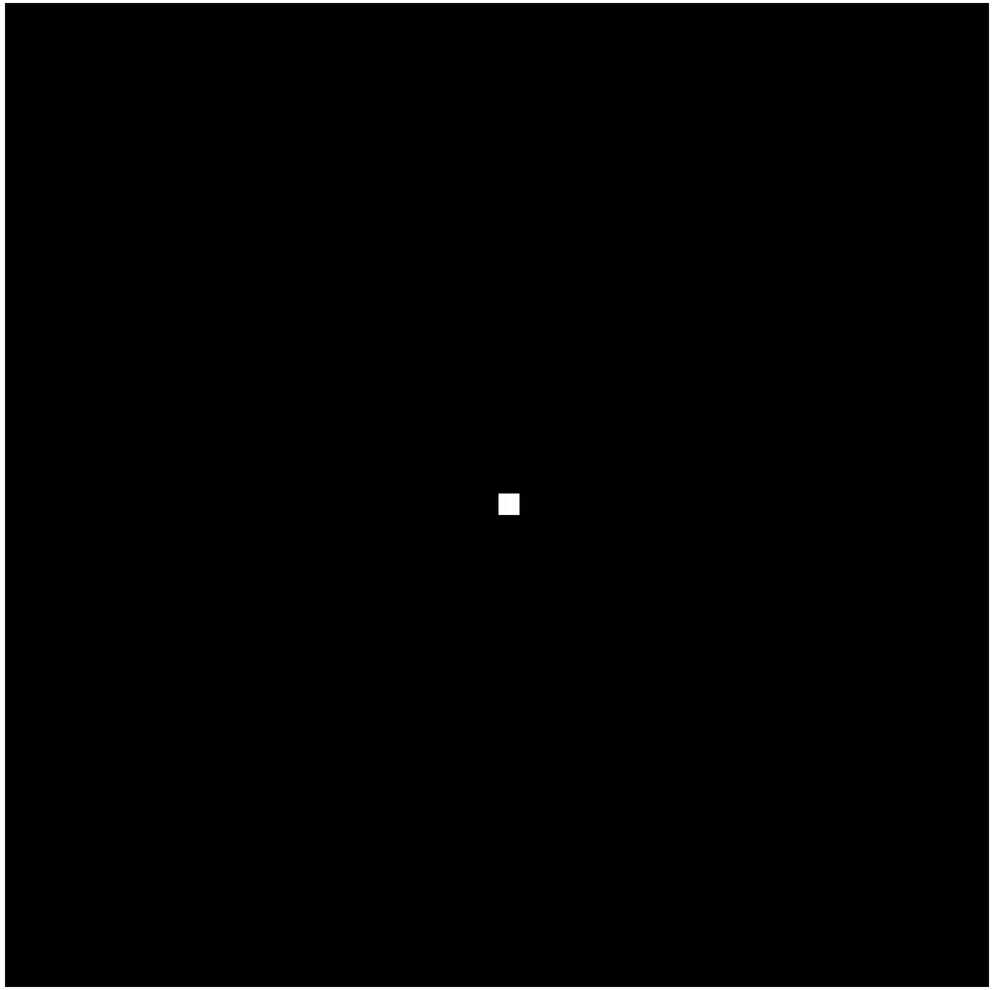
- Class 1: Convergent: All initial conditions eventually evolve into a homogeneous, stable state.
- Class 2: Periodic
- Class 3: Chaotic: Produces complex, pseudo-random patterns.
- Class 4: Computable (Turing Complete)

https://writings.stephenwolfram.com/2017/05/a-new-kind-of-science-a-15-year-view/

Complexity emerges even in 1D!



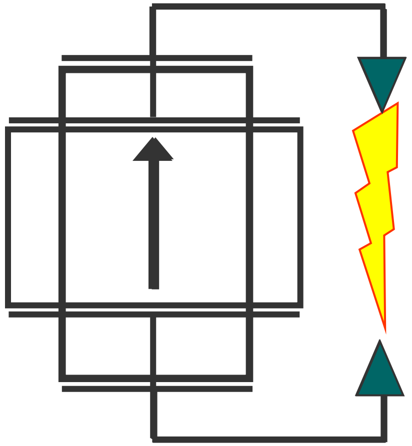
Dynamic Processes



https://scijinks.gov/snowflakes/

Ferroelectrics

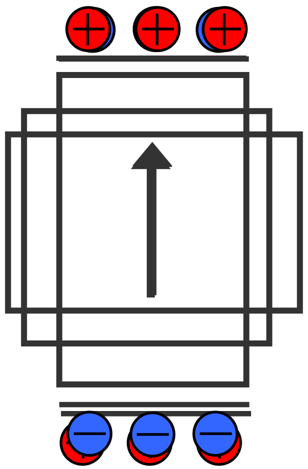
Direct piezoelectric effect



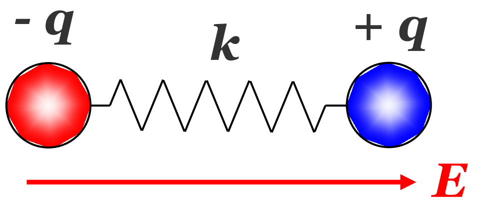
Charge = Force • d_{33}

In crystals, d_{33} ranges
from ~2 pm/V (quartz) to ~500 pm/V (PZT)

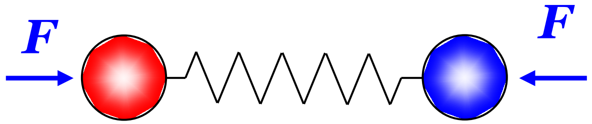
Inverse piezoelectric effect



Strain = Bias • d_{33}



External electric field



External force

Electrostatic force: $F_{el} = 2qE$

Change in bond geometry:

$$dl = (F + F_{el})/k = F/k + 2qE/k$$

- Electromechanical coupling is ubiquitous in systems with polar bonds, if not forbidden by symmetry
- Surfaces, interfaces, and low dimensional systems with broken symmetry will have unusual forms of electromechanical coupling

Estimate for single chemical bond:

$l = 1A$

$q = 0.3e$

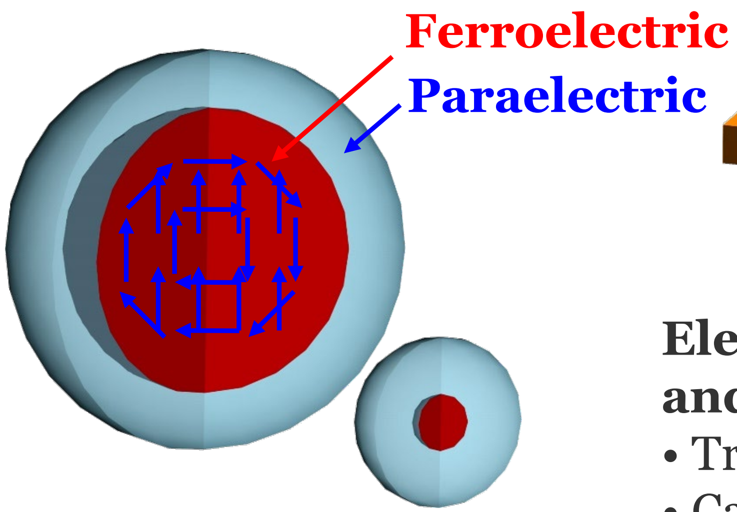
$k = 100\,N/m$

$d = 9.6\,pm/V$

or

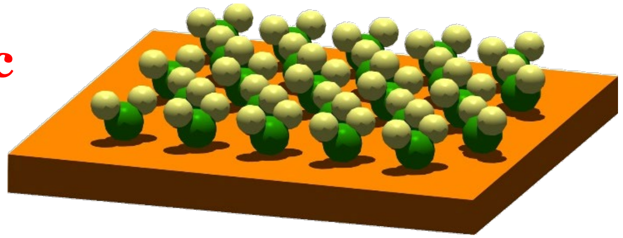
$d = 9.6\,C/N$

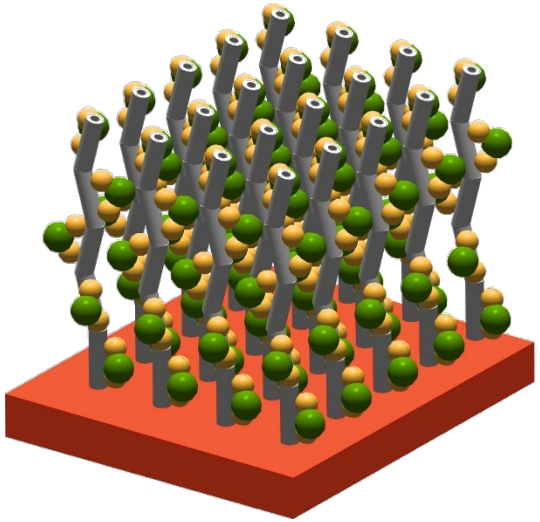
Classically, surface and dimensionality effects are considered as purely detrimental to ferro- and piezoelectricity.



Surface piezoelectricity:

- Ordered dipolar water layers
- Polar surfaces



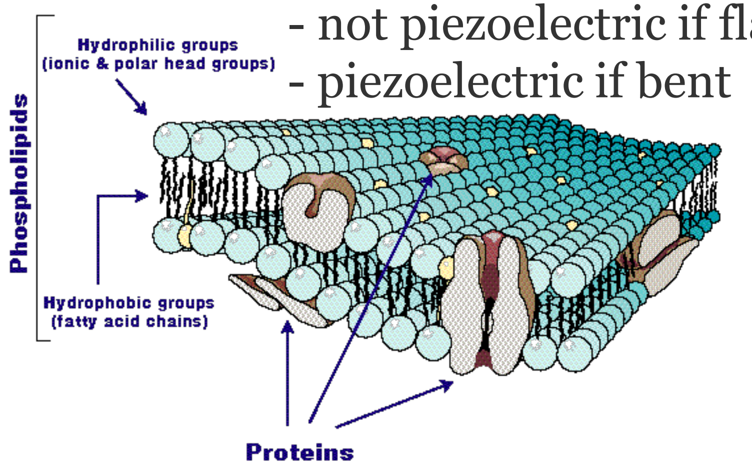


Electromechanics of composites and complex materials:

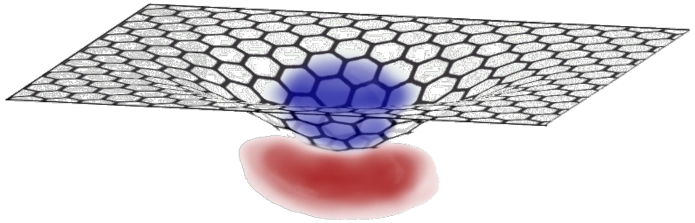
- Triboelectricity,
- Cavitation,
- Sonochemistry
- Sonoluminescence

Flexoelectricity in membranes:

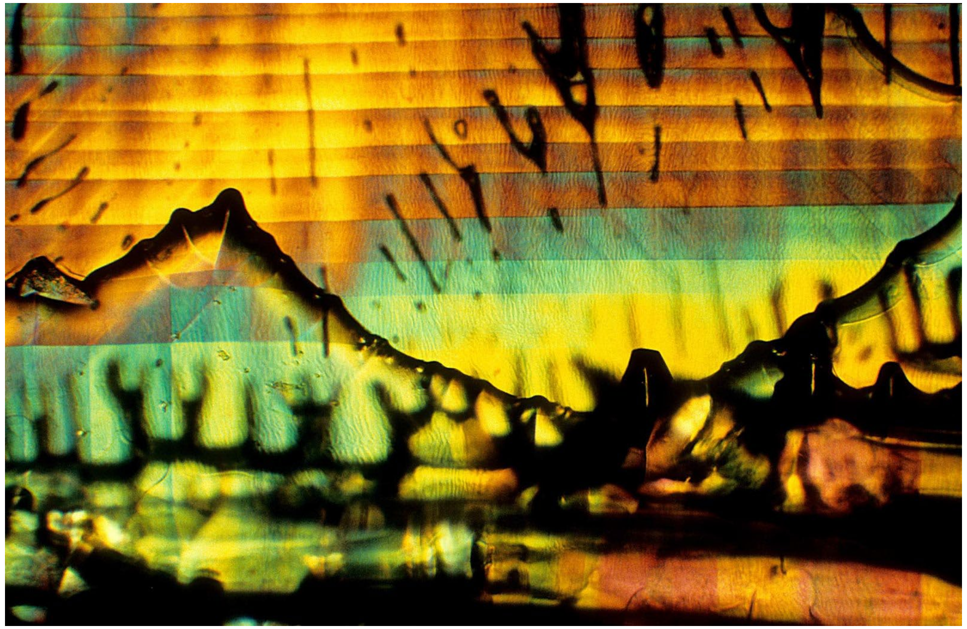
- not piezoelectric if flat
- piezoelectric if bent

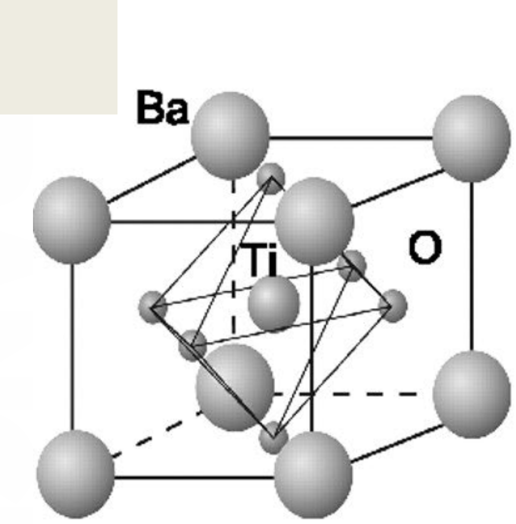


Flexoelectricity also exists in quantum systems:

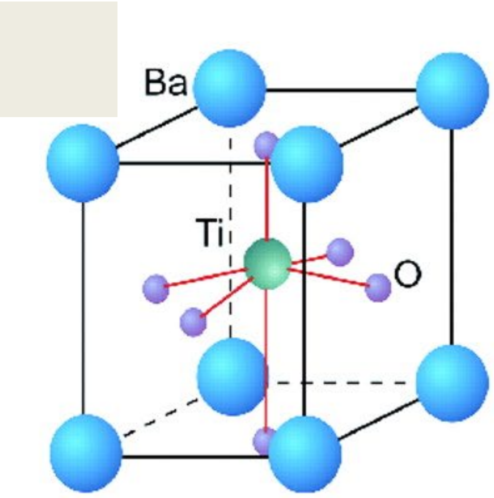


Ferroelectrics

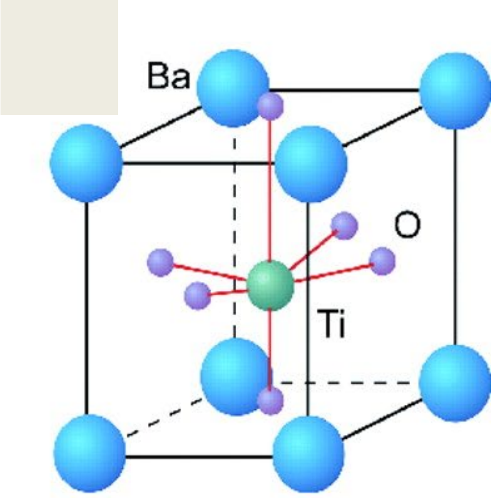




Cubic phase



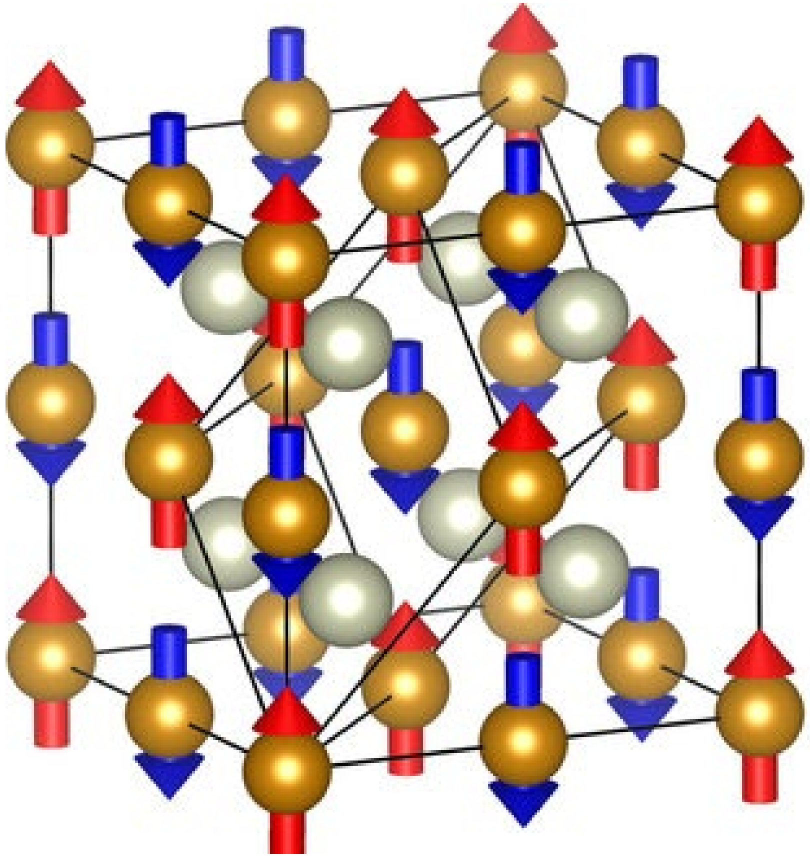
P_{up}



P_{down}

https://www.nikonsmallworld.com/galleries/1982-photomicrography-competition/single-crystal-of-barium-titanate-with-impurities-mounted-in-immersion-oil

How Can we Model Magnetism?



- Each atom has a localized spin
- Spins interact with their nearest neighbors
- All dynamics can be represented via spin interactions

https://www.researchgate.net/publication/306187646_Impact_of_lattice_dynamics_on_the_phase_stability_of_metamagnetic_FeRh_Bulk_and_thin_films/figures?lo=1

Ising Model?

Ising model represents a system of spins (magnetic dipoles) on a lattice.

Without external magnetic field, the energy reads

$$E = -J \sum_{<ij>} s_i s_j$$

J > 0: ferromagnetic, sum over neighbors only

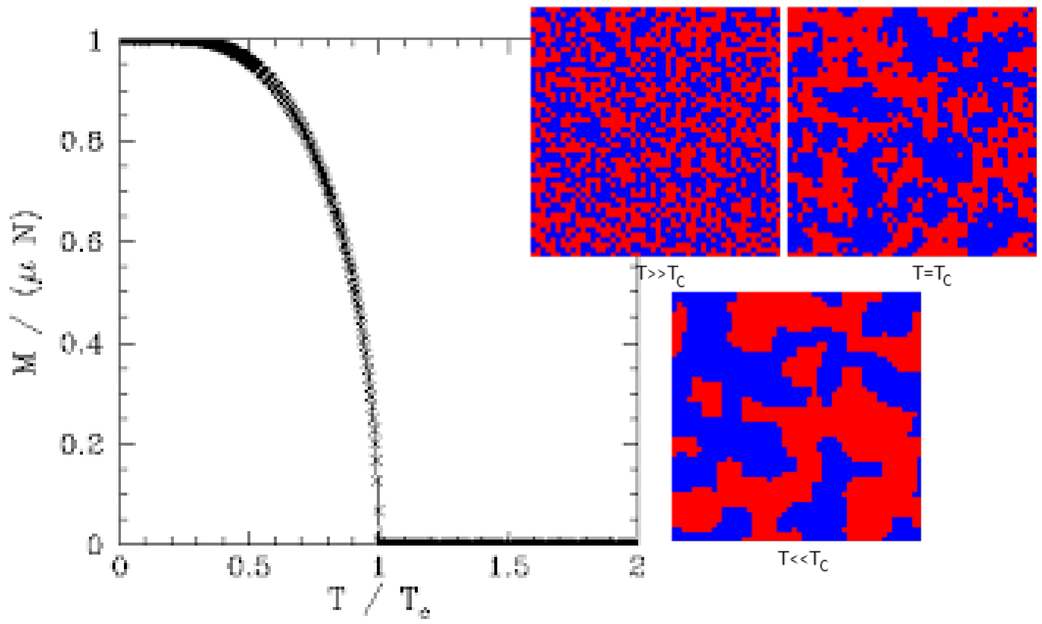
Magnetisation:

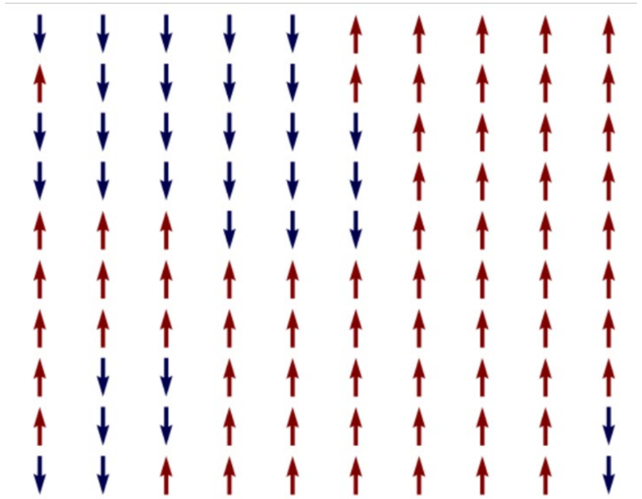
$$M = \sum_i s_i$$

Below the Curie temperature

$$\frac{k_B T_C}{J} = \frac{2}{\ln(1+\sqrt{2})}$$

exhibits spontaneous magnetization |M|>0





From the course by Volodymyr Vovchenko, https://github.com/vlvovch/PHYS6350-ComputationalPhysics

1. Ising Model

- **Spins:** Discrete spin-½ variables σi=±1 (up or down).
- **Interactions:** Nearest-neighbor coupling Jσiσj.
- **Physical Analogs:** Ferromagnetic and antiferromagnetic materials.
- **What the Model Describes:** Phase transitions, critical phenomena.
- **Salient Properties:**
    - Exhibits a phase transition at critical temperature.
    - Exact solution in 2D (Onsager solution), but not in 3D.
    - Used in statistical mechanics, neural networks, and even finance.

2. Heisenberg Model (Describes Real Magnetic Materials)

- **Spins:** Continuous 3D spin vectors Si=(Six,Siy,Siz)
- **Interactions:** Neighboring spins interact via dot product J Si·Sj.
- **Physical Analogs:** Ferromagnetic and antiferromagnetic materials.
- **What the Model Describes:** Classical and quantum magnetism.
- **Salient Properties:**
    - Unlike the Ising model, allows full rotational symmetry.
    - Used for **spin waves** and **magnon excitations**.
    - Has quantum versions: **XXX, XXZ, and XYY models**.

3. Potts Model (Generalization of Ising Model)

- **Spins:** Discrete variables with q possible states (e.g., $\sigma_i = 1, 2, \ldots, q$)
- **Interactions:** Neighboring spins interact if they are the same, $J\delta_{\sigma_i,\sigma_j}$
- **Physical Analogs:** Multistate magnetic systems, biological clustering, social dynamics.
- **What the Model Describes:** Generalized phase transitions, percolation, graph coloring.
- **Salient Properties:**
  - For q=2, it reduces to the Ising model.
  - For q=1, it maps onto percolation problems.
  - Used in image segmentation and materials science.

4. Ashkin-Teller Model (Coupled Ising Models)

- **Spins:** Two coupled Ising spins per site, σ_i and τ_i, each taking ±1 values.
- **Interactions:**
  - Standard Ising interactions $J_\sigma \sigma_i \sigma_j$ and $J_\tau \tau_i \tau_j$.
  - Coupling term $J_{\sigma\tau} \sigma_i \tau_i \sigma_j \tau_j$
  - **Physical Analogs:** DNA denaturation, coupled neural networks.
- **What the Model Describes:** Phase transitions in **competing interactions**.
- **Salient Properties:**
  - Reduces to the **4-state Potts model** when parameters match.
  - Used in biological and statistical models beyond magnetism.
  - Demonstrates **multicritical behavior**.

5. XY Model (For Superfluidity & Vortices)

- **Spins:** Continuous spin vectors $S_i=(\cos\theta_i,\sin\theta_i)$
- **Interactions:** Neighboring spins interact via cosine function $J\cos(\theta_i-\theta_j)$
- **Physical Analogs:** Superfluidity, superconductivity, 2D quantum gases.
- **What the Model Describes:** Vortex-antivortex pairs, Kosterlitz-Thouless transition.
- **Salient Properties:**
  - No long-range order in 2D but has a **topological phase transition**.
  - Describes phase transitions in liquid crystals.
  - Relevant in modern quantum simulations.

6. Blume-Capel Model (Spin-1 Generalization of Ising)

- **Spins:** Spin-1 variables $S_i=-1,0,+1$
- **Interactions:**
  - Standard Ising-like exchange interaction JS_iS_j
  - Additional single-site anisotropy ΔS_i^2 (favoring spin-zero states).
- **Physical Analogs:** Multistate magnetic systems, liquid-gas transitions.
- **What the Model Describes:** First-order vs. second-order phase transitions.
- **Salient Properties:**
  - Introduces **single-ion anisotropy** (favoring zero-spin states).
  - Has a tricritical point where **first-order** and **second-order** transitions meet.
  - Used to describe **binary alloy systems and phase separation**.

Why is it even reasonable?

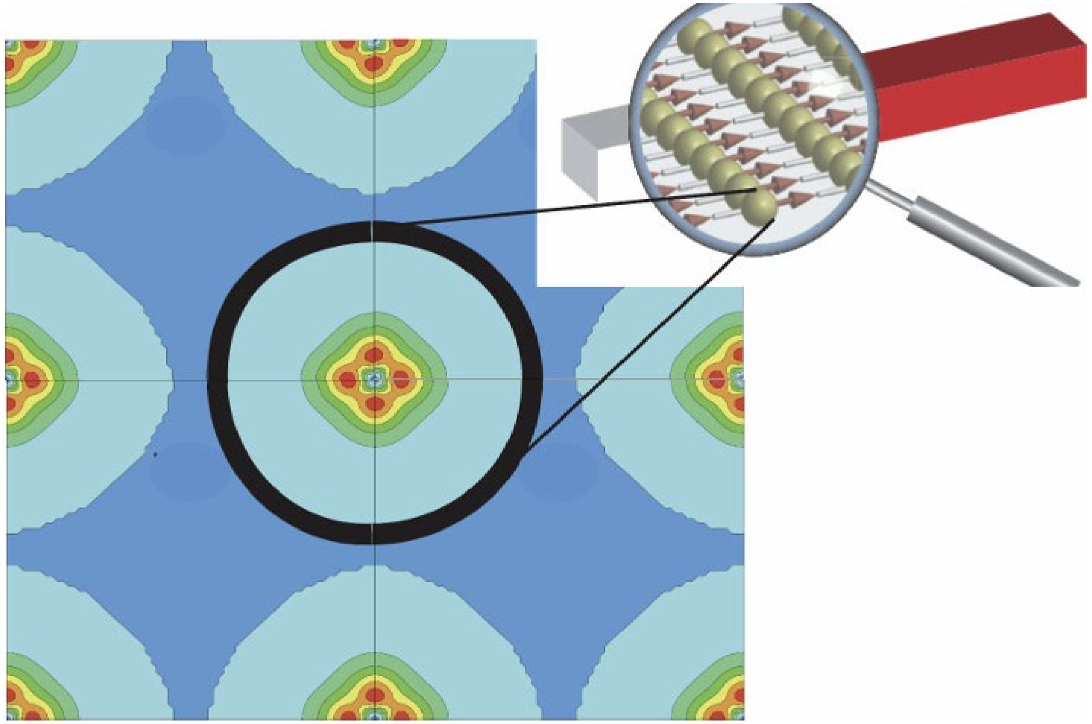


FIG. 3. Magnetization density of bcc Fe from theoretical calculations based on DFT. Adapted from Eriksson *et al.*, 2017.

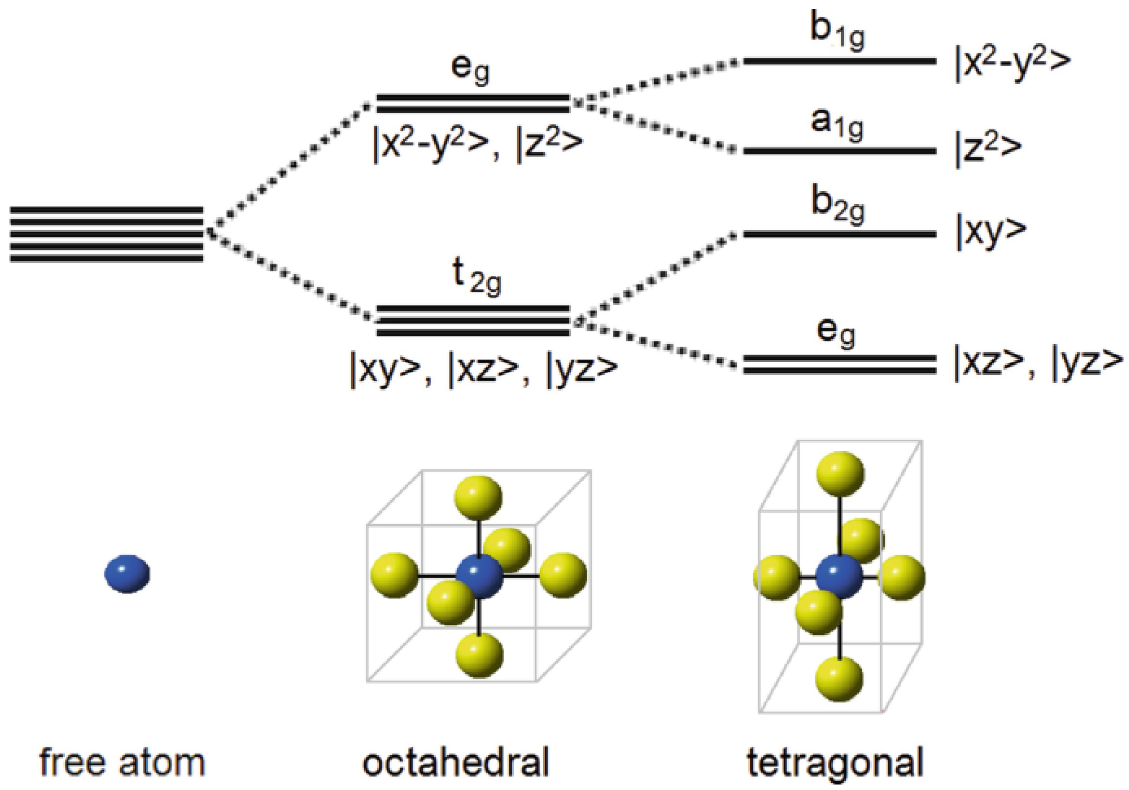
Heisenberg Hamiltonian

$$\mathcal{H}_H = \sum_{\langle ij \rangle} \mathcal{J}_{ij} \vec{S}_i \cdot \vec{S}_j,$$

Dzyaloshinski – Moriya Interactions

$$\mathcal{H}_{\mathrm{DM}} = \sum_{\langle ij \rangle} \vec{\mathcal{D}}_{ij} \cdot (\vec{S}_i \times \vec{S}_j).$$

Computation is very complex!



https://link.springer.com/referenceworkentry/10.1007/978-3-030-63210-6_3

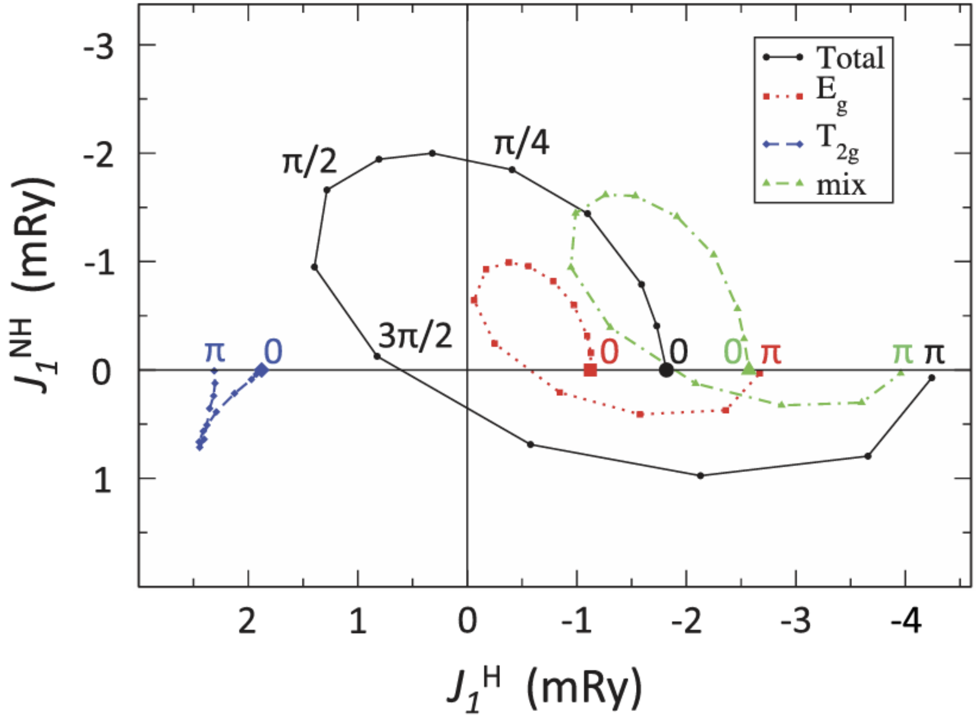


FIG. 14. First-nearest-neighbor Heisenberg and non-Heisenberg interatomic exchange parameters in bcc Fe when one spin is rotated by a finite θ_i running from zero to π at site i in a ferromagnetic background in the case of bcc Fe (Szilva *et al.*, 2017). $J_1^{\mathrm{H}} = J_1^{(2)} + A_1^{(2)xx}$ and $J_1^{\mathrm{NH}} = -2A_1^{(2)zx}$; see Eqs. (5.47) and (5.49). The black (solid) curve stands for the total value while the red (dotted), blue (dashed), and green (dash-dotted) lines show its symmetry decomposition in the d channel defined by Eq. (7.5).

As is Experimental Validation

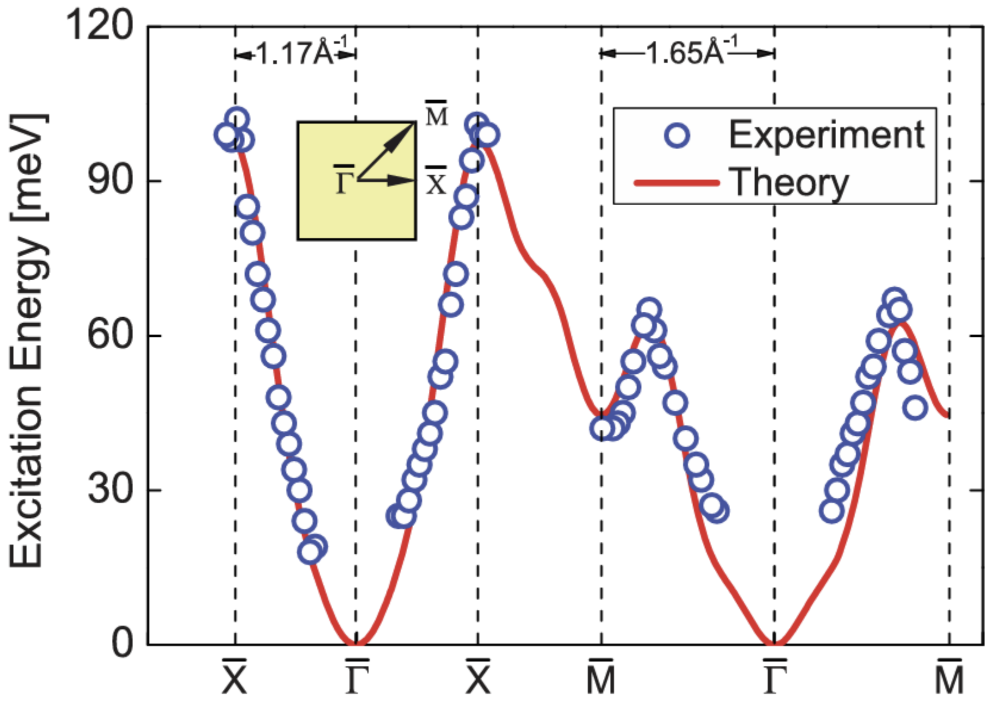


FIG. 19. Computed and measured acoustic magnon dispersions in Fe/Rh(001). Inset shows the parts of the Brillouin zone used in the plot. From Meng *et al.*, 2014.

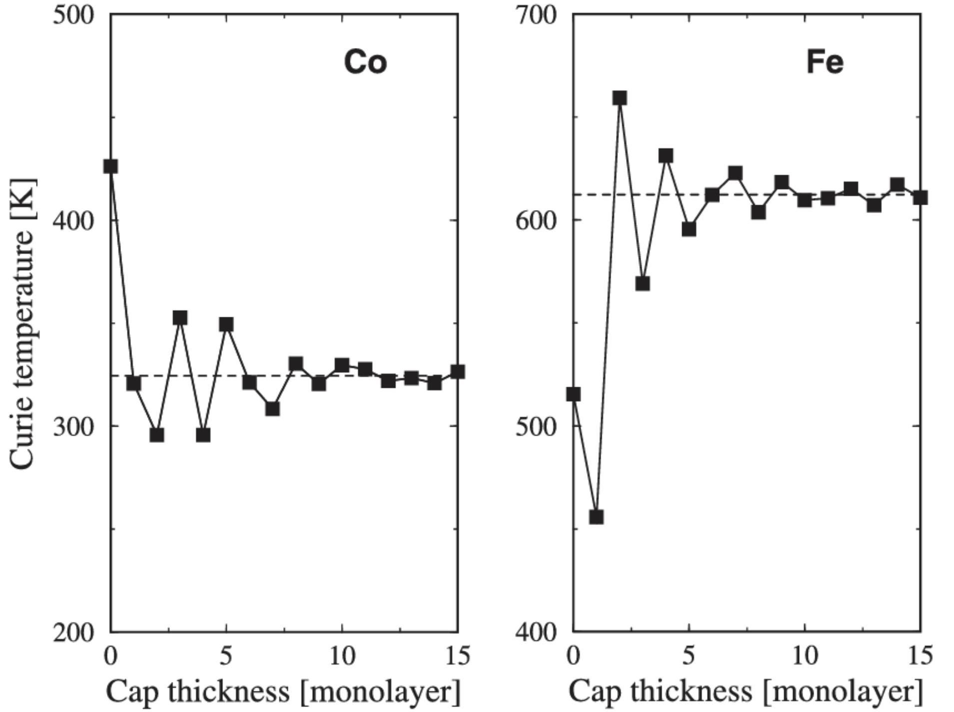
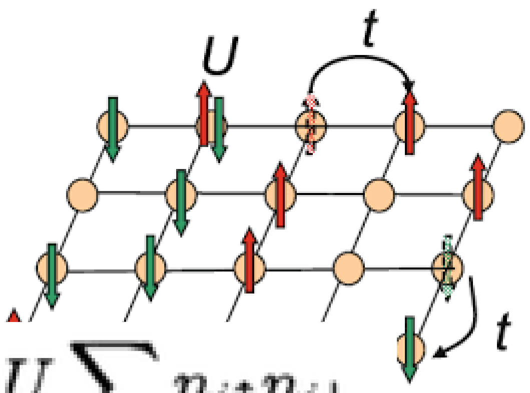


FIG. 18. RPA-derived estimates of the T_c of (left panel) Co and (right panel) Fe monolayers on a Cu(001) substrate, covered by a Cu layer of varying thickness. From Pajda *et al.*, 2000.

But there are more models!

The **Hubbard model** is a fundamental theoretical model used to describe interacting electrons in a lattice. It is widely applied to understand strongly correlated electron systems, magnetism, and high-temperature superconductivity.



Mathematical Formulation

•The Hamiltonian for the **Hubbard Model** :

$$H = -\tilde{t} \sum_{i,j,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow},$$

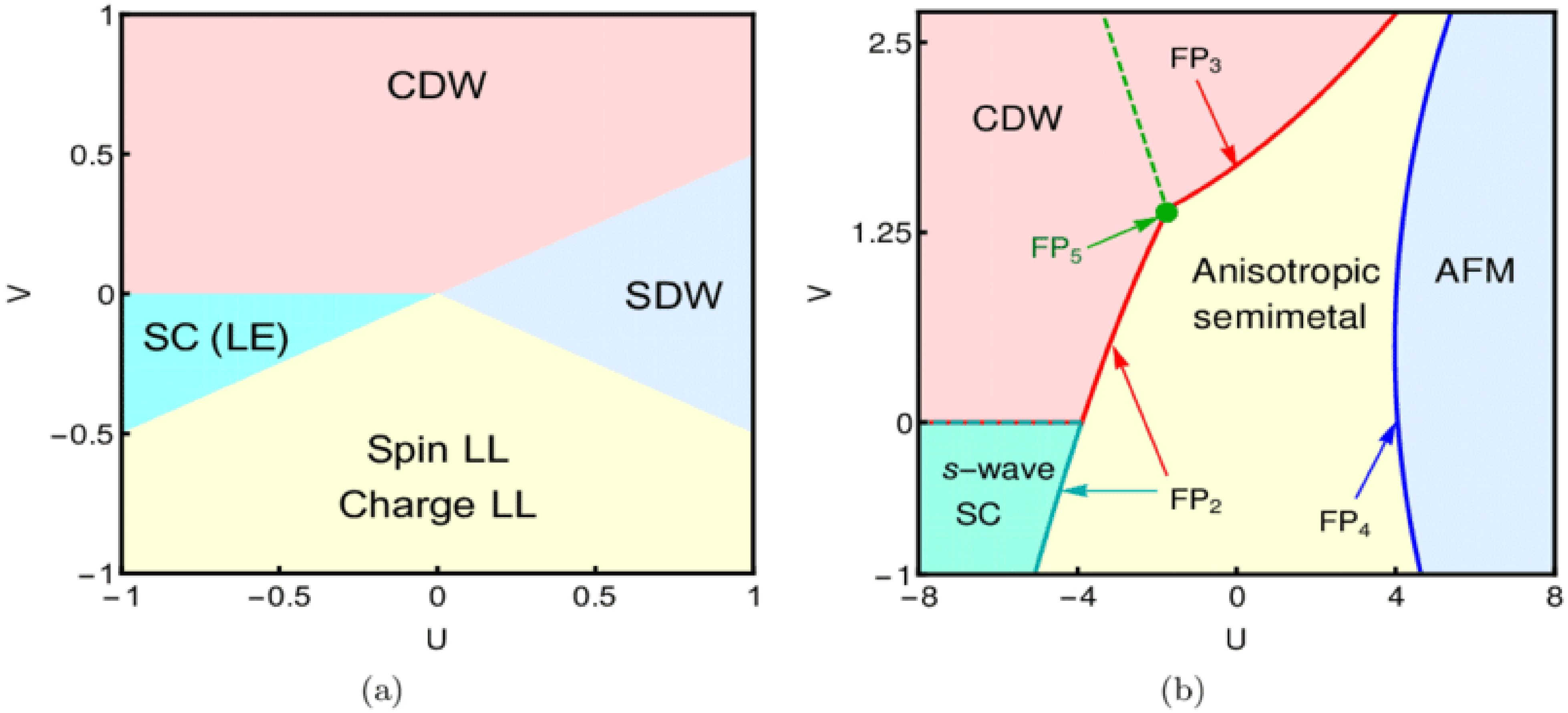
- t = hopping amplitude (electron movement between sites).
- U = on-site Coulomb repulsion (penalty for double occupancy).

•**Weak Interaction (U≪t) → Metallic Behavior**
- Electrons move freely, forming a **Fermi liquid**.

•**Strong Interaction (U≫t) → Mott Insulator**
- Electrons localize due to repulsion, leading to an **insulating state**

•**Magnetism and Spin Physics**
- At **half-filling** (one electron per site), the Hubbard model reduces to the **Heisenberg model**, predicting **antiferromagnetic ordering** for strong U

Can be used to describe complex systems!



https://www.researchgate.net/publication/317284336_Quantum_multicriticality_near_the_Dirac_semimetal-band_insulator_critical_point_in_two_dimensions_A_controlled_ascent_from_one_dimension/figures?lo=1

Overall, its not all about formulae!

Short-Form Physical Laws (Symbolic Expressions)

- Many fundamental physical laws can be compactly written as mathematical equations.
  - **Newton's Laws**: F=ma (simple equation but powerful predictive capability).
  - **Maxwell's Equations**: Compact set of equations describing electromagnetism.
  - **Schrödinger Equation**: Governs quantum mechanics with relatively few terms.
- Often derived from symmetry principles, conservation laws, or variational principles.
- Easily generalizable and applicable across different systems.

Emergent Complexity from Simple Models

- Some models have very few parameters but give rise to complex behavior.
  - **Ising Model**: Defined by simple spin interactions but exhibits phase transitions.
  - **Navier-Stokes Equations**: Governing fluid dynamics, but leading to turbulence.
  - **Cellular Automata** (e.g., Conway's Game of Life): Simple update rules create highly complex patterns.
- No compact symbolic equation fully describes emergent behavior.
- Understanding often requires numerical simulations, renormalization group theory, or statistical mechanics