Spin Glass Systems Using Edward-Anderson Model

"*The history of spin glass may be the best example I know of the dictum that a real scientific mystery is worth pursuing to the ends of the Earth for it's own sake, independently of any obvious practical importance or intellectual glamor*"
– Philip Anderson

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January 3, 2022

What is spin glass?

And Why is it spinning?

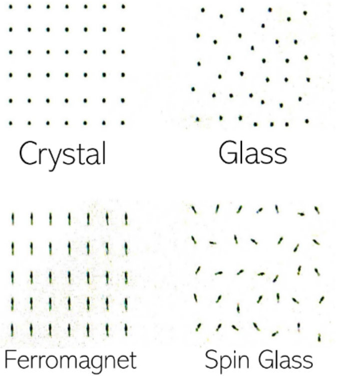


Figure: **Spin Glass is a "general" class of magnetic systems having random interaction.** Therefore, they are Disordered (glass) Magnets (spins). This can happen due to disorder in the lattice or disorder in the interactions itself. The alloys like Cu_yMn_x *or* Au_yFe_x show this property.

Frustration

Randomness seen geometrically

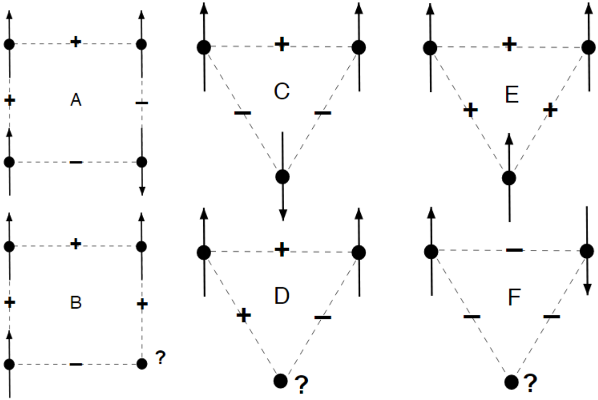


Figure: There is no configuration which satisfies every bond

Frustration

Randomness seen through Energy Landscape

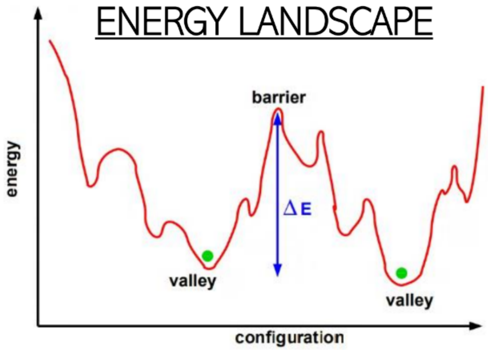


Figure: There is no pattern for global ground state since many asymmetric lower energy states are present in the energy landscape.

Modelling of Spin-Glass System

Edward-Anderson Model

Spin Glass Ising Model Hamiltonian:

$$H = -\sum_{<i,j>} J_{ij} s_i s_j + \sum_i h_i s_i$$

Bimodal interaction with no external field

$$H = -\sum_{<i,j>} J_{ij} s_i s_j$$

where both J_{ij} & $s_i \in \{-1, 1\}$

Assumptions

what kind of materials it represent?

1. 3-Dimensional lattice space
2. Ising Spins can only point to two directions.
3. Fixed Lattice sites (mixer of only two molecules)
4. Nearest neighbour interactions.
5. Same kind of antiferromagnetism and ferromagnetism is shown by equal number of molecules of each kind.
6. No Net Magnetisation
7. Quenched disorder ($T_{measurement} << T_{fluctuations}$)
8. No external magnetic field

Phase Transition

What kind of transition may these materials show?

This question was first answered by EA model only in which they defined their order parameter as

Edwards-Anderson Order Parameter $q \equiv \frac{1}{N}\sum_{i=1}^{N}(\langle\sigma_i\rangle)^2 \neq 0$

Origin of the expression:

High-temperature paramagnetic phase $\langle\sigma_i\rangle = 0 \quad M \equiv \frac{1}{N}\sum_{i=1}^{N}\langle\sigma_i\rangle = 0$

Low-temperature spin glass phase $\langle\sigma_i\rangle \neq 0 \quad M \equiv \frac{1}{N}\sum_{i=1}^{N}\langle\sigma_i\rangle = 0$

Overlap between two replicas of spin, a and b, for J disorder at i^{th} lattice site is $q_{J,i}^{a,b}$.

$$q^{a,b} = \frac{1}{N}\sum_i [q_i^{a,b}] = \frac{1}{N}\sum_i q_{J,i}^{a,b} = \frac{1}{V}\sum_i \langle\sigma_{i,J}^{a}\sigma_{i,J}^{b}\rangle$$

Quantum Spin Glasses

Justification for semi-classical treatment

Decoherence in any quantum system leads it to behave like a semi-classical one. The connection to a heat bath of very large D.O.F. makes the system too noisy at freezing temperature T_f ($\approx 30K$).

You can associate an energy to this slow frequency of noise (ideally 0).

Since, we deal with spin glasses near $T_f >> \frac{\hbar\omega_{noise}}{k_B}$ which makes the quantum fluctuations irrelevant.

Metropolis Algorithm and Simulations Obstacles

Ergodicity and Detailed Balance

If we try to implement the numerical simulation of Spin Glasses using conventional tools like Markov Chains we face a couple of challenges.

1. Algorithm will give you results for a unique J everytime.
2. Ergodicity breaking

AIM

An algorithm which can sample over the whole of the state space without getting stuck in the metastable regions formed by local basins of low energy which also takes in account of different **J**s.

Ergodicity Breaking

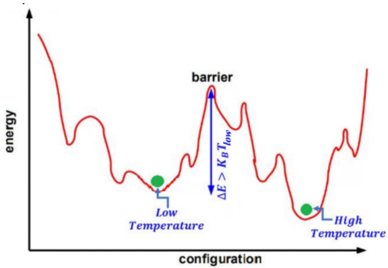
Are we implementing Physical World?

But still, in reality too, we have ergodicity breaking so *really* why do we care if it can't traverse whole space?

1. It is much better to find some observable property of our model which is independent of the algorithm we use, so that we are free to choose any algorithm we think that will be efficient.
2. We are mimicking experimentalists.
3. But this is not unique to Spin-Glass. Normal ordered Magnetic also shows the same ergodicity breaking but in symmetric pure states.

Parallel Tempering

How do we overcome Ergodicity breaking



The metropolis Detailed Balance is maintained through the following flip probability.

$$P_f(\Delta E) = \begin{cases} e^{-(\beta_{low} - \beta_{high})\Delta E} & \Delta E > 0 \\ 1 & \Delta E \leq 0 \end{cases}$$

Swapping

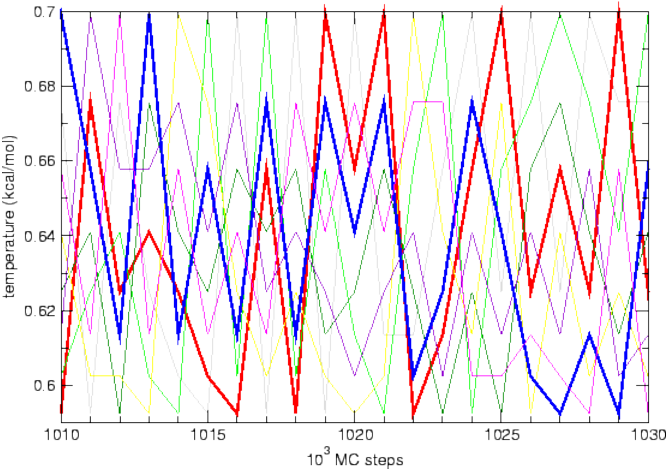
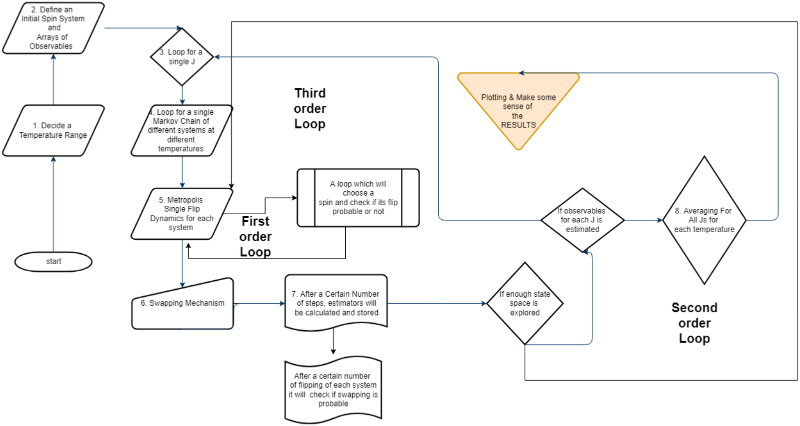


Figure: Over the course of Simulation, spin replicas will get swapped in different state space and further dynamic

Final Algorithm



Results

(one of them)*

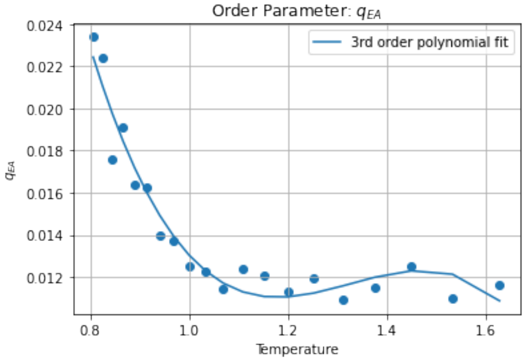


Figure: There is a rise in order parameter near $1.1 \left(\in [0.9, 1.2] \right)$ units, which marks the phase transition of spin glass. This was done for **N**$= 15 * 15 * 15$, averaged over 1000 J random distributions. The *thermalization* is done over $3.375M$ Monte-Carlo sweeps in which states were swapped after every 10 spin flips for individual temperature replicas.

Caveats and Conclusion

- Different models have different problems, definitions and give different results.
- NP-complete problem and thus it is difficult to simulate on a *classical* computers.
- Lattice size is way too small for the system to be considered macroscopic.
- Not many theoretical results are there (Parisi's Solution of SK model), just numerical simulations which are unreliable.
- Geometric optimisations can be implemented.
- Promising Computational Physics problem; many controversial results, far from completely understood.
- Recent studies (H. Rieger, A. P. Young (1996)) have shown the emergence of Quantum Spin Glasses

Motivation

Why Spin Glass interested me?

Universality —— *Complexity* —— *Emergence*

Classical Example: Waves are emergent phenomena

Other Projects

and further

1. Computational Projects
    1.1 **Simulation of Meteorite Shower, 2021**: Analysed perturbing system of Haley's comet with planetary interactions through **N-body** numerical methods and presented error analysis.
    1.2 **Design of an Log-Periodic modified antenna, 2020**: Optimisation of LPDA dipoles on EM simulators for SKA project competition.
    1.3 **Simulation of Lennard-Jones potential between two particles on IBM Quantum Lab, 2019**: Optimised a general Quantum Simulation algorithm for LJP using symmetries in Hamiltonian. Mapping of eigenstates, operators on Qubits. Pedagogical Project. https://arxiv.org/abs/2101.10202
2. Other Initiative: Compphy
3. Relevant Courses: Condensed Matter Physics (#2), Quantum Mechanics (#4), Nanomaterial and Nanoscience, Statistical Mechanics (#2).

Thank You!