Sadakathullah Appa College

MY LORD
VOUCHSAFE ME WISDOM

THE PHASE TRANSITIONS IN THE HARD CORE LATTICE GAS

ASWEEL AHMED A JALEEL

10th Indian Statistical Physics Community Meeting

ICTS | INTERNATIONAL CENTRE for THEORETICAL SCIENCES

TATA INSTITUTE OF FUNDAMENTAL RESEARCH

23 -25 MAY 2025

Hard Core Lattice Gases (HCLG)

A regular grid

Particles can be deposited or evaporated

No two particles can occupy

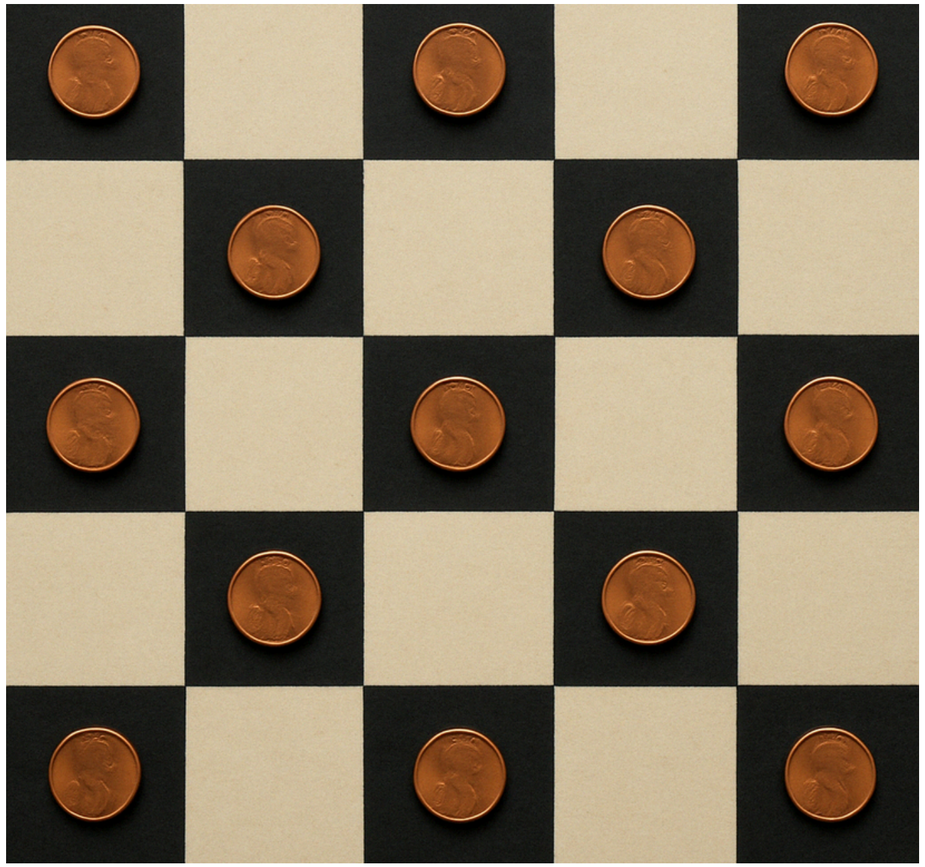


Image of coins on a checkerboard

k-NN Model

First k next-nearest neighbors of a particle are excluded from being occupied by another particle.

1-NN

Nearest-neighbor exclusion

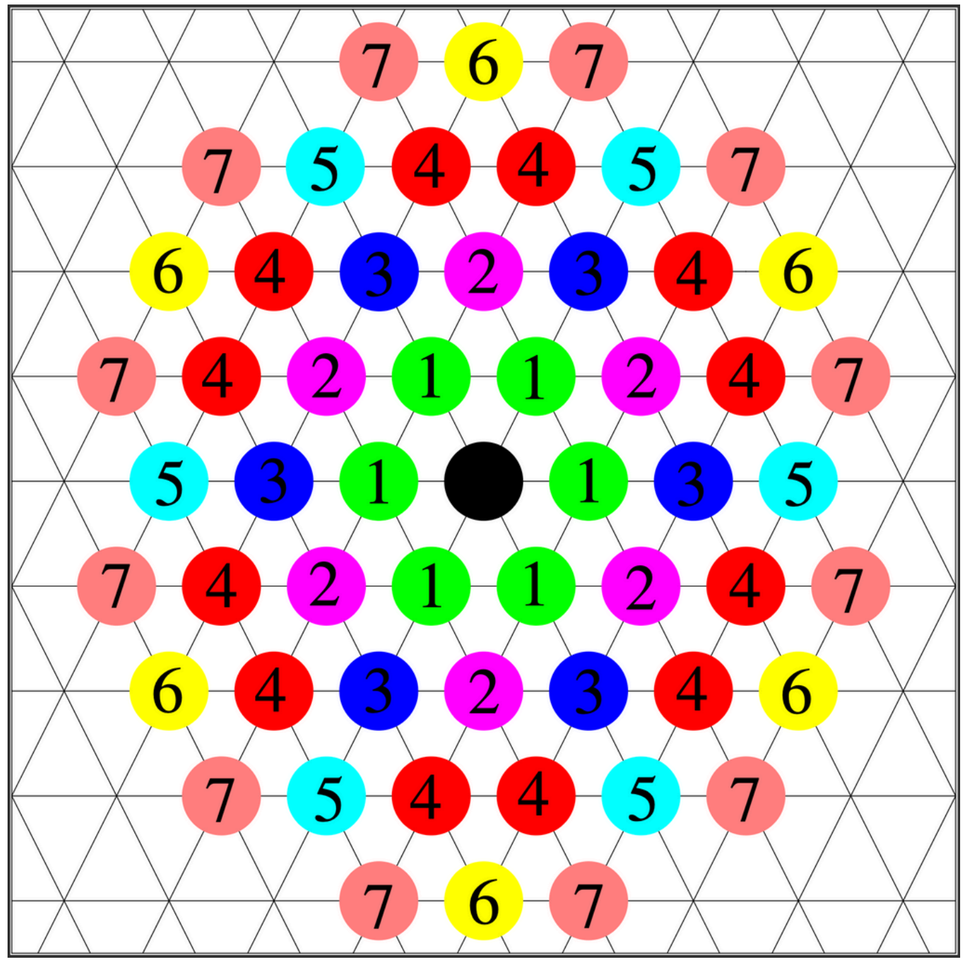
2-NN

Next nearest-neighbor exclusion

On the square lattice, the model has been studied for k < 12

Jaleel et.al., Phys. Rev. E, 106: 044136 , 2022.
Jaleel et.al., J. Chem. Phys. 155, 224101, 2021

k-NN Model on Triangular Lattice



Monte Carlo algorithm

Strip Cluster Wang-Landau algorithm (SCWL)

Rejection-free cluster moves

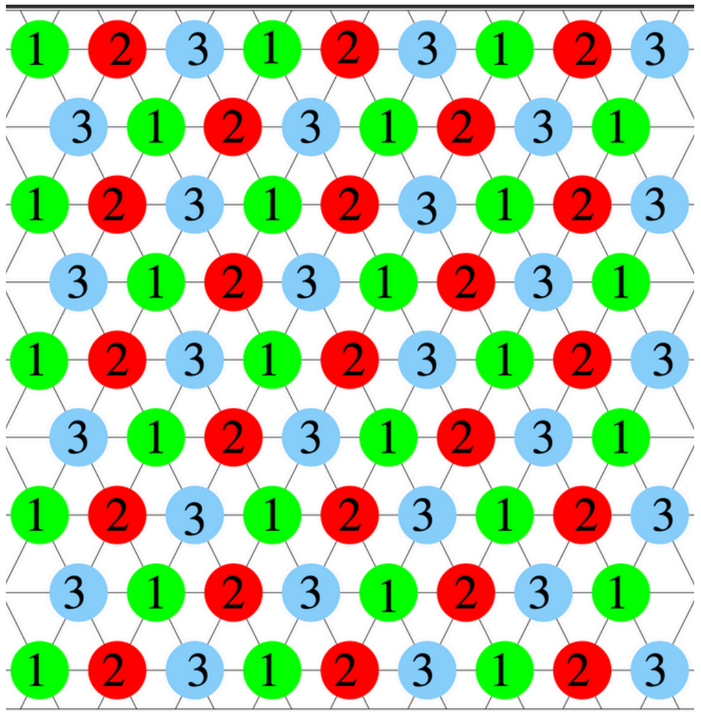
Wang-Landau flat histogram

Jaleel et.al., Phys. Rev. E, 106: 044136 , 2022.
Jaleel et.al., Phys. Rev. E, 104:045310, 2021.

Density of states $g(N, L)$

N Number of particles

Entropy $S(N) = \ln g(N, L).$



1-NN

Benchmark

Critical parameters

$$\mu_c = \ln[\frac{1}{2}(11+5\sqrt{5})]$$

$$2.4060$$

$$\frac{1}{\nu} = 1.2$$

$$\frac{\gamma}{\nu} = 1.733$$

$$\frac{\beta}{\nu} = 0.133$$

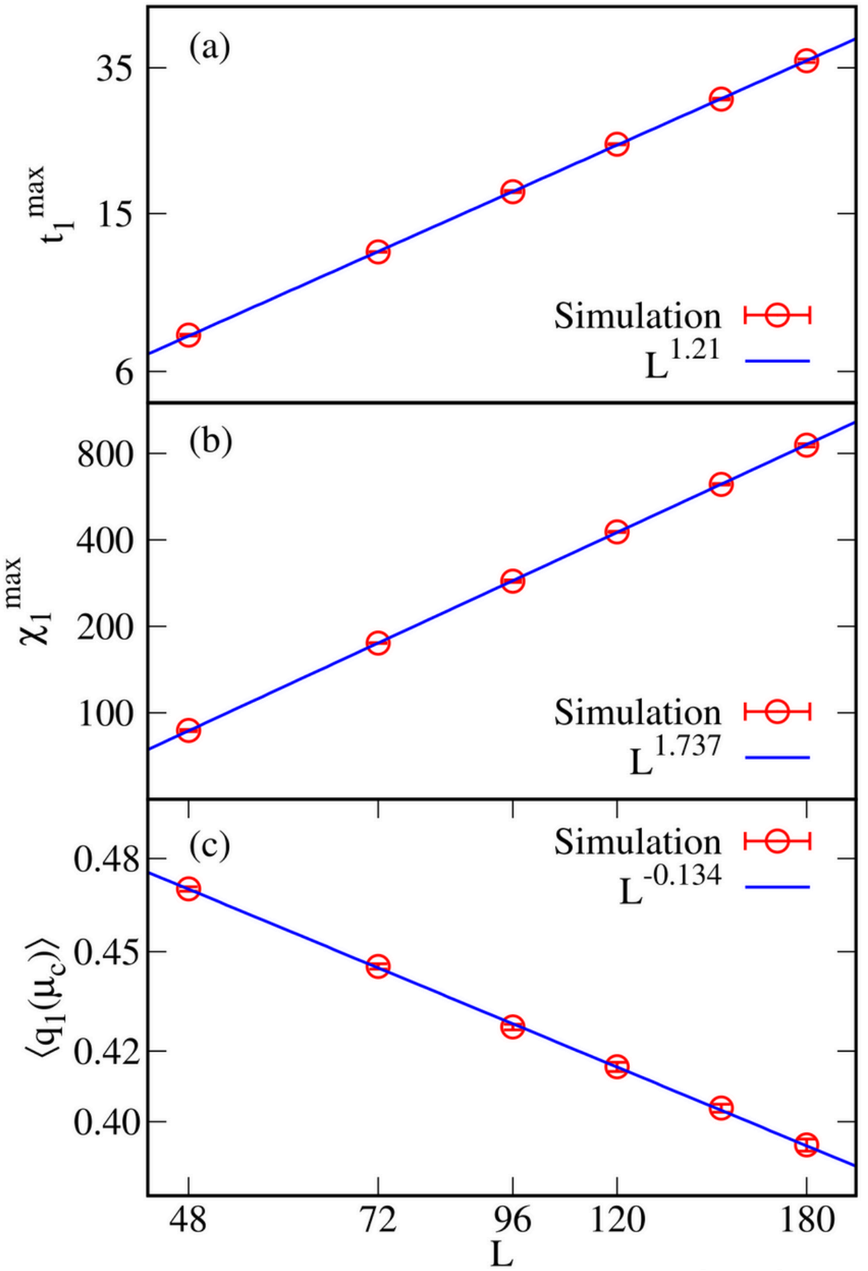
Hard Hexagon Model

Single continuous phase transition

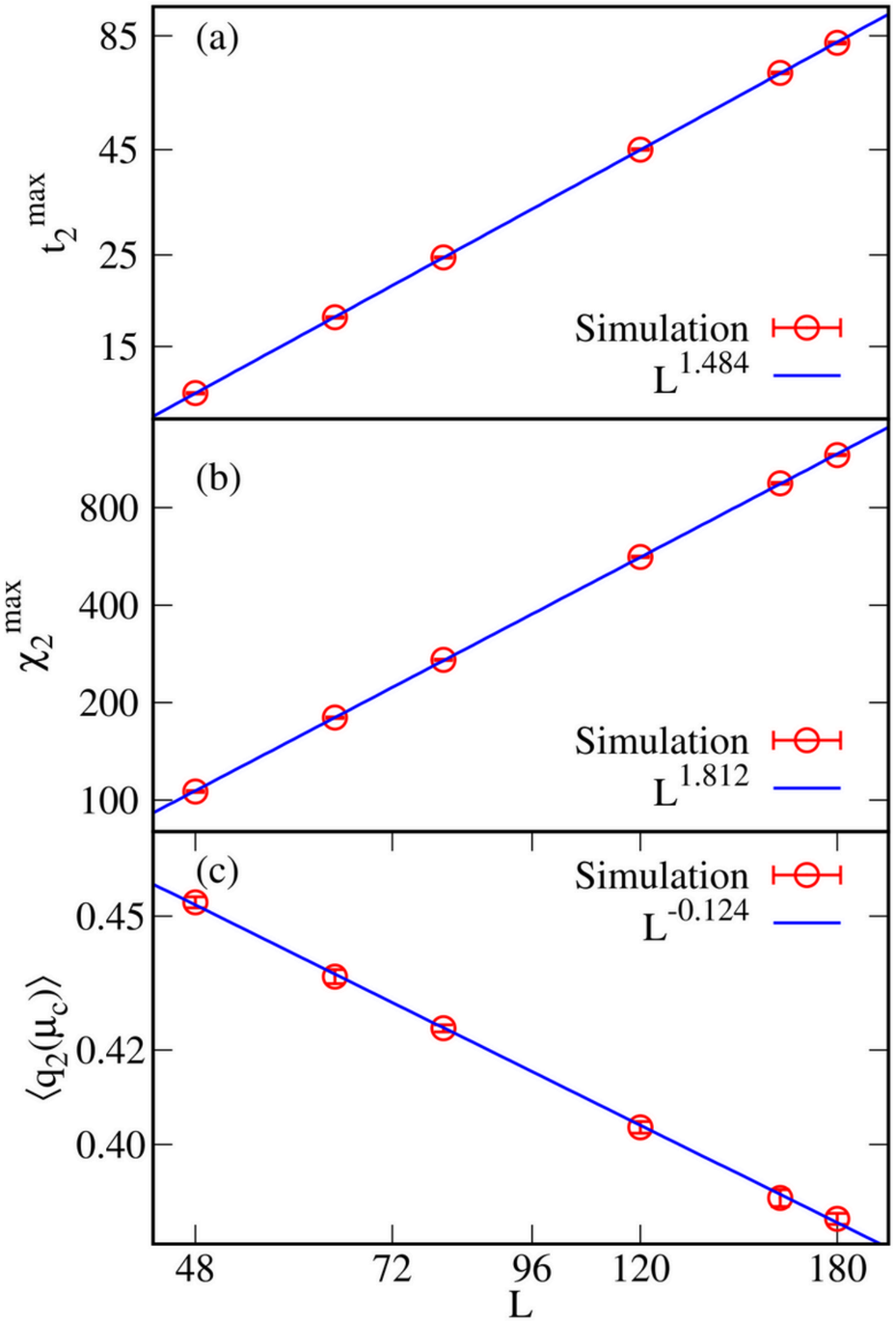
Three-state Potts model universality class.

Baxter, J. Phys. A: Math. Gen. 13, L61 (1980).

Baxter, Exactly Solved Models in Statistical Mechanics



$$\mu_c = 2.4064(1)$$



2-NN Benchmark

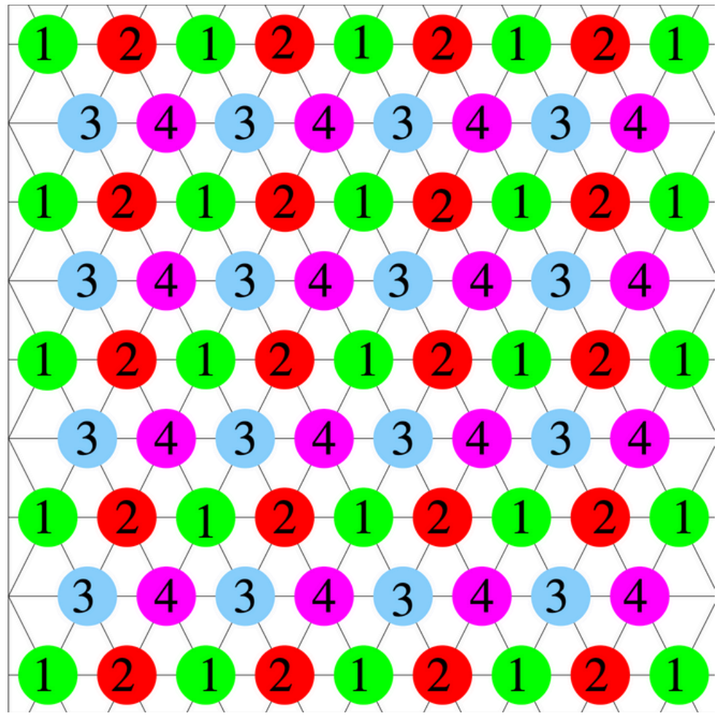
$$\frac{1}{\nu} = 1.5$$

$$\frac{\gamma}{\nu} = 1.75$$

$$\frac{\beta}{\nu} = 0.125$$

$$\mu_c = 1.7568(4)$$

$$\rho_c = 0.7419(5)$$



Single continuous phase transition

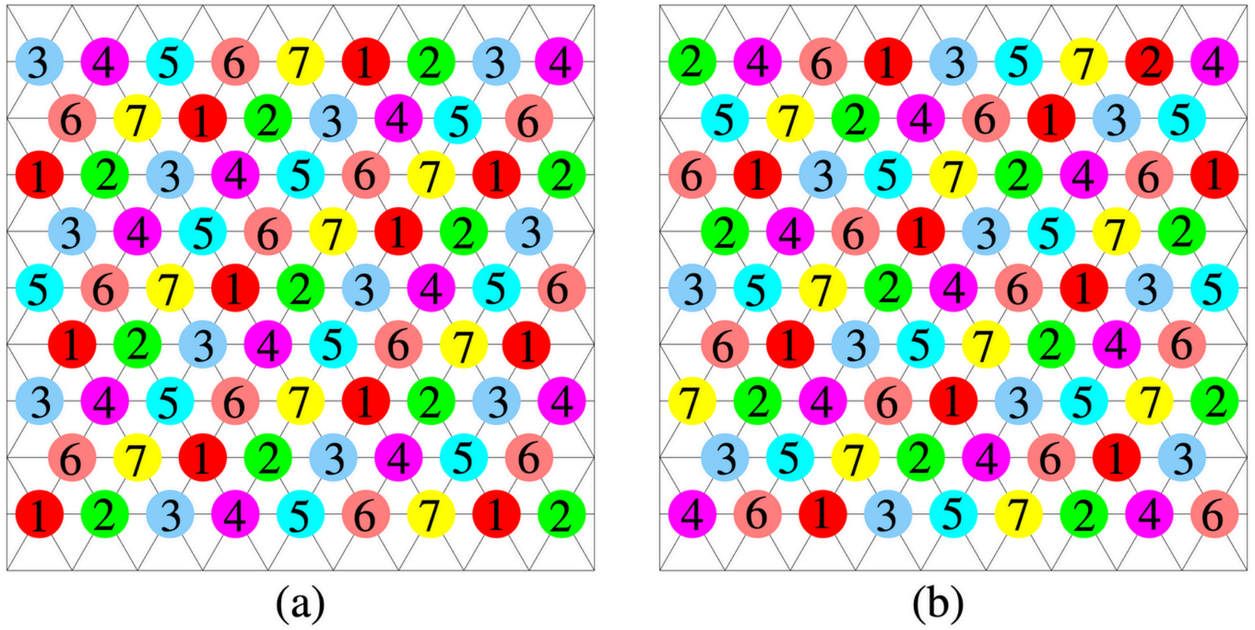
Four-state Potts model

3-NN

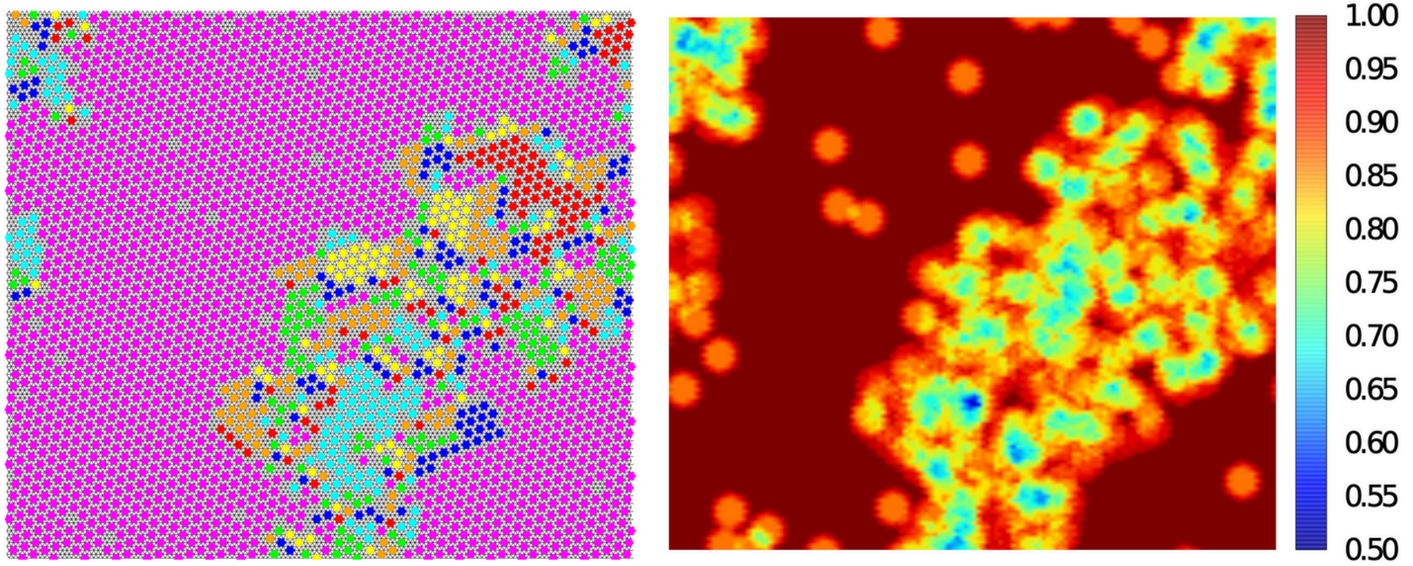
Two transitions?

First from a low density fluid phase to an intermediate density hexatic phase and second from a hexatic phase to a high density solid-like sublattice phase

S. Darjani et. al. J. Chem. Phys. 151, 104702 (2019)

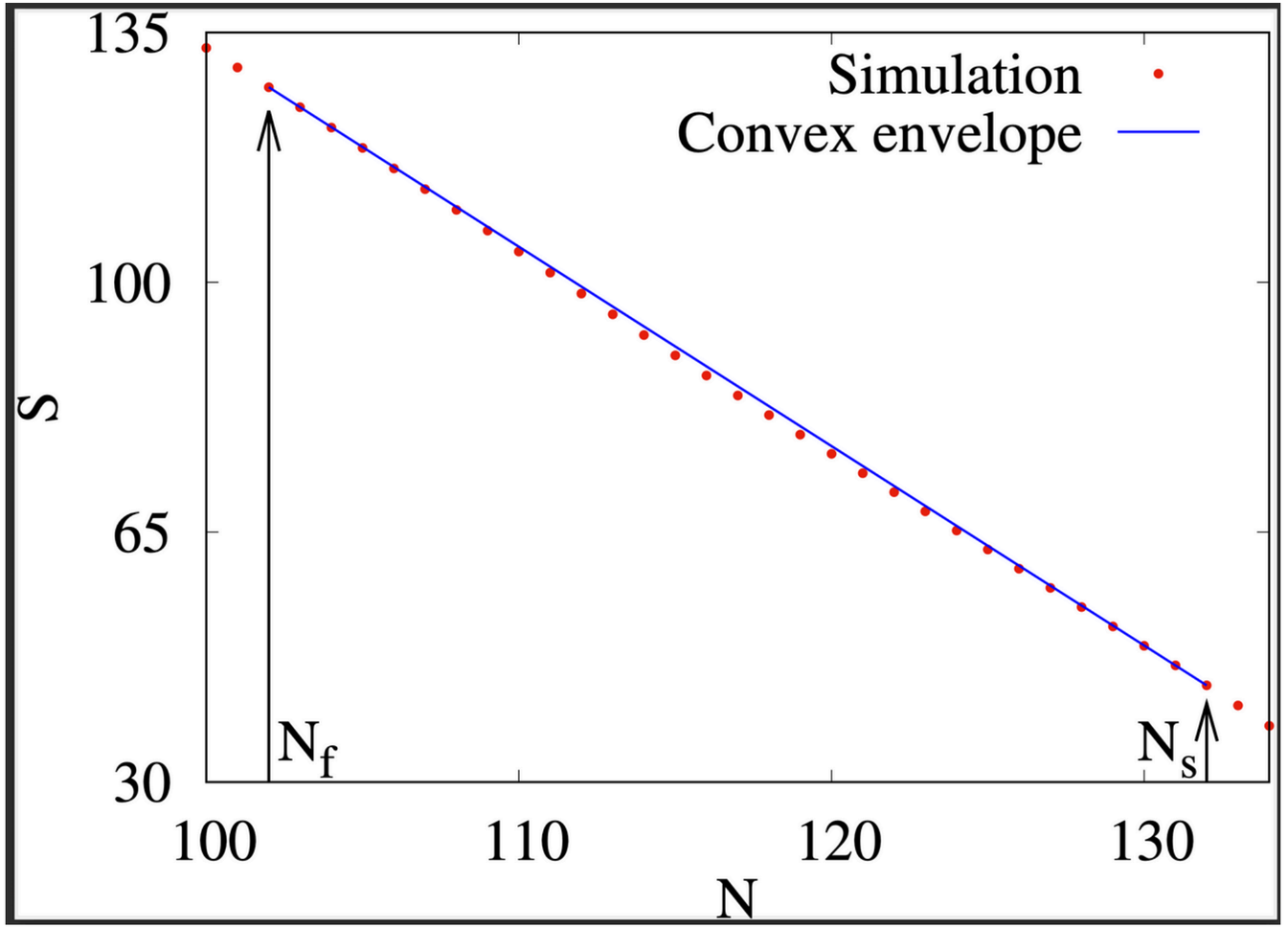


Jaleel et.al., J. Chem. Phys. 155, 224101, 2021



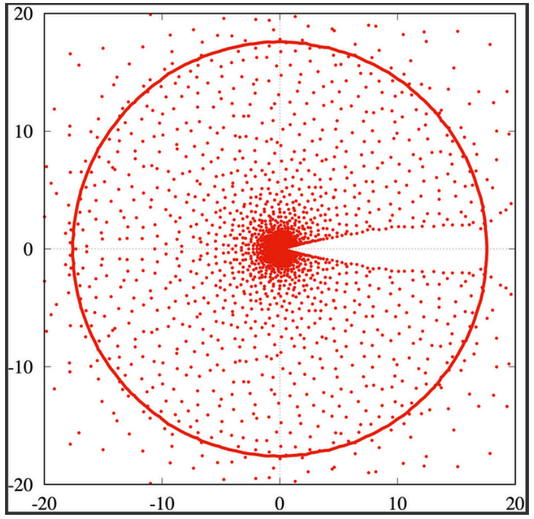
Non convexity in Entropy

$$\mu_c(L) = -\frac{S(N_s) - S(N_f)}{N_s - N_f}$$

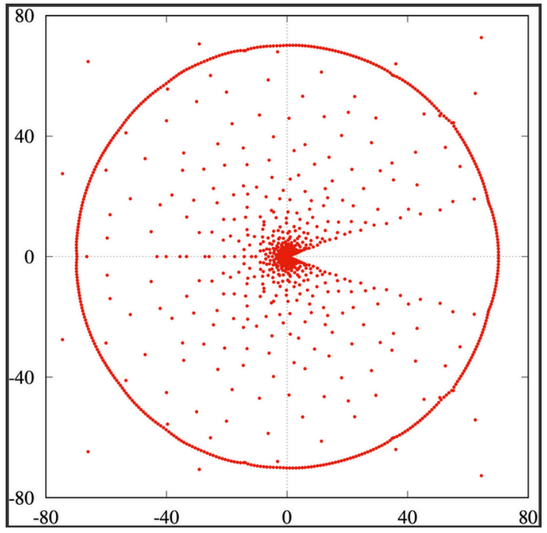


The non-convex part of the entropy and the corresponding convex envelope construction

Summary

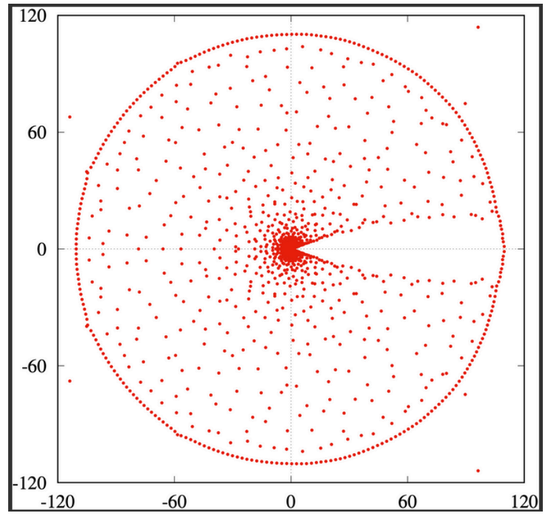


4-NN

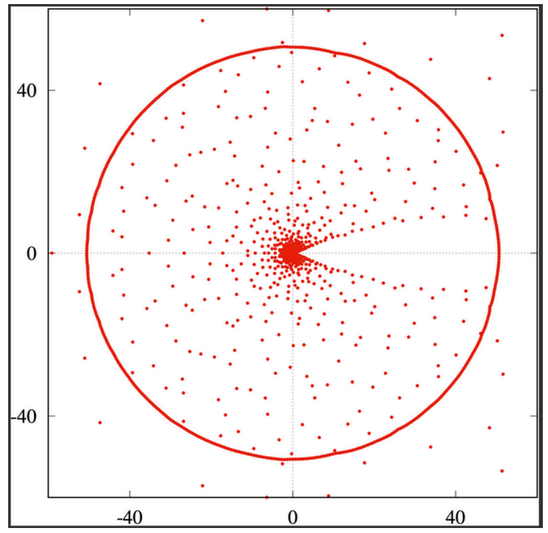


6-NN

k	ρ_f	ρ_s	μ_c	P_c
1	–	0.82917	2.4060	
2	–	0.7419(5)	1.7568(4)	
3	0.8482(1)	0.9839(2)	4.4641(3)	0.6397(1)
4	0.7404(2)	0.9067(2)	2.8696(2)	0.3262(2)
5	0.916(3)	0.988(3)	4.720(3)	0.3942(2)
6	0.7898(1)	0.9818(2)	4.2574(4)	0.3287(1)
7	0.7469(4)	0.9709(3)	3.9315(6)	0.2471(1)



5-NN



7-NN

Ongoing work

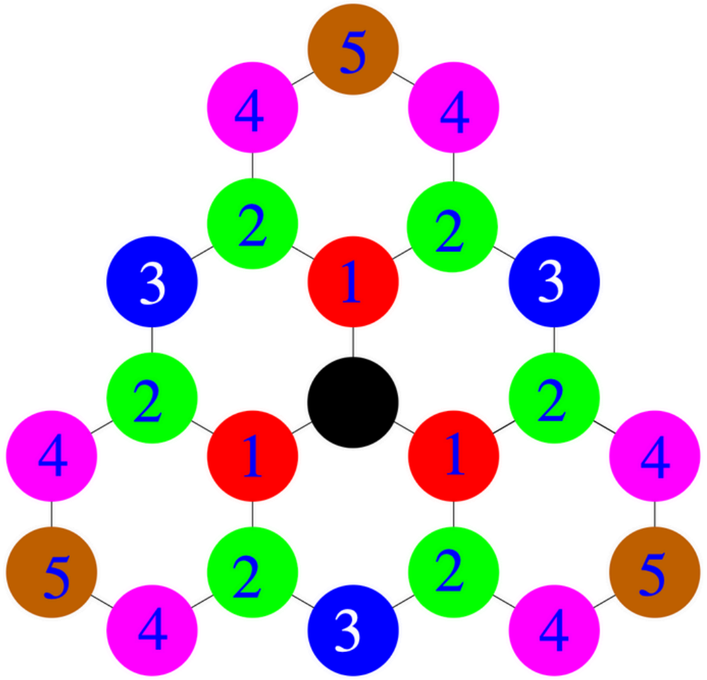
Honeycomb lattice

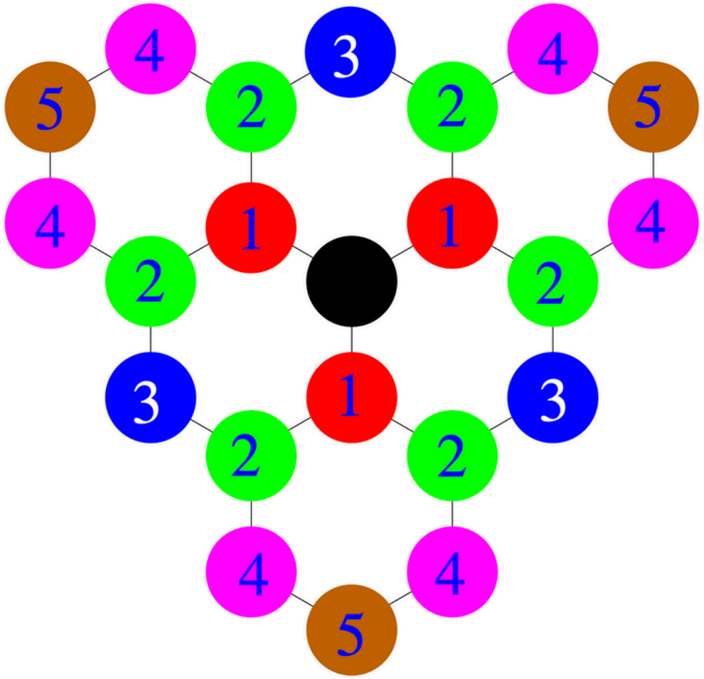
1-NN

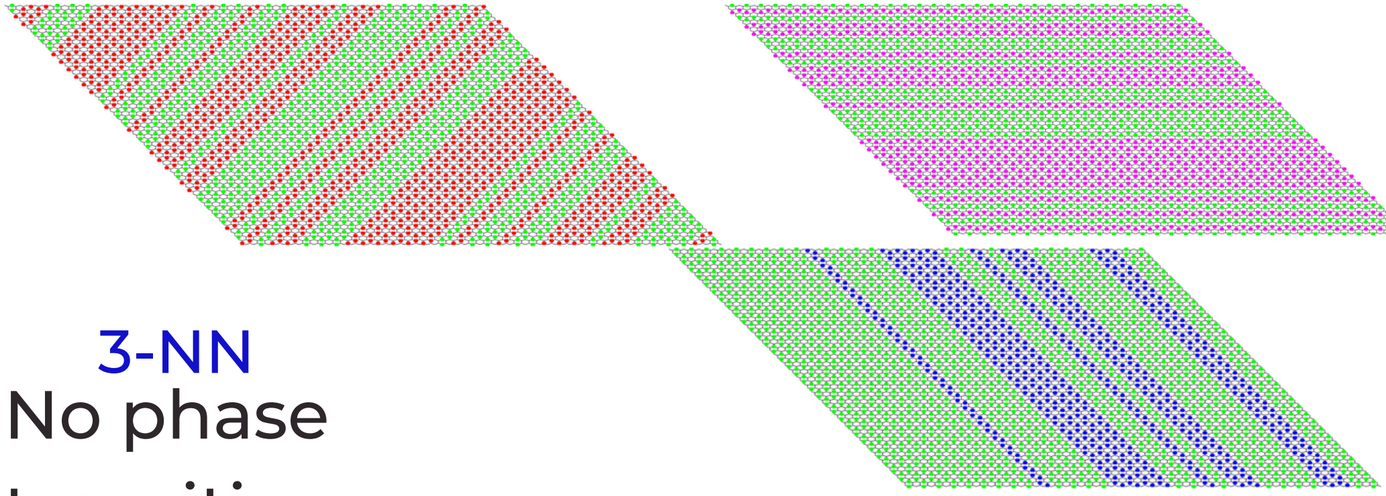
2D Ising model universality class

2-NN

exponential growth of ground state degeneracy







3-NN

No phase transition

Acknowledgement

Rajesh

Jetin

Dipanjan

THANK YOU