Limiting shapes of Ising droplets, fingers, and corners

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Plan and Motivation

- Evolving limiting shapes in the context of Ising model endowed with T=0 spin-flip dynamics.
- In 2D, limiting shapes can be examined through a mapping onto 1D lattice gases. Fluctuations can be also explored using this connection.
- Ising model with NN couplings maps onto simple exclusion processes (SEPs); increasing the range of interactions still leads to tractable lattice gases.
- In 3D, limiting shapes are still inaccessible.

The Ising System

Ising Hamiltonian $\mathcal{H} = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j$ $\sigma_i = \pm 1$ $\uparrow\downarrow$

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$\uparrow\uparrow$ $\quad$ $\downarrow\downarrow$ $\qquad\qquad$ $\uparrow\downarrow$

E=-1 $\qquad\qquad$ E=+1

Glauber dynamics at T=0

Pick a random spin and compare the outcome after reversing the spin

$$\text{if } \Delta E < 0 \qquad \text{flip spin}$$

$$\text{if } \Delta E > 0 \qquad \text{don't flip}$$

$$\text{if } \Delta E = 0 \qquad \text{flip with prob. } 1/2$$

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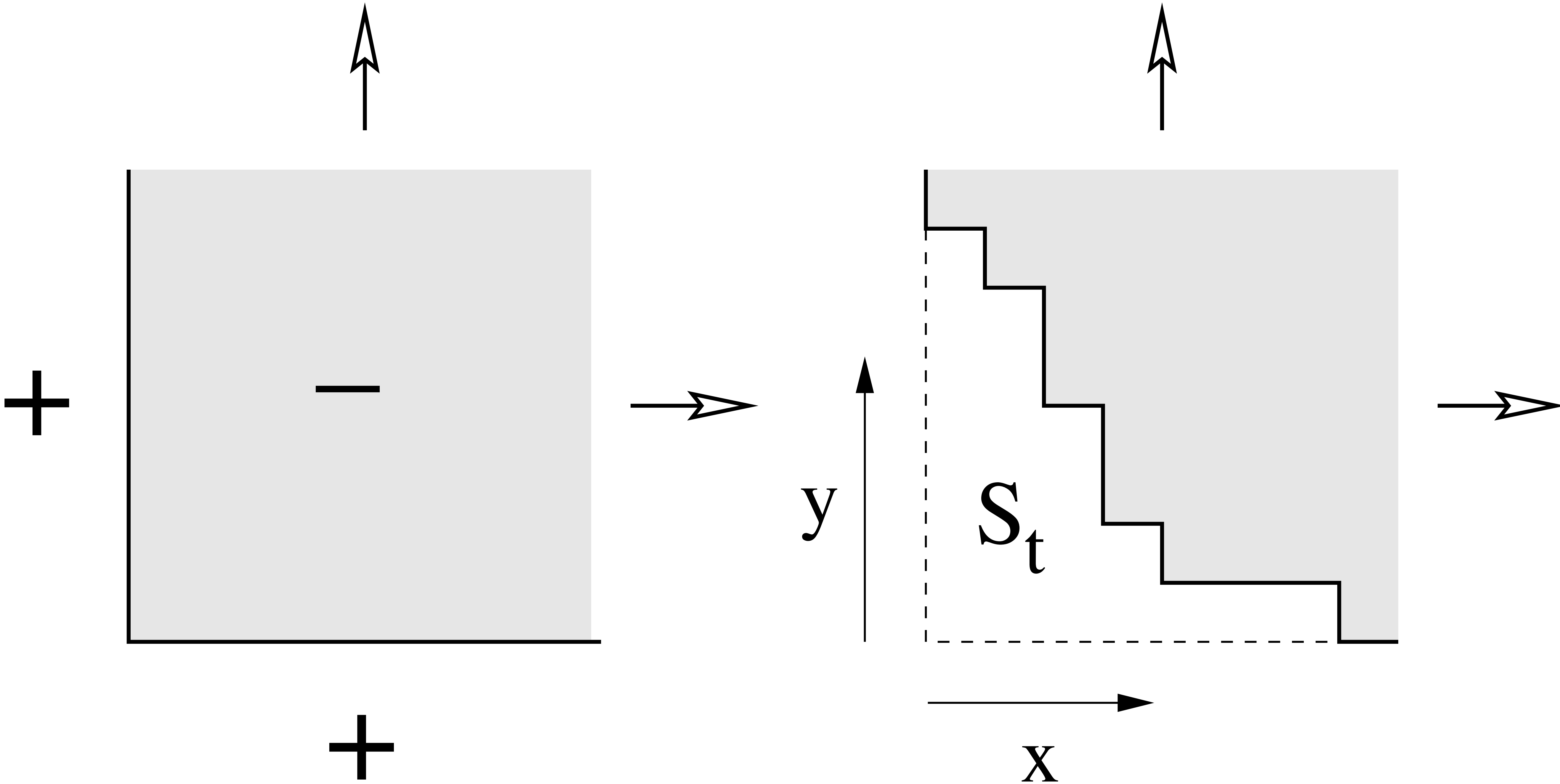
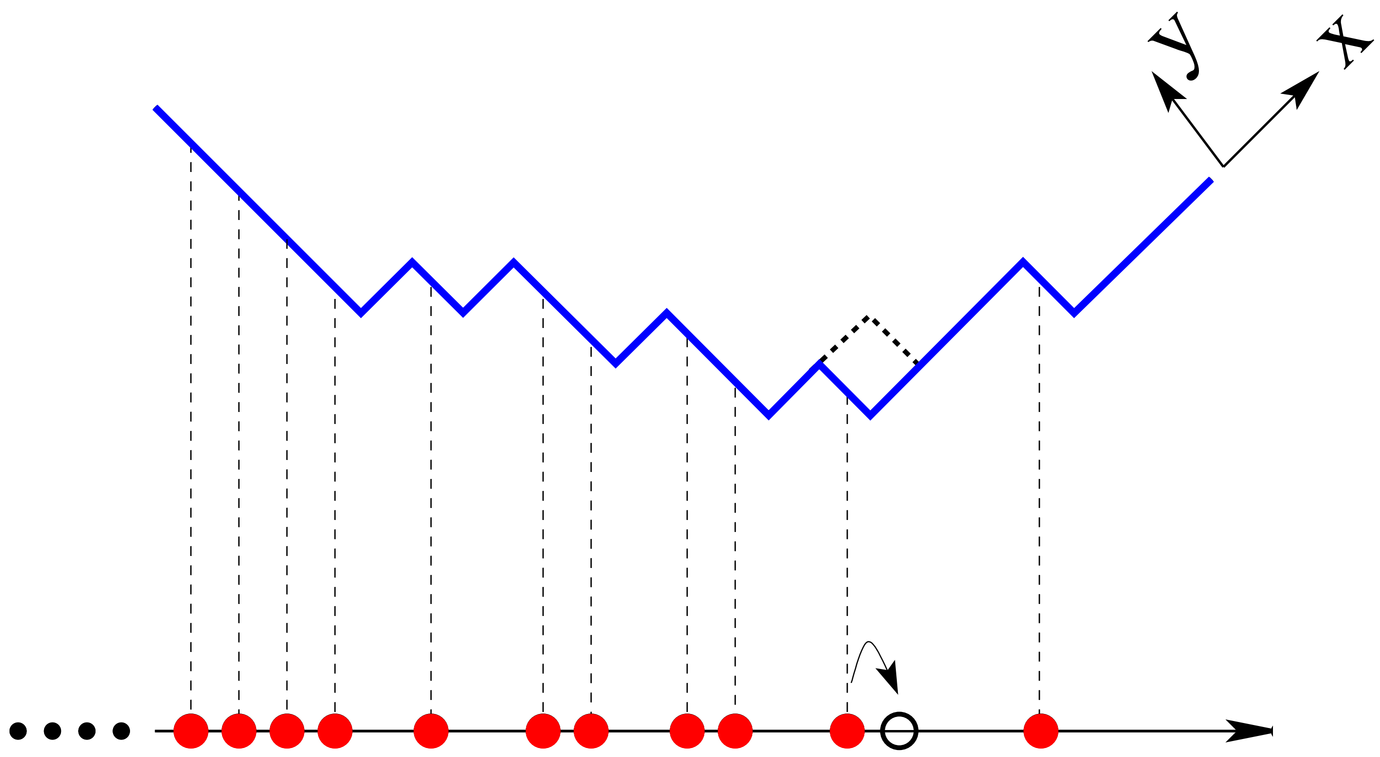
or any rate >0



+
−
+
y
S_t
x

SEP Correspondence



$$\frac{\partial n}{\partial t} = \frac{\partial^2 n}{\partial z^2} \quad \longrightarrow \quad n(z,t) = \frac{1}{2}\,\mathrm{erfc}\left(\frac{z}{\sqrt{4t}}\right)$$

$$y(x,t) = \int_{x-y}^{\infty} dz\; n(z,t)$$

$$(\xi,\eta) = (4t)^{-1/2}(x,y)\,, \quad \eta = \frac{1}{\sqrt{4\pi}}\, e^{-(\xi-\eta)^2} - \frac{\xi-\eta}{\sqrt{\pi}}\int_{\xi-\eta}^{\infty} d\zeta\, e^{-\zeta^2}$$

$$x = y = \sqrt{t/\pi}$$

Fluctuations of the Area

$$\langle A \rangle = t$$

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$$\langle A^3 \rangle_c = C_3 t^2, \qquad C_3 = \frac{6\sqrt{3}}{\pi} - 2$$

$$\langle A^4 \rangle_c = C_4 t^{5/2}$$

$$C_4 = \tfrac{32}{5\pi^{3/2}} \left[(5\sqrt{2}-4)\pi + 12 - 12\sqrt{2}\arccos\left(\tfrac{5}{3\sqrt{3}}\right) - 9\sqrt{2}\arccos\left(\tfrac{1}{3}\right)\right]$$

PLK, K. Mallick, and T. Sadhu, J. Phys. A **48**, 015005 (2015)

Diffusion Equation (Hydrodynamics)

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left[D(\rho)\, \frac{\partial \rho}{\partial x} \right]$$

All microscopic details of lattice gas dynamics are absorbed into a single number, the diffusion coefficient $\mathbf{D}(\rho)$

Large Deviations: Recap

$$\partial_t \rho = \nabla \cdot [D(\rho)\nabla\rho] + \nabla \cdot \left[\sqrt{\sigma(\rho)}\,\boldsymbol{\eta}(\mathbf{x},t)\right]$$

Langevin description (fluctuating hydrodynamics).
Another formalism is a macroscopic fluctuation theory:

$$\partial_t q = \nabla \cdot [D(q)\nabla q - \sigma(q)\nabla p]$$

$$\partial_t p = -D(q)\nabla^2 p - \frac{1}{2}\sigma'(q)(\nabla p)^2$$

In addition to the diffusion coefficient, we need another transport coefficient: mobility $\sigma(\rho)$

Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim (2001–2015)

Our Problem: Large Deviations of the Area

$$p(x,T) = \lambda \; x \qquad \text{and} \qquad q(x,0) = \Theta(-x)$$

$$\mu(\lambda) = \ln\langle \exp[\lambda A] \rangle = \lambda \langle A \rangle_c + \tfrac{\lambda^2}{2!} \langle A^2 \rangle_c + \tfrac{\lambda^3}{3!} \langle A^3 \rangle_c + \cdots$$

$$\mu(\lambda) = \int_0^T dt \int_{-\infty}^{\infty} dx \left[\lambda \; x \; \partial_t q - \tfrac{\sigma(q)}{2} \left(\partial_x p \right)^2 \right]$$

$$A = \int_{-\infty}^{\infty} dx \, x [q(x,T) - q(x,0)]$$

Perturbation Analysis

$$q = q_0 + \lambda q_1 + \lambda^2 q_2 + \cdots$$

$$p = \lambda p_1 + \lambda^2 p_2 + \cdots$$

$$\langle A \rangle_c = \int_0^T dt \int_{-\infty}^{\infty} dx \; x \partial_t q_0$$

$$\langle A^2 \rangle_c = \int_0^T dt \int_{-\infty}^{\infty} dx \; \sigma_0$$

$$\langle A^3 \rangle_c = 3 \int_0^T dt \int_{-\infty}^{\infty} dx \; \sigma_1$$

$$\langle A^4 \rangle_c = 12 \int_0^T dt \int_{-\infty}^{\infty} dx \left[\sigma_2 - \sigma_0 (\partial_x p_2)^2 \right]$$

Formulas for $\langle A^n \rangle_c$ **assume** that $D = 1$.

Ising Model

The corresponding lattice gas, SEP, is characterized by

$$D(q) = 1, \qquad \sigma(q) = 2q(1-q)$$

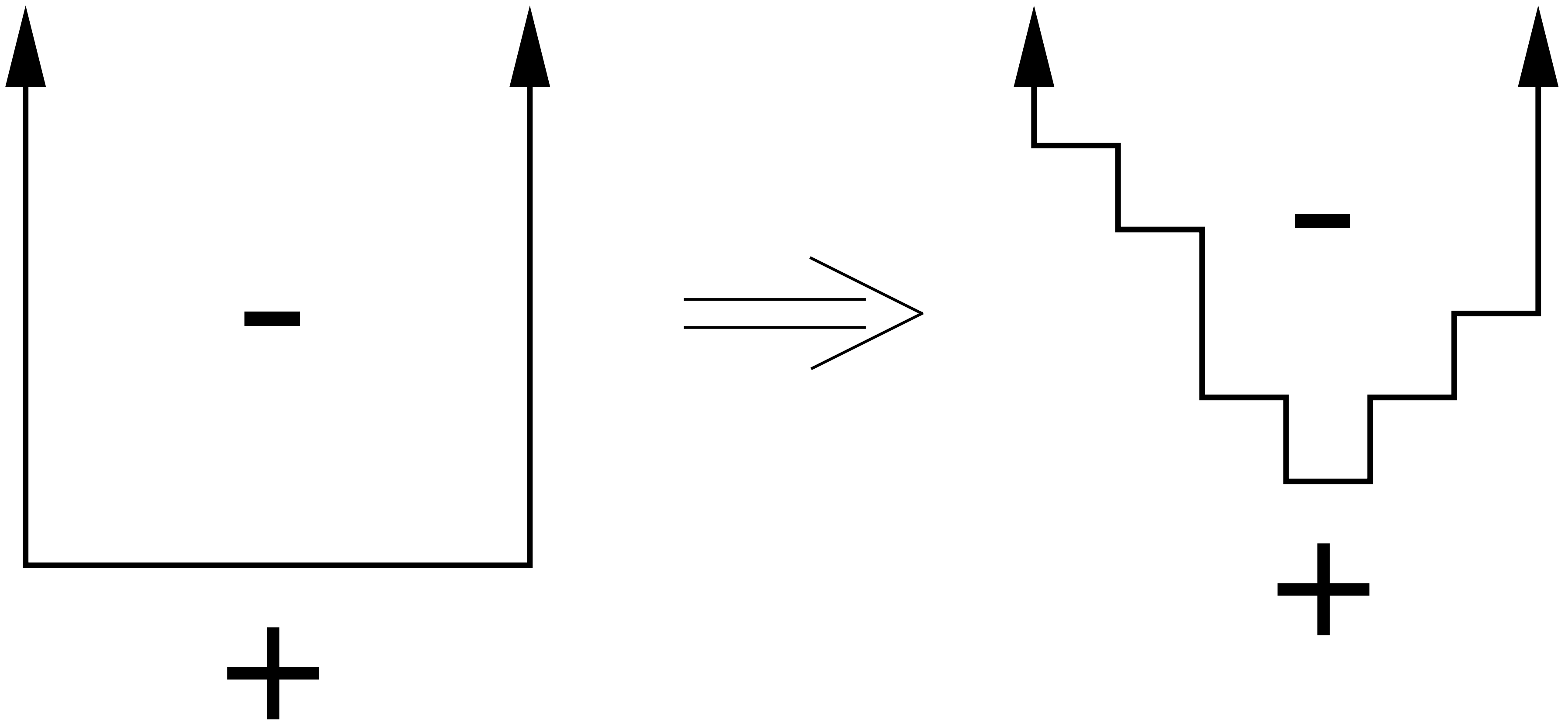
$$\sigma_0 = 2q_0 \left[1 - q_0\right]$$

$$\sigma_1 = 2q_1 \left[1 - 2q_0\right]$$

$$\sigma_2 = 2q_2 \left[1 - 2q_0\right] - 2q_1^2$$

In the following: Only Limiting Shapes

Ising Finger



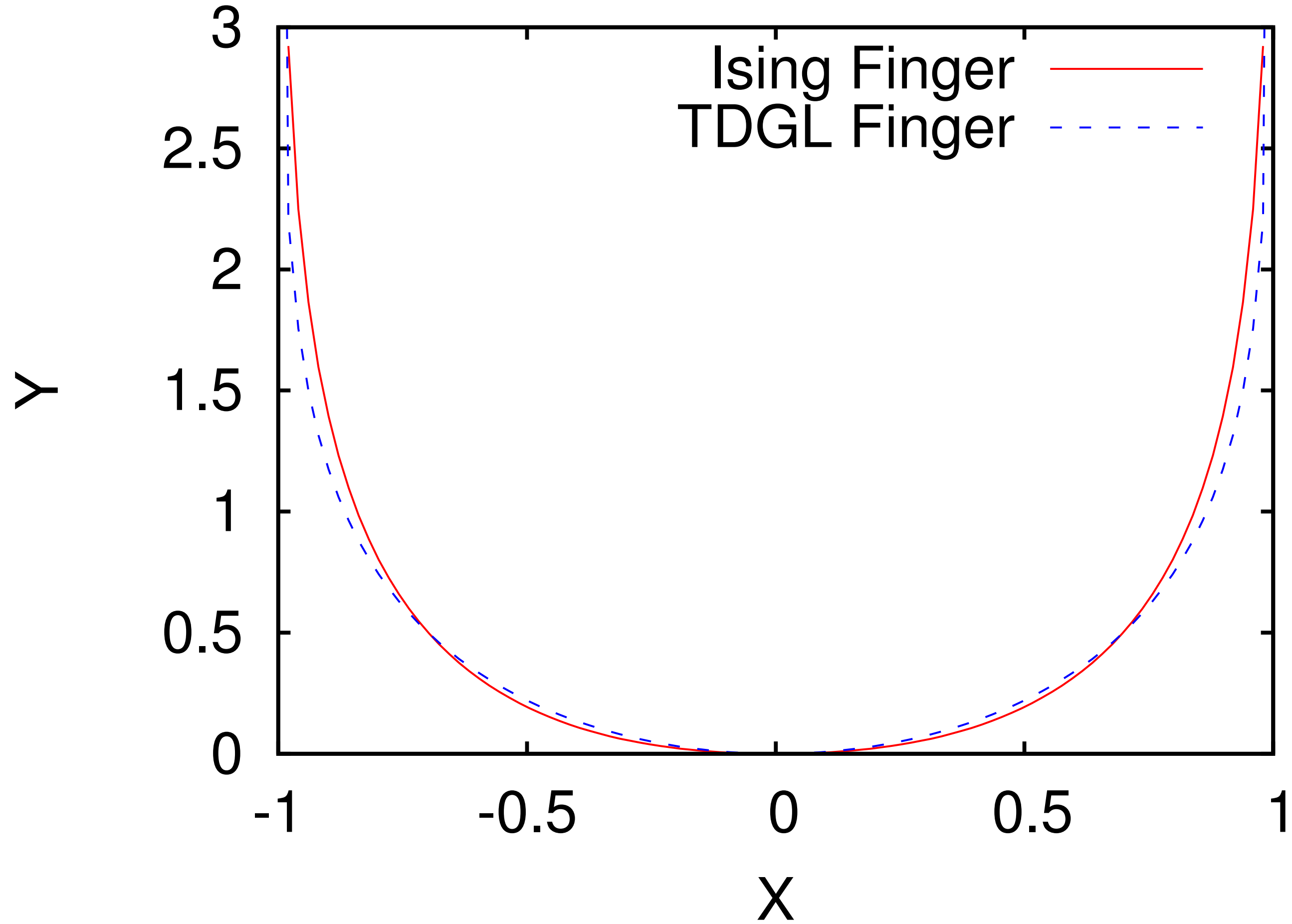
$$y_t = \frac{y_{xx}}{(1+y_x)^2} = v \qquad (0 < x < L)$$

$$y(0) = 0, \quad y(L) = \infty \quad \longrightarrow \quad v = \frac{1}{L}$$

Ising Finger

$$Y = -\ln(1-X) - X\,, \quad (X,Y) = \left(\frac{x}{L}, \frac{y}{L}\right)$$

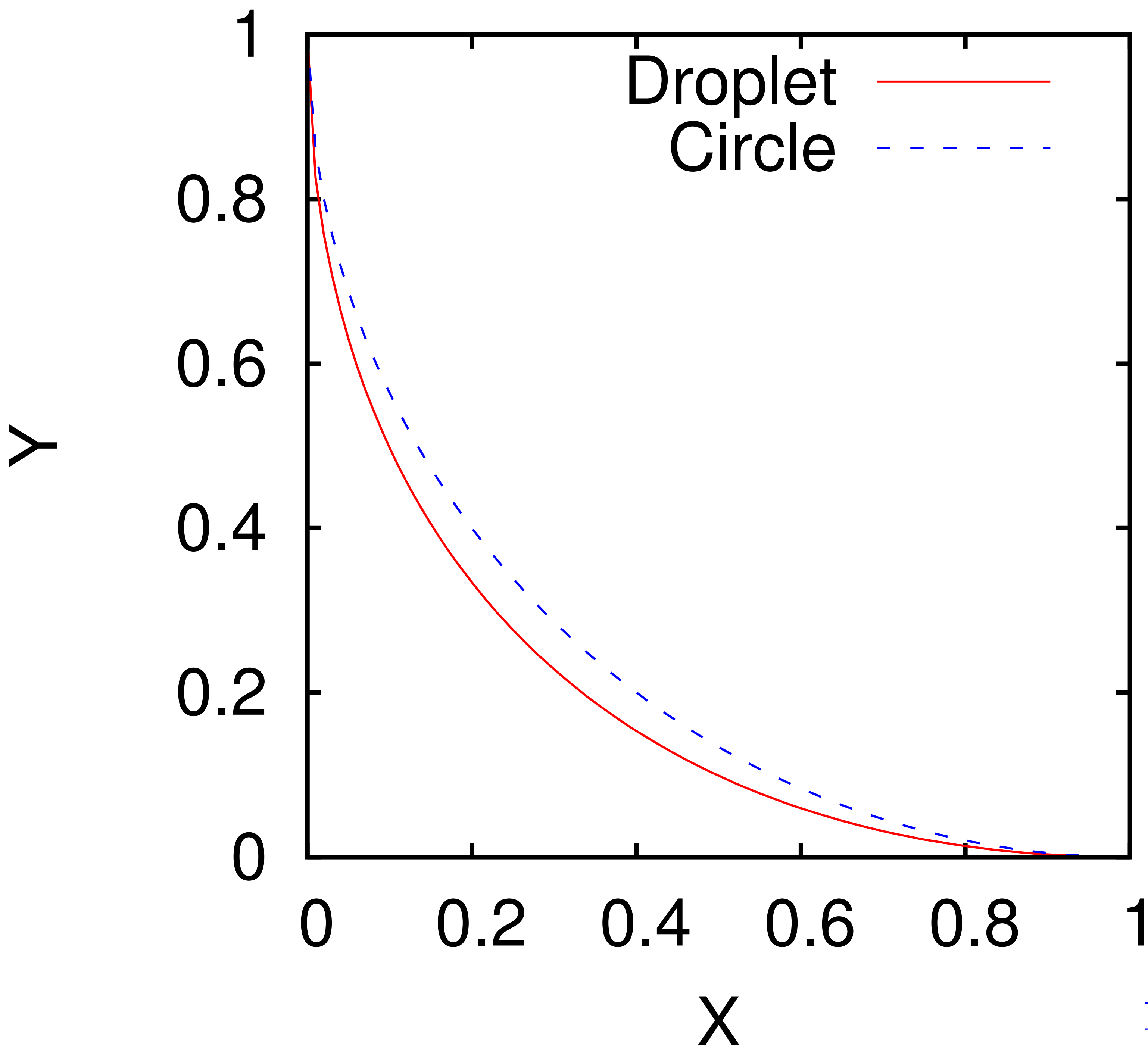
$$Y = -\frac{2}{\pi}\ln\left[\cos\left(\frac{\pi X}{2}\right)\right] \quad \text{for} \quad \text{TDGL}$$



TDGL finger:
Mullins (1956)
Saffman-Taylor finger (1958)
Dendritic crystal growth (80s)
grim reaper (differential geometers)

Ising finger: PLK (2012)

Ising Droplet



Karma and Lobkovsky (PRE, 2005)
PLK (PRE, 2012)
Lacoin, Simenhaus, Toninelli (JEMS, 2014)

Ising Droplet

$$\frac{\partial n}{\partial t} = \frac{\partial^2 n}{\partial z^2}\,, \quad -L(t) \le z \le L(t)$$

Stefan problem
(boundary is determined in the process of solution)

$$n(-L(t), t) = 1, \qquad n(L(t), t) = 0$$

$$n(z, t) = N(Z), \quad Z = z/L(t)$$

$$N(Z) = 2b\int_Z^1 dv\, e^{bv^2 - b}, \quad 1 = 4b\int_0^1 dv\, e^{bv^2 - b}$$

IM with NNN couplings: Repulsion Process (RP)

$$\mathcal{H} = -J \sum_{|\mathbf{i}-\mathbf{j}|=1} s_{\mathbf{i}} s_{\mathbf{j}} - J_1 \sum_{|\mathbf{i}-\mathbf{j}|=2} s_{\mathbf{i}} s_{\mathbf{j}} \qquad |\mathbf{i}| = |i_1| + |i_2|$$

$$\ldots \bullet\bullet\bullet\bullet\bullet\circ\circ\circ\circ\circ \ldots \Longrightarrow \ldots \bullet\bullet\bullet\bullet\circ\bullet\circ\circ\circ\circ \ldots$$

SEP: $\bullet\bullet\bullet\bullet\circ\bullet\circ\circ\circ\circ \Longrightarrow \begin{cases} \bullet\bullet\bullet\bullet\bullet\circ\circ\circ\circ\circ \\ \bullet\bullet\bullet\circ\bullet\bullet\circ\circ\circ\circ \\ \bullet\bullet\bullet\bullet\circ\circ\bullet\circ\circ\circ \end{cases}$

RP: $\bullet\bullet\bullet\bullet\circ\bullet\circ\circ\circ\circ \Longrightarrow \begin{cases} \bullet\bullet\bullet\circ\bullet\bullet\circ\circ\circ\circ \\ \bullet\bullet\bullet\bullet\circ\circ\bullet\circ\circ\circ \end{cases}$

Repulsion Processes

PLK arXiv:1303.3641 (JSTAT, 2013)
PLK and Jason Olejarz arXiv:1303.5128 (PRE, 2013)

- Exclusion processes (no multiple occupancy)
- Repulsion between neighboring particles (the simplest RP)
- Generally the range of repulsion interaction is arbitrary but finite (with rapidly decreasing strengths)
- Zero-temperature dynamics (energy raising hops are forbidden).

Simplest RP: Definition

$$\mathcal{H}_1 = J_1 \sum n_i n_{i+1} \qquad n_i = \begin{cases} 1 & \text{site } i \text{ is occupied} \\ 0 & \text{site } i \text{ is empty} \end{cases}$$

There is an energy cost when particles occupy adjacent sites.

A zero-temperature dynamics associated with above Hamiltonian.

A hop to a neighboring **empty** site is performed with rate

$$\begin{cases} 2 & \#(\text{NN pairs of particles decreases}) \\ 1 & \#(\text{NN pairs of particles remains the same}) \\ 0 & \#(\text{NN pairs of particles increases}) \end{cases}$$

Generalized RPs: Definition

$$\mathcal{H}_2 = J_1 \sum n_i n_{i+1} + J_2 \sum n_i n_{i+2}$$

Zero temperature dynamics is the same for all $J_1 > J_2 > 0$.

Only the number of NN pairs of particles matters if it changes.
If it remains the same, the number of NNN pairs of particles matters.

$$\mathcal{H}_m = J_1 \sum n_i n_{i+1} + \ldots + J_m \sum n_i n_{i+m}$$

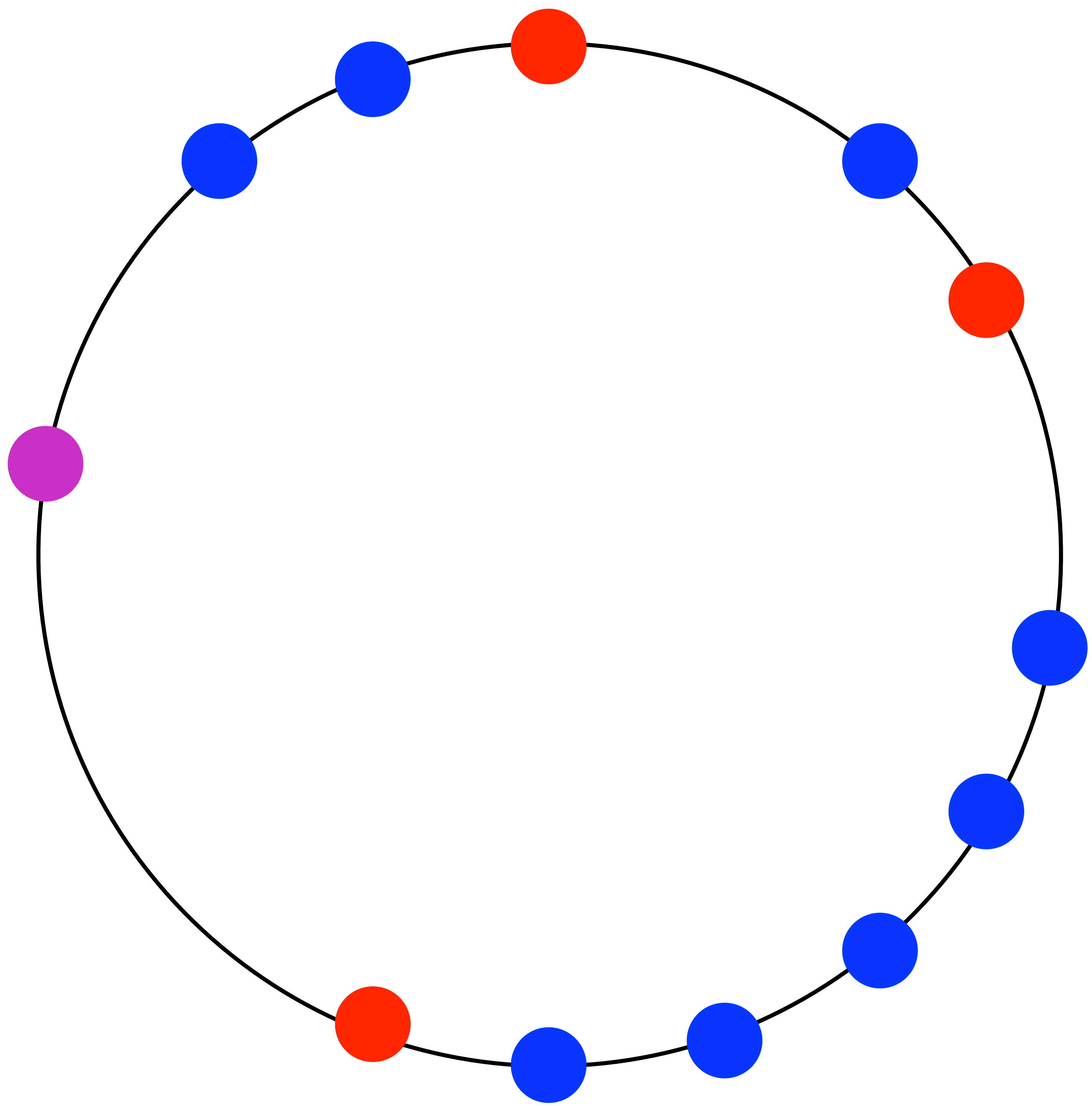
$$J_k > J_{k+1} + \ldots + J_m, \qquad k = 1, \ldots, m-1$$

Then the magnitudes of J's are irrelevant and
we can treat interactions in a lexicographic order.

Understanding of Equilibrium States is the key

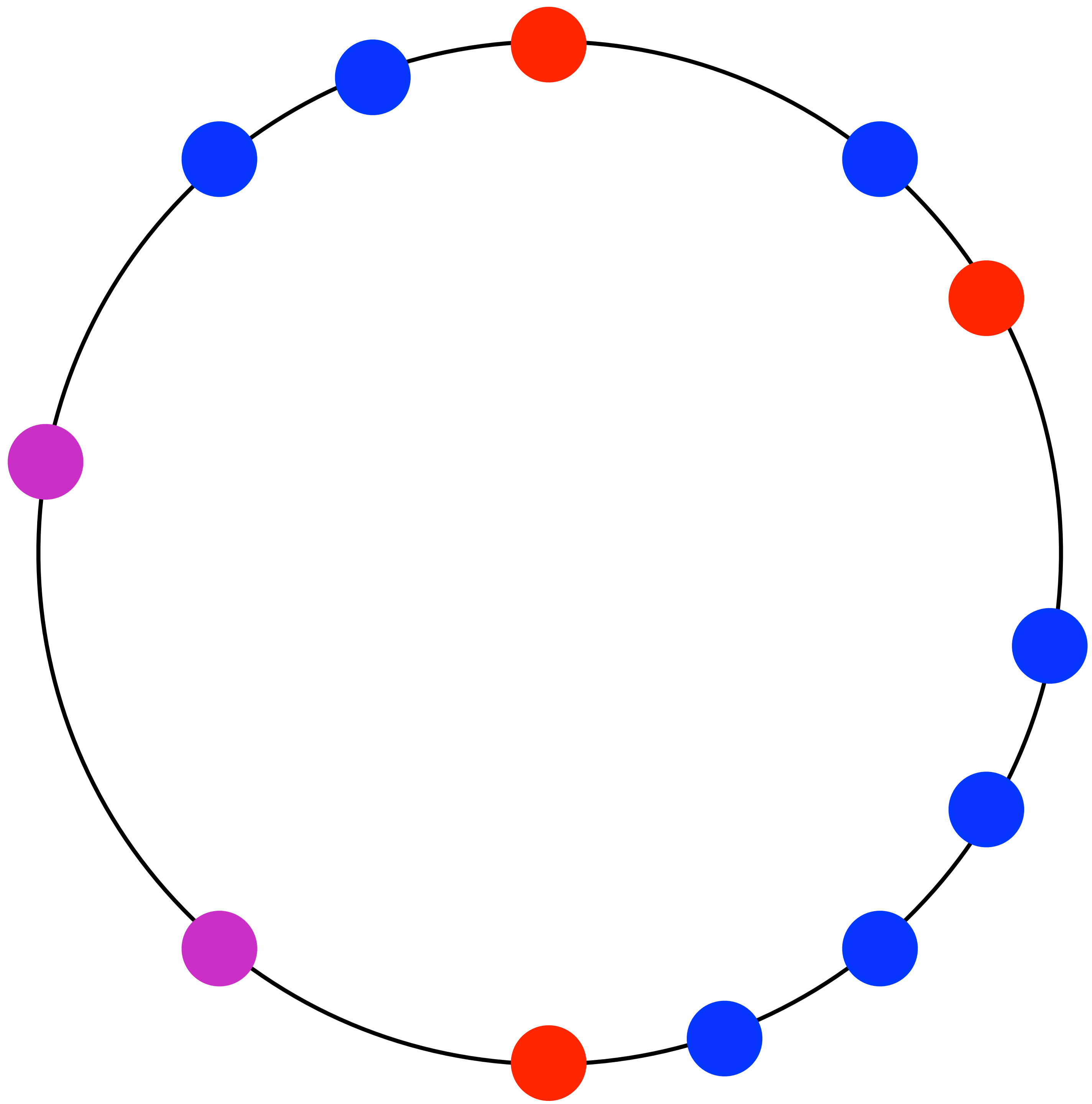
- Let's consider the asymmetric RP and try to classify the equilibrium states.
- The same results are valid for the symmetric RP.
- Similar arguments apply to generalized RPs.

Finite Ring (density > 1/2)



4 islands

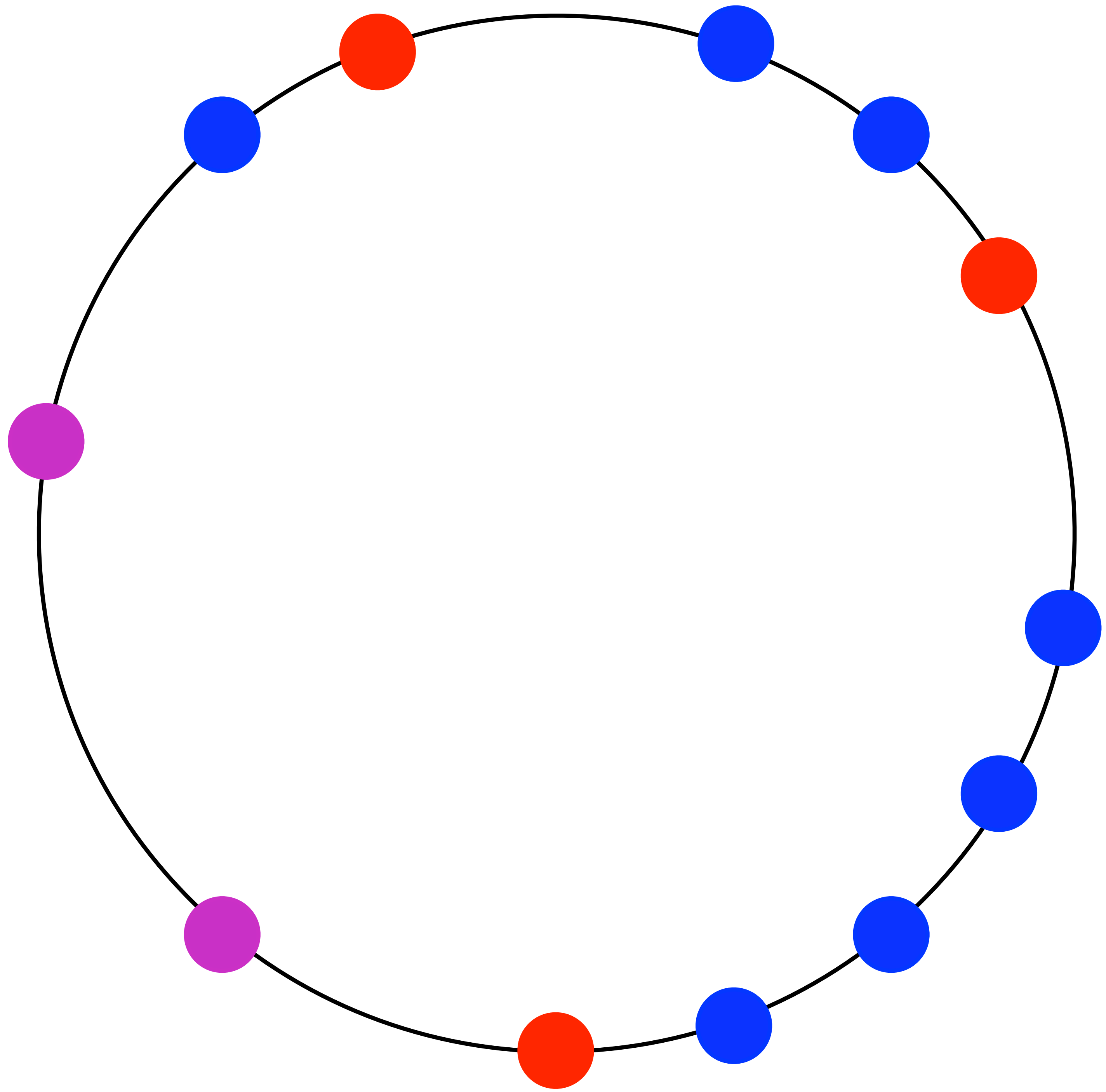
Finite Ring (density > 1/2)



5 islands

Finite Ring (density > 1/2)

5 islands



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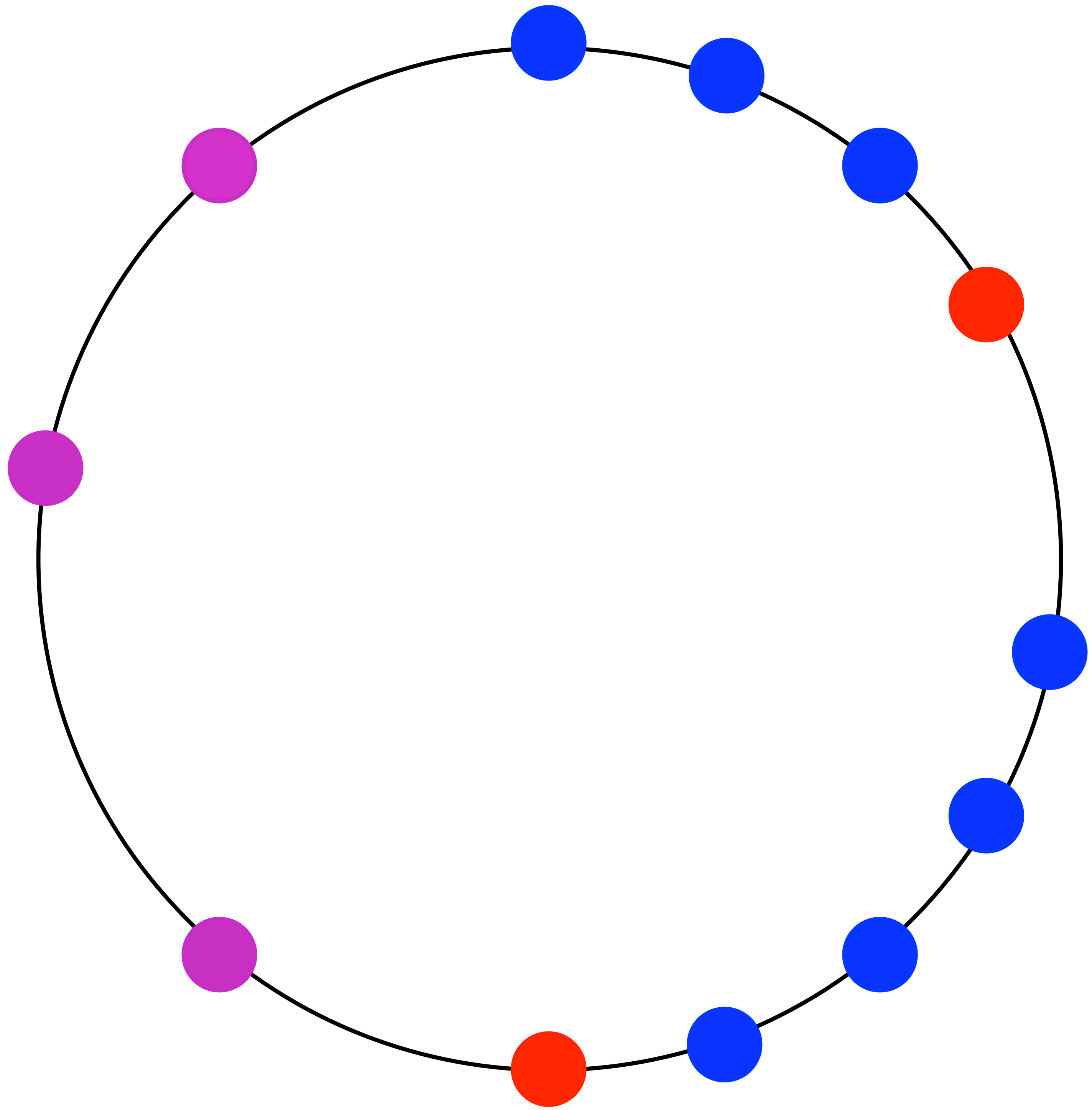

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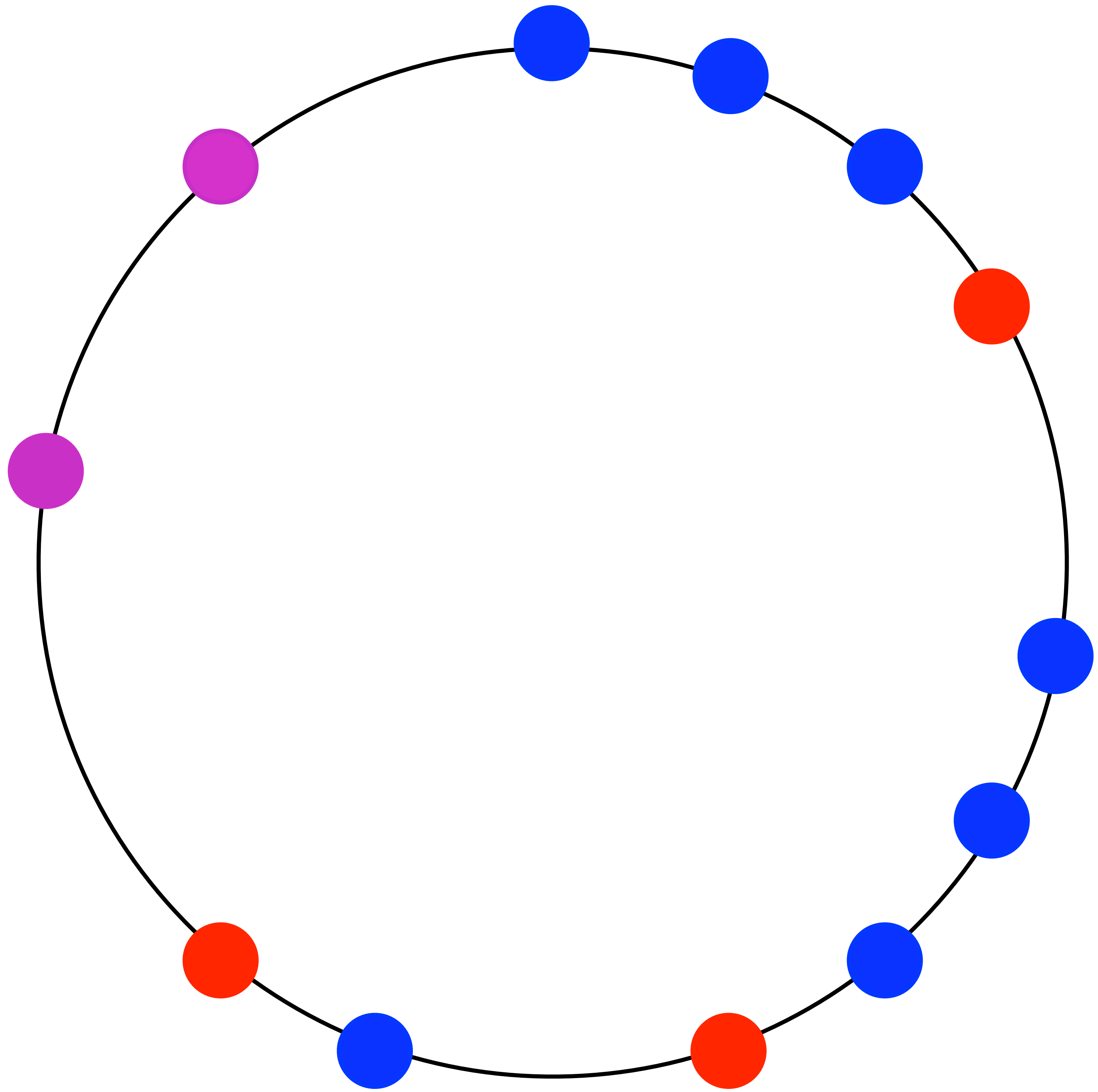

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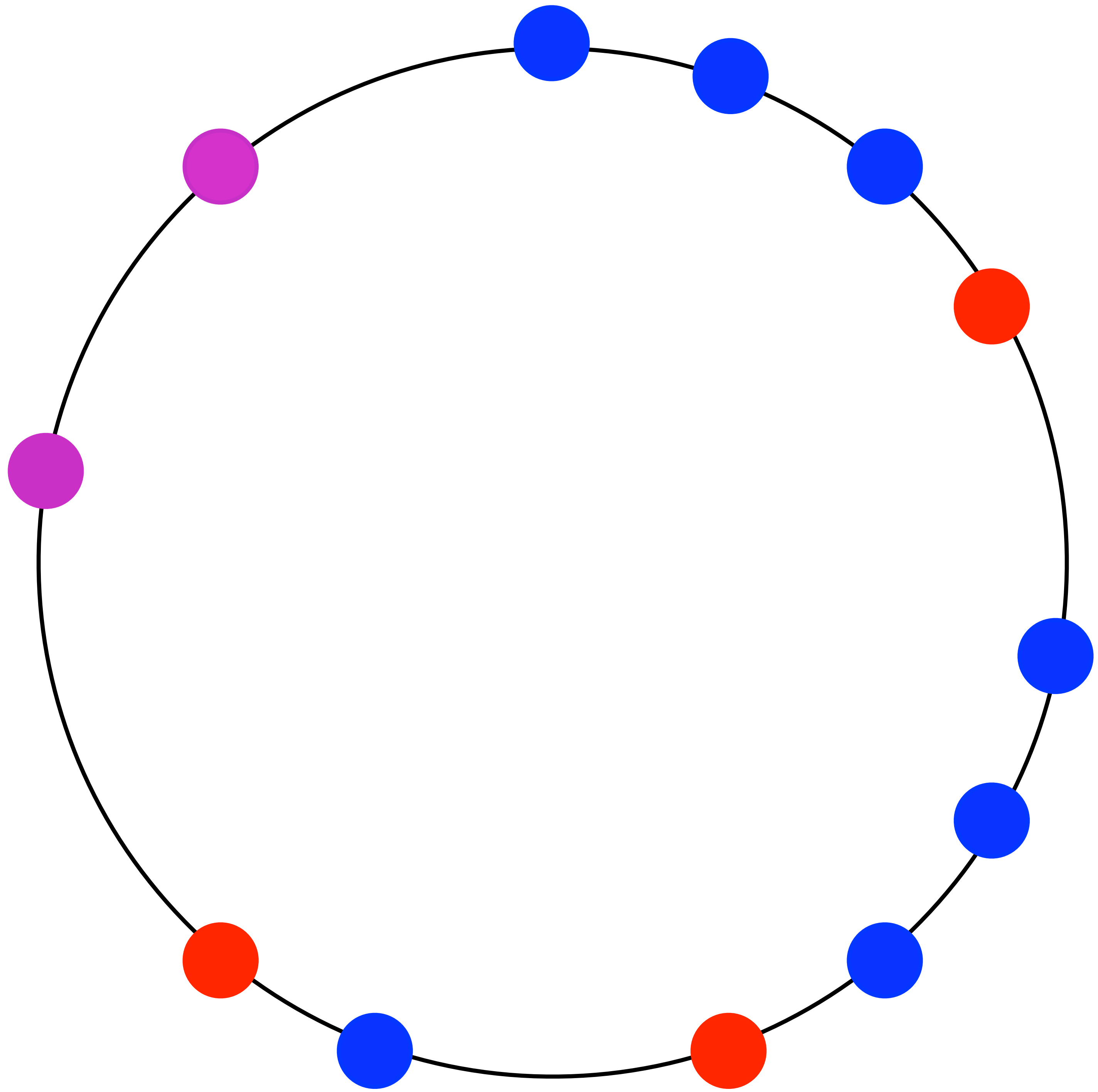

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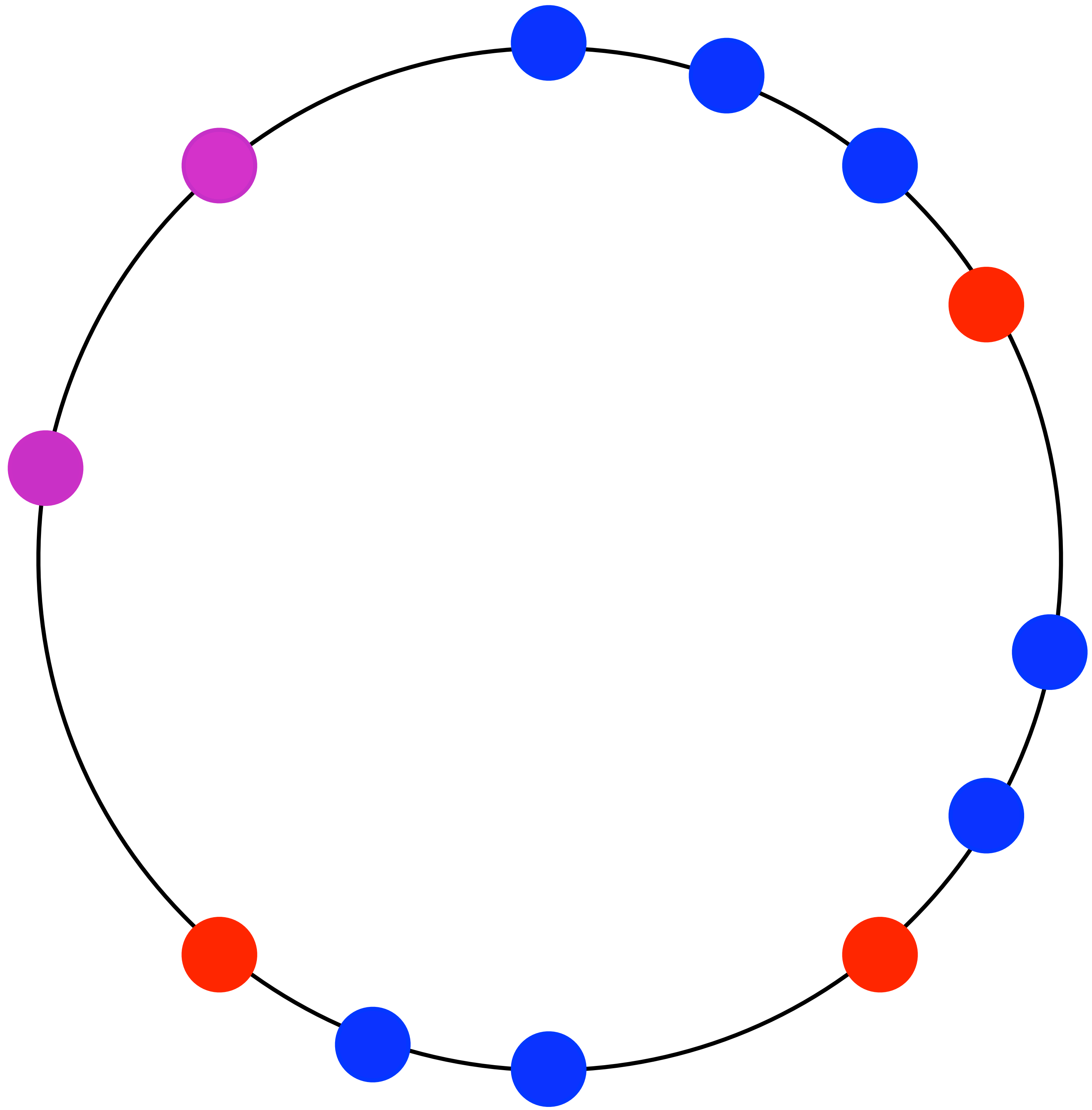

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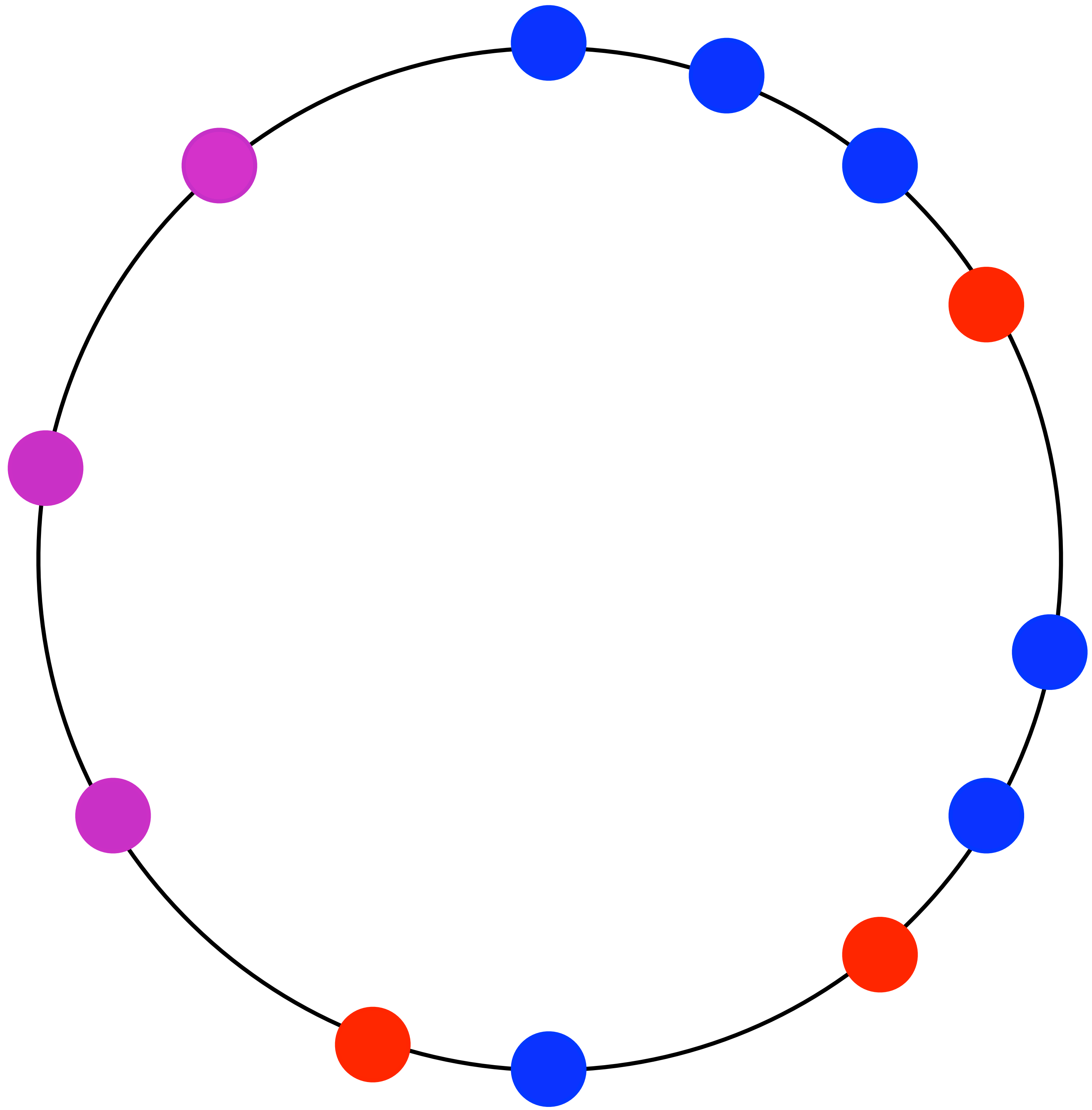
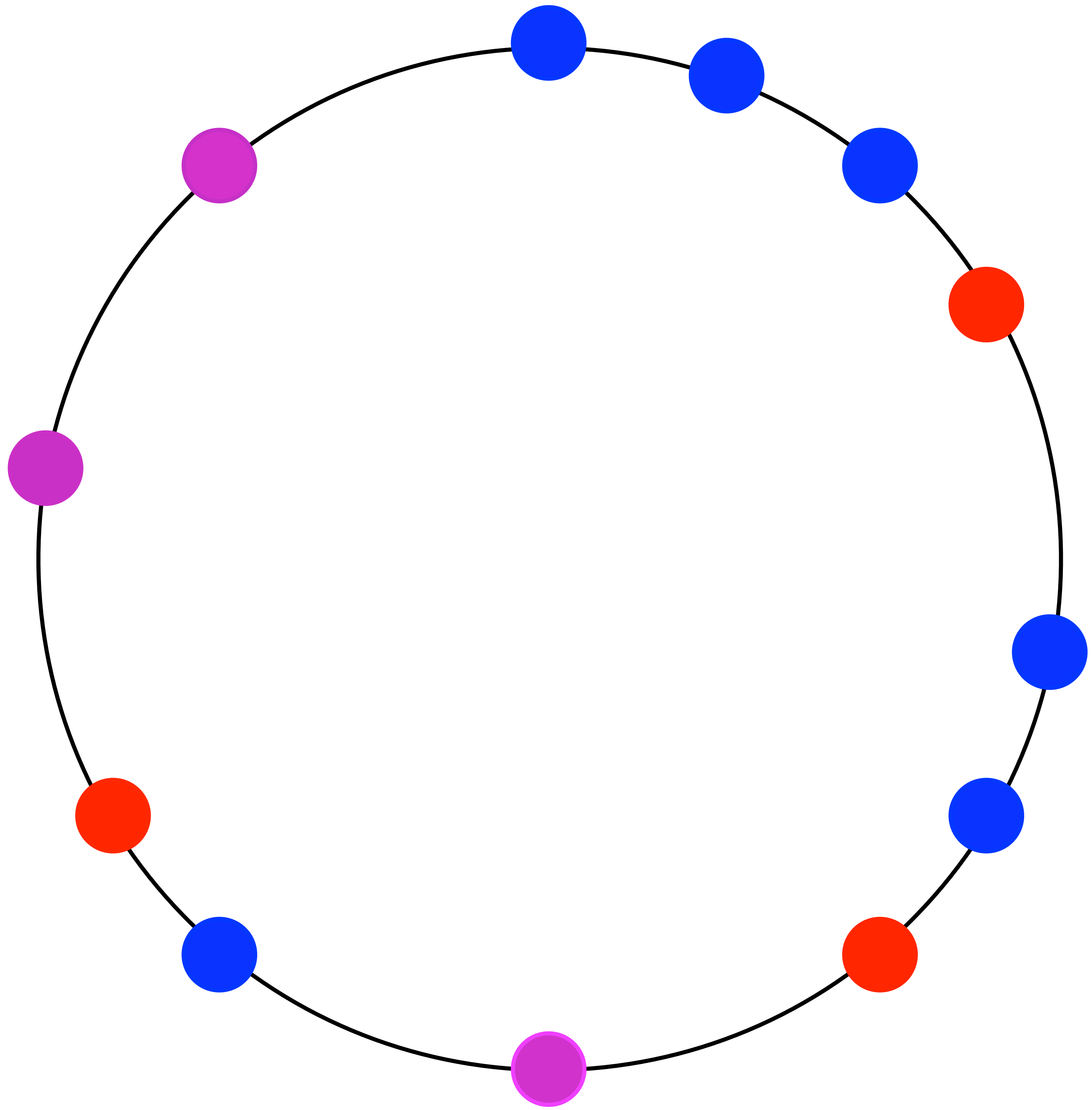


6 islands

Finite Ring (density > 1/2)

6 islands



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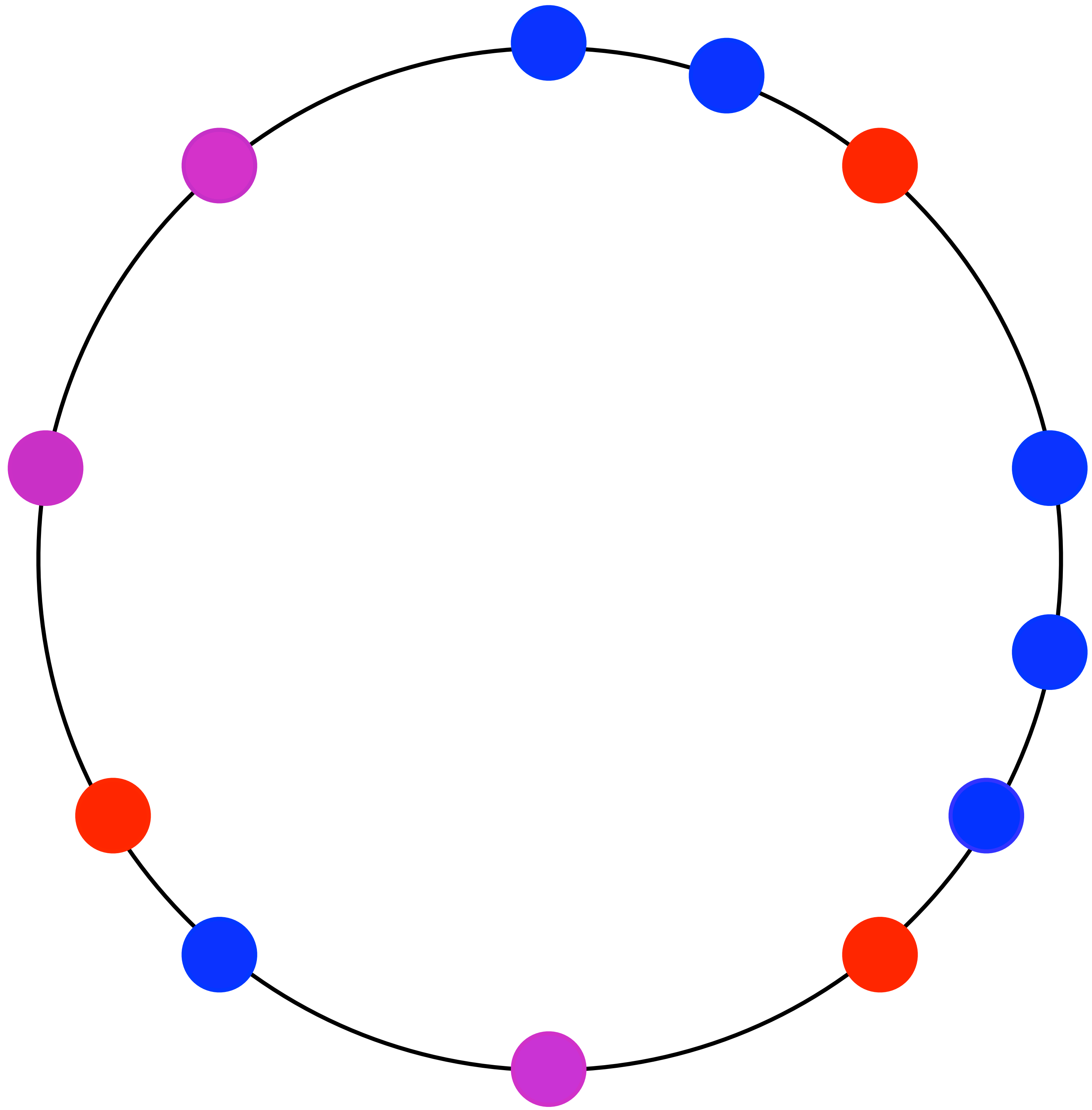

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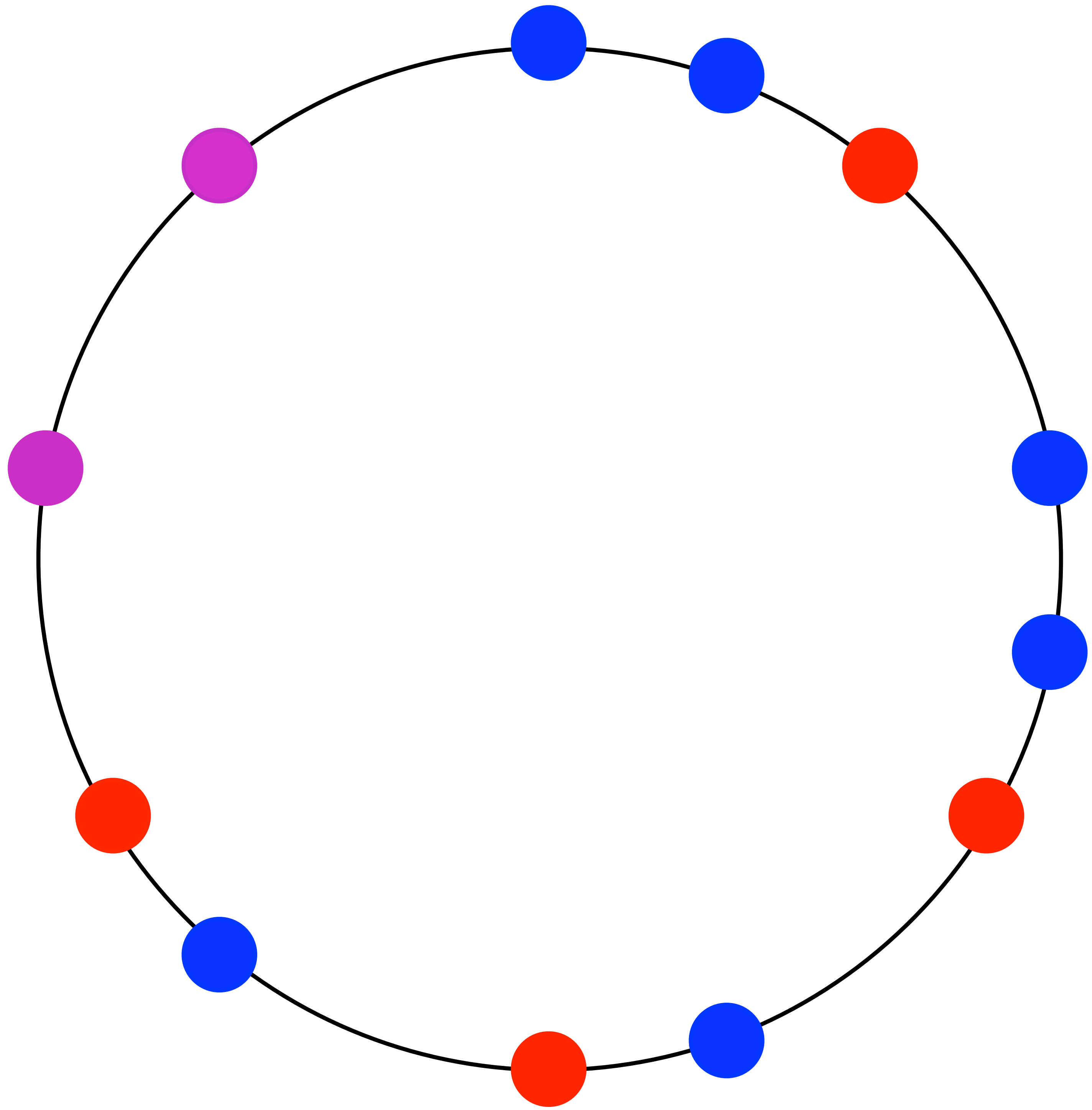

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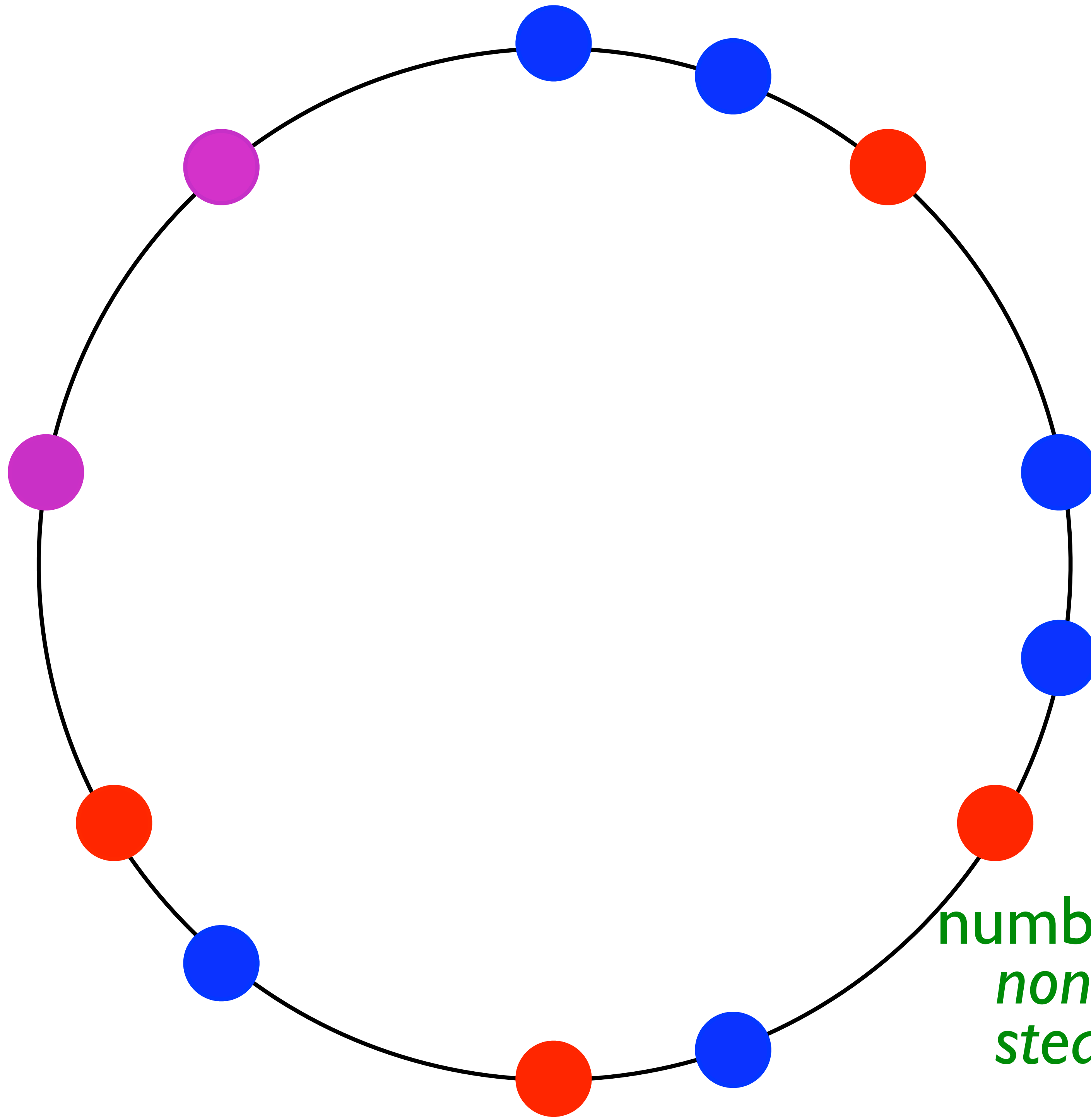
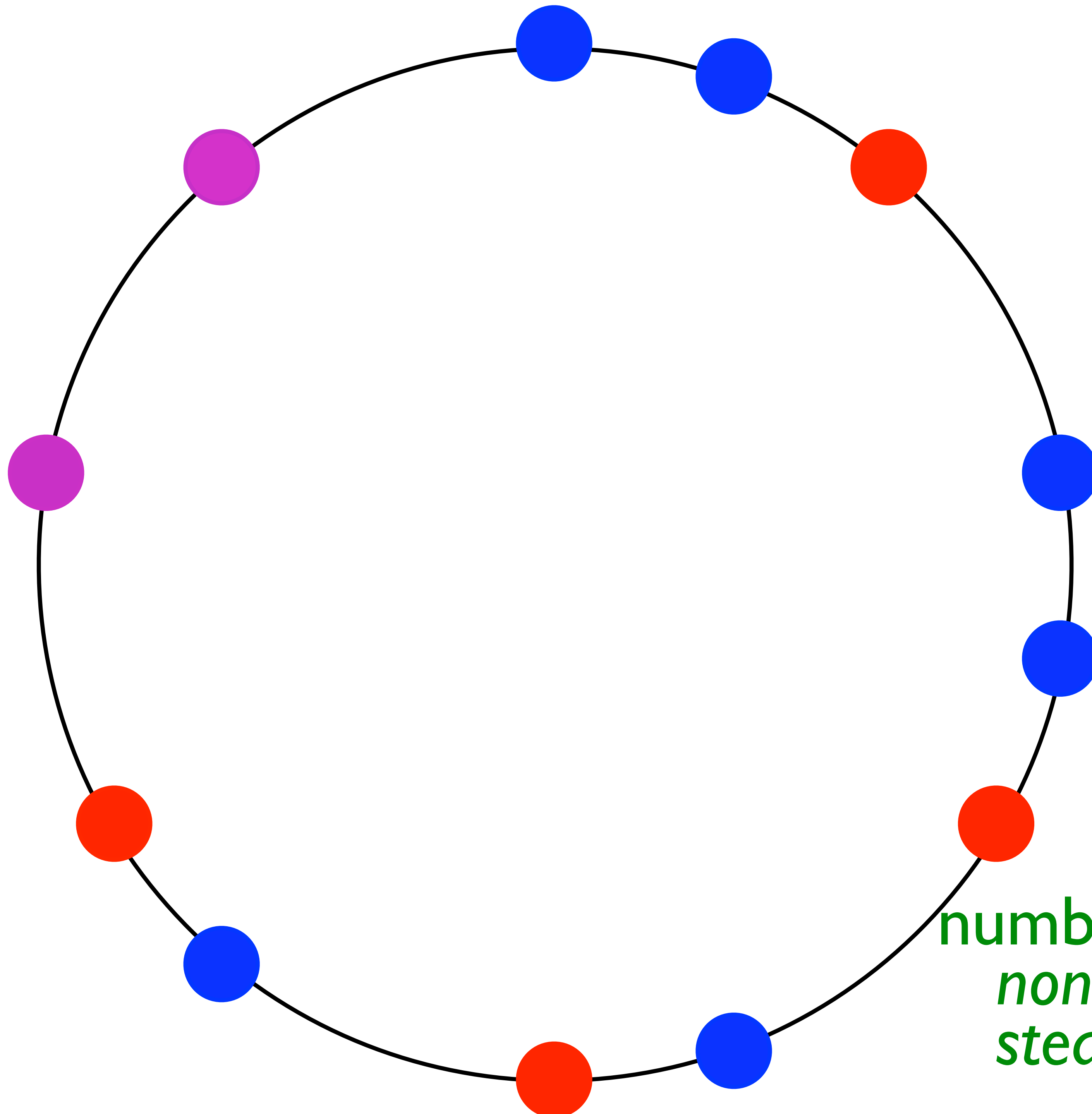


6 islands

number of islands:
non-decreasing until a steady state is achieved

Finite Ring (density > 1/2)



6 islands

number of islands:
non-decreasing until a steady state is achieved

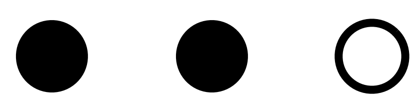
isolated vacancies

Equilibrium States on the Ring

claim: all maximal-island states are equiprobable

$$P(C)\sum_{C'} R(C\to C') = \sum_{C'} P(C')\,R(C'\to C)$$

# of active leading triplets



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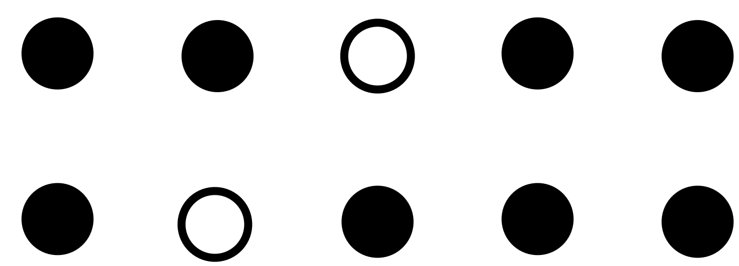


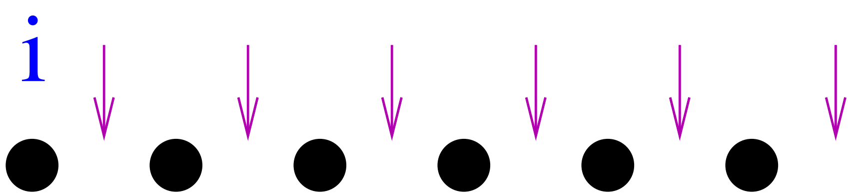
equilibrium states: P(C)= constant

Equilibrium States on the Ring

$$P(C) = \mathcal{C}^{-1}$$

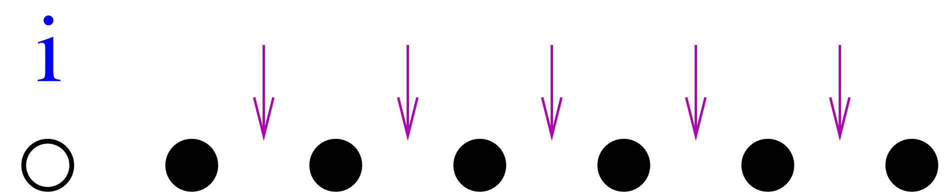
$\mathcal{C} =$ number of maximal-island configurations with N particles & V vacancies

if site i occupied:



N particles
N possibilities for V vacancies

if site i empty



N particles
N-1 possibilities for V vacancies

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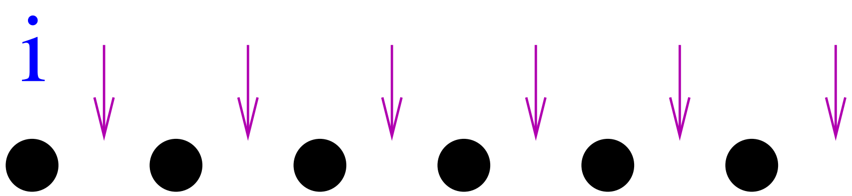

N particles
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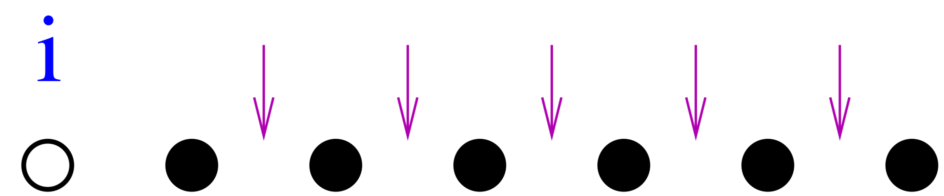


N particles
N-1 possibilities for V vacancies

$$\mathcal{C} = \binom{N}{V} + \binom{N-1}{V-1}$$

Steady States (SSs) for GRPs

When $\rho < \frac{1}{3}$, the steady states are maximal-island configurations with islands of vacant sites of length ≥ 2:

● ○ ○ ● ○ ○ ○ ● ○ ○ ○ ○ ● ○ ○ ● ○ ○ ○ ○

The total number of admissible maximal-island configurations is

$$\mathcal{C} = \frac{L}{N}\binom{V-N-1}{N-1}, \quad \rho < \frac{1}{3}$$

When $\frac{1}{3} < \rho < \frac{1}{2}$, admissible maximal-island configurations have islands of vacant sites of length 1 or 2:

● ○ ○ ● ○ ○ ● ○ ● ○ ○ ● ○ ○ ● ○ ● ○ ● ○

$$\mathcal{C} = \frac{L}{N}\binom{N}{V-N}$$

Generally for the GRP with Hamiltonian

$$\mathcal{H}_m = J_1 \sum n_i n_{i+1} + \ldots + J_m \sum n_i n_{i+m}$$

the steady state current in the low-density region ($\rho < \frac{1}{2}$) is given by

$$J(\rho) = \begin{cases} \frac{\rho[1-(m+1)\rho]}{1-m\rho} & 0 < \rho < \frac{1}{m+1} \\ \frac{[(k+1)\rho-1][1-k\rho]}{\rho} & \frac{1}{k+1} < \rho < \frac{1}{k} \end{cases}$$

where $k = 2, 3, \ldots, m$.

In the high-density region ($\frac{1}{2} < \rho < 1$) we determine the steady state current from the mirror symmetry $J(\rho) = J(1-\rho)$.

Correlation Functions

We consider only the simplest RP and the low-density phase.

$$\langle n_i n_j \rangle_c \equiv \langle n_i n_j \rangle - \rho^2 = \rho(1-\rho)\left(-\frac{\rho}{1-\rho}\right)^{|j-i|}$$

$$\langle n_i n_j n_k \rangle = \frac{\langle n_i n_j \rangle \langle n_j n_k \rangle}{\langle n_j \rangle} \qquad \text{for all } i \leq j \leq k.$$

This is reminiscent to the Kirkwood's superposition approximation.

$$\left\langle \prod_{a=1}^{k} n_{i_a} \right\rangle = \frac{1}{\rho^{k-2}} \prod_{a=1}^{k-1} \langle n_{i_a} n_{i_{a+1}} \rangle$$

Diffusion Coefficient

The idea is to apply a Green-Kubo formula (Spohn, 1991). Schematically it reads

$$D(\rho) = \frac{J(\rho)}{\chi(\rho)} - \int_0^\infty dt\, C(t)$$

This integral contribution has never been computed, apart from a few cases where it has been proven to be zero. This occurs for a $1d$ lattice gase if the current can be written in a gradient form. The RP satisfies this requirement.

Thus we need to compute:

The current $J(\rho)$ in the **asymmetric** version (known).

The compressibility $\chi(\rho) = \sum_{\ell=-\infty}^{\infty} \langle n_0 n_\ell \rangle_c$

Compressibility

For the simplest RP: $\chi(\rho) = \rho(1-\rho)|1-2\rho|$

Generally one gets (in the low-density regime):

$$\chi = \begin{cases} \rho[1-(m+1)\rho][1-m\rho] & 0 < \rho < \frac{1}{m+1} \\ \rho[(k+1)\rho - 1][1-k\rho] & \frac{1}{k+1} < \rho < \frac{1}{k} \end{cases}$$

$$D(\rho) = \begin{cases} (1-m\rho)^{-2} & 0 < \rho < \frac{1}{m+1} \\ \rho^{-2} & \frac{1}{m+1} < \rho < \frac{1}{2} \\ (1-\rho)^{-2} & \frac{1}{2} < \rho < \frac{m}{m+1} \\ (m\rho - m + 1)^{-2} & \frac{m}{m+1} < \rho < 1 \end{cases}$$

What have we learned?

- We must understand the structure of equilibrium states and be able to compute simple correlation functions. This is why we cannot say anything about RPs in two dimensions.
- The Green-Kubo formula is applicable since the gradient condition holds for the RPs.

Back to Limiting Shapes: Corner Problem and RP

PLK, J. Stat. Mech. (2013)

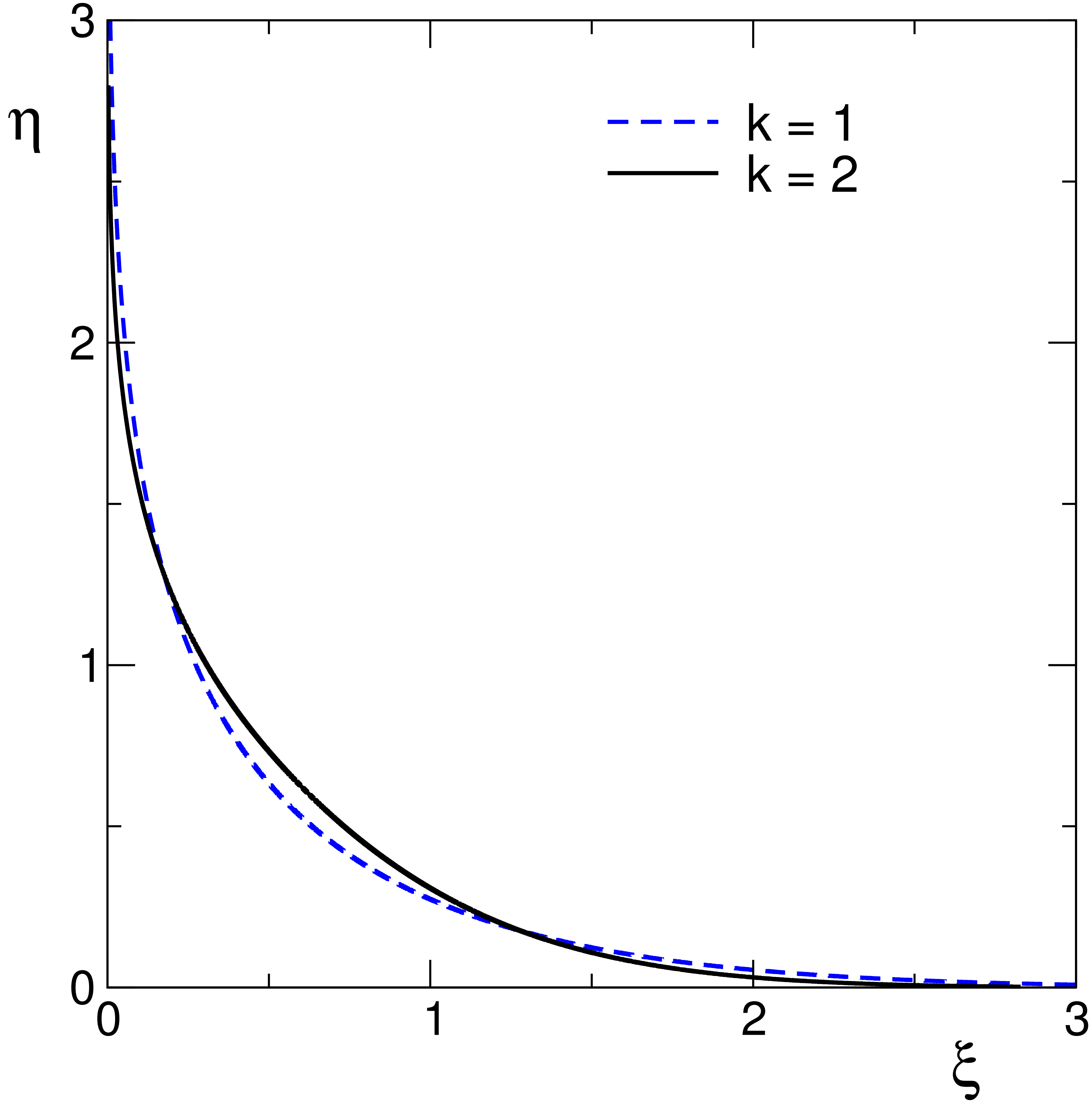
$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial z}\left[D(\rho)\,\frac{\partial \rho}{\partial z}\right]$$

$$D(\rho) = \begin{cases} (1-\rho)^{-2} & 0 < \rho < \frac{1}{2} \\ \rho^{-2} & \frac{1}{2} < \rho < 1 \end{cases}$$

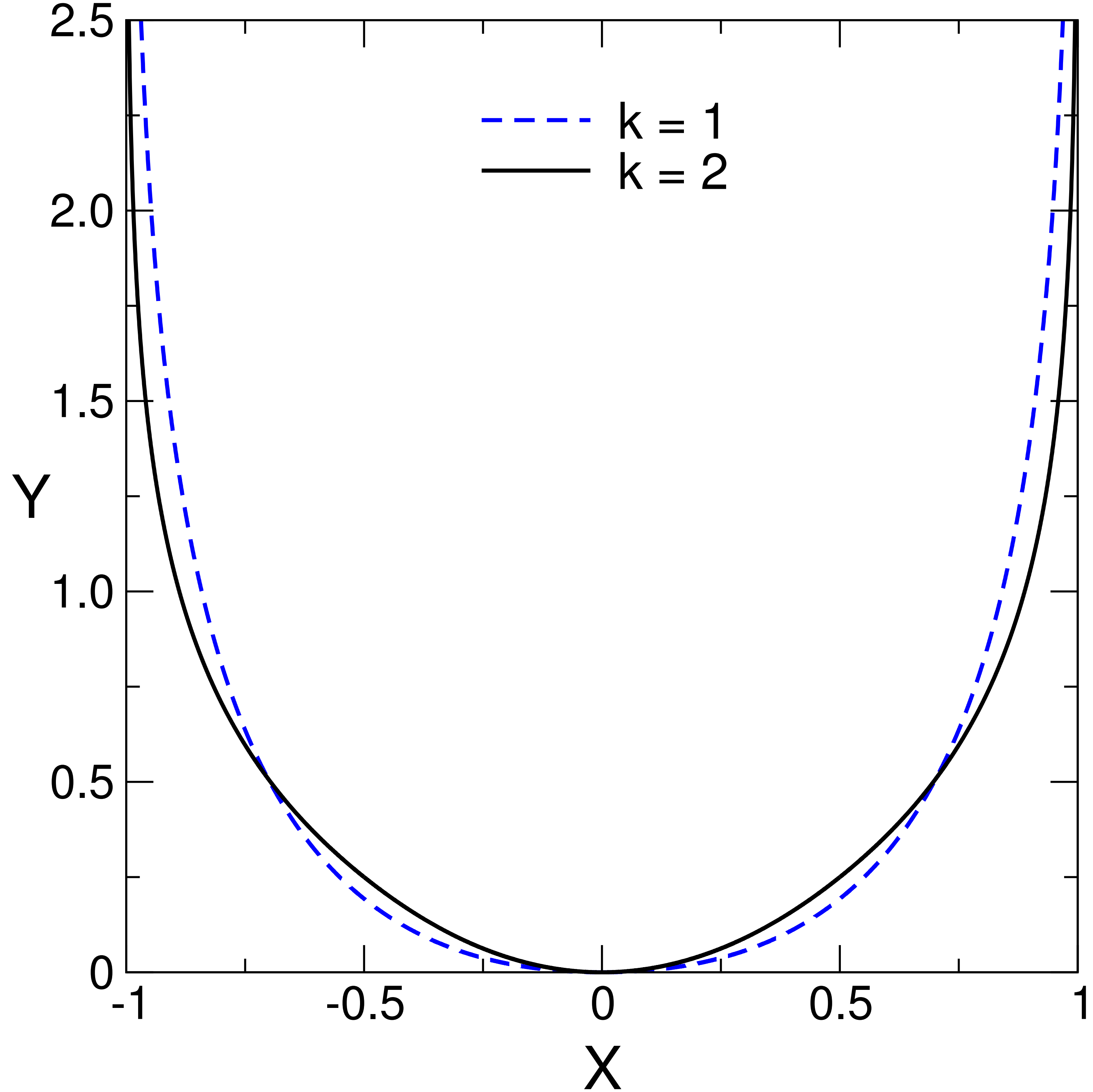
$$\rho(z, t=0) = \begin{cases} 1 & z < 0 \\ 0 & z > 0 \end{cases}$$

$$\rho(z,t) = f(\zeta), \quad \zeta = \frac{z}{\sqrt{4t}}$$

PLK and Jason Olejarz, PRE (2013)



Ising Finger



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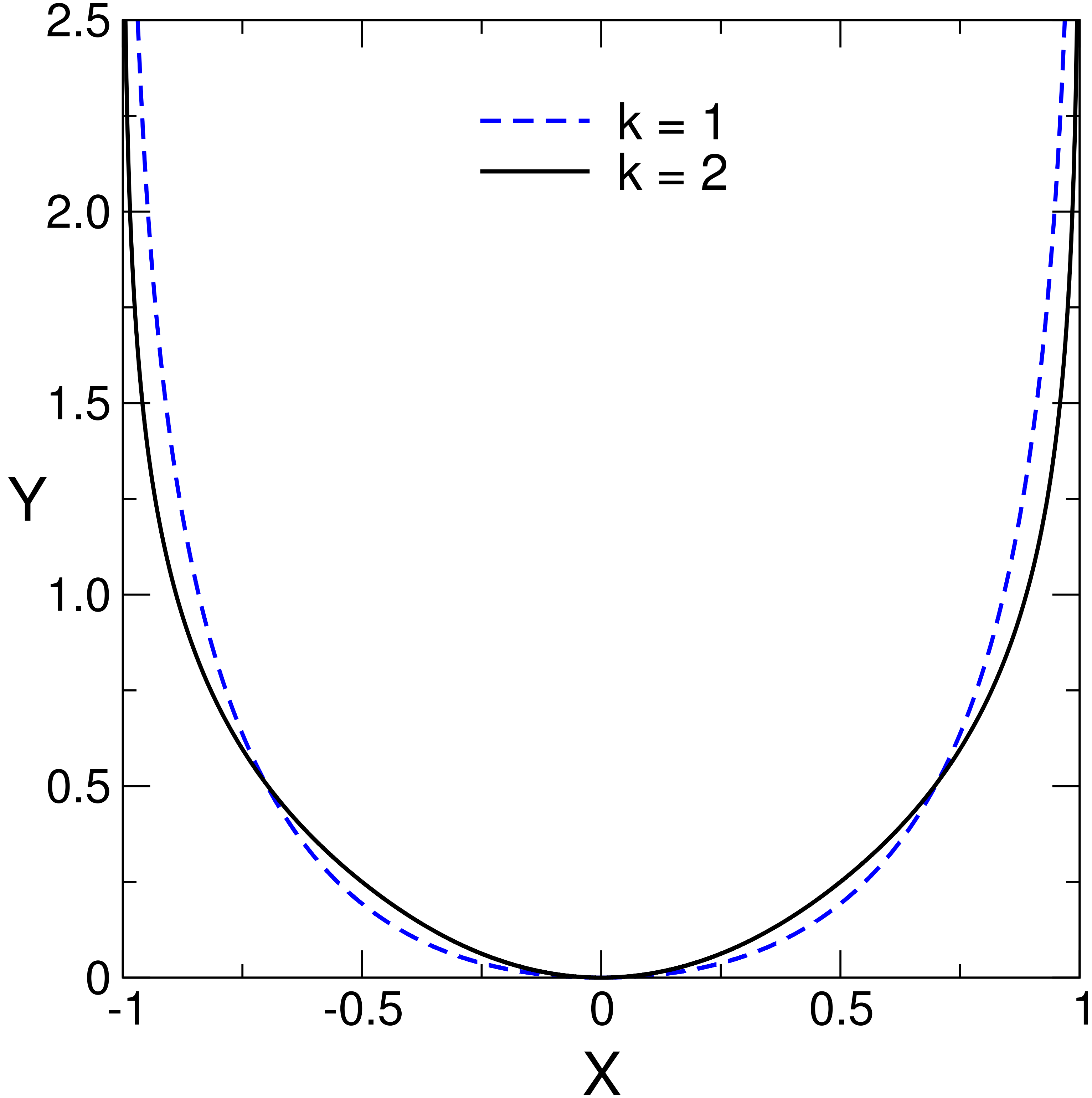
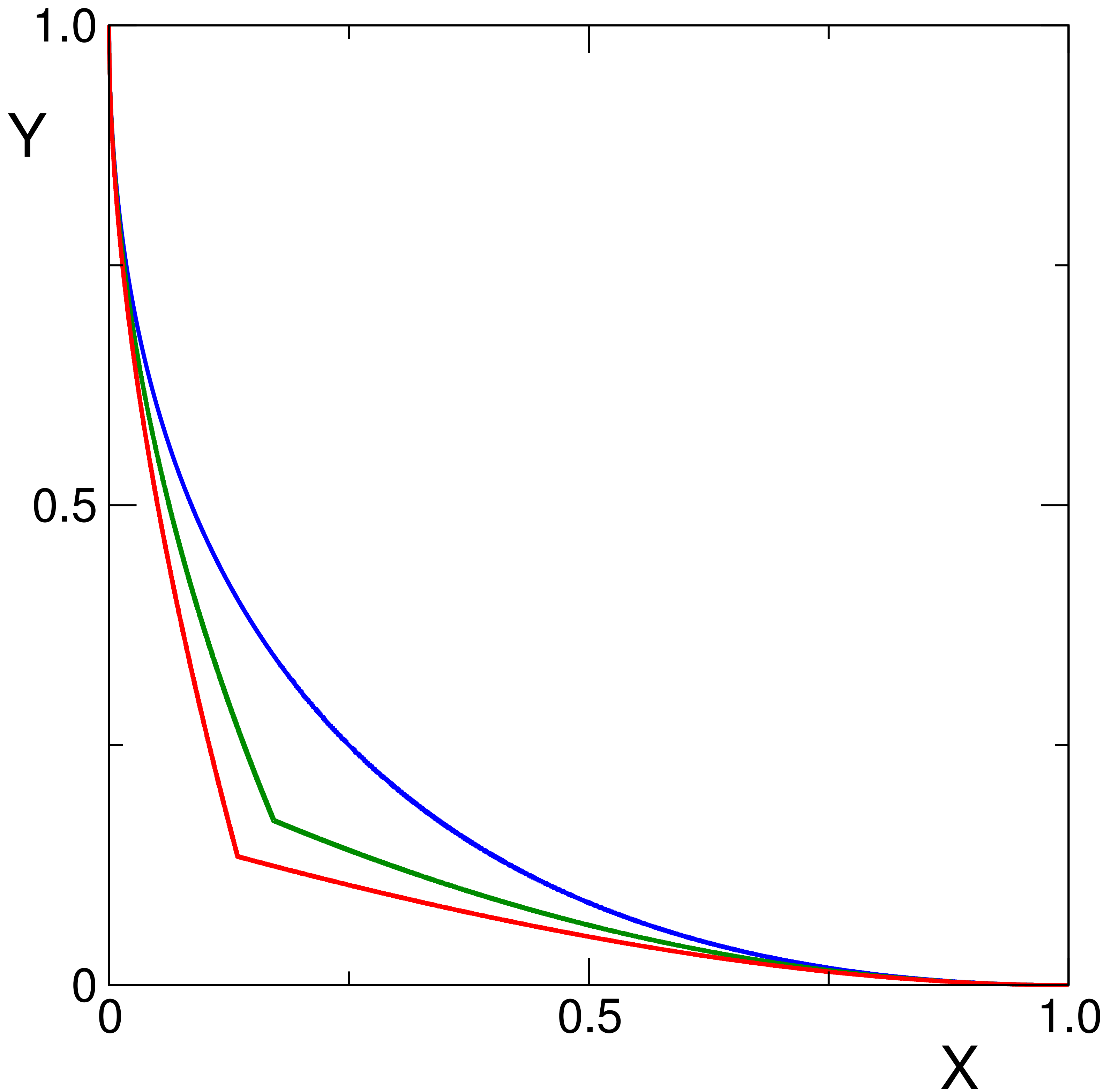


$$y_t = \frac{y_{xx}}{(1+y_x)^2}\,, \quad y_x > 0$$

$$y_t = y_{xx}\,, \qquad 0 < y_x < 1$$

$$y_t = \frac{y_{xx}}{y_x^2}\,, \qquad 1 < y_x < \infty$$

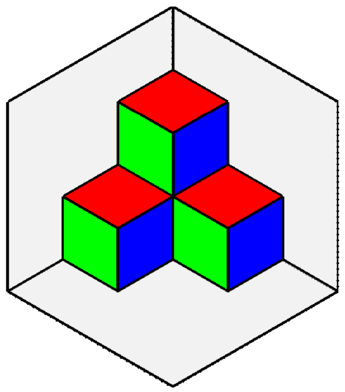
Corner in a Magnetic Field



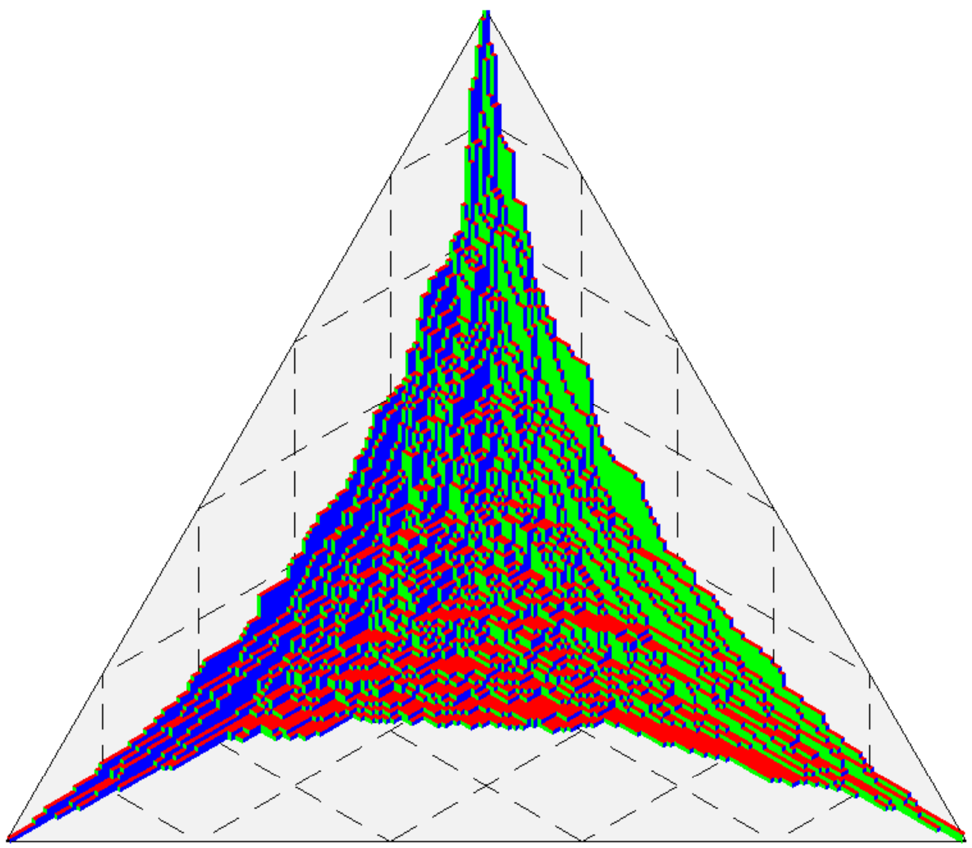
Magnetic Field => Totally Asymmetric RPs

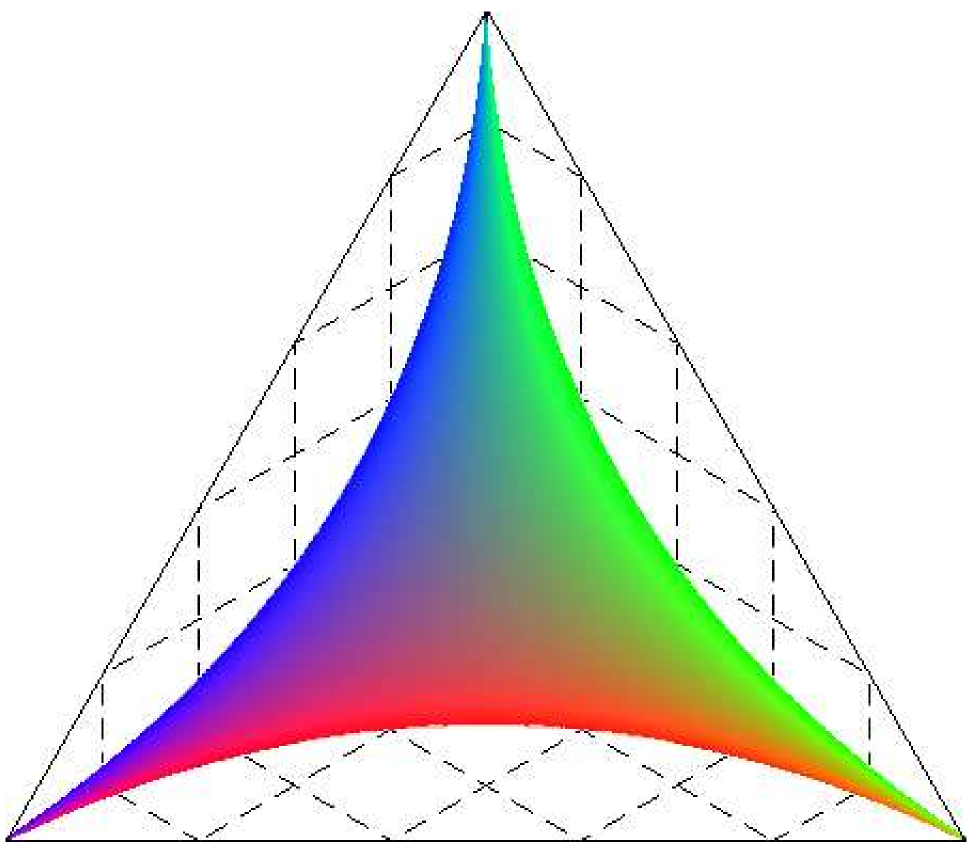
$$\frac{\partial\rho}{\partial t}+\frac{\partial J}{\partial z}=0 \qquad J(\rho)=\begin{cases}\frac{\rho(1-2\rho)}{1-\rho} & 0<\rho<\frac{1}{2}\\ \frac{(1-\rho)(2\rho-1)}{\rho} & \frac{1}{2}<\rho<1\end{cases}$$

$$J(\rho)=\begin{cases}\frac{\rho(1-3\rho)}{1-2\rho} & 0<\rho<\frac{1}{3}\\ \frac{(1-2\rho)(3\rho-1)}{\rho} & \frac{1}{3}<\rho<\frac{1}{2}\\ \frac{(2\rho-1)(2-3\rho)}{1-\rho} & \frac{1}{2}<\rho<\frac{2}{3}\\ \frac{(1-\rho)(3\rho-2)}{2\rho-1} & \frac{2}{3}<\rho<1\end{cases}$$



Pure Growth in 3D





$$z_t = \frac{z_x}{z_x - 1}\,\frac{z_y}{z_y - 1}\left[1 - \frac{1}{z_x + z_y}\right]$$

Arguments in favor of the evolution equation

In two dimensions the correct equation is $y_t = \frac{1}{1 - \frac{1}{y_x}}$

In three dimensions one guesses $z_t = \frac{1}{1 - \frac{1}{z_x}} \frac{1}{1 - \frac{1}{z_y}}$

It reduces to correct equations on $x = 0$ and $y = 0$

But is not invariant under $x \leftrightarrow z$ (or $y \leftrightarrow z$)

An equation with required properties is

$$z_t = \frac{1 - \frac{1}{z_x + z_y}}{\left(1 - \frac{1}{z_x}\right)\left(1 - \frac{1}{z_y}\right)}$$

Too many equations...

$$z_t = \frac{1 - \frac{1}{z_x + z_y}}{\left(1 - \frac{1}{z_x}\right)\left(1 - \frac{1}{z_y}\right)}$$

$$\frac{1}{z_t} = 1 - \frac{1}{z_x} - \frac{1}{z_y} \qquad \longrightarrow \qquad \sqrt{x} + \sqrt{y} + \sqrt{z} = \sqrt{t}$$

The former equation is also solvable by method of characteristics, or treating it as a Hamilton-Jacobi equation.

In the $(1,1,1)$ direction:
$$\begin{array}{ll} x = y = z = t \times 0.126 & \text{(simulations)} \\ x = y = z = t/8 & \text{(first eq)} \\ x = y = z = t/9 & \text{(second eq)} \end{array}$$

Higher Dimensions

$$(2D) \quad h_t = \frac{1}{1 - \frac{1}{h_x}}$$

$$(3D) \quad h_t = \frac{1 - \frac{1}{h_x + h_y}}{\left(1 - \frac{1}{h_x}\right)\left(1 - \frac{1}{h_y}\right)}$$

Higher Dimensions

$$(2D) \quad h_t = \frac{1}{1 - \frac{1}{h_x}}$$

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$$(4D) \quad h_t = \frac{\left(1 - \frac{1}{h_x + h_y}\right)\left(1 - \frac{1}{h_y + h_z}\right)\left(1 - \frac{1}{h_z + h_x}\right)}{\left(1 - \frac{1}{h_x}\right)\left(1 - \frac{1}{h_y}\right)\left(1 - \frac{1}{h_y}\right)\left(1 - \frac{1}{h_x + h_y + h_z}\right)}$$

Evolution equations in the Ising case

$$(2D) \quad h_t = \frac{1}{\left(1 - \frac{1}{h_x}\right)^2} \frac{h_{xx}}{h_x^2}$$

$$(3D) \quad h_t = \left[\frac{\left(1 - \frac{1}{h_x + h_y}\right)}{\left(1 - \frac{1}{h_x}\right)\left(1 - \frac{1}{h_y}\right)}\right]^2 \left[\frac{h_{xx}}{h_x^2} - \frac{h_{xy}}{h_x h_y} + \frac{h_{yy}}{h_y^2}\right]$$

Broad Lessons

- Lattice gas techniques are useful in studying limiting shapes. These techniques are very general, but efficient results are established in models which could be mapped onto simple lattice gases.
- A by-product is a class of new `integrable' lattice gases, repulsion processes.
- No serious advance in three and higher dimensions; an infinite set of amusing evolution equation, but no derivation of these equations.


The End