Diffusive Lattice Gases: Transport Coefficients and Large Deviations

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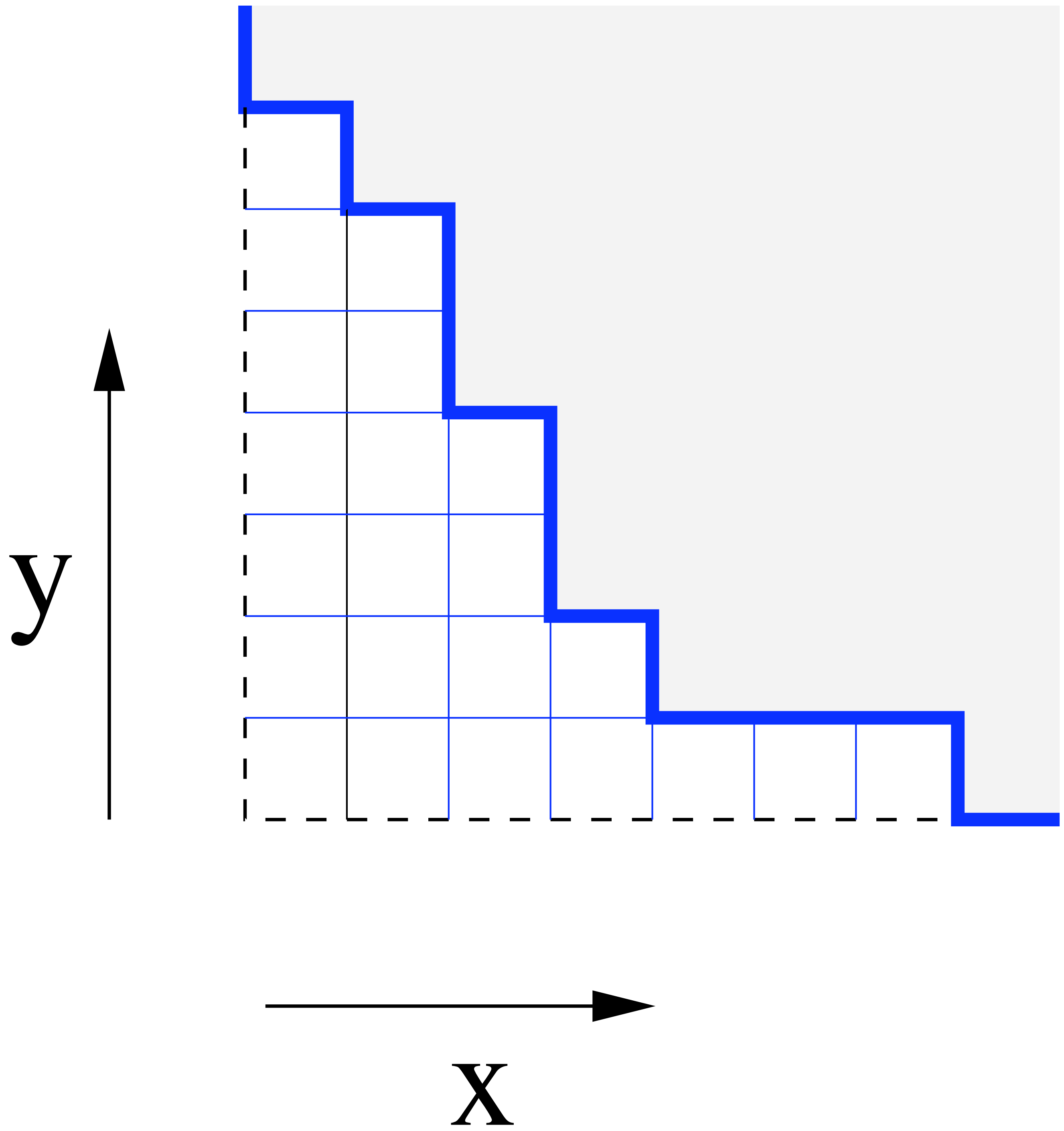
Plans and Motivation

- Tractable lattice gases: Repulsion Processes (RPs), Exclusion Processes with Avalanches (EPA), etc.
- Lattice gases shed light on fundamental issues such as derivation of hydrodynamic equations for dense gases, large deviations, etc.
- Many of these insights were gained from simplest models like simple exclusion processes (SEPs); the hope is to learn more by using RPs as a vehicle.

Emergence of RPs

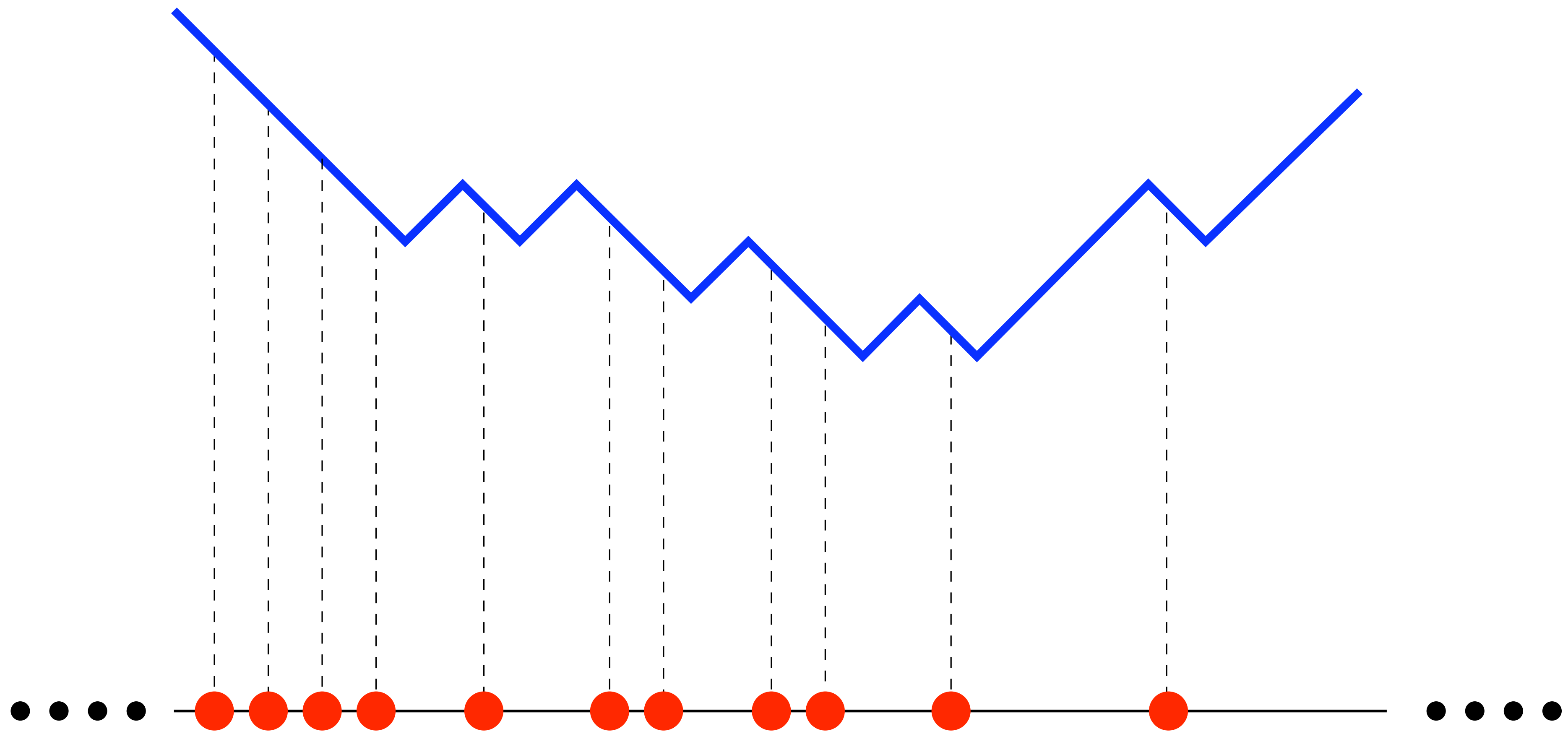
- 2D Ising Model with a zero temperature spin-flip (Glauber) dynamics.
- Evolution of an interface is described by the SEP (in one basic example).
- RPs emerge when we consider Ising models with long-ranged interactions.

Simplest Ising Interface



Equivalent to *Asymmetric* Exclusion Process

downslope → particle
upslope → hole



Ising Model with NNN interactions (RP)

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

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

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

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

Repulsion Process, Hydrodynamic Approach

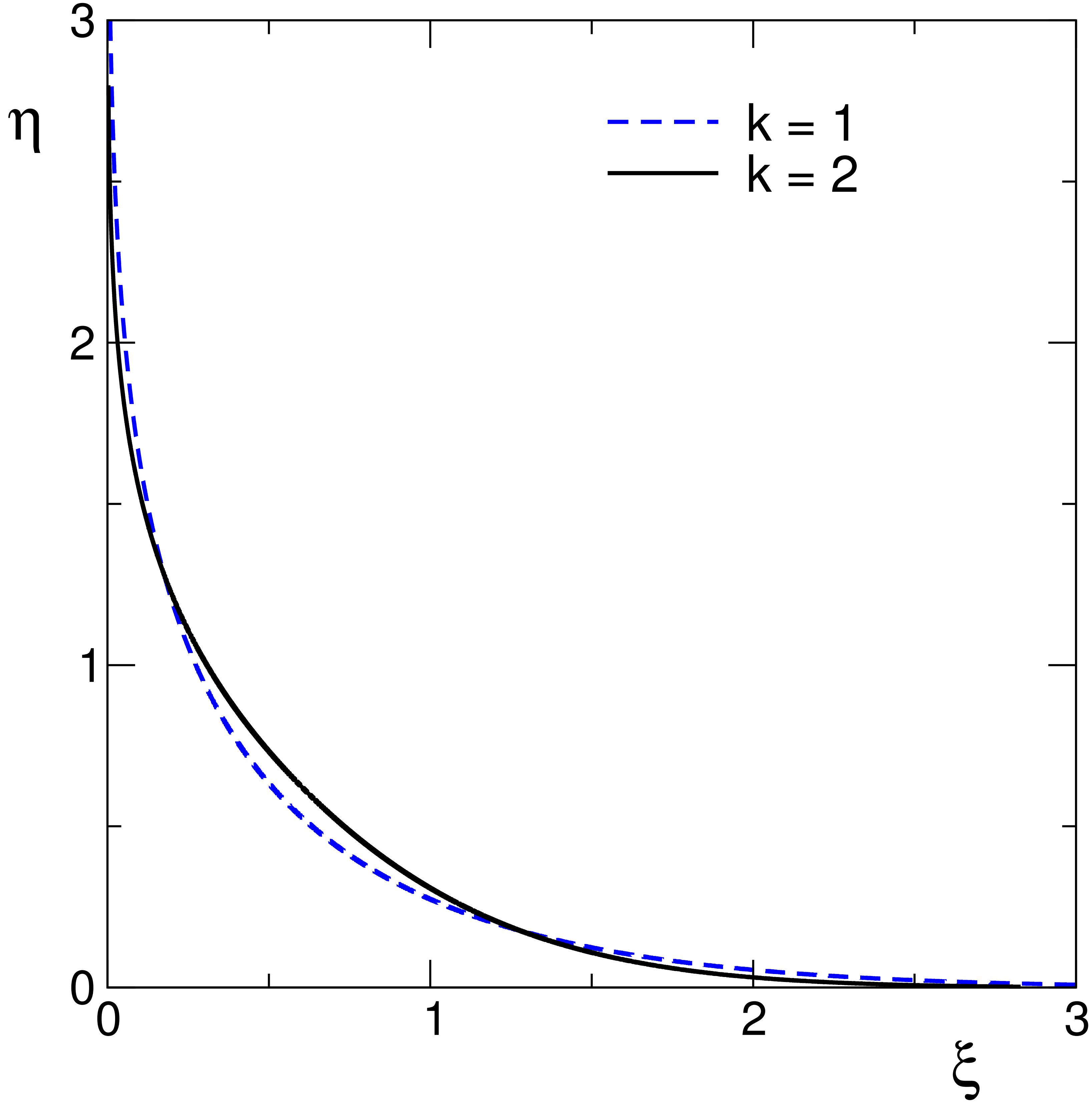
PLK, J. Stat. Mech. (2013)

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

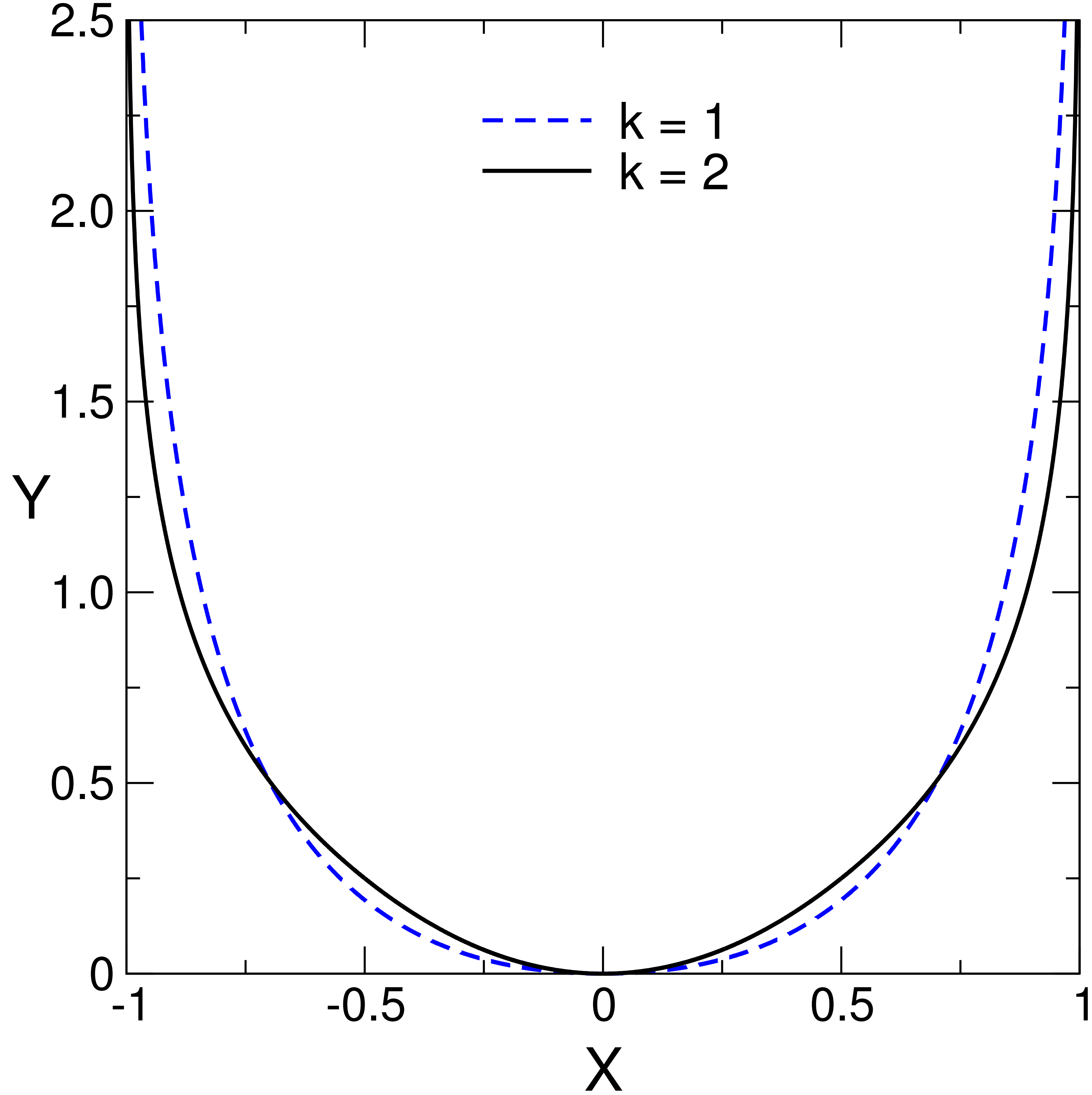
$$D(\rho) = \begin{cases} (1-\rho)^{-2} & 0 < \rho < \frac{1}{2} \\ \rho^{-2} & \frac{1}{2} < \rho < 1 \end{cases}$$

$$\rho(z, t=0) = \begin{cases} 1 & z < 0 \\ 0 & z > 0 \end{cases} \qquad\qquad \rho(z,t) = f(\zeta), \quad \zeta = \frac{z}{\sqrt{4t}}$$

PLK and Jason Olejarz, PRE (2013)



Ising Finger



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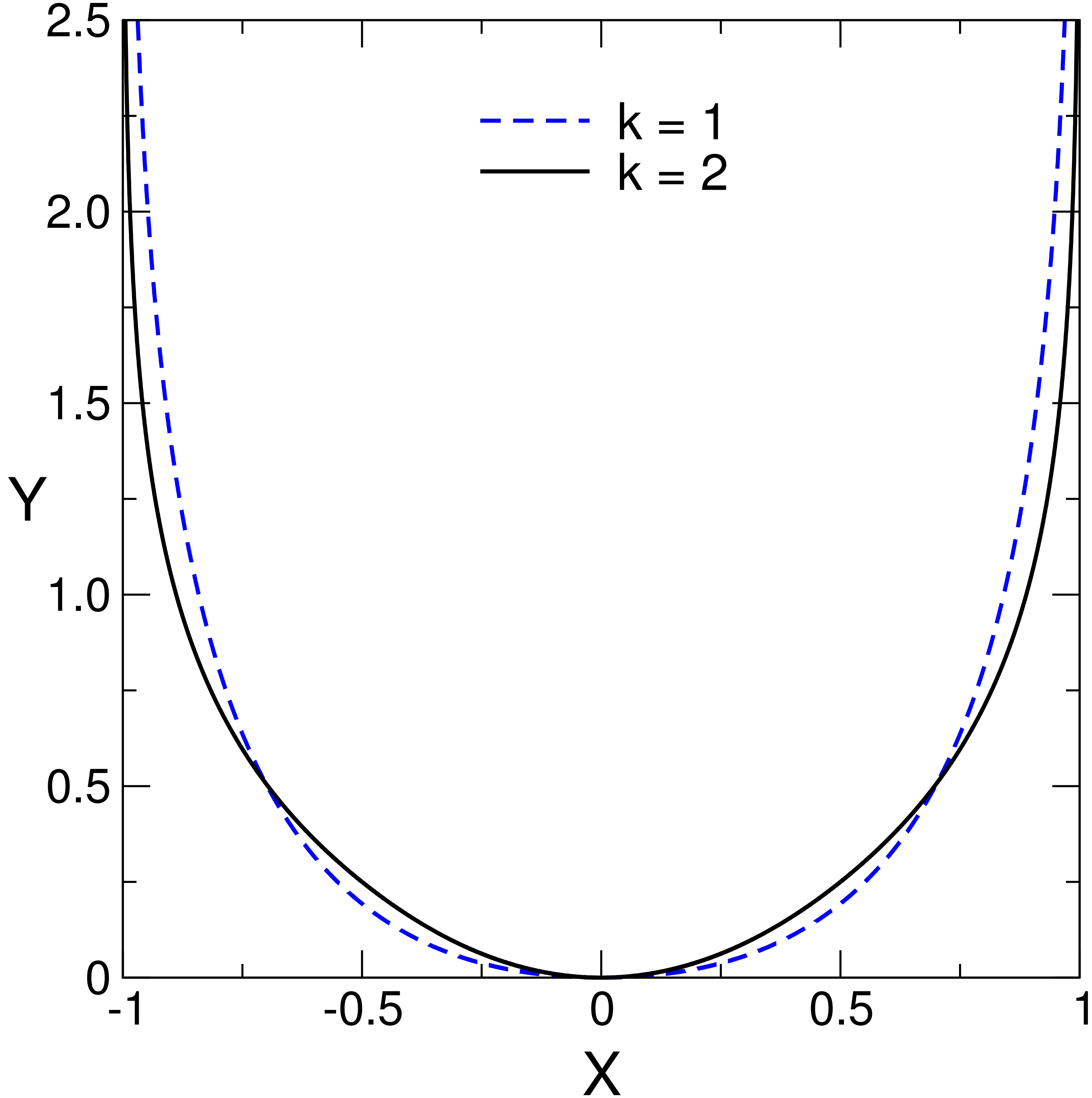
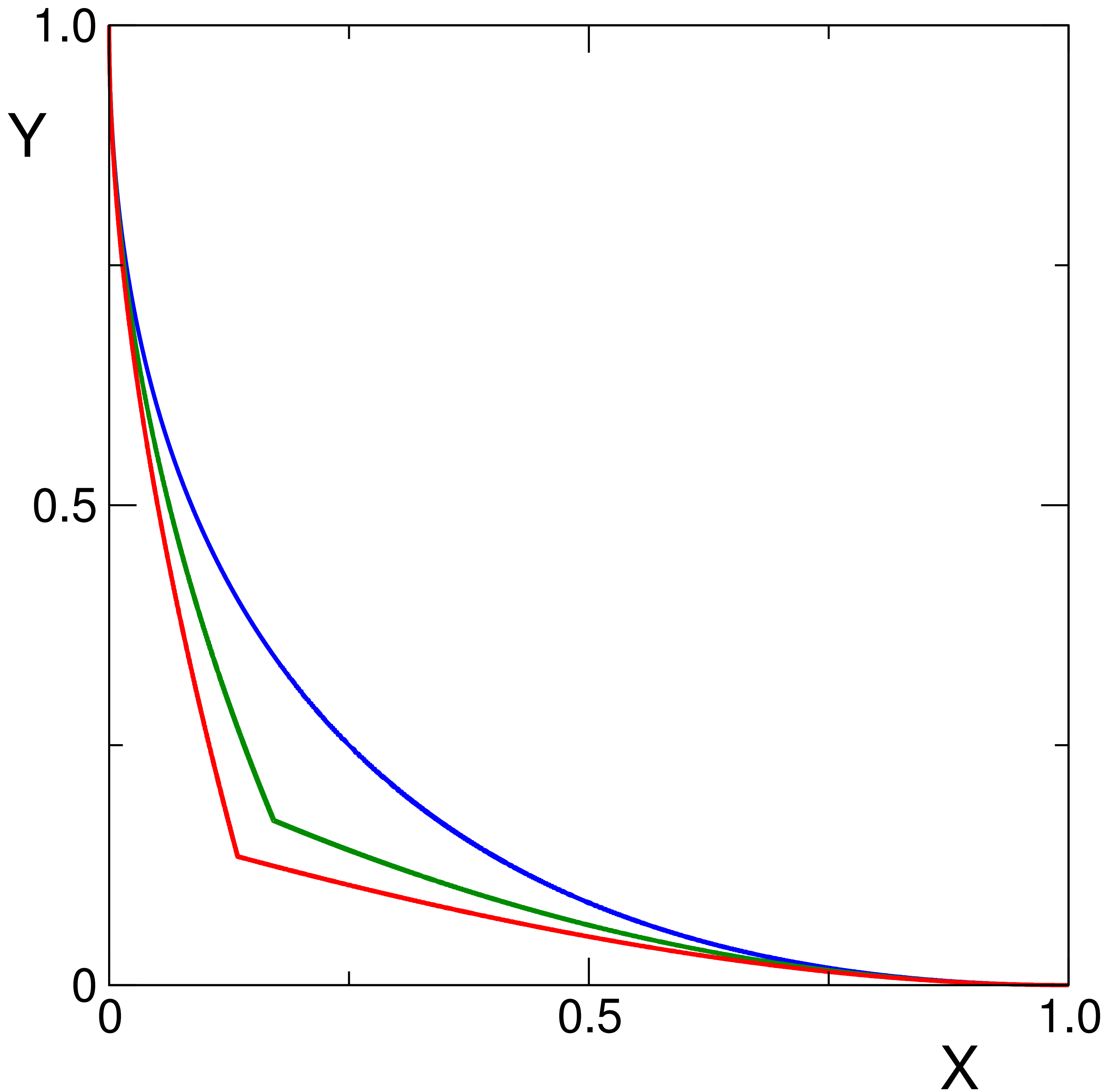


$$y_t = \frac{y_{xx}}{(1+y_x)^2}\,, \quad y_x > 0$$

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

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

Corner in a Magnetic Field



Magnetic Field => Totally Asymmetric RPs

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

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

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.

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

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

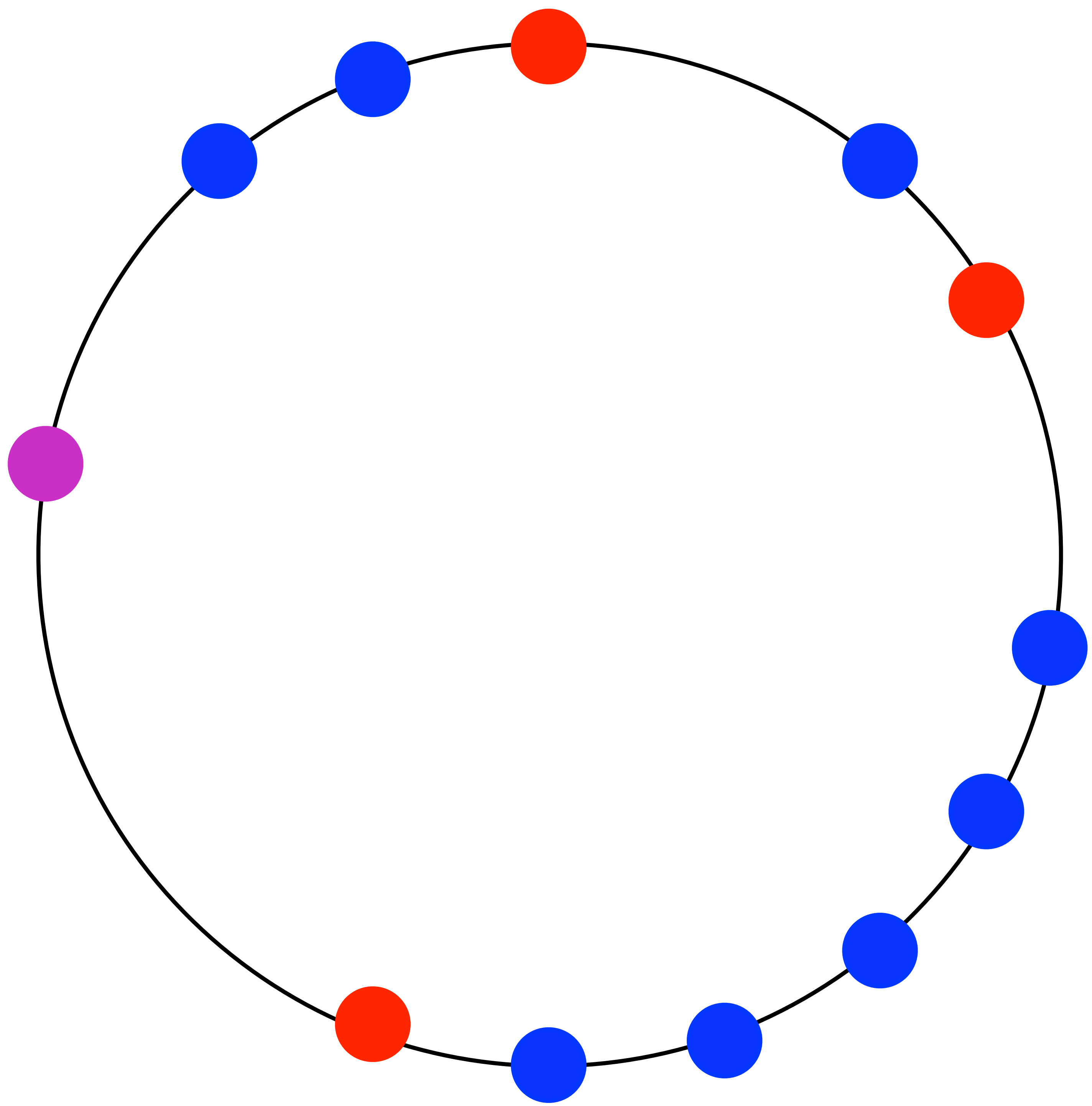
Then the magnitudes of J's are irrelevant and
we can treat interactions in a lexicographic order.

Steady States

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

Finite Ring (density > 1/2)

4 islands



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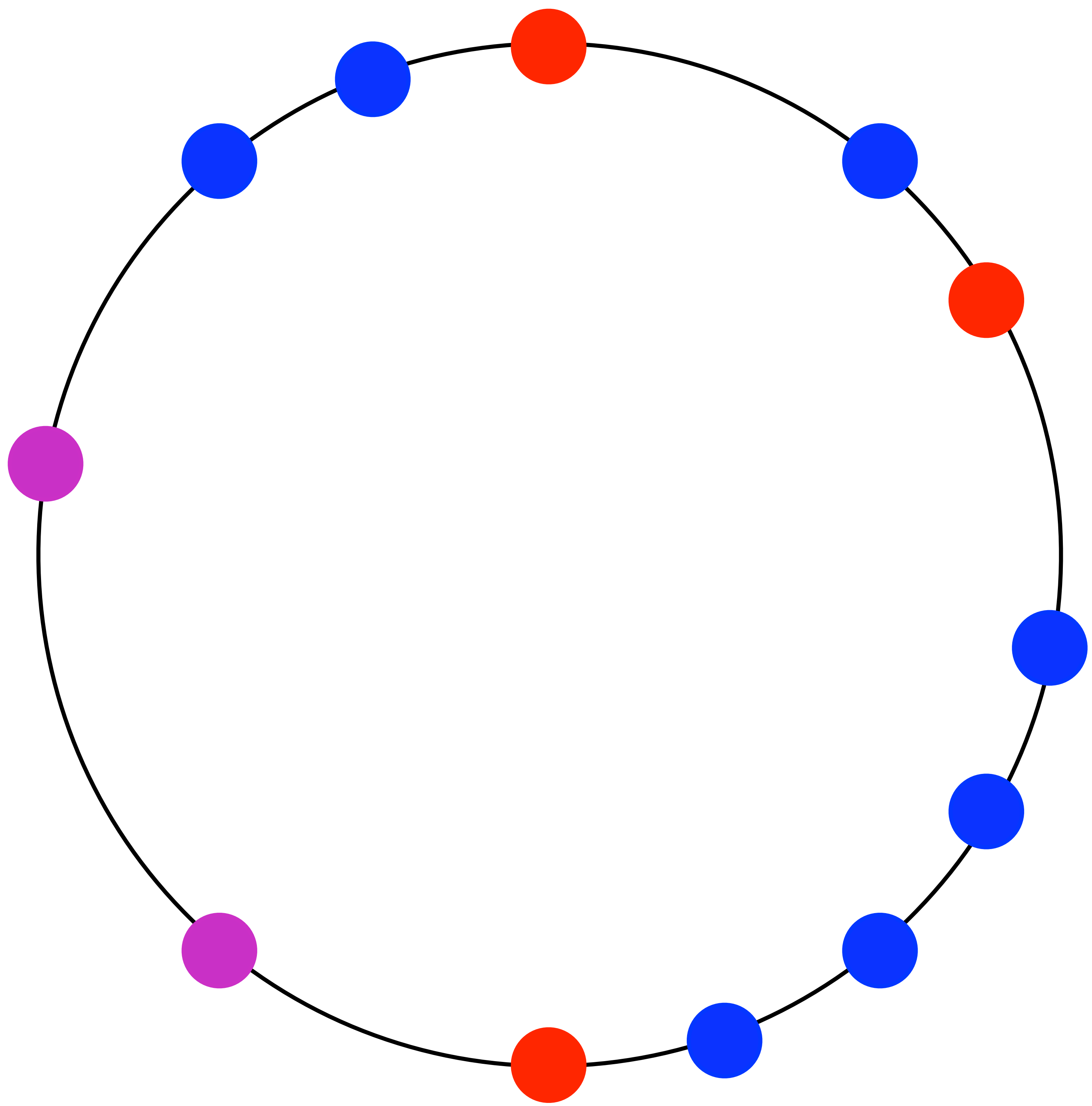

5 islands

Finite Ring (density > 1/2)

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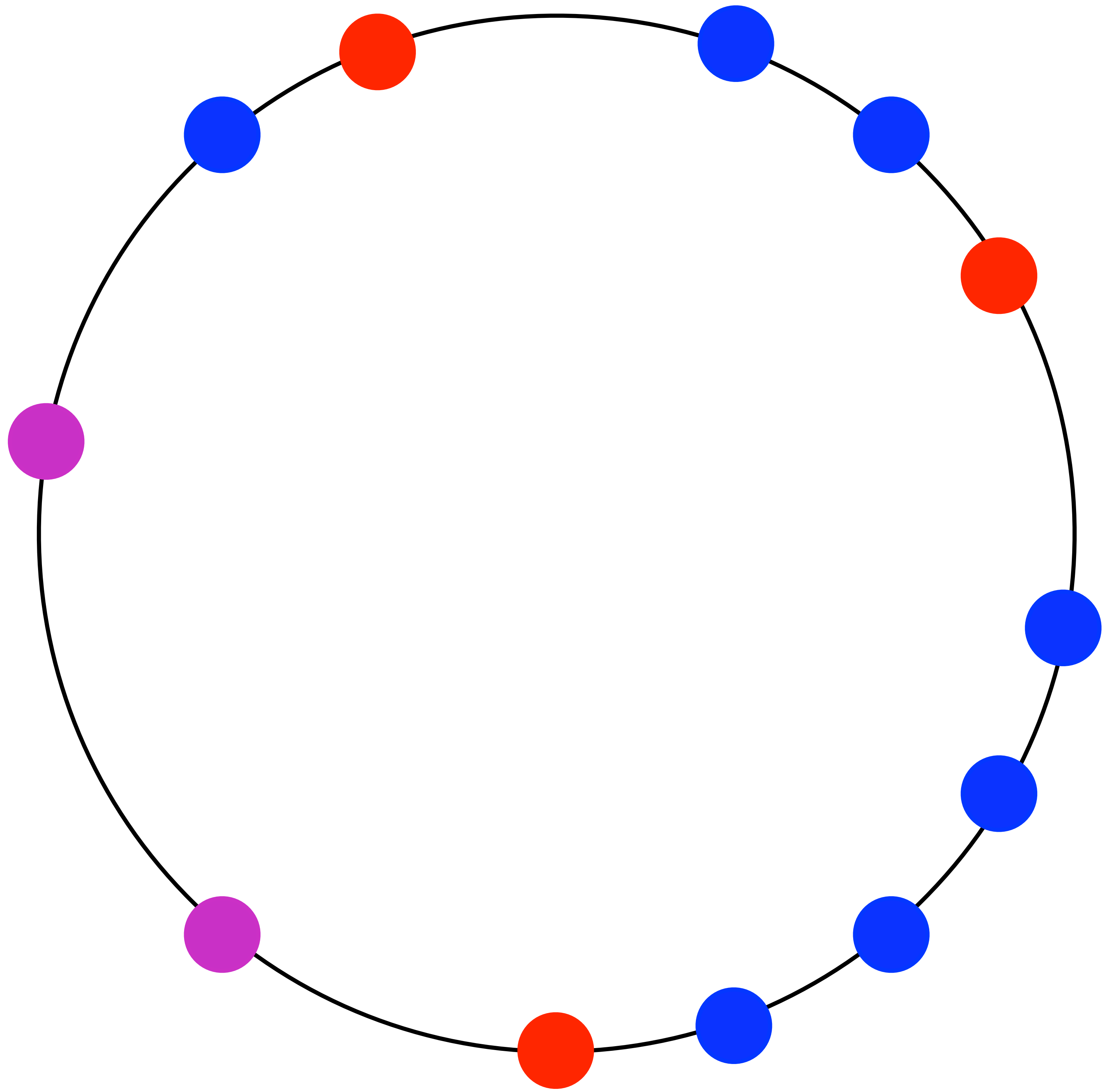

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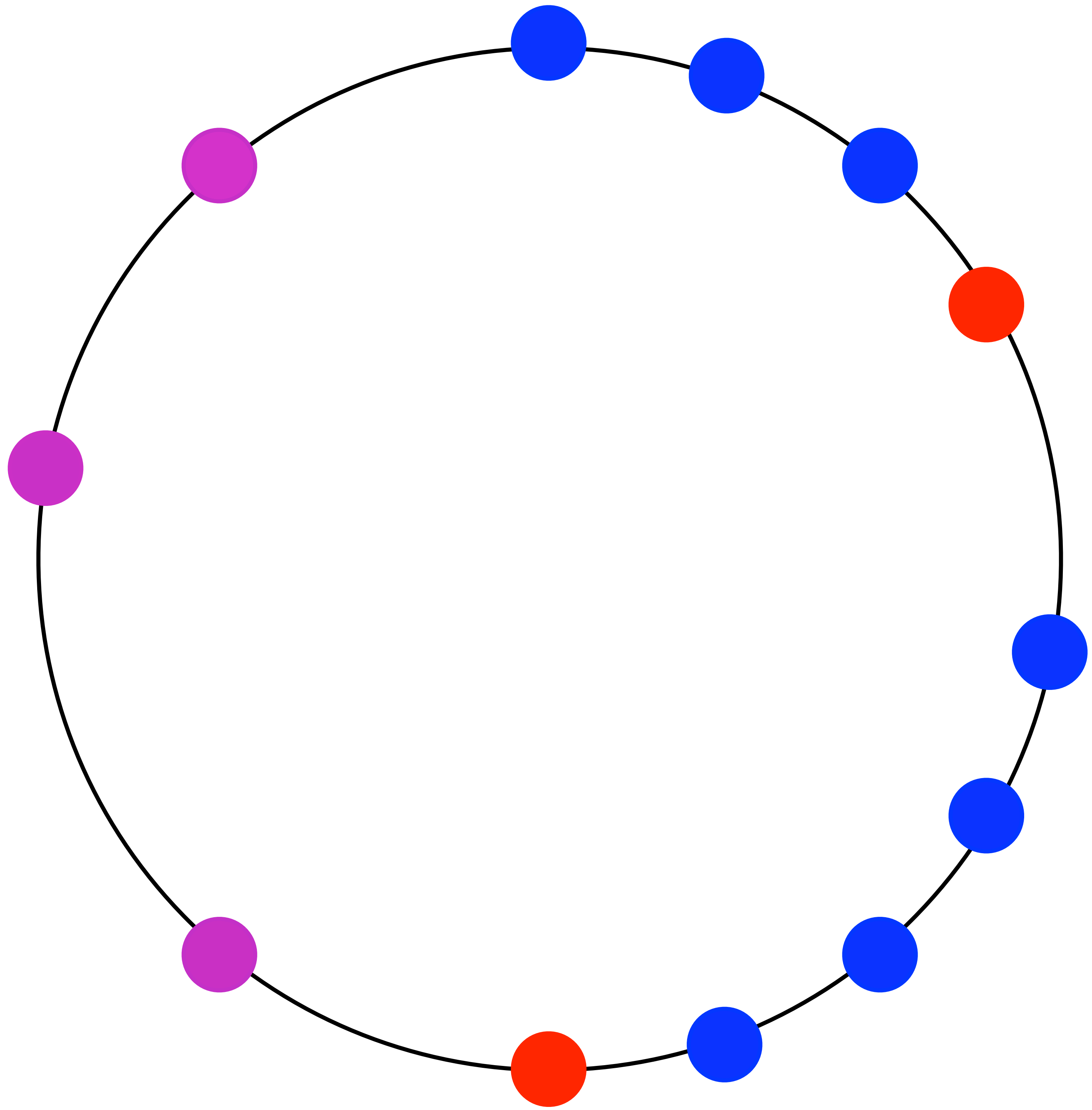

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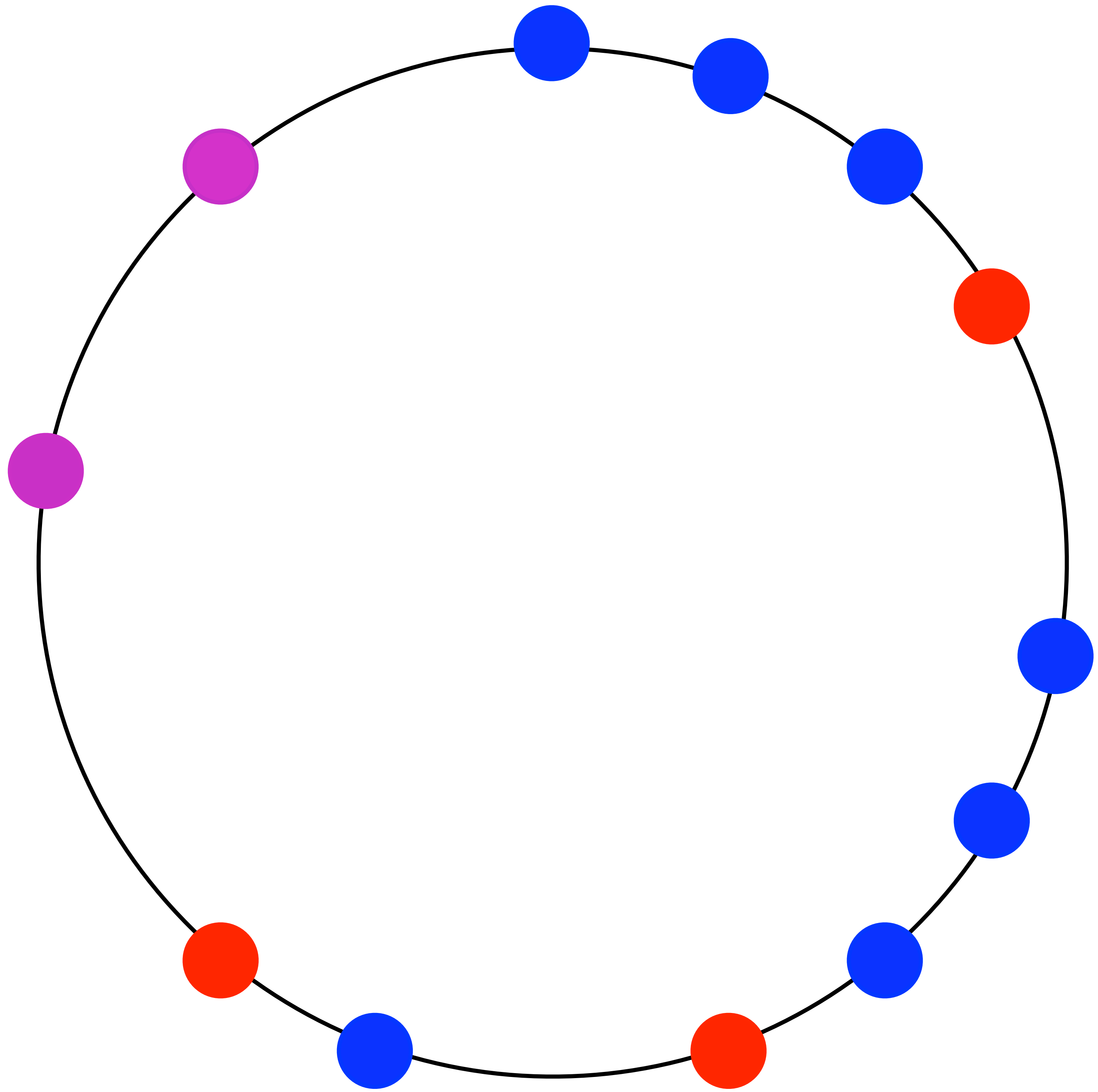

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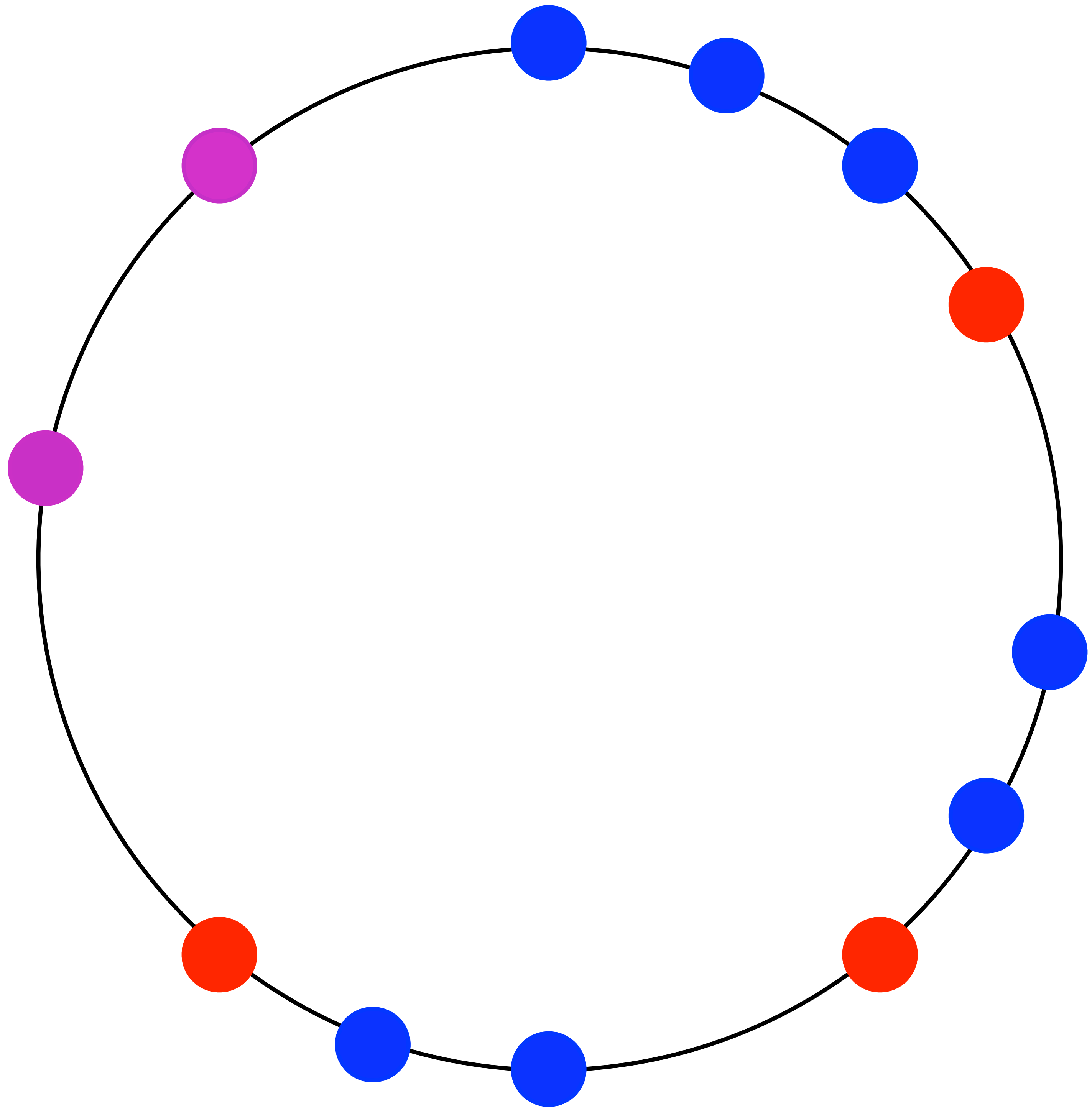
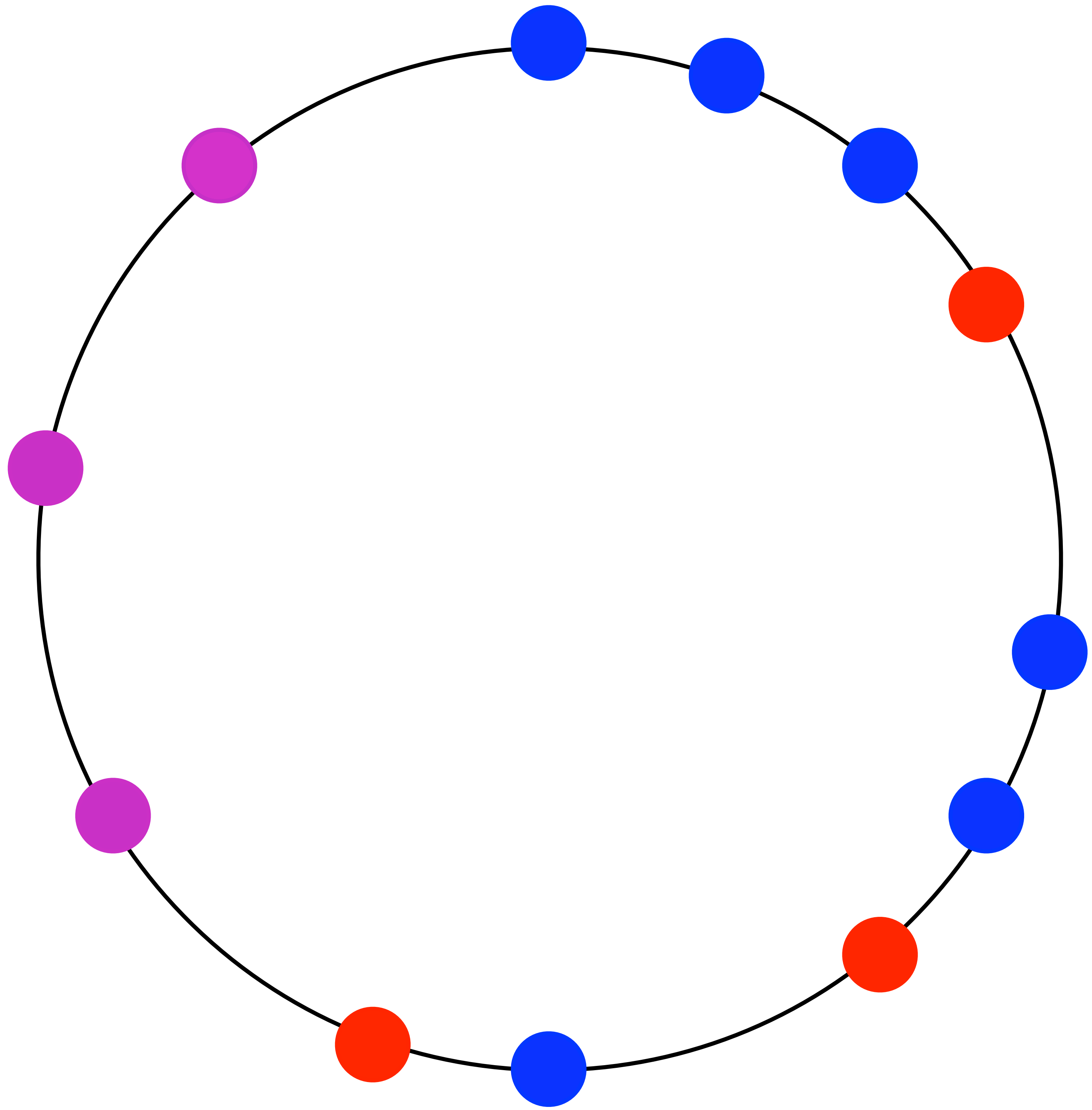


5 islands

Finite Ring (density > 1/2)

6 islands



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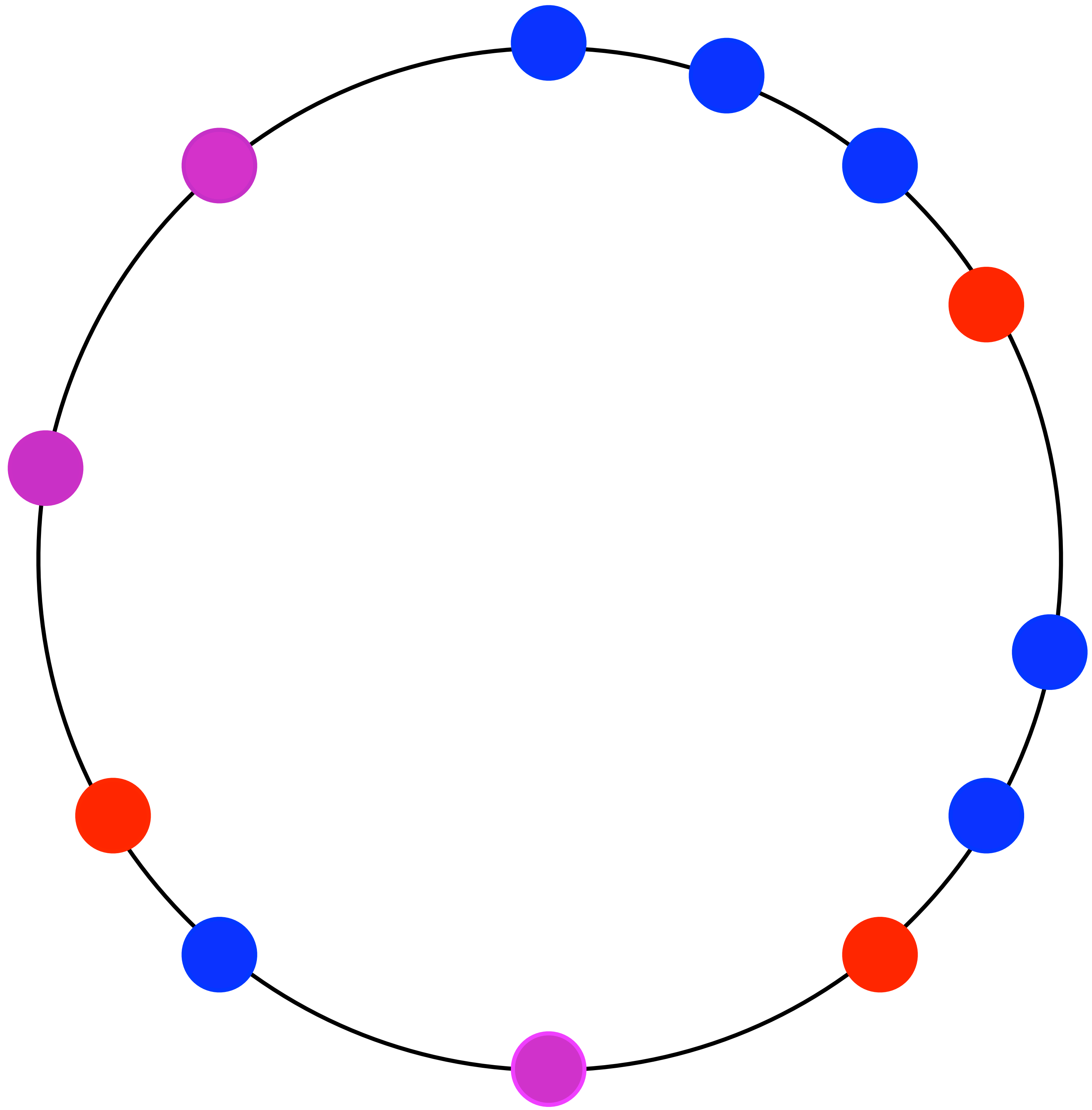
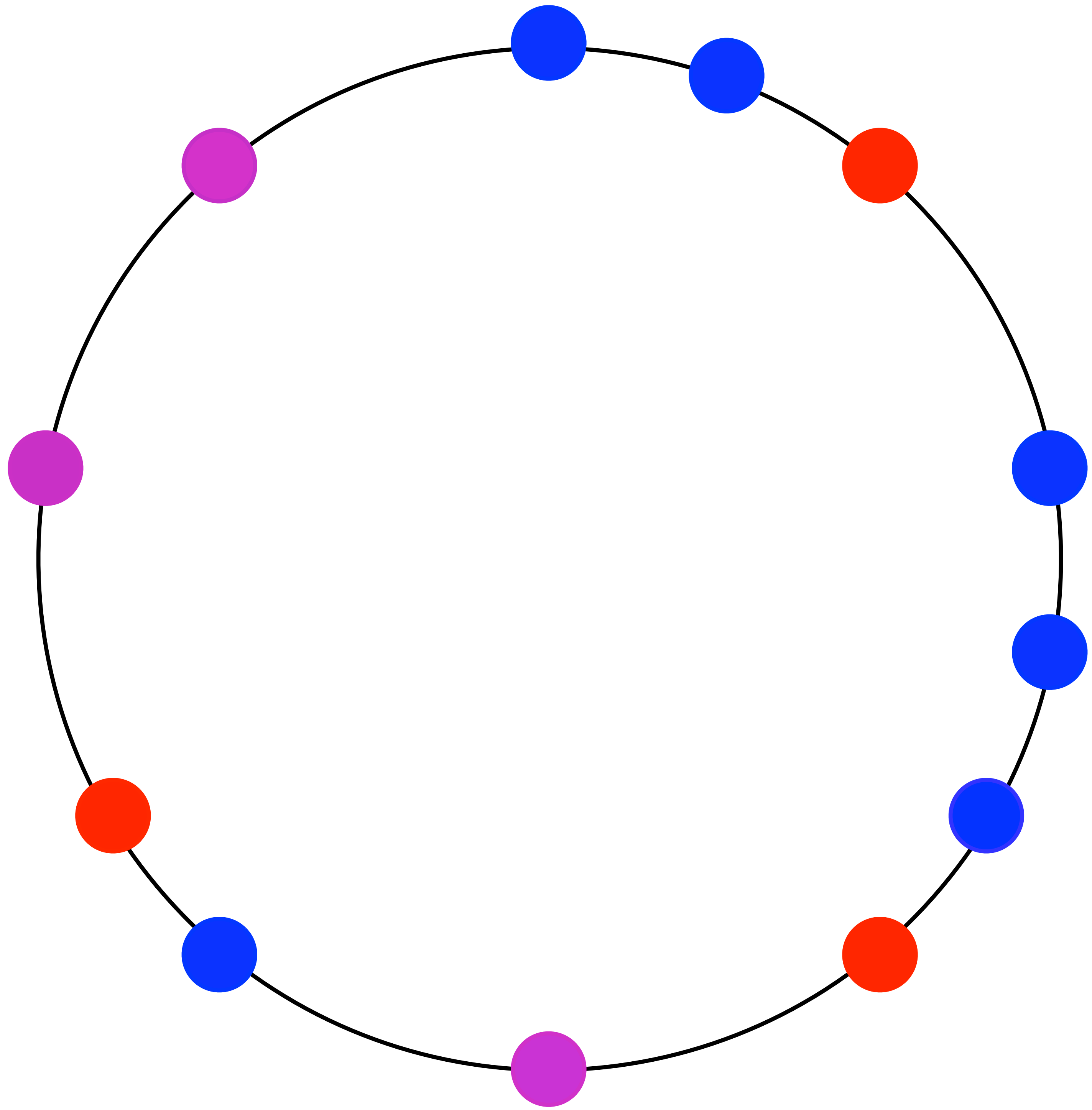


Finite Ring (density > 1/2)



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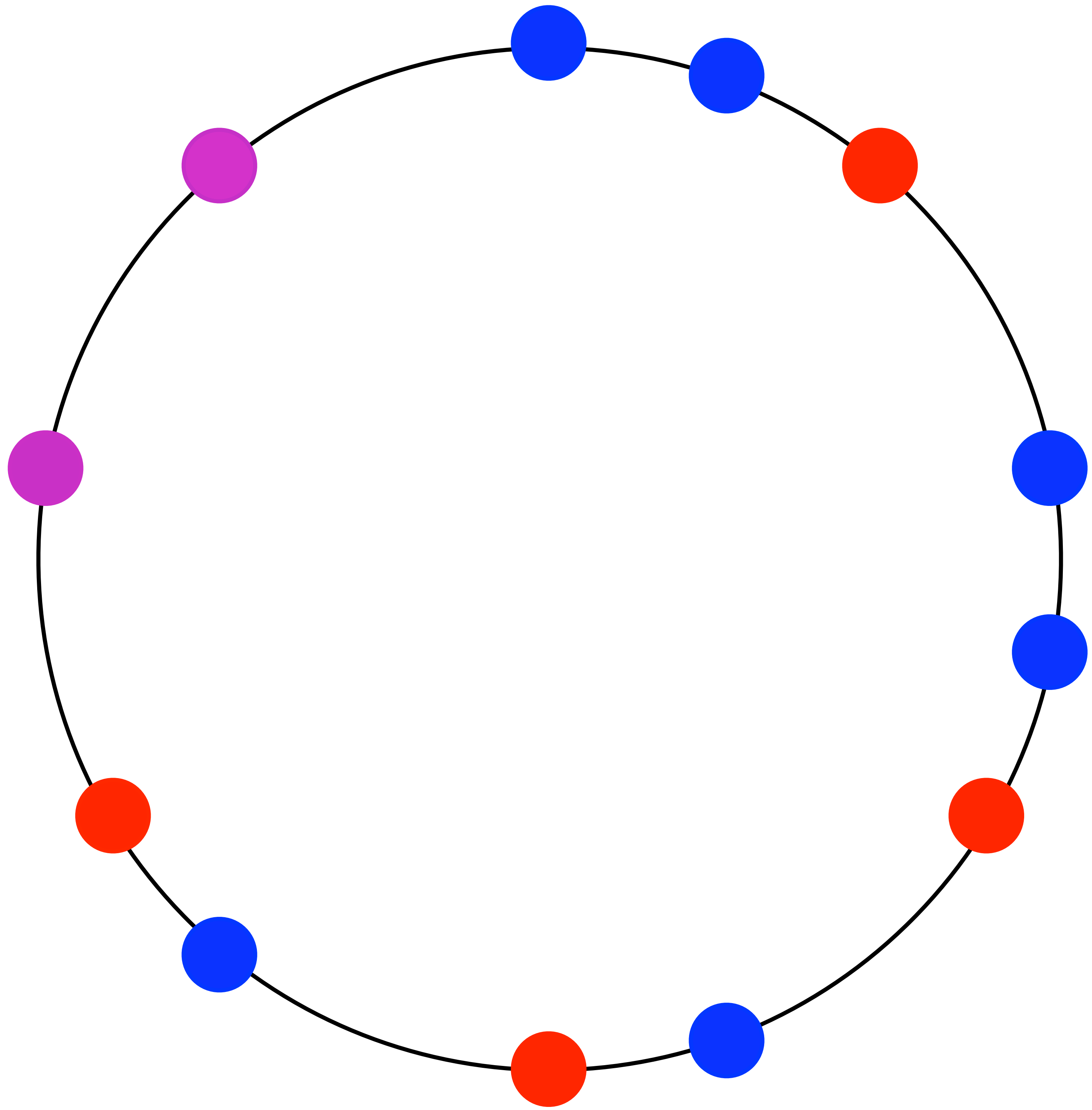

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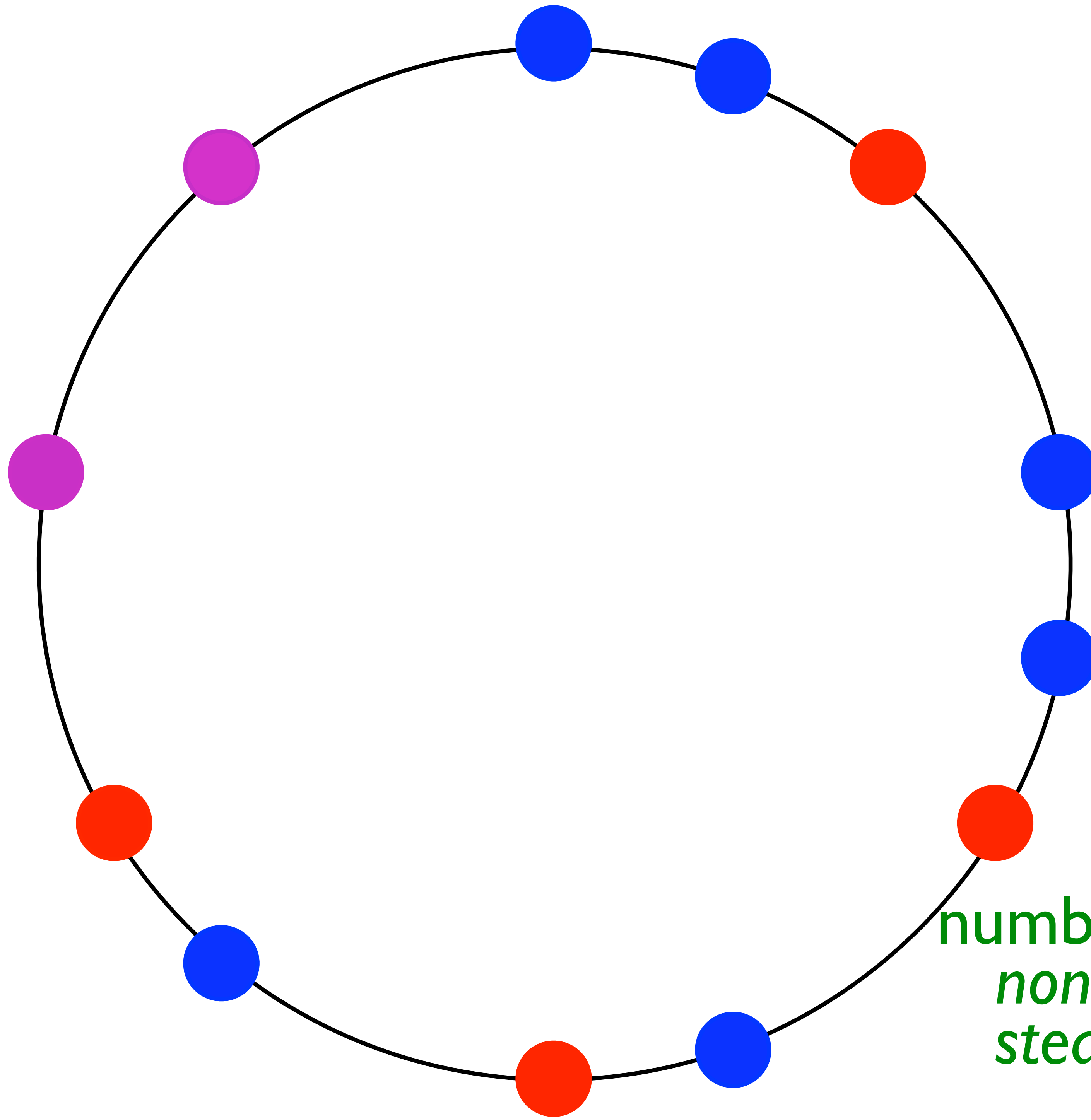
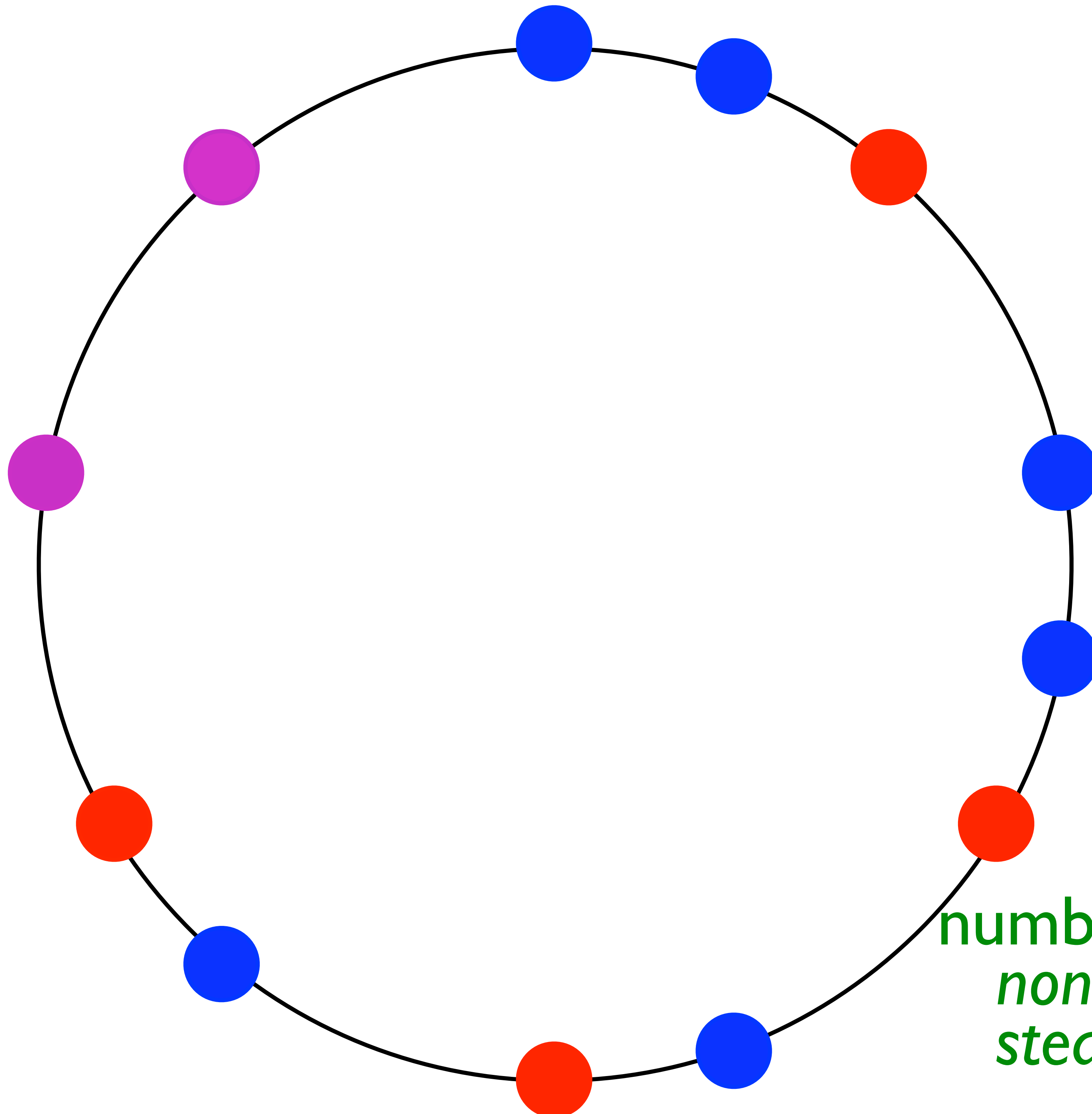


6 islands

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

Steady State 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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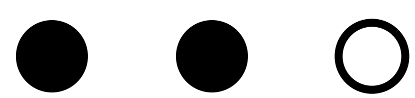

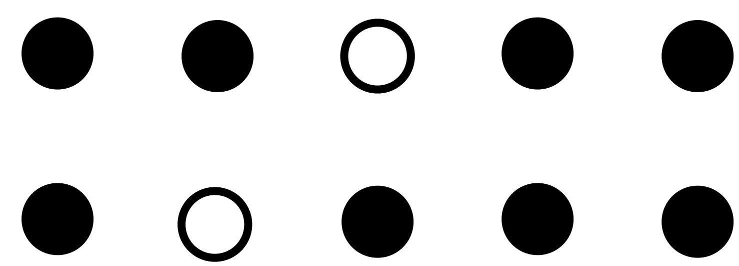

steady state for P(C)= constant

Steady State on the Ring

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

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

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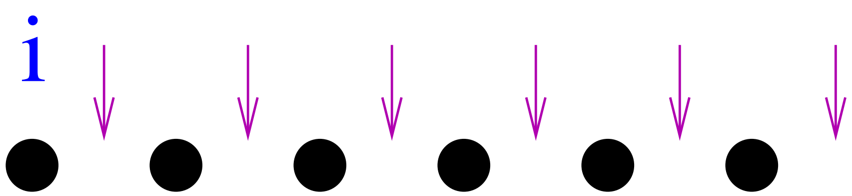
if site i occupied:



N particles
N possibilities for V vacancies

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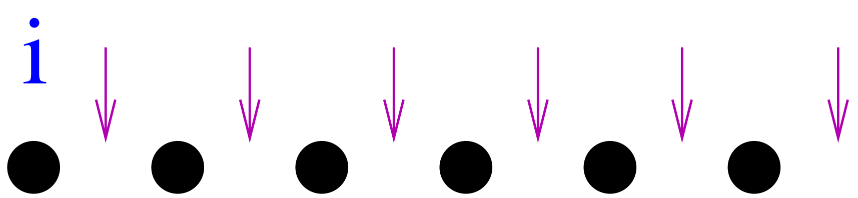
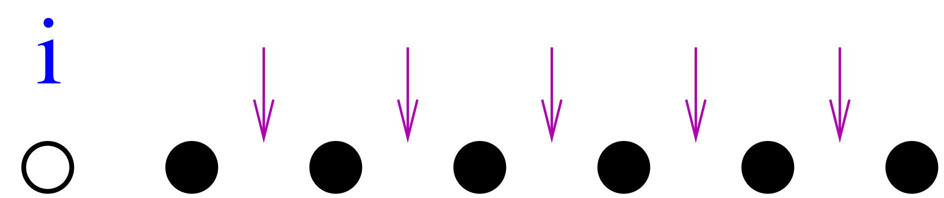


N particles
N possibilities for V vacancies

if site i empty



N particles
N-1 possibilities for V vacancies

Steady State on the Ring

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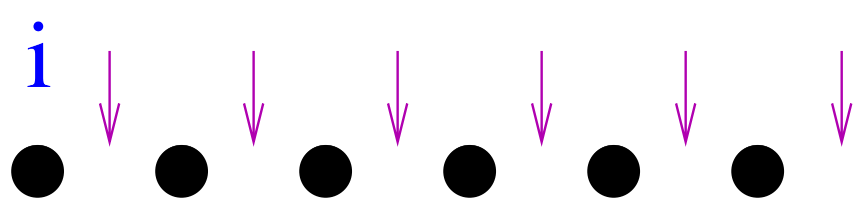
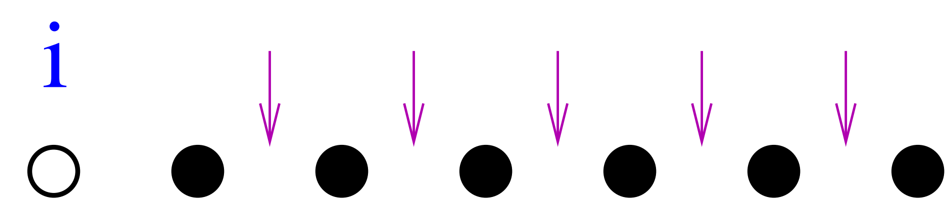
$\mathcal{C} =$ number of maximal-island configurations with N particles & V vacancies

if site i occupied:



N particles
N possibilities for V vacancies

if site i empty



N particles
N-1 possibilities for V vacancies

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

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):

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

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

Self-Diffusion

We tag a particle and probe its long time behavior. For the $1d$ RP (and other $1d$ lattice gases with nearest-neighbor hopping and exclusion), the mean-square displacement of the tagged particle grows as

$$\langle X^2(t)\rangle = \mathcal{D}(\rho)\sqrt{t}$$

For the simplest RP

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

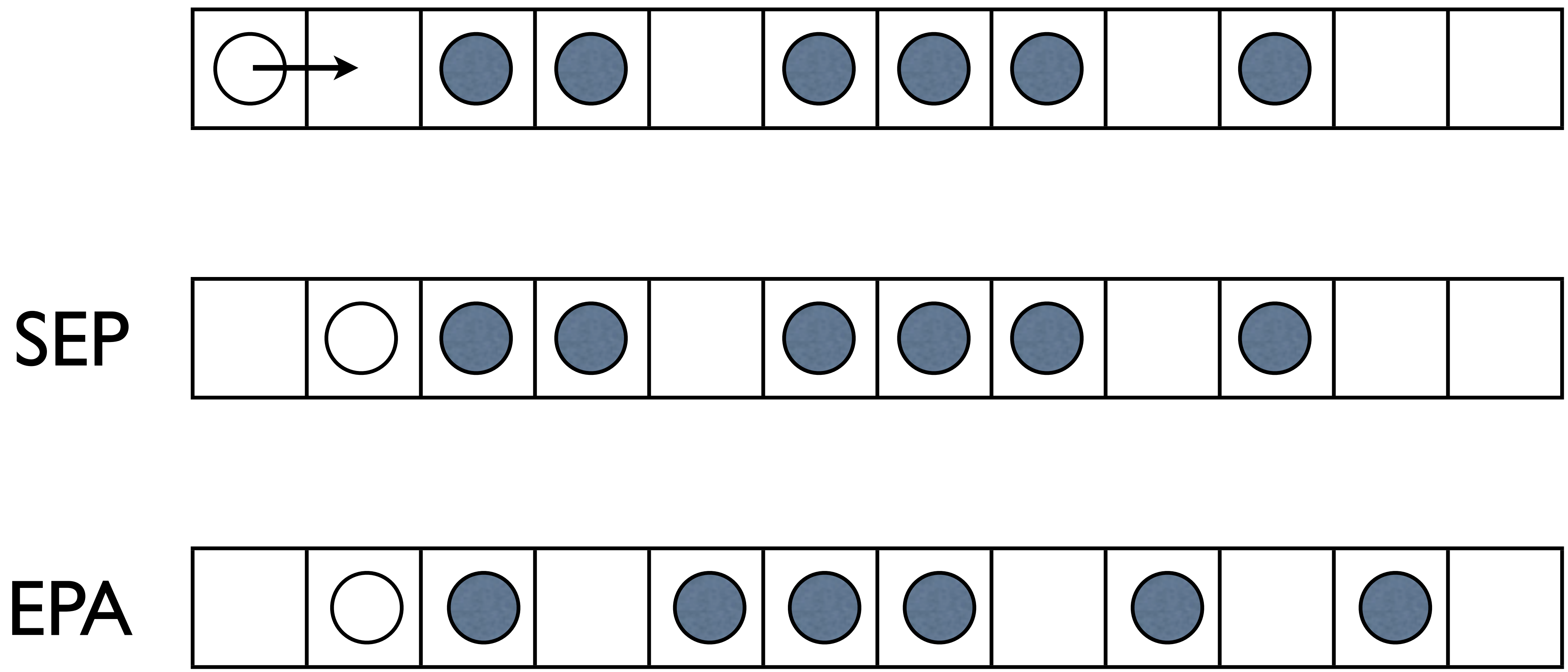
The self-diffusion coefficient vanishes at half-filling: $\mathcal{D}(\frac{1}{2}) = 0$.

The mean-square displacement still grows algebraically at half-filling:

$$\langle X^2(t)\rangle\Big|_{\rho=1/2} \sim t^{1/4}$$

Exclusion Process with Avalanches

- Particles hop to nearest neighbors, only to empty sites (exclusion).
- If a hopping particle joins an island, the front particle from this island hops in the same direction.
- This 2nd hop may trigger the 3rd, etc. No limits on the duration of the avalanche.
- More details: U. Bhatt and PLK, arXiv:1406.1937



A particle (empty disc) hops to the vacant site on the right. This completes the hopping event in the case of SEP. In the case of EPA, the initial hop triggers an avalanche with three induced hops. The initial configuration has 4 islands. After the hopping event there are 3 islands for the SEP and 4 islands for the EPA: In the latter case, the total number of islands cannot decrease.

Steady states

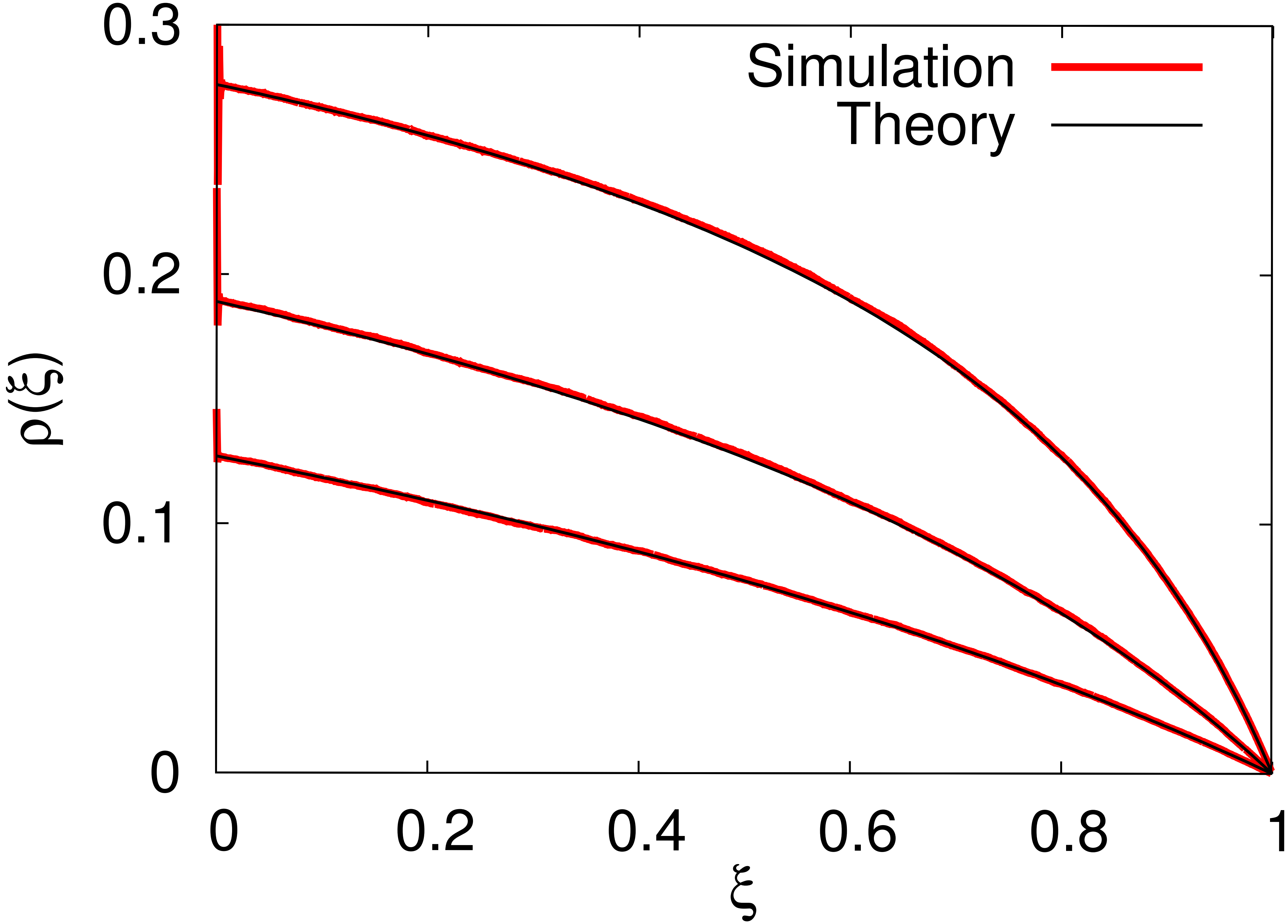
- The same as for the simplest RP: The number of islands is maximal, and these steady states have equal weight.
- The EPA is well defined when the density is less than 1/2; otherwise a never-ending avalanche will emerge.
- All the correlation functions are the same as for the simplest RP.

Basic Results

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

$$D = (1 - 2\rho)^{-3}$$

$$\mathcal{D} = \frac{2}{\sqrt{\pi}} \frac{1-\rho}{\rho\sqrt{1-2\rho}}$$



Density ρ versus the scaled spatial coordinate $\xi = x/L$. Theoretical predictions are in excellent agreement with simulation results in the bulk.

Conclusions

- Transport coefficients depend on the density. They can be computed for a few tractable lattice gases.
- More precisely, the diffusion coefficient has been computed. Then it is easy to find the mobility.
- The self-diffusion coefficient is much harder to compute, it is unknown even for the SEP in two dimensions. In one dimension with NN hopping and exclusion constraint, the self-diffusion coefficient vanishes. The tagged particles exhibits an anomalous behavior, which is quantitatively understood for simplest lattice gases.

Thank you !