Two-Dimensional Asymmetric Simple Exclusion Process (ASEP)

Dmytro Goykolov

This work was done as thesis project
at the University of Kentucky, USA
Supervisor: Dr. Joseph Straley.

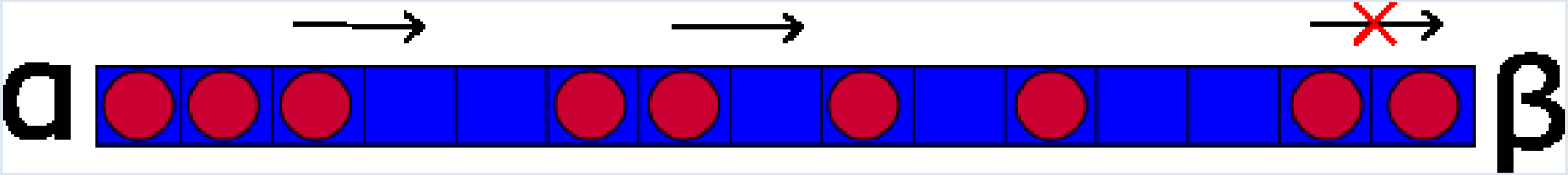
Institute of Physics, Academy of Science
Of Czech Republic

October 7, 2008

Introduction. 1D Model

Applications:

- protein synthesis
- conductivity in zeolites
- traffic flow



Introduction. 1D Model

Parameters of the model:

- **α** - density of the particles at the source reservoir
- **β** – density of the particles at the sink reservoir
- **ρ** – density of the particles in the system
- **j** – current density (defined as the number of particles that cross vertical cross-section of the lattice)

Introduction. 1D Model

Phase diagram:

High density phase

($\beta \leqslant 1/2, \beta < \alpha$)

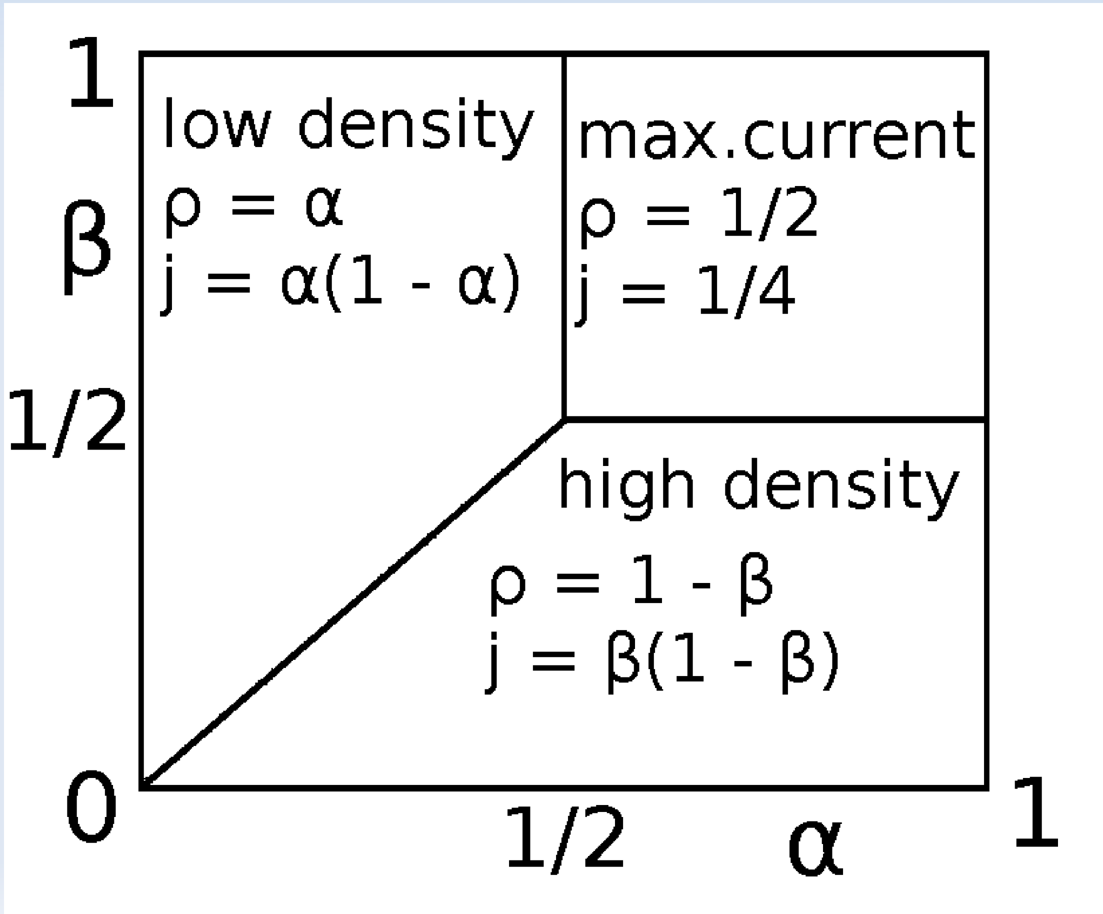
Low density phase

($\alpha \leqslant 1/2, \beta > \alpha$)

Max. current phase

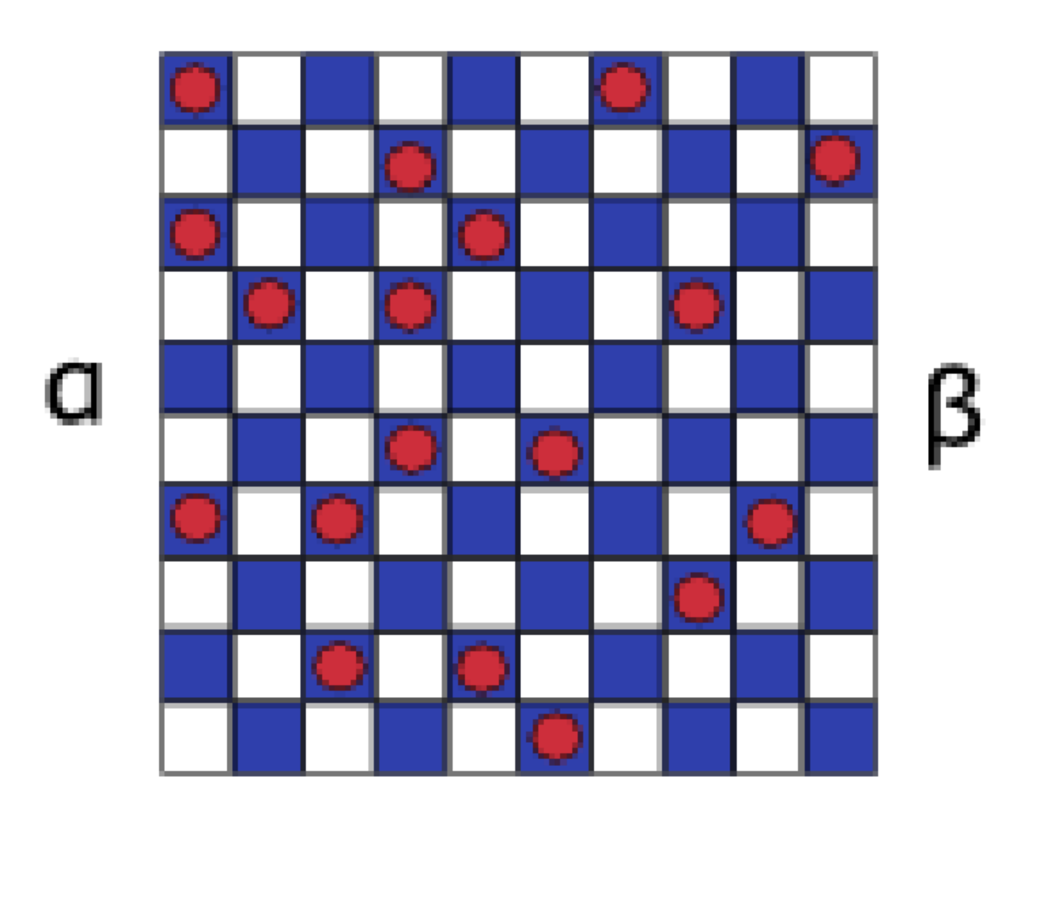
($\alpha \geqslant 1/2, \beta \geqslant 1/2$)

Current – density relationship: $j = \rho(1-\rho)$



Introduction. 2D Model

- Square NxN lattice
- Particles move upward-right or downward-right
- Particle supply on the left edge and particle extraction on the right edge
- Periodic boundary conditions in vertical direction



Introduction. 2D Model

Applications:

- useful instrument to describe different flow models
- gel electrophoresis
- models of traffic flow and traffic jams

Two-dimensional model is not studied as deeply as one-dimensional.

2D Regular Model

Assumptions:

- no correlations between the particles
- replace actual particle density (0 or 1) by ensemble average
- system is in the steady state (current of particles is constant)
- density of the particles slowly changes with distance in horizontal direction
- density is uniform along the vertical direction

2D Regular Model

The change of the particle density due to imbalance in arrival and departure of the particles:

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= \frac{1}{2}(\rho(x-1, y-1)+\rho(x-1, y+1))(1-\rho(x, y)) \\ &- \frac{1}{2}\rho(x, y)(1-\rho(x+1, y+1)+1-\rho(x+1, y-1))\end{aligned}$$

2D Regular Model

Expand density into a power series, ignoring terms of order O(3):

$$\frac{\partial \rho}{\partial t} = -\rho_x + 2\rho\rho_x + \frac{1}{2}\rho_{xx}$$

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0$$

$$j = -\frac{1}{2}\rho_x + \rho(1-\rho) \xrightarrow{\text{Homogeneous system}} j = \rho(1-\rho)$$

2D Regular Model

Solving previous equation for $\rho(x)$

$$\frac{1}{2}\rho_x = \rho - \rho^2 - j$$

for $j < \frac{1}{4}$

$$\rho(x) = \frac{1}{2} + \frac{1}{2}\sqrt{1-4\mathrm{j}}\,\tanh\left[2(x-C)\sqrt{1-4\mathrm{j}}\right]$$

Describes density in high or low density phases or on the coexistence line

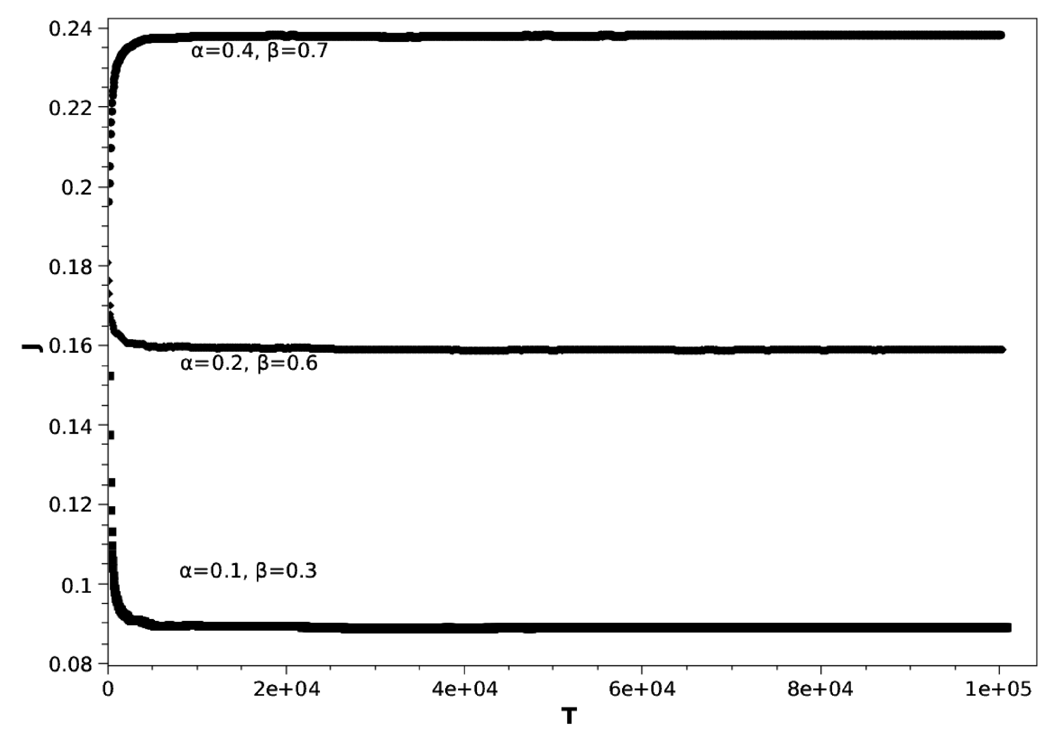
for $j \geqslant \frac{1}{4}$

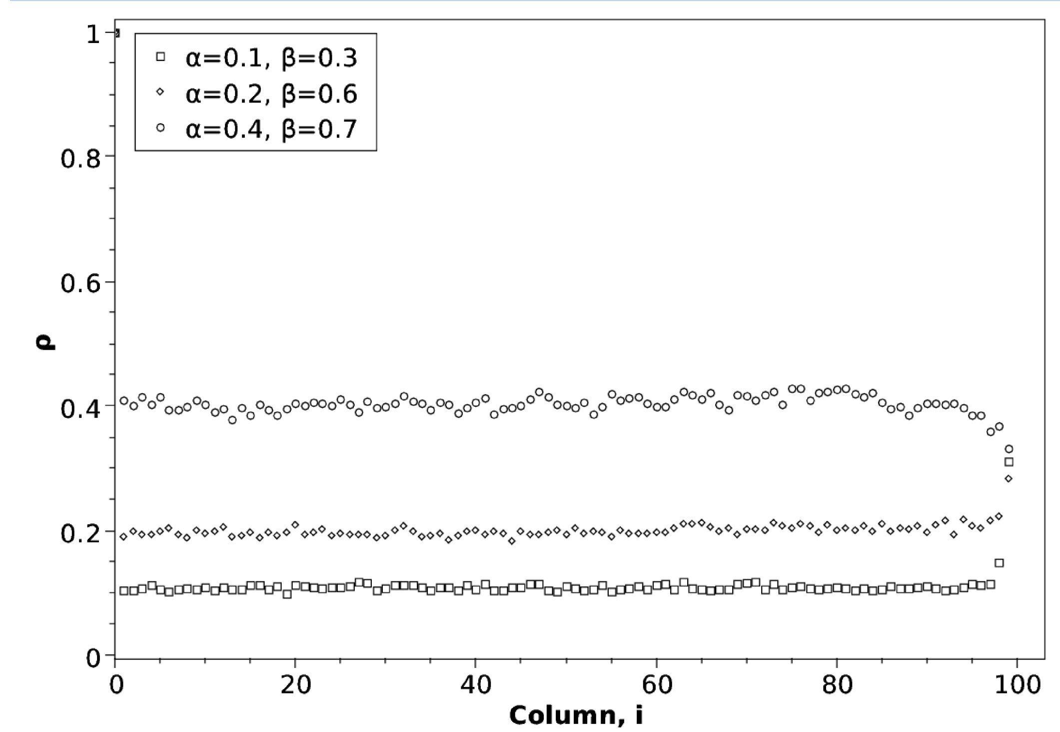
$$\rho(x) = \frac{1}{2} - \frac{1}{2}\sqrt{4\mathrm{j}-1}\,\tan\left[(x-C)\sqrt{4\mathrm{j}-1}\right]$$

Describes the phase of maximal current

2D Regular Model

Low density phase





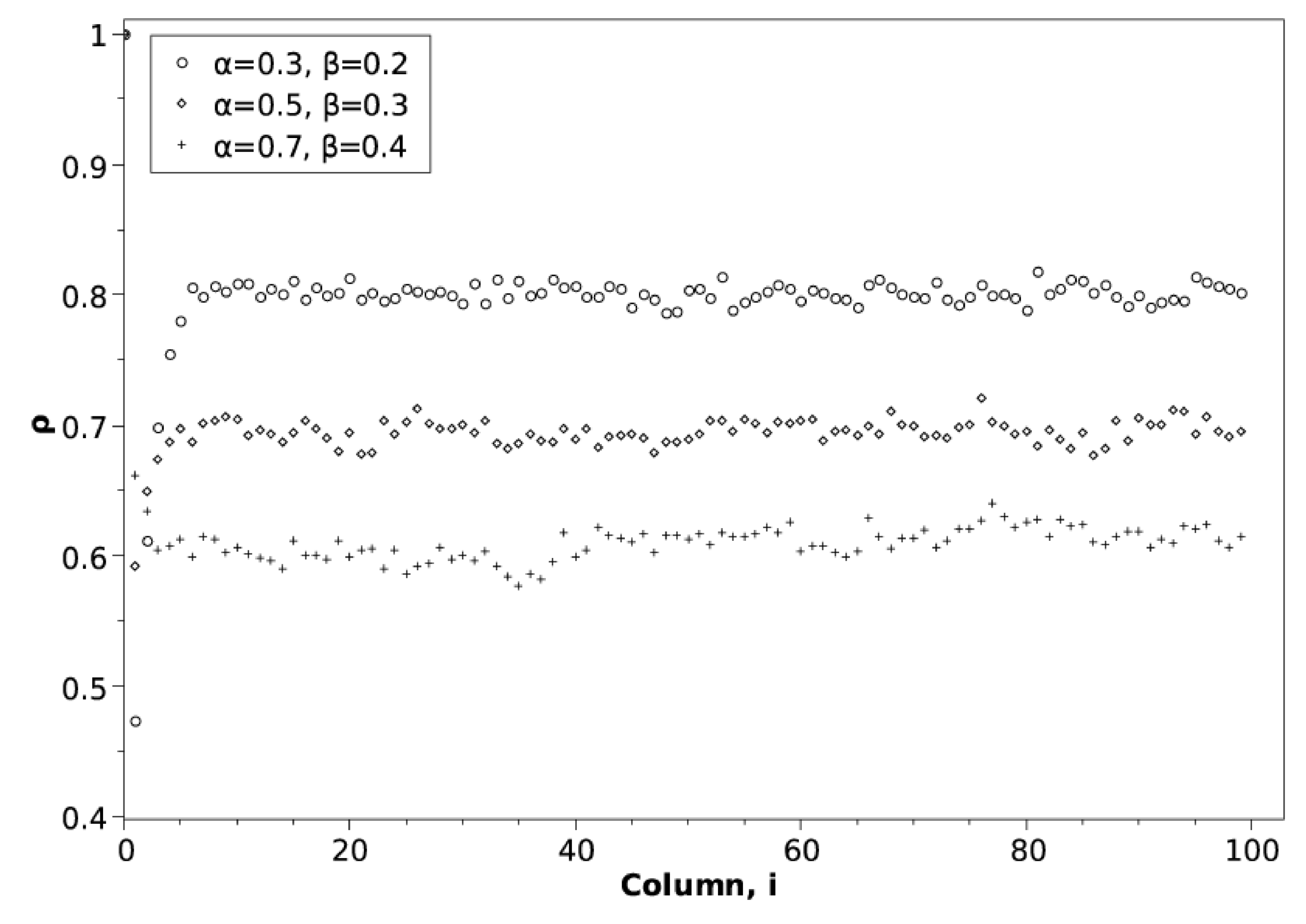
For $\alpha=0.2, \beta=0.6$

MFT: $\rho_{MFT}=\alpha=0.2, j_{MFT}=-\frac{1}{2}\rho'+\alpha(1-\alpha)\approx0.158$

Simulation: $\rho_S\approx0.207, j_S\approx0.159\pm0.0099$

2D Regular Model

High density phase



$$\alpha = 0.3, \beta = 0.2$$

MFT:

$$\rho = 1 - \beta = 0.8$$

$$j = -\frac{1}{2}\rho' + \beta(1-\beta)$$

$$j \approx 0.1575$$

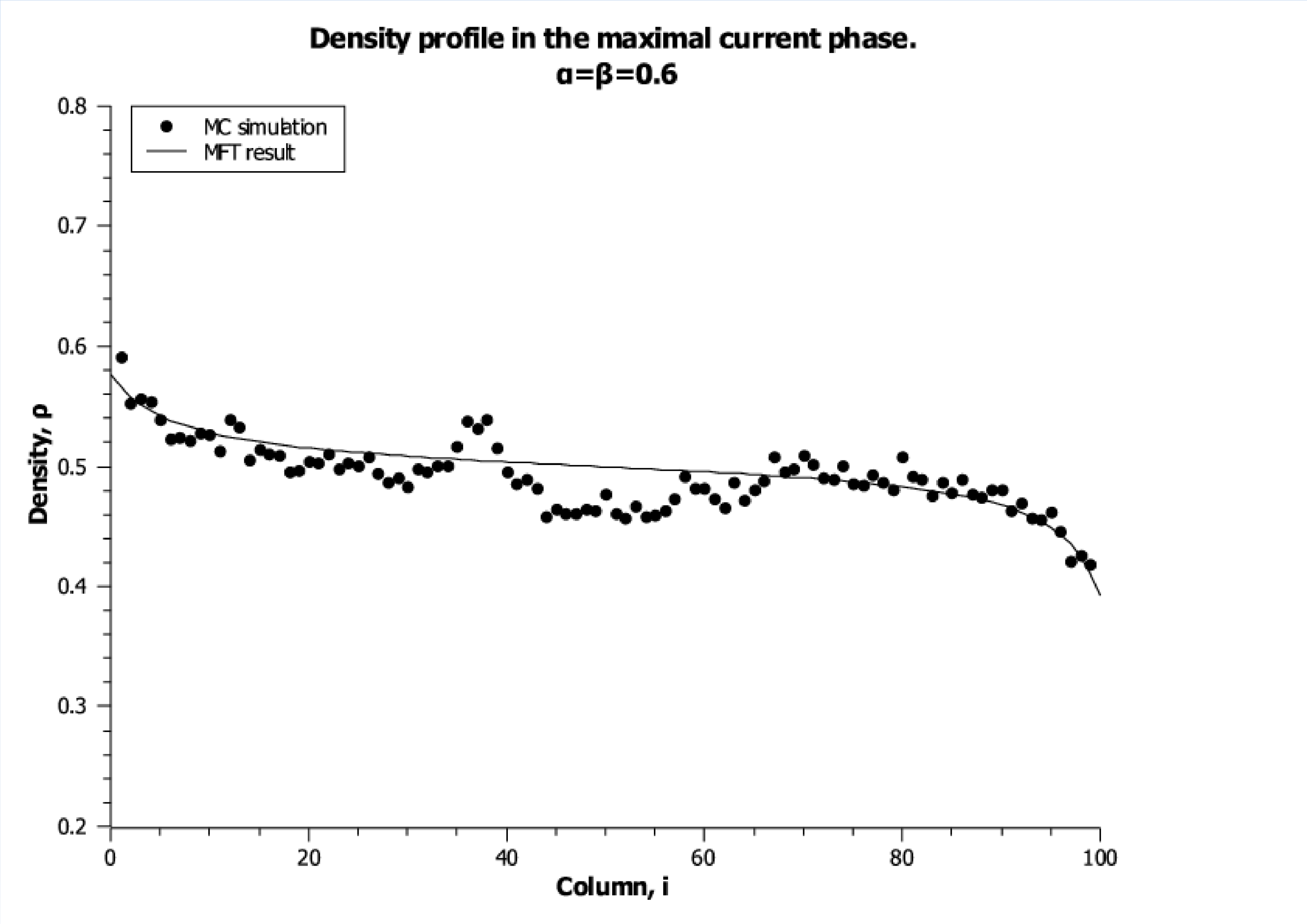
Simulation:

$$\rho_S = 0.79 \pm 0.0037$$

$$j_S = 0.16 \pm 0.004$$

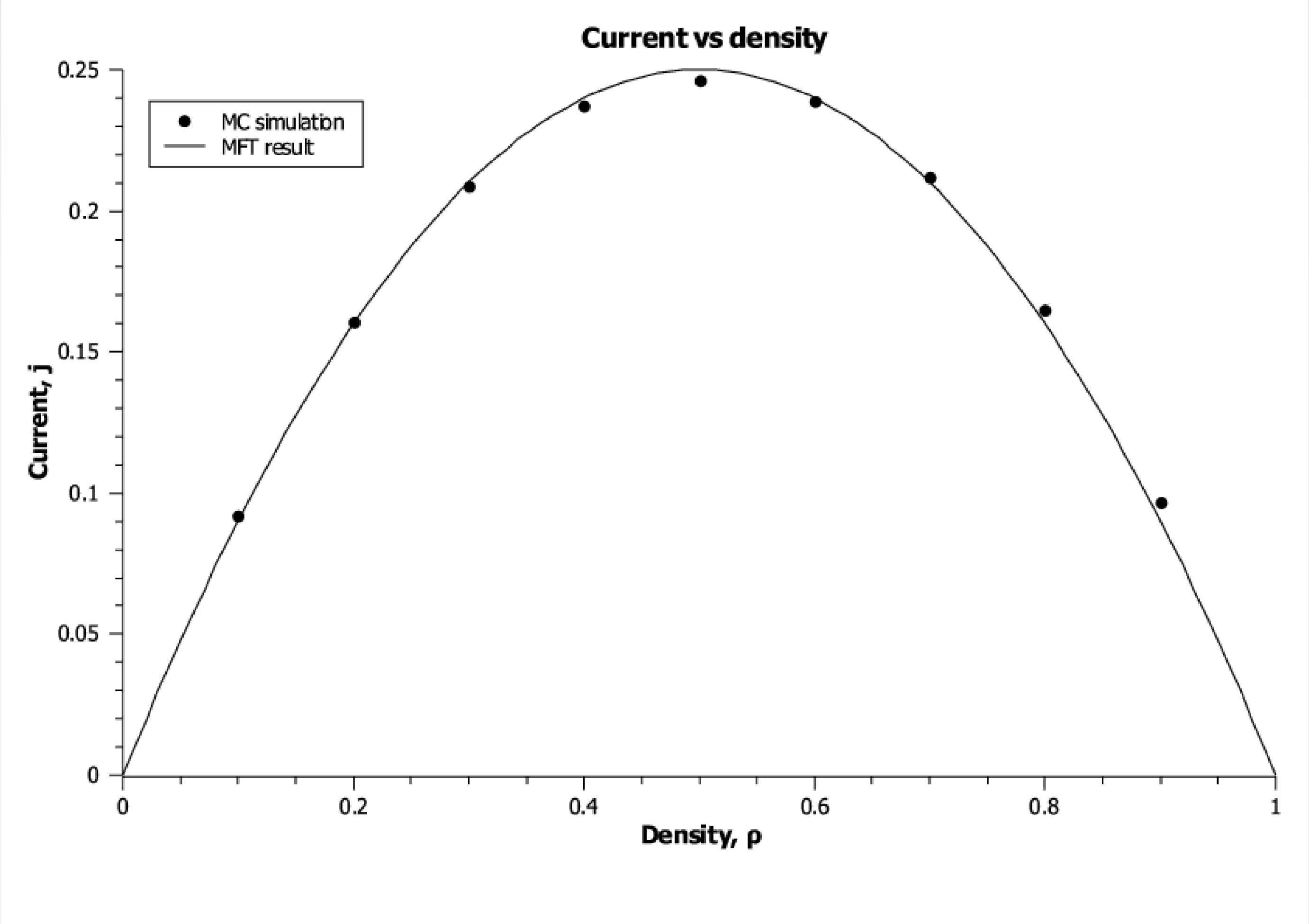
2D Regular Model

Maximal current phase



2D Regular Model

Dependency of current on the particle density



2D Regular Model

Coexistence line in closed systems with a barrier.

Barrier – there is a probability $\gamma \leq 1$ that a particle at the right edge will hop to an empty site on the left edge.

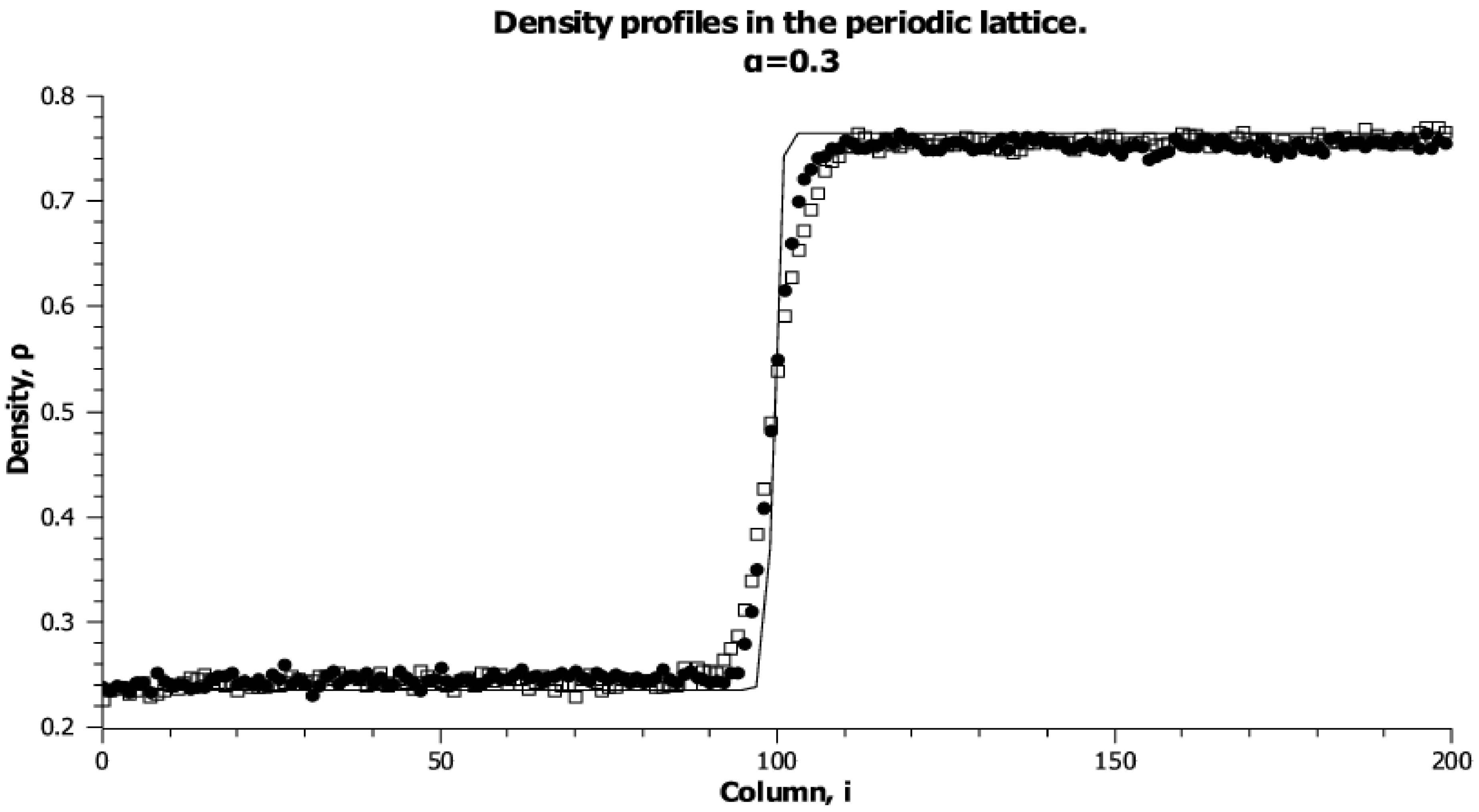
Density at the left side - ρ

Density at the right side - $1-\rho$

$$\rho(1-\rho)=\gamma(1-\rho)(1-\rho)$$

$$\rho=\frac{\gamma}{1+\gamma}$$

2D Regular Model

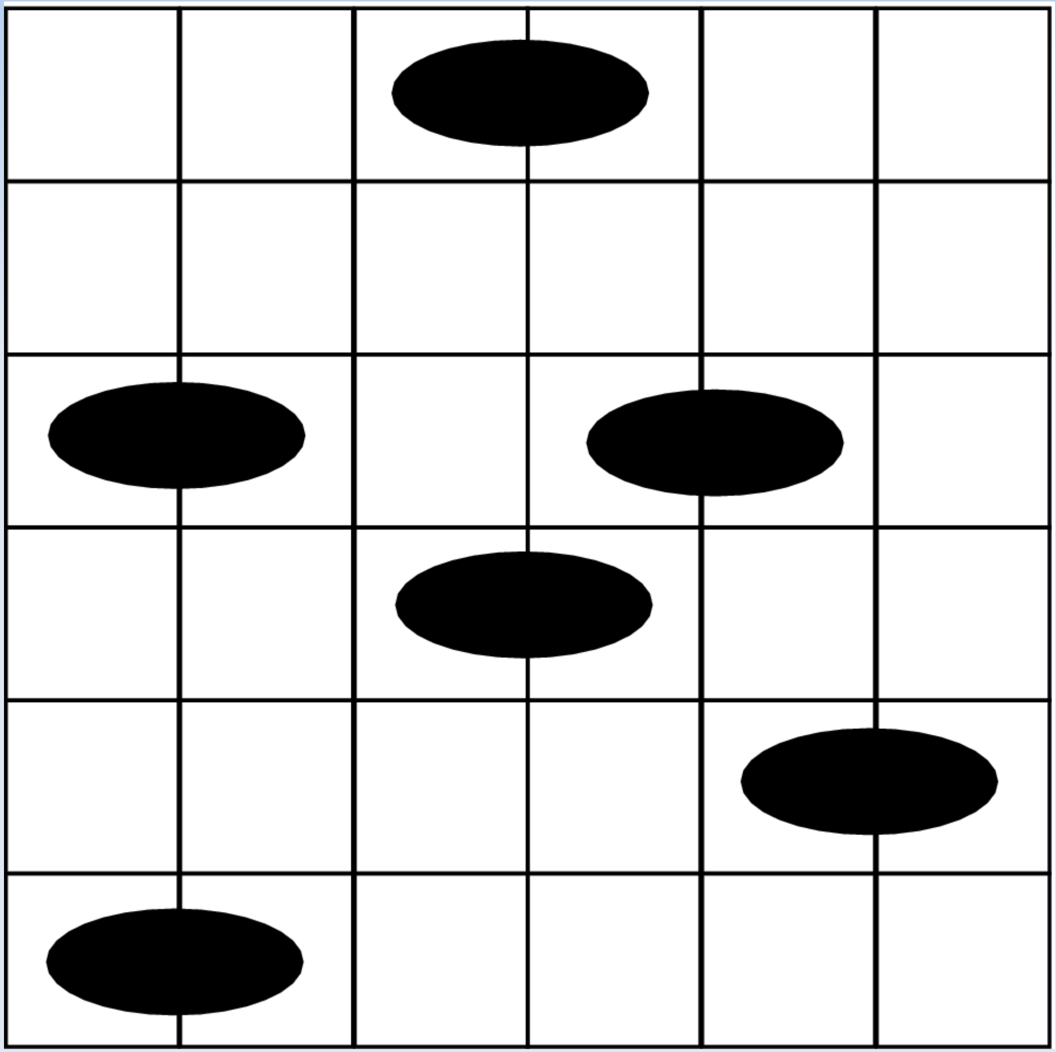


Extended particles. Model 1

Particles occupy two horizontal adjacent cells

There are no two different sub lattices

Three possible directions of jump



Extended particles

Mean-field theory:

– no correlations between particles

– replace actual particle density with its average value

– define $\rho(x, y)$ as probability that particle occupies sites (x, y) and (x+1,y)

– define two types of density:

- density of the particles
- coverage density ($\rho_c = 2\rho_p$)

Extended particles

Define functions:

- *F(n)* – probability that the particle is followed by *n* or more vacancies:

$$F(0)=1$$

$$F(n+1)=qF(n)$$

$$F(n)=q^n$$

- *Q(n)* – probability that there is a row of exactly *n* vacancies:

$$Q(n)=F(n)-F(n+1)=(1-q)q^n$$

Extended particles

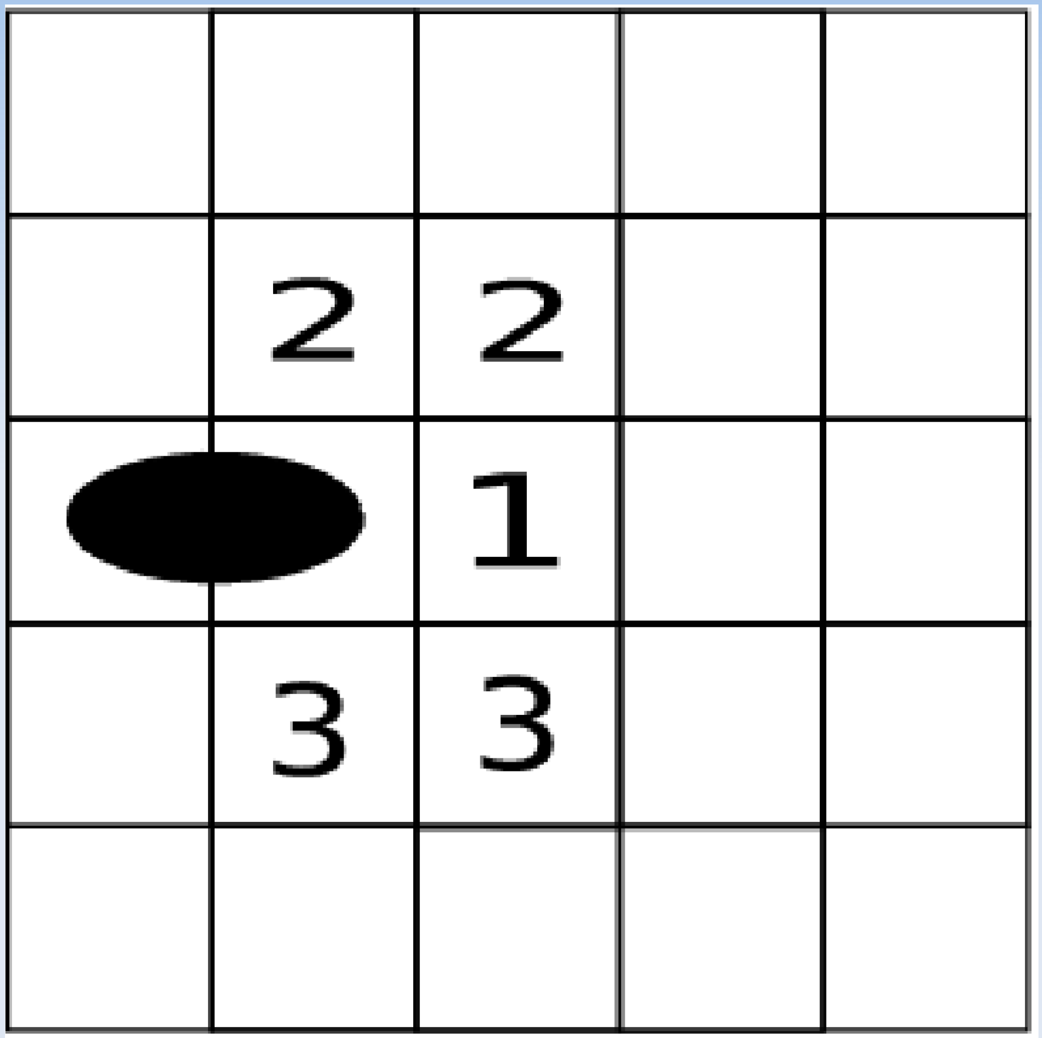
- Average spacing between particles:

$$D = 2 + \sum_{n=0}^{\infty} nQ(n) = \frac{2-q}{1-q}$$

- By definition $D = \frac{1}{\rho}$

$$q = \frac{1-2\rho}{1-\rho}$$

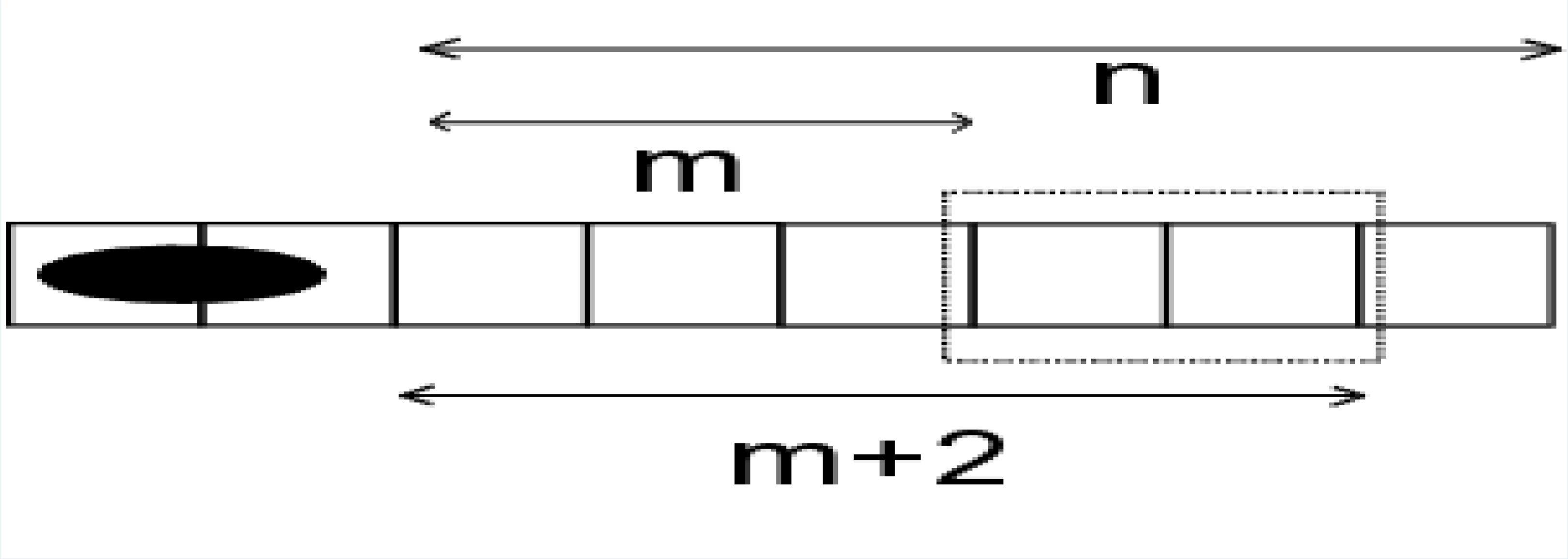
Extended particles



Probability to jump to *1*: $\rho F(1)$

Extended particles

Jump to positions *2* and *3* requires two adjacent vacancies. Probability of this configuration:



$$P = \rho \sum_{m=0}^{\infty} F(2+m) = \frac{(1-2\rho)^2}{1-\rho}$$

Extended particles

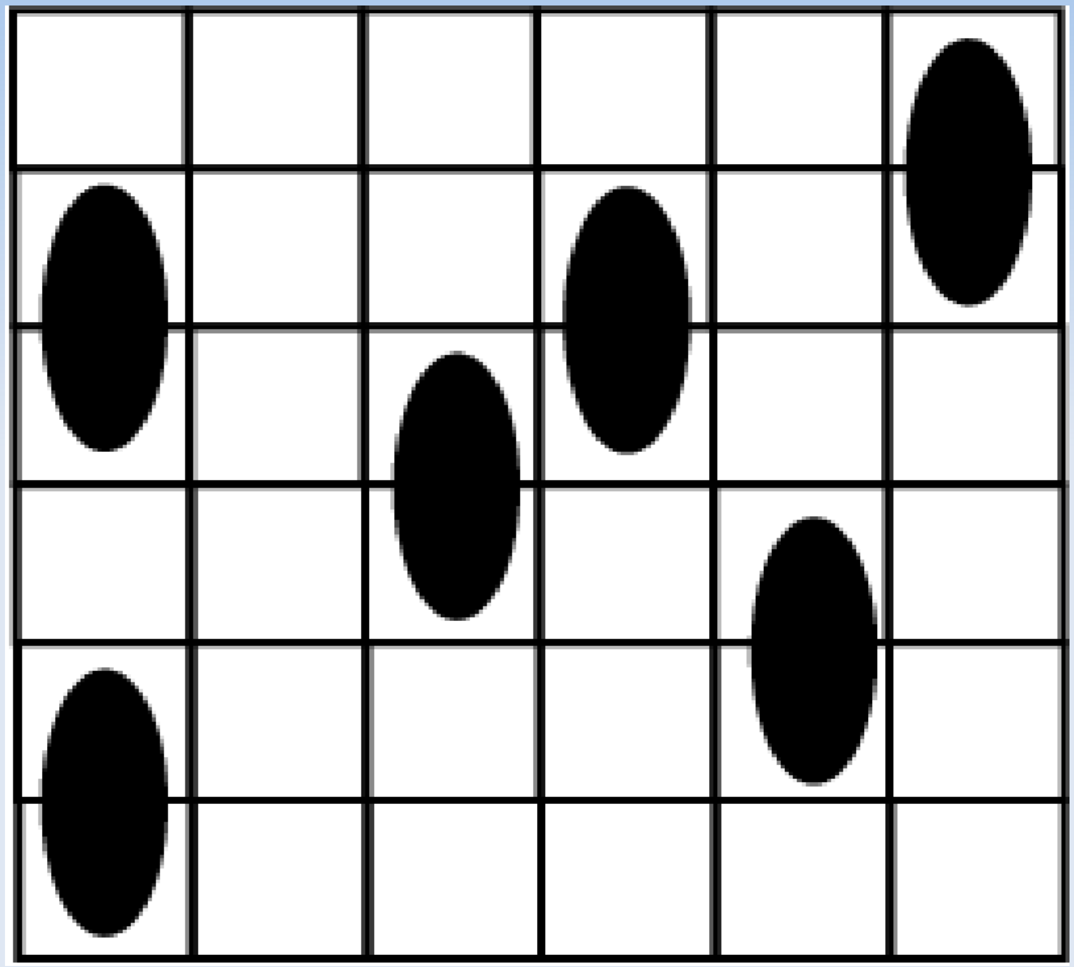
Current density:

$$j = \frac{1}{3}\rho F(1) + \frac{2}{3}\rho P = \frac{\rho(1-2\rho)(3-4\rho)}{3(1-\rho)}$$

Since extended particles are twice as massive as regular particles:

$$j = \frac{2\rho(1-2\rho)(3-4\rho)}{3(1-\rho)}$$

Extended particles. Model 2



Particles occupy sites (x, y) and $(x, y+1)$

Extended particles

Using functions defined earlier – *F(n)* and *Q(n)*:

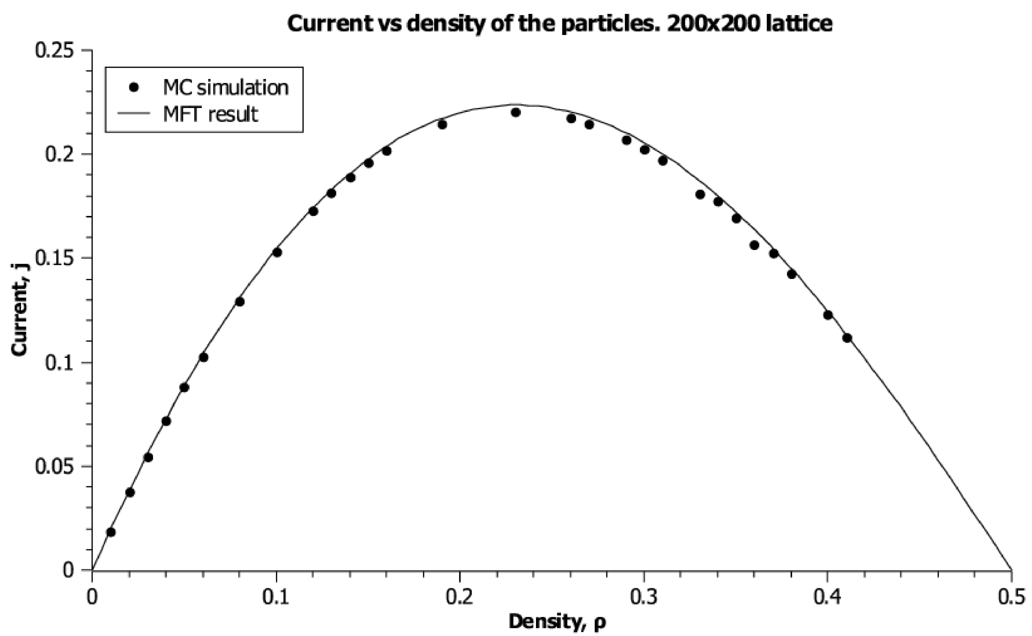
$$j = \rho \frac{(1-2\rho)^2}{1-\rho}$$

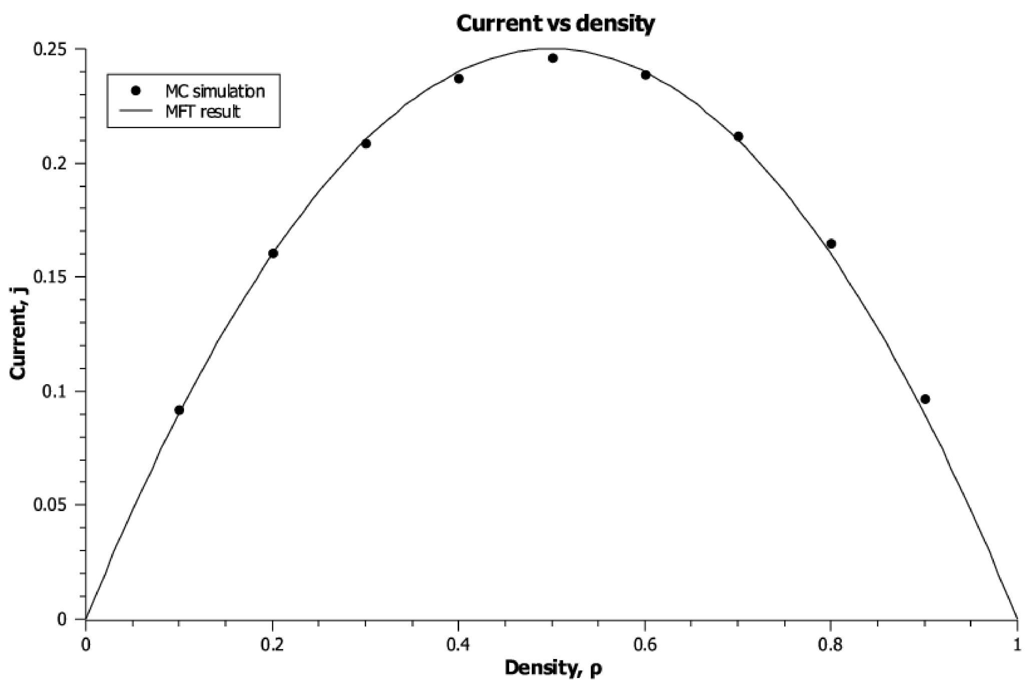
In order to get mass current density we multiply this equation by 2:

$$j = 2\rho \frac{(1-2\rho)^2}{1-\rho}$$

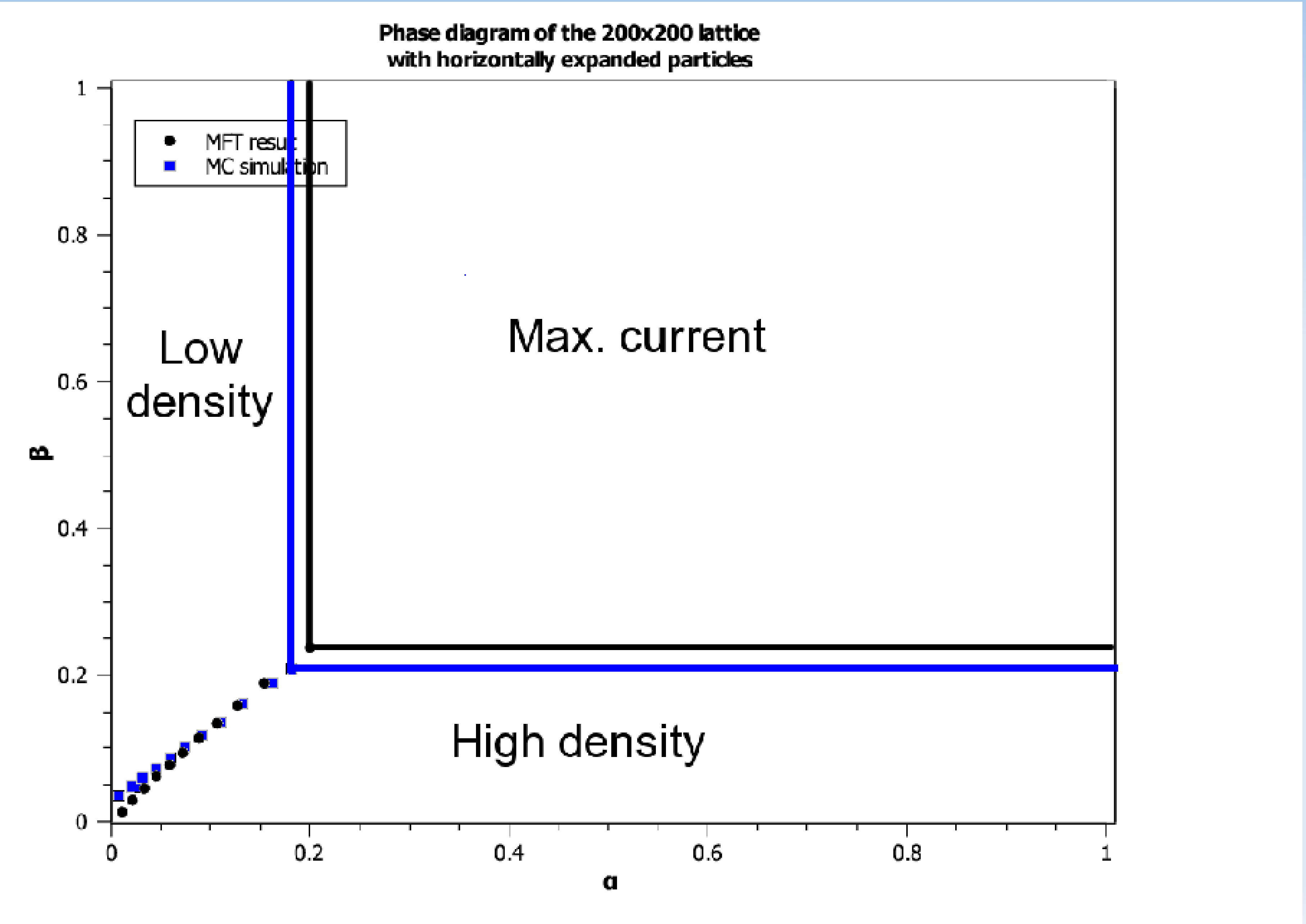
Extended particles

Horizontally extended particles:



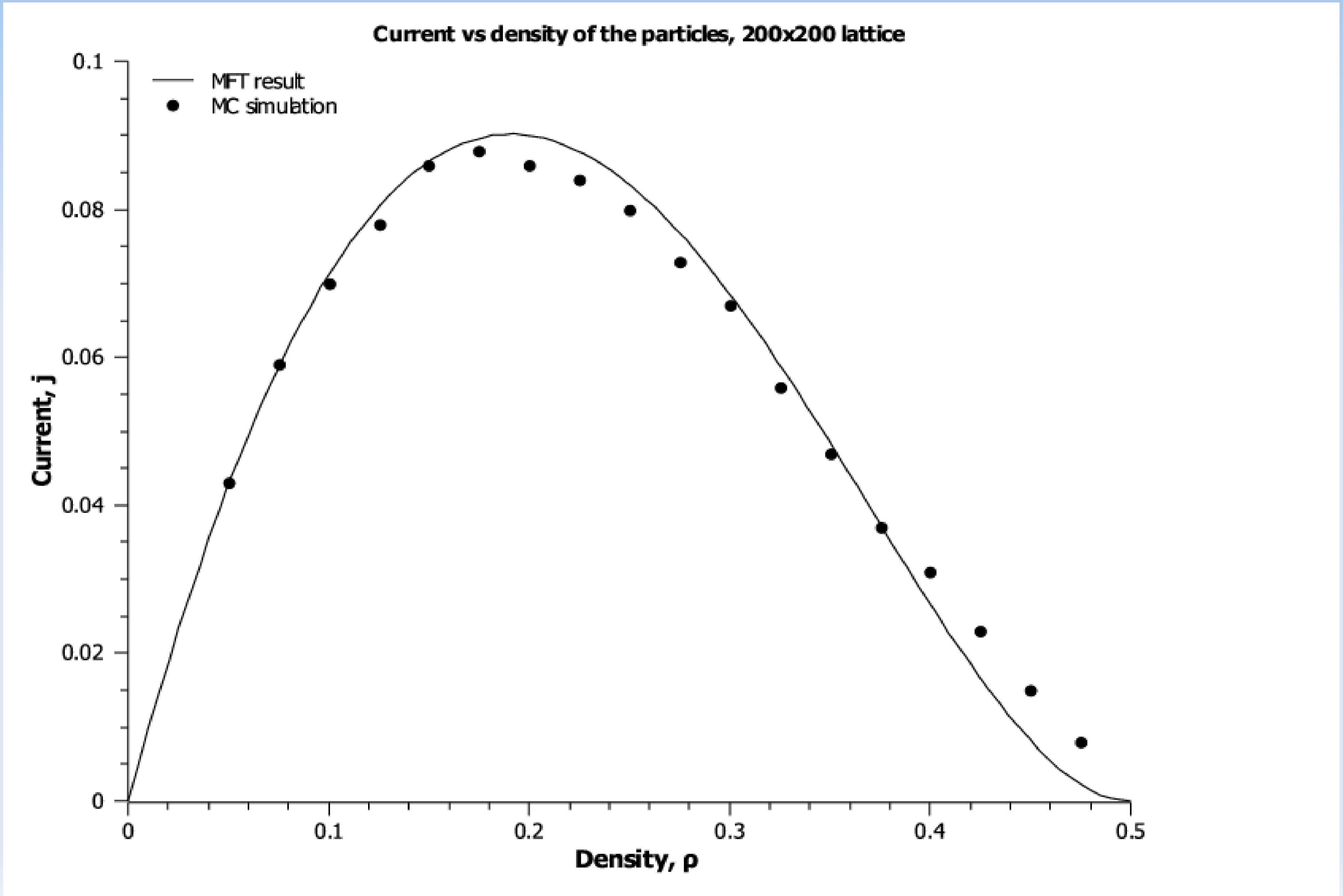


Extended particles

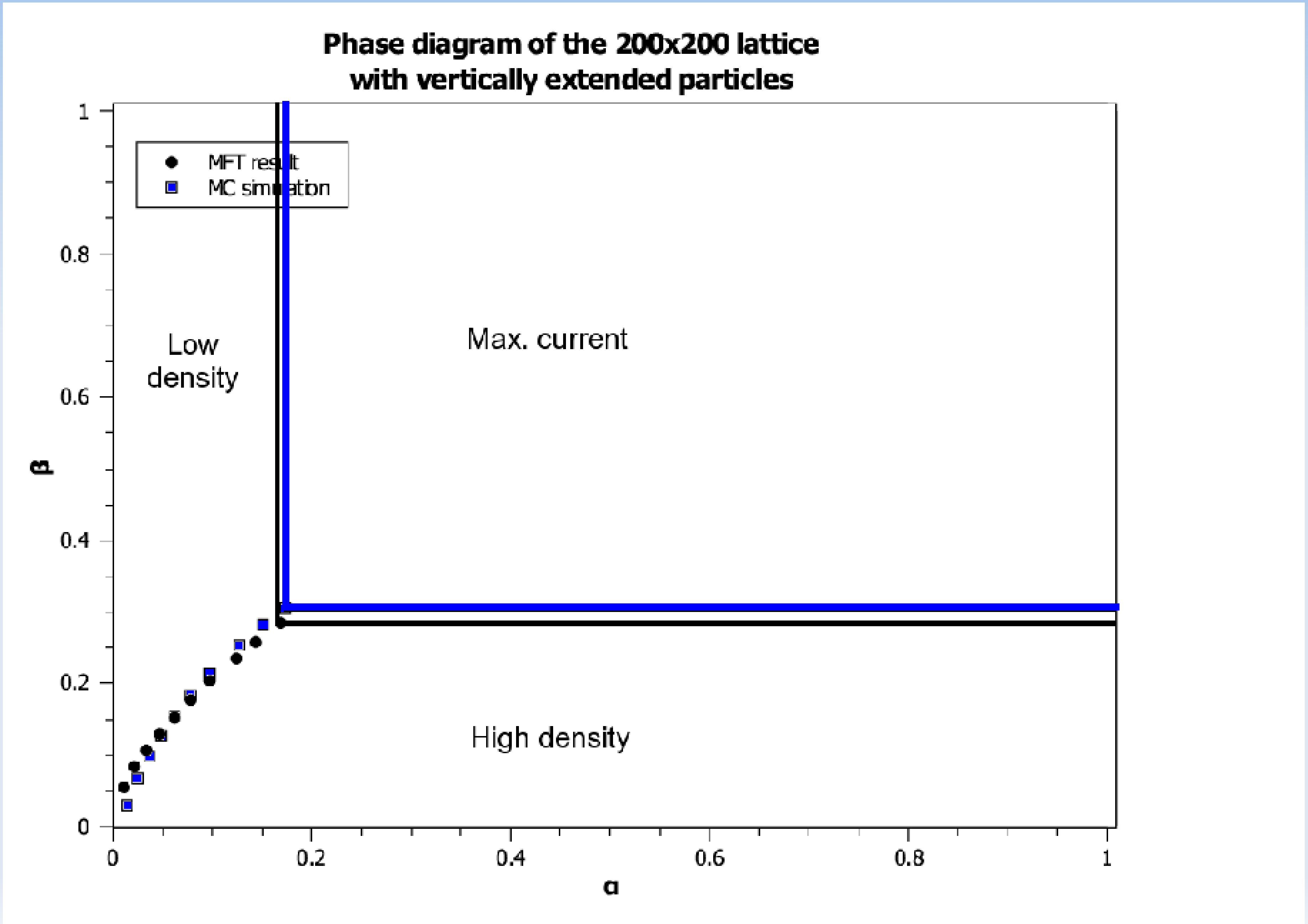


Extended particles

Vertically extended particles:



Extended particles



Vertical particle drift

Particles occupy one lattice site

Breaking $y \to -y$ symmetry of particle flow:

- probability to jump upward-right is *p*
- probability to jump downward-right is *1-p*

Vertical particle drift

Assumptions:

- No correlations between particles
- Substitute probability of the site to be occupied by its average value (average density)
- Density slowly changes in space
- To get current through *(x, y)*:
  - calculate current components through the planes located half a lattice spacing away
  - calculate average

Vertical particle drift

Right plane:

$$
\begin{aligned}
j_x(x+\frac{1}{2}) &= (1-p)\rho(x,y)(1-\rho(x+1,y+1)) \\
&+ p\rho(x,y)(1-\rho(x+1,y-1)) \\
j_y(x+\frac{1}{2}) &= (1-p)\rho(x,y)(1-\rho(x+1,y+1)) \\
&- p\rho(x,y)(1-\rho(x+1,y-1))
\end{aligned}
$$

Left plane:

$$
\begin{aligned}
j_x(x-\frac{1}{2}) &= (1-p)\rho(x-1,y-1)(1-\rho(x,y)) \\
&+ p\rho(x-1,y+1)(1-\rho(x,y)) \\
j_y(x-\frac{1}{2}) &= (1-p)\rho(x-1,y-1)(1-\rho(x,y)) \\
&- p\rho(x-1,y+1)(1-\rho(x,y))
\end{aligned}
$$

Vertical particle drift

Horizontal component of the current:

$$j_x = \rho(1-\rho) - \frac{1}{2}\frac{\partial\rho}{\partial x} - \frac{1}{2}(1-2\mathrm{p})\frac{\partial\rho}{\partial y}$$

Vertical component of the current:

$$j_y = (1-2\mathrm{p})\rho(1-\rho) - \frac{1}{2}\frac{\partial\rho}{\partial y} - \frac{1}{2}(1-2\mathrm{p})\frac{\partial\rho}{\partial x}$$

Vertical particle drift

Away from the boundaries and domain walls:

$$j_x = \rho(1-\rho)$$

$$j_y = (1-2\mathrm{p})\rho(1-\rho)$$

Critical values:

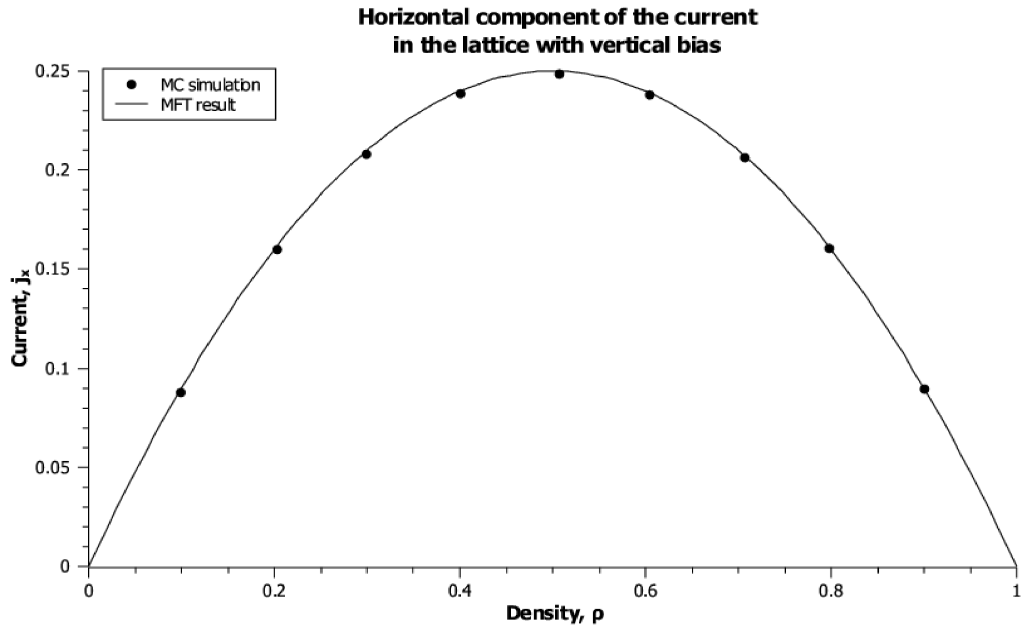
$$\rho_c = \frac{1}{2}$$

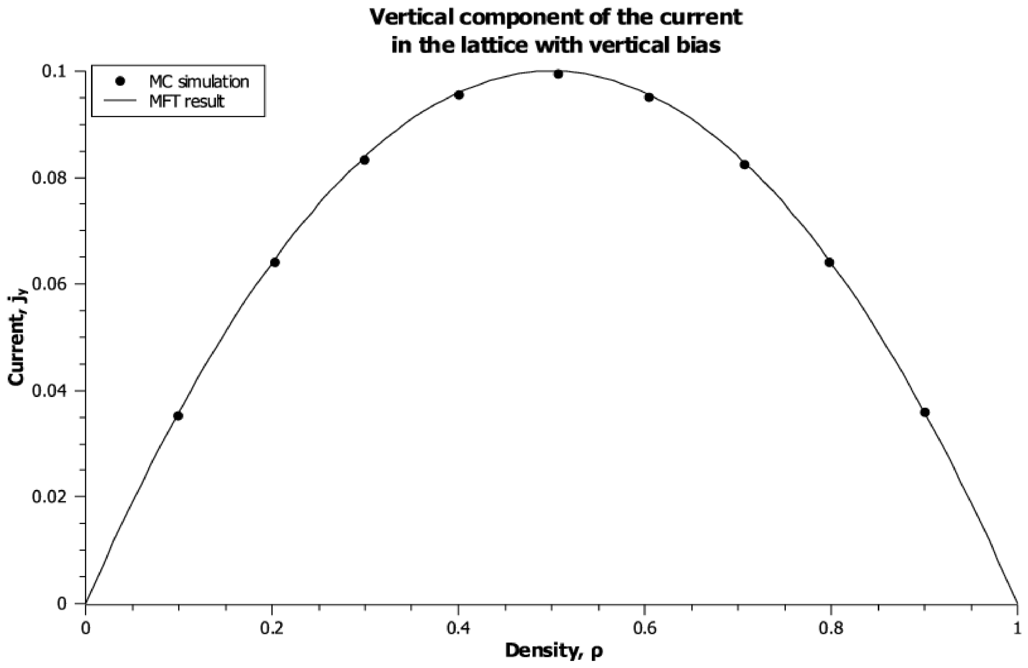
$$j_x^{max} = \frac{1}{4}, \quad j_y^{max} = \frac{1}{4}(1-2\mathrm{p})$$

Vertical particle drift.

Horizontal current component

Vertical current component





System with an obstacle

- Introduce an obstacle into the system – set of fixed particles:
- Spatial inhomogeneity $\rightarrow$ current inhomogeneity
- Non-uniform density distribution:
  - “traffic jam” in front of the obstacle
  - “shadow” behind the obstacle

System with an obstacle

Using the same MFT assumptions:

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= [\rho(x-1,y-1)+\rho(x-1,y+1)][1-\rho(x,y)] \\ &- \rho(x,y)[2-\rho(x+1,y-1)-\rho(x+1,y+1)]\end{aligned}$$

Assume that system is in steady state and expand density into the power series:

$$0=\frac{\partial^2 \rho}{\partial x^2}+\frac{\partial^2 \rho}{\partial y^2}-2\frac{\partial \rho(1-\rho)}{\partial x}$$

System with an obstacle

Density is uniform far from an obstacle (ρ_∞):

$$-S\frac{\partial \delta(x)\delta(y)}{\partial x}=\frac{\partial^2 f}{\partial x^2}+\frac{\partial^2 f}{\partial y^2}-2\mathrm{c}\frac{\partial f}{\partial x}$$

Where $f=\rho-\rho_\infty$ and $c=1-2\rho_\infty$

LHS – dipole source of strength *S*

$$\rho(x,y)=\rho_\infty+S\frac{\partial}{\partial x}(e^{cx}K_0(c\sqrt{x^2+y^2}))$$

$K_0=\int_0^\infty \frac{\cos(rt)\,dt}{\sqrt{t^2+1}}$ modified Bessel function of the second kind

For large argument: $K_0(r)\approx\frac{e^{-r}}{\sqrt{r}}$

System with an obstacle

For *x < 0*: $\rho(x,0) \approx \rho_\infty + Sce^{-2c|x|}$

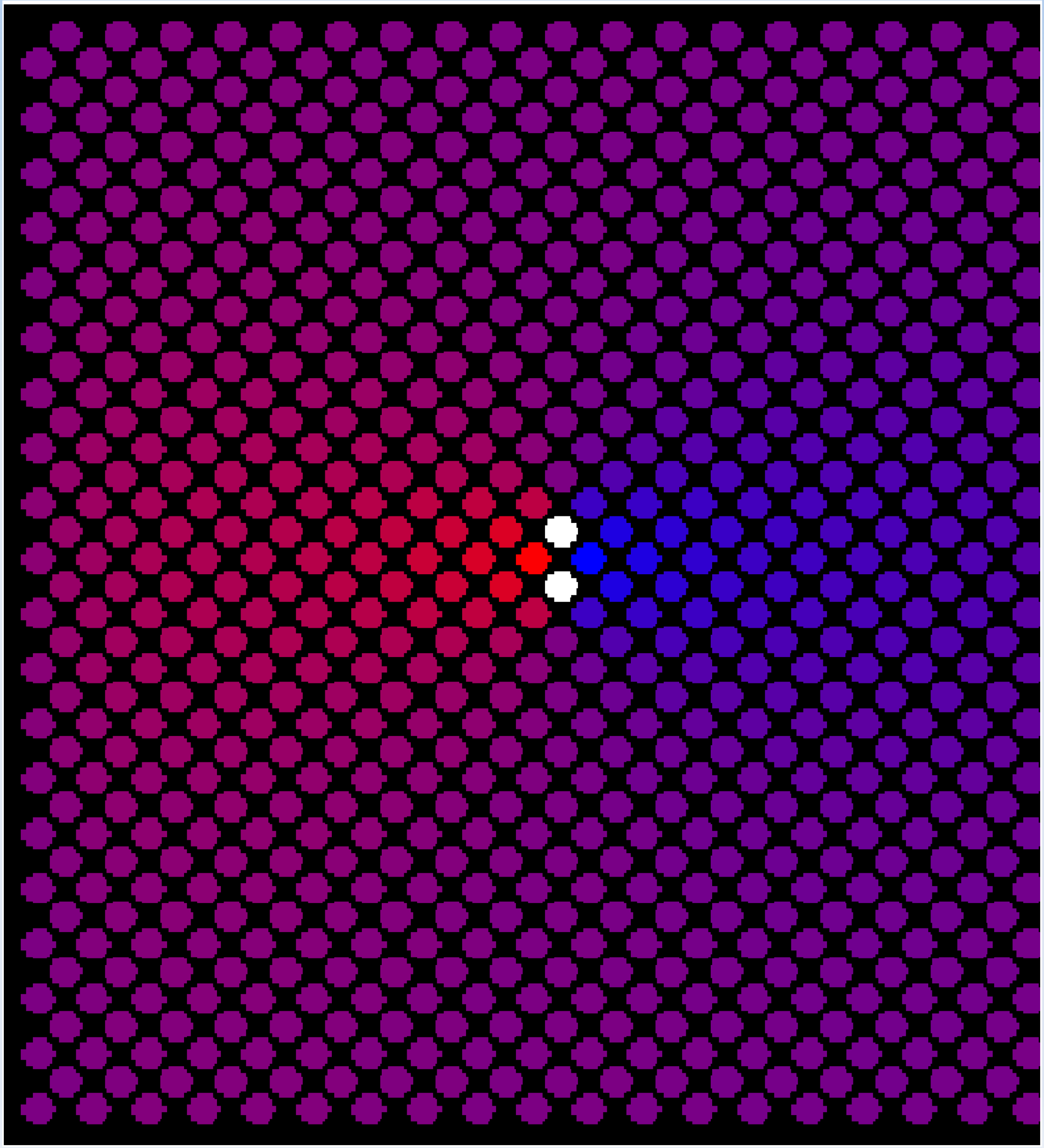
For *x > 0*: $\rho(x,0) \approx \rho_\infty - Sc(cx)^{-3/2}$

In transverse direction: $\rho(0,y) \approx \rho_\infty + Sce^{-|cy|}$

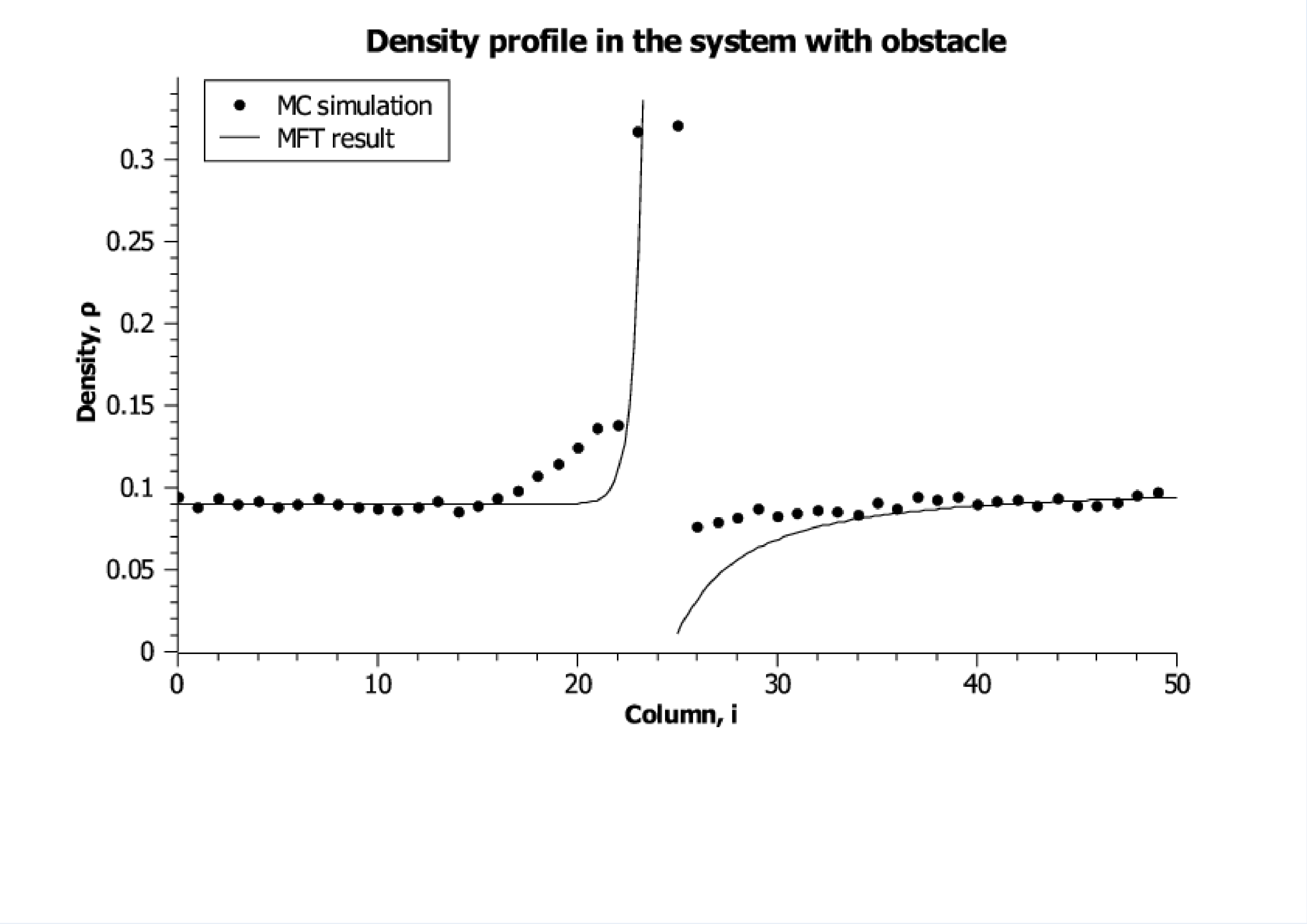
In front of the obstacle density changes from $\rho < 1/2$ to $\rho > 1/2$. There is characteristic length:

$$\xi = \frac{1}{c} = \frac{1}{1 - 2\rho_\infty}$$

System with an obstacle



System with an obstacle



Summary:

- **Regular 2D ASEP model:**
  - relationship between current and density
  - expressions for density profiles in all three phases and on the coexistence line
  - *results closely resemble results for 1D model*
- **2D ASEP with large particles:**
  - relationship between current and density
  - because of the broken particle – hole symmetry, results differ from those of regular 2D model

Summary:

- **2D ASEP with vertical particle drift:**
  - relationship between current and density for both current components (vertical and horizontal)
- **2D ASEP with immovable obstacle:**
  - density profiles in the vertical and horizontal directions

Open questions:

- **Regular 2D ASEP:** behavior and width of the domain wall

- **System with the extended particles:** particles of different size; mixture of particles with different size.

- **System with the immovable obstacle.** shape and characteristic dimensions of the region of increased density in front of the obstacle and “shadow” behind it; current in the system.