Driven Colloids I: Ratchets

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Outline

- Ratchets: Out of equilibrium by definition
  - Requirements for ratchet: Break enough symmetry

- Soft matter simulations – brief description

- Ratchet example 1: Quasi-1D ratchet
  - Collective interactions produce ratchet reversals

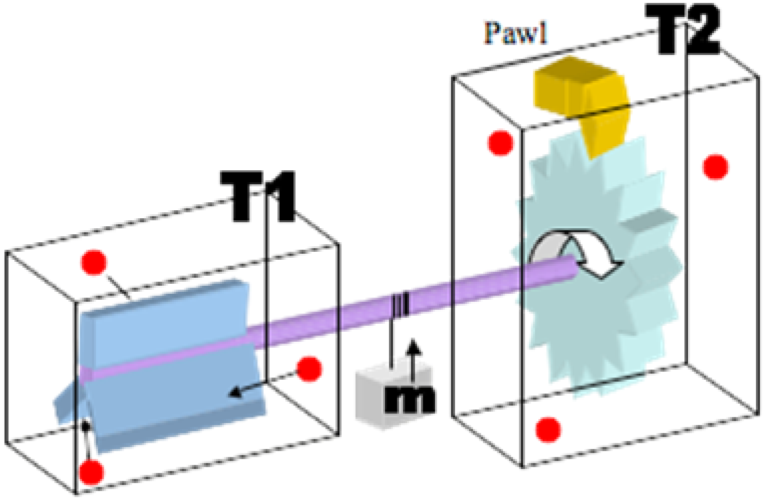
- Ratchet example 2: Colloidal logic
  - Alternative logic architecture requires a ratchet device to operate

- Ratchet example 3: Bacteria ratchet
  - Not "Maxwell's demon" but a simple Brownian ratchet

For an excellent review of ratchets, see P. Riemann, Phys. Rep. 361, 57 (2002)

Ratchets

- “Ratchet effect:” the emergence of directed transport in a spatially periodic system.
- Classic example: The Feynman-Smoluchowski ratchet
  - Asymmetric teeth
  - Pawl should move in only one direction
  - Rectification of thermal fluctuations, right? Wrong!
  - Not enough symmetries are broken



Ratchets and symmetry

- Necessary but not sufficient conditions for a ratchet:
  - Broken spatial symmetry (can also be statistical)
    - No dx s.t. V(-x) = V(x+dx) for all x
  - Broken temporal symmetry (ditto)
- Feynman ratchet breaks only spatial symmetry
- Perturbations of the system must be non-equilibrium in order to produce a ratchet effect.

Ways to break symmetry

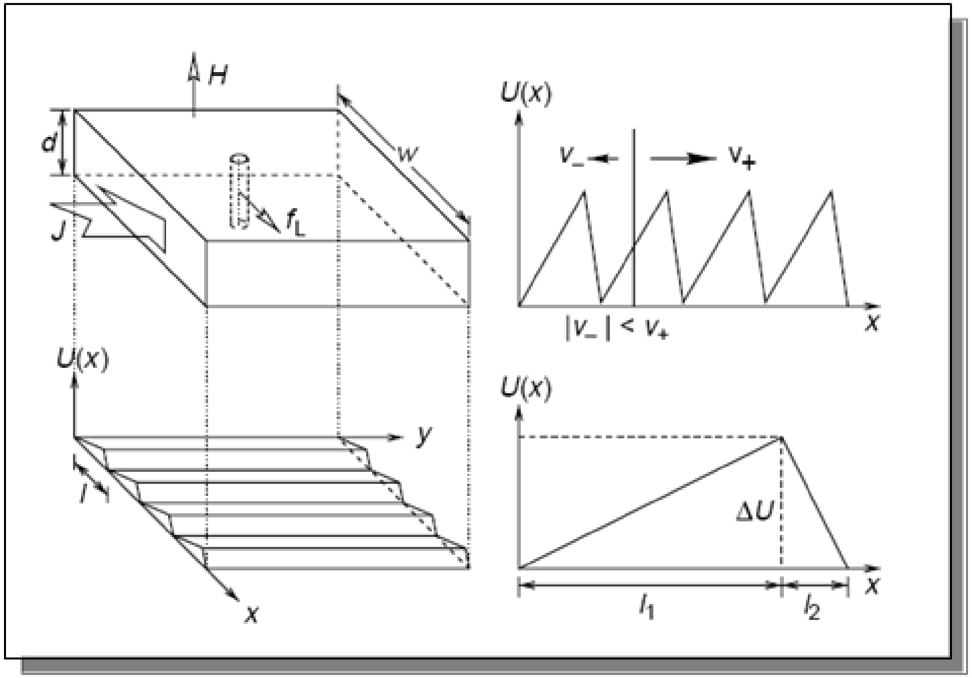
- Spatial:
  - Asymmetric sawtooth potential
  - Spatially dependent friction coefficient
- Temporal:
  - “Flashing” potential
  - Tilting potential
  - Asymmetric ac drive: zero net mean, but different amount of time spent at each force
  - Broken detailed balance: self-propelled particles

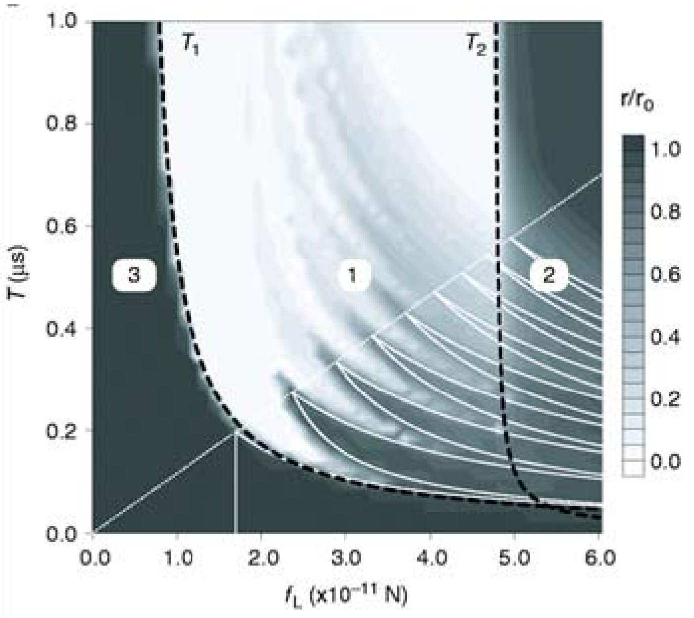
Ratchet Example 1: Quasi-1D (Vortex)

- **Ratchet effect for vortices on a one-dimensional asymmetric periodic substrate**
- **Normal ratchet effect occurs in the limit of noninteracting vortices**
- **Ratchet reversal appears due to vortex-vortex interactions as vortex density changes**
- **Ratchet behaviour connected with local vortex structure**

Ratchet effect

The simplest vortex ratchet proposal was for a simple periodic, asymmetric 1D substrate. Can this system exhibit reversal effects and other collective dynamical effects?



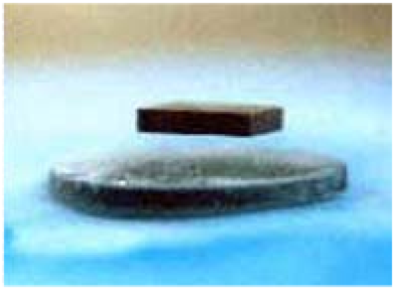


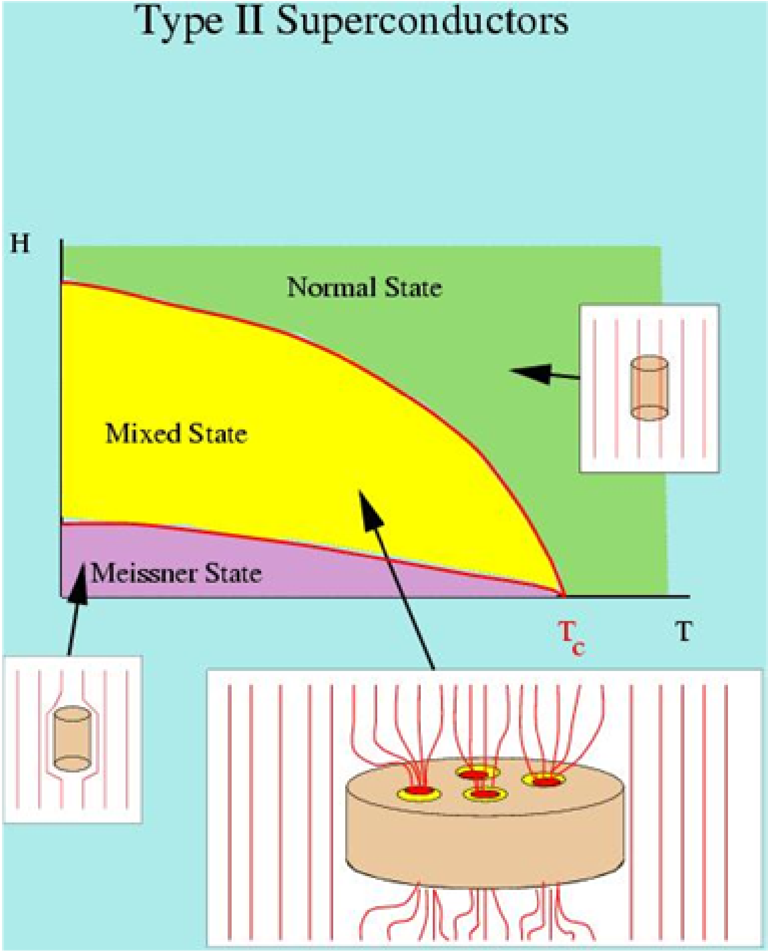
C.S. Lee, B. Janko, I. Derenyi, A.L. Barabasi, Nature 400, 337 (1999)

Soft matter: Superconducting Vortices

Superconductor:
- Perfect transport of current
- Complete expulsion of magnetic field.

Vortex: localized magnetic field line

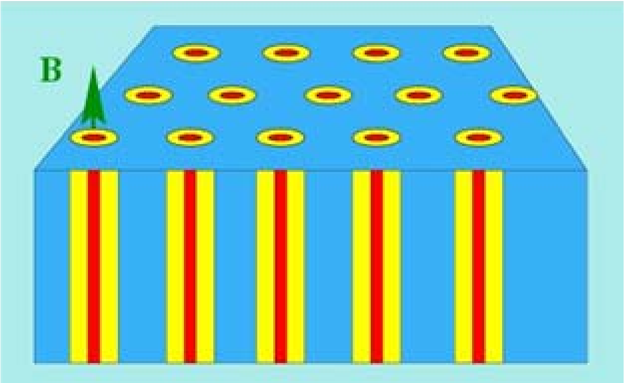


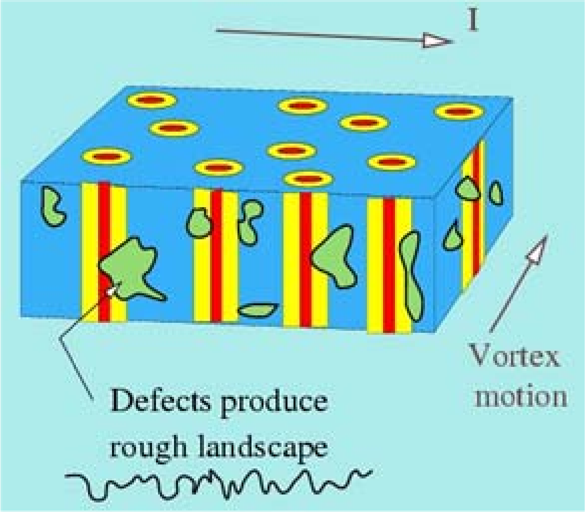


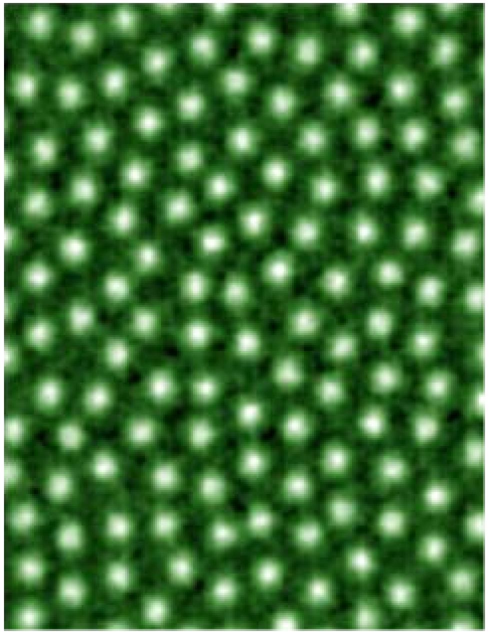
Vortices in Superconductors

- Vortices repel each other and form a soft triangular lattice.
- Vortex has line energy due to superconductivity suppression at the vortex core.
- Interaction with defects in the material can produce pinning.

- Pinning (quenched disorder) can be altered through sample treatment.
- Strength of vortex interaction can be tuned by changing magnetic field.





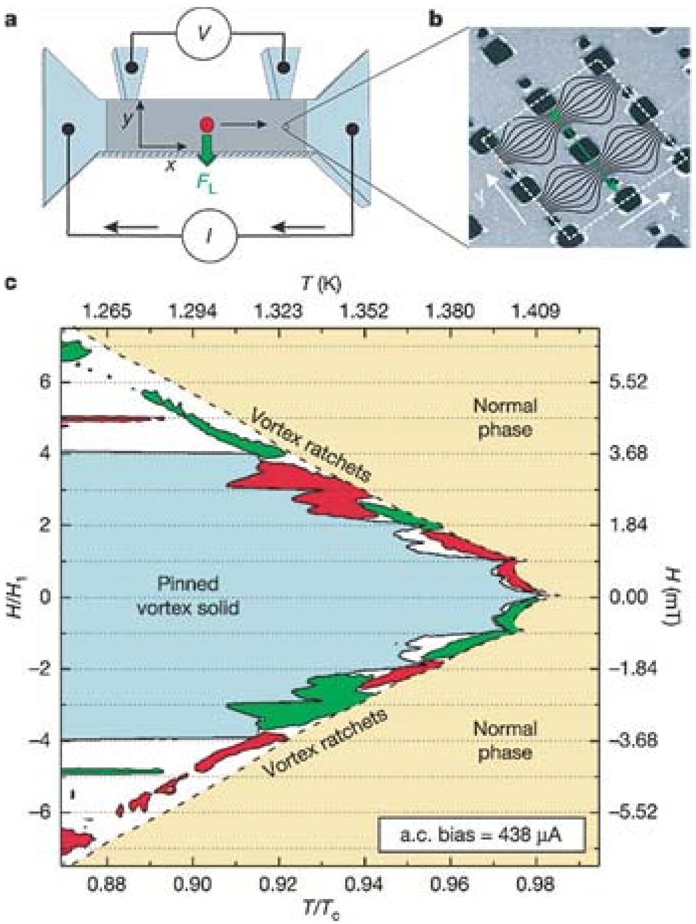


Vortices in Nb
TH Johansen, Oslo
Vortex spacing ~ 1 μm

Ratchet effect and reversed ratchet effect

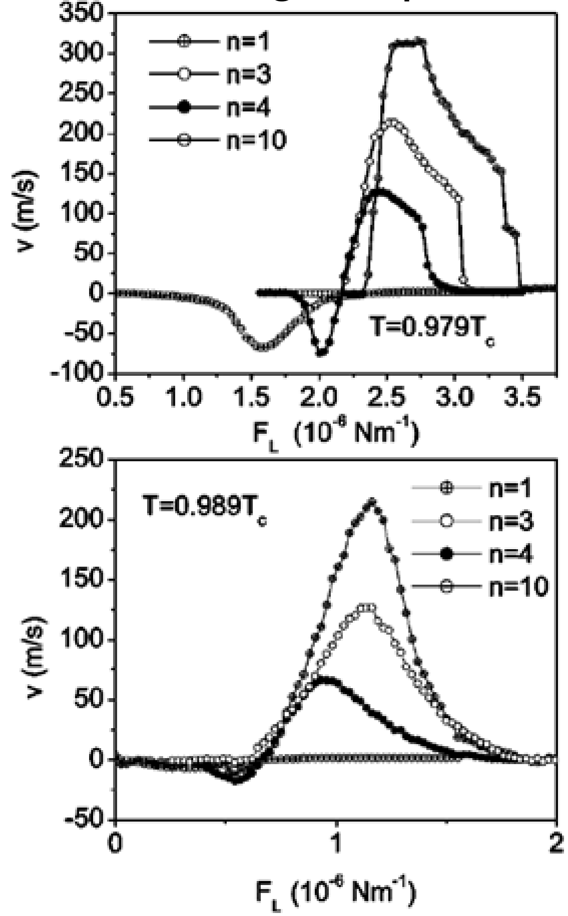
- **Seen for 2D periodic pinning structures.**

Asymmetric squares



C. De Souza Silva et al, Nature 440, 651 (2006)

Triangular pins



J.E. Villegas et al, PRB 71, 024519 (2005)

Dynamics of Vortices

- Motion of vortices are dominated by the following motion equation with vortices treated as over-damped (damping constant η) massless particles:

$$\eta \frac{d\mathbf{r_i}}{dt} = \mathbf{f_i}^{\mathbf{vv}} + \mathbf{f_i}^{\mathbf{T}} + \mathbf{f_i}^{\mathbf{p}} + \mathbf{f_i}^{\mathbf{d}}$$

  - Vortex-vortex interaction force:

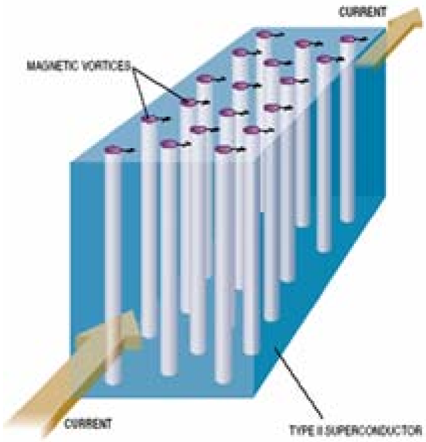
$$\mathbf{f_i}^{\mathbf{vv}} = \sum_{j \neq i}^{N_v} \frac{\phi_0^2}{2\pi\mu_0\lambda^3} \cdot K_1\left(\frac{r_{ij}}{\lambda}\right)\hat{\mathbf{r}}_{\mathbf{ij}}$$

  - Thermal force arises from random Langevin kicks

$$\left\langle \mathbf{f_i}^{\mathbf{T}} \right\rangle = 0 \qquad \text{and} \qquad \left\langle \mathbf{f_i}^{\mathbf{T}}(t) \cdot \mathbf{f_j}^{\mathbf{T}}(t') \right\rangle = 2\eta k_B T \delta(t - t')\delta_{ij}$$

Dynamics of Vortices (continued)

- $$\eta \frac{d\mathbf{r_i}}{dt} = \mathbf{f_i^{vv}} + \mathbf{f_i^{T}} + \mathbf{f_i^{p}} + \mathbf{f_i^{d}}$$

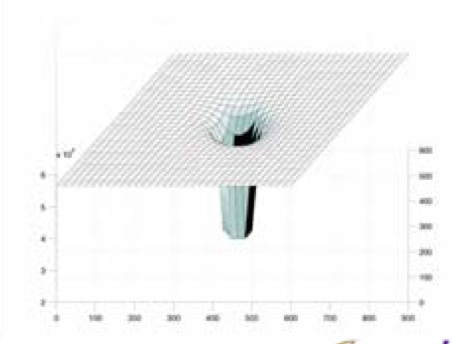


  - Lorentz driving force from an external applied current:

$$\mathbf{f_i^{d}} = (\mathbf{J} \times \hat{\mathbf{h}})\phi_0 d$$

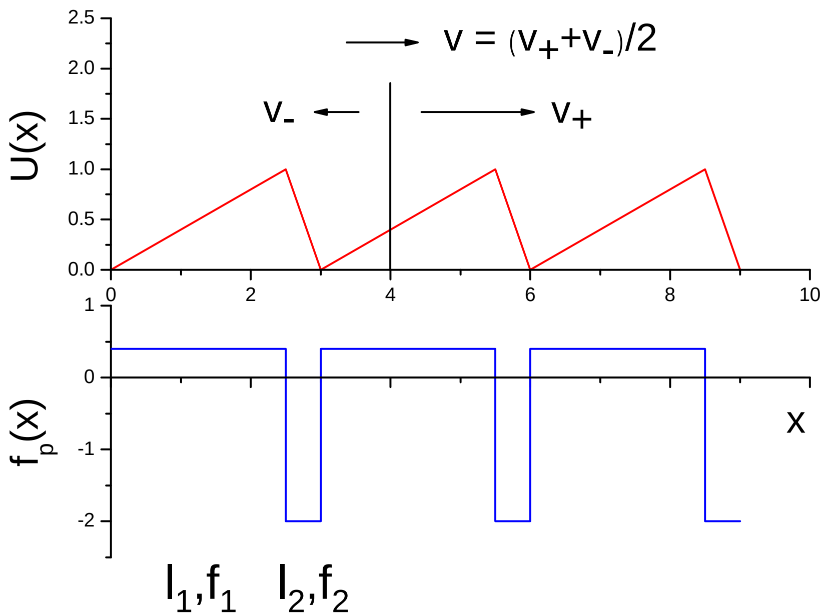
  - Flux-Pinning : magnet flux (vortex) can be trapped or “pinned” inside a superconducting material when there are **defects** in the crystalline structure of the superconductor

$$\mathbf{f_i^{p}} = -\nabla U(\mathbf{r})$$

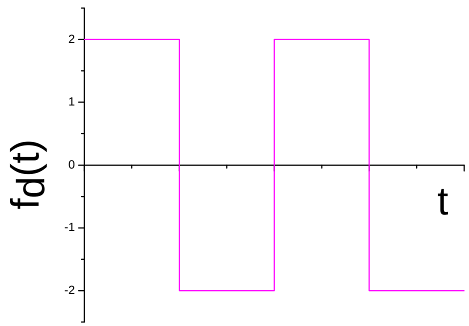


Asymmetric 1D periodic pinning potential

- **1D periodic potential of the type proposed by C.S. Lee et al, 1999.**
- **Study ratchet effect for increasing vortex density**
- **Study vortex ordering and correlate with ratchet effect and reversals.**



Apply an ac drive

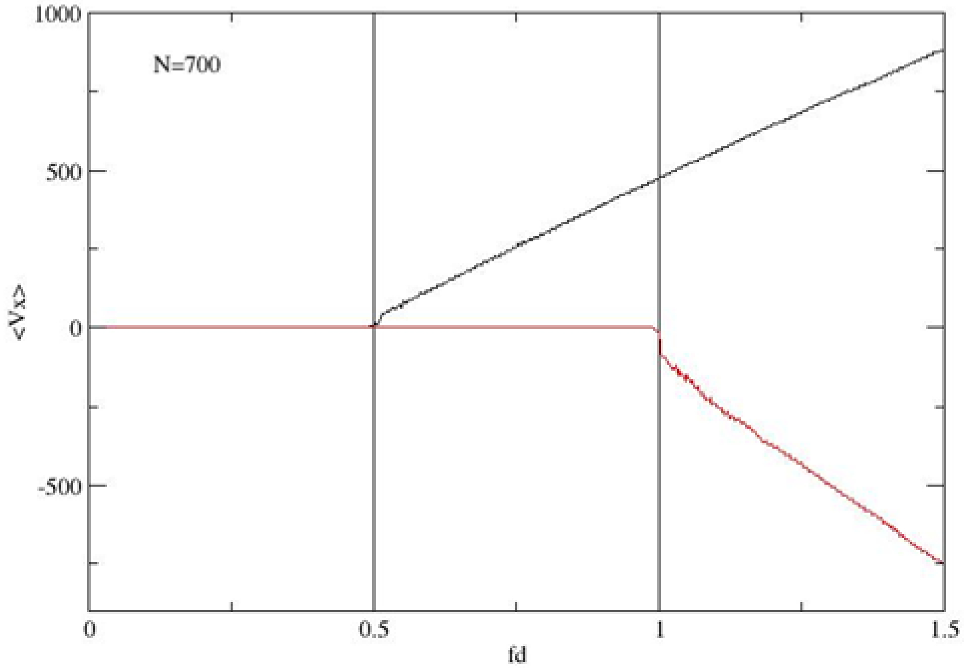


Magnitude fd

Period T

Ratchet Effect
DC Current

- Study the **net velocity** (displacement) when **positive** (toward soft edge) or **negative** (toward hard edge) DC current is applied



Three phases:

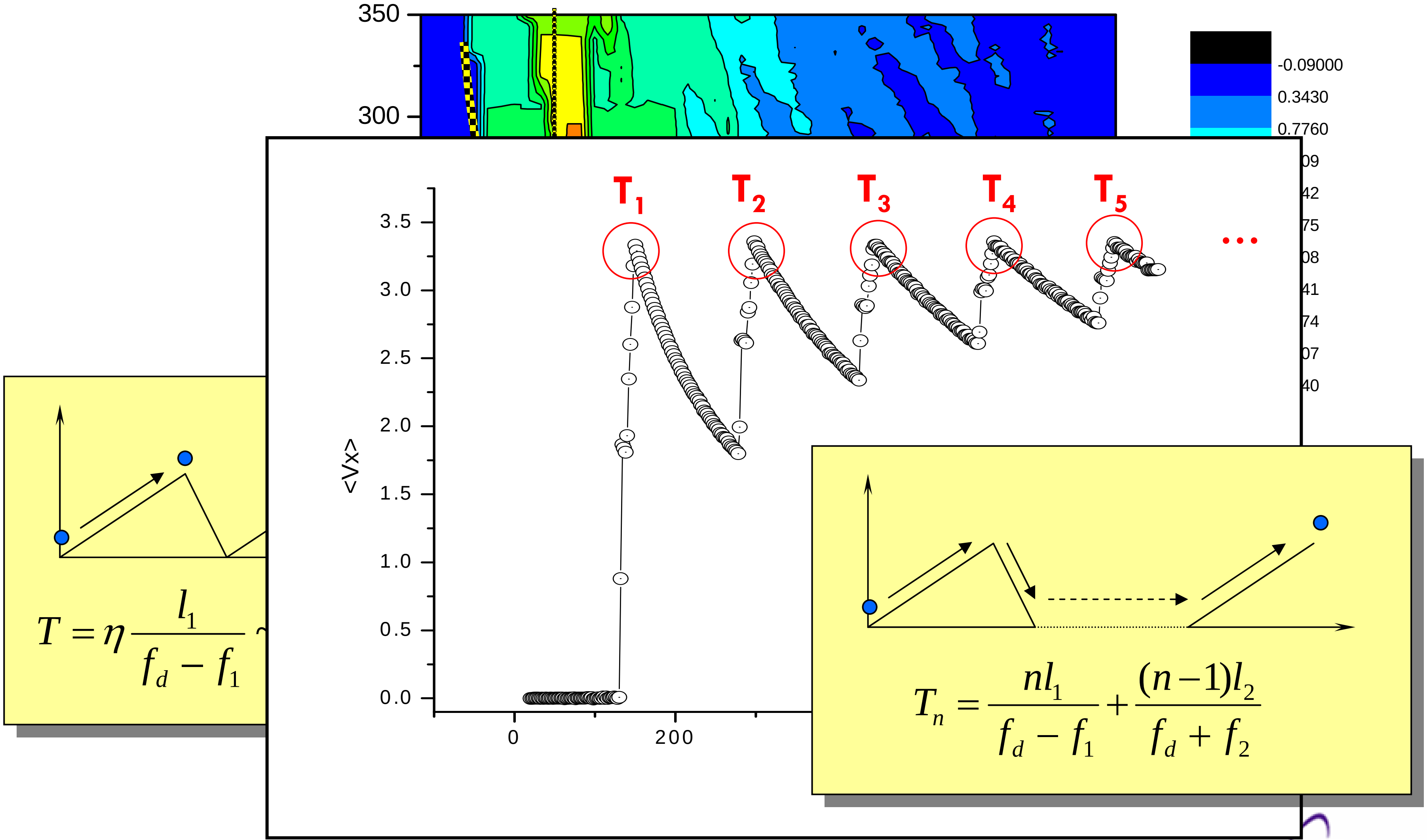
➢ $|f_d|<0.5$,
No ratchet effect

➢ 0.5<|fd|<1.0,
Positive net velocity

➢ |fd|>1.0,
Reduced ratchet effect

Ratchet Effect

ac current with different frequencies and amplitude



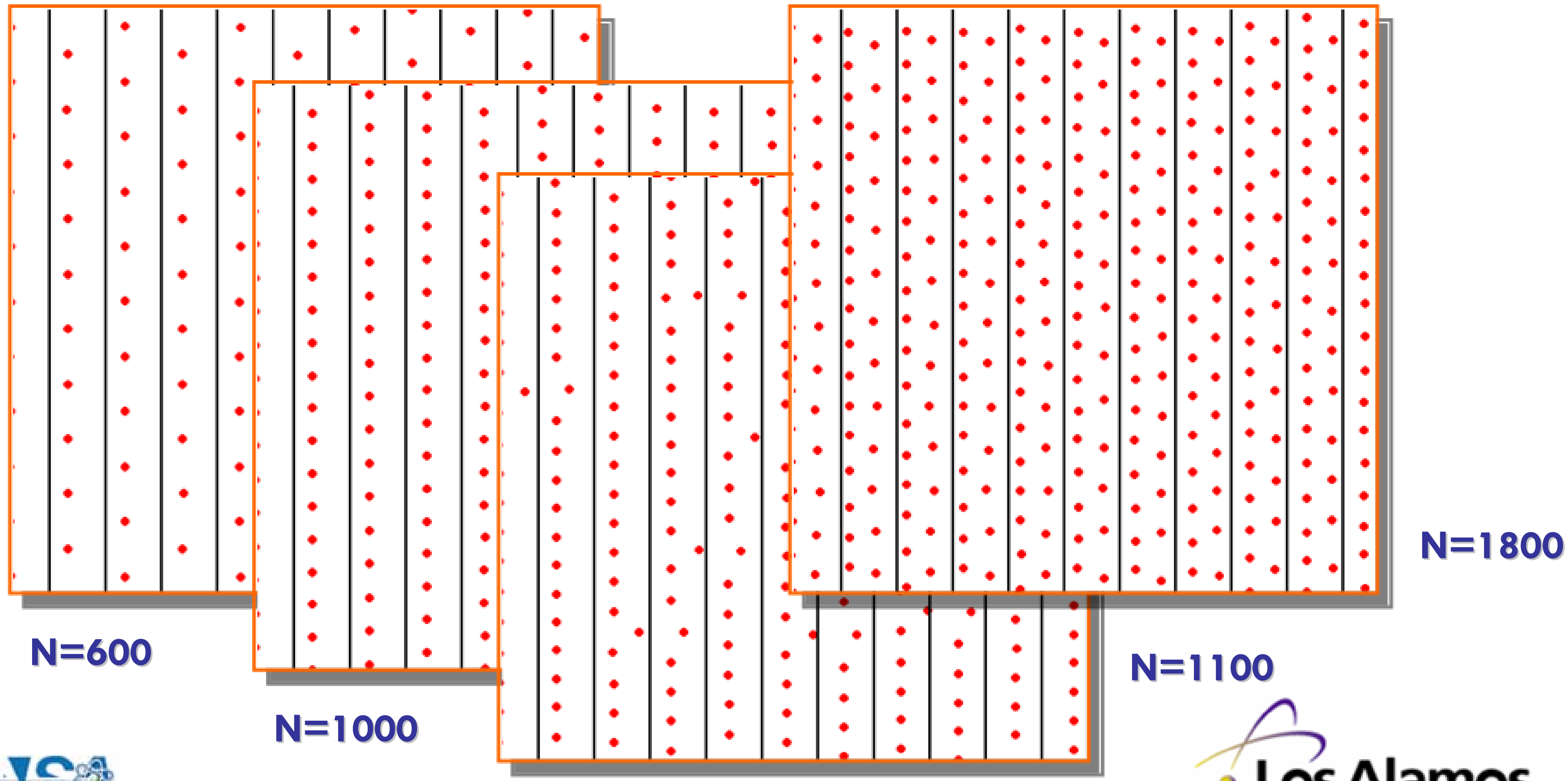
$$T = \eta \frac{l_1}{f_d - f_1}$$

$$T_n = \frac{nl_1}{f_d - f_1} + \frac{(n-1)l_2}{f_d + f_2}$$

Ratchet Effect

Introducing vortex-vortex interactions

- So far we used low vortex density; thus, the vortex-vortex interactions can be neglected
- What if we increase the vortex density?



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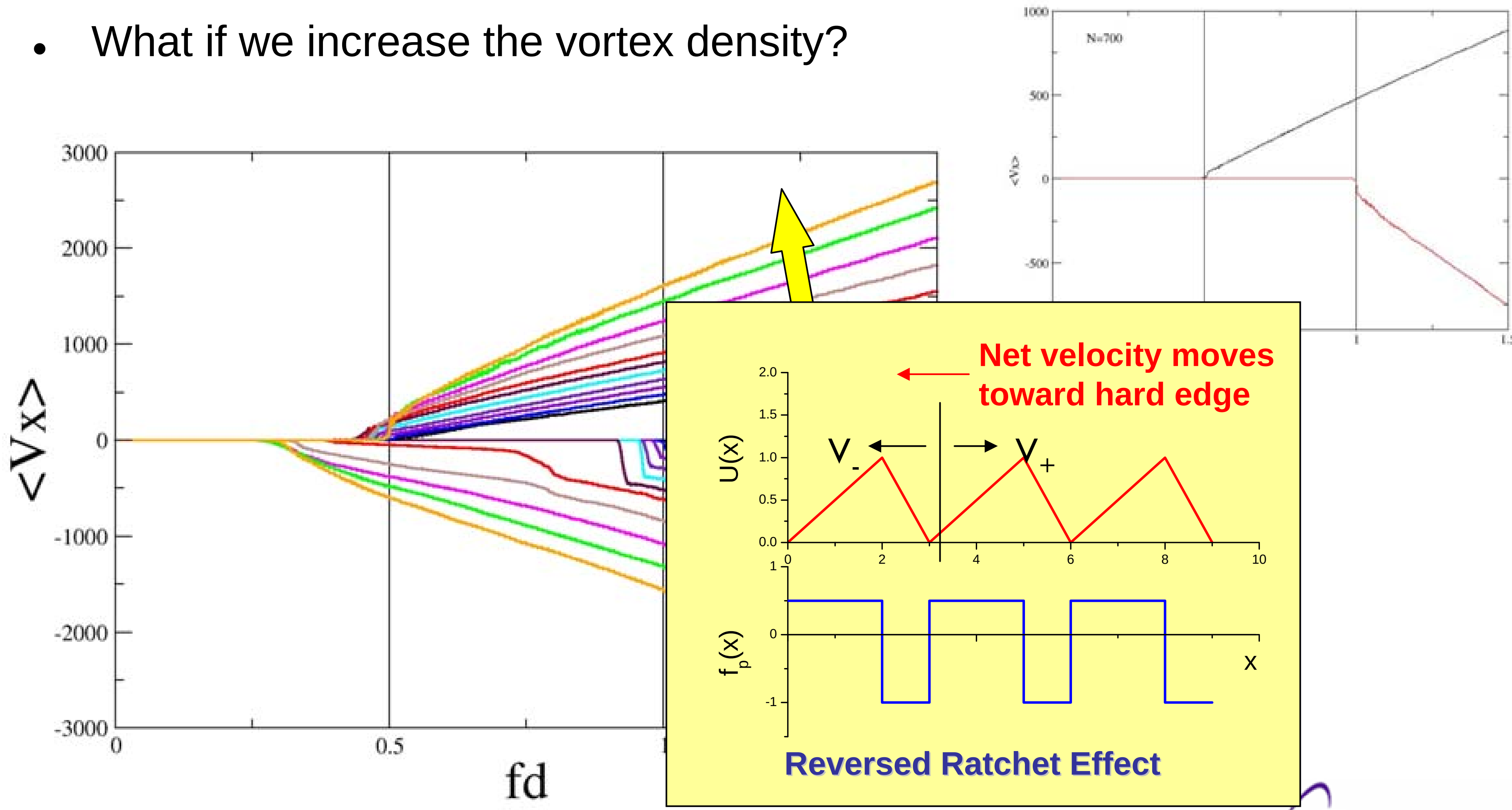
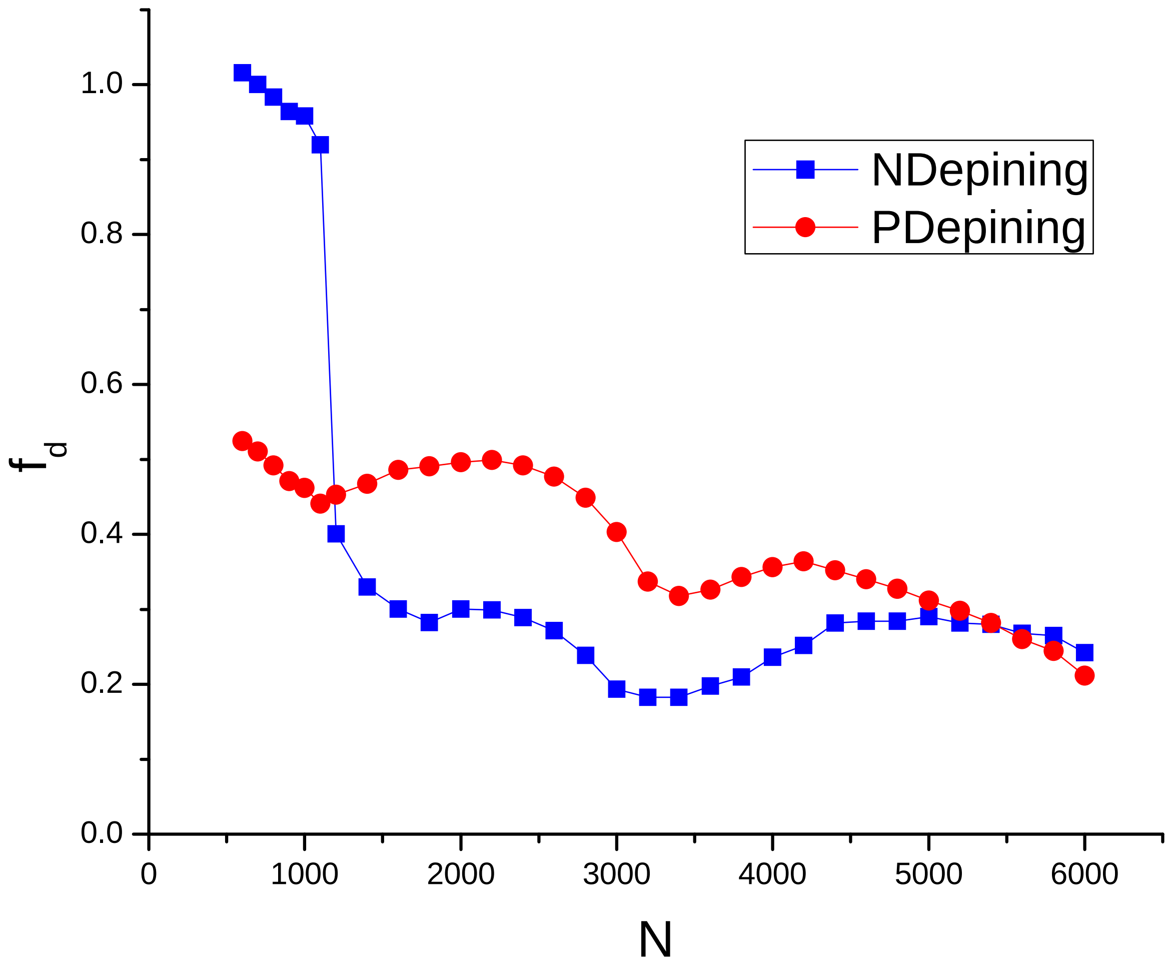


Ratchet Effect

Vortex-vortex interactions and reversed ratchet effect

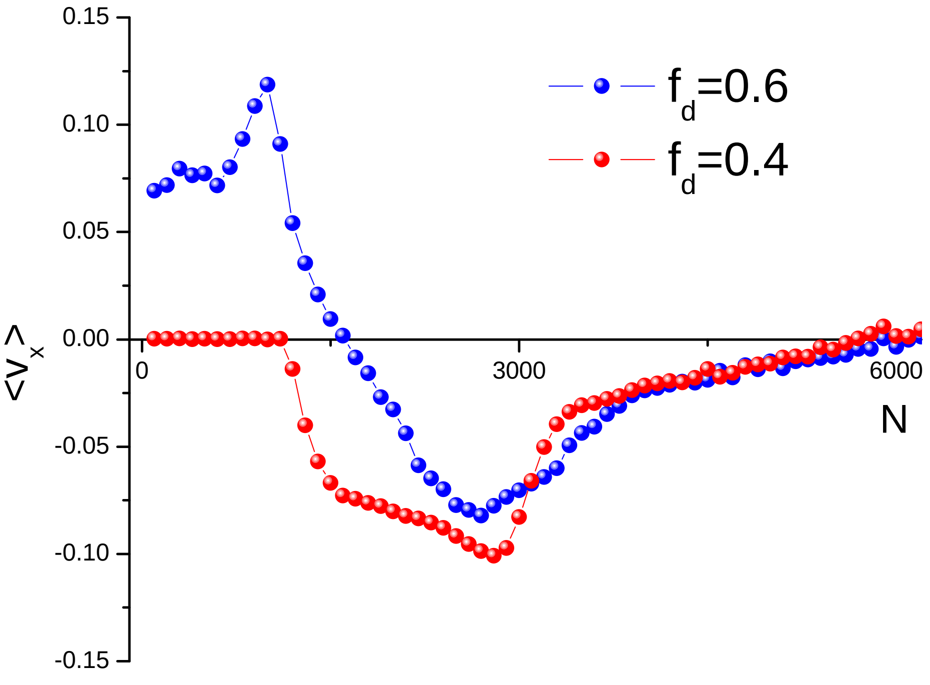
- Depinning forces

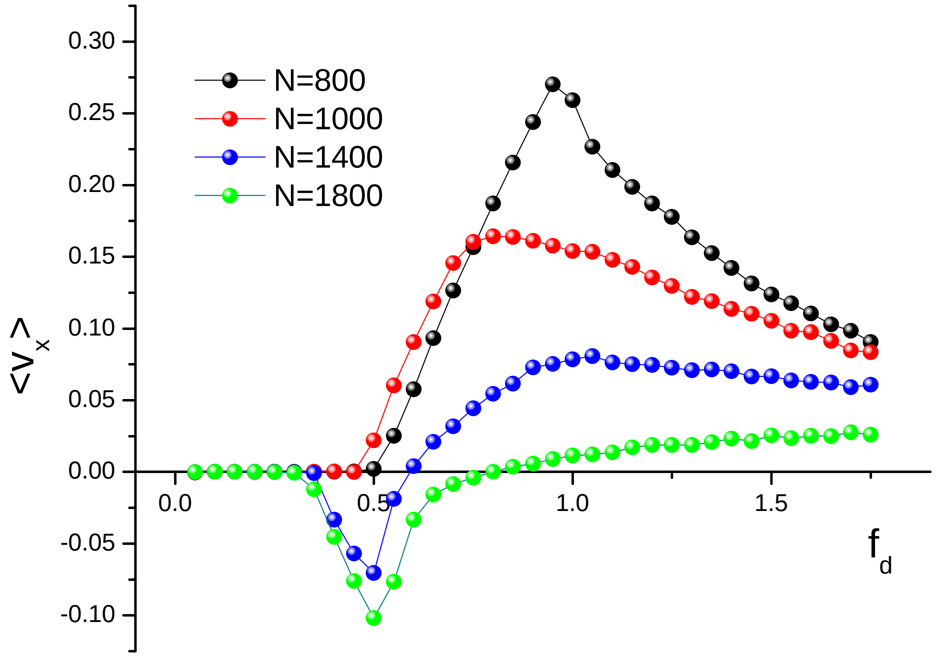


Ratchet Effect

Vortex-vortex interactions and reversed ratchet effect

- Ratchet displacement: ac drive

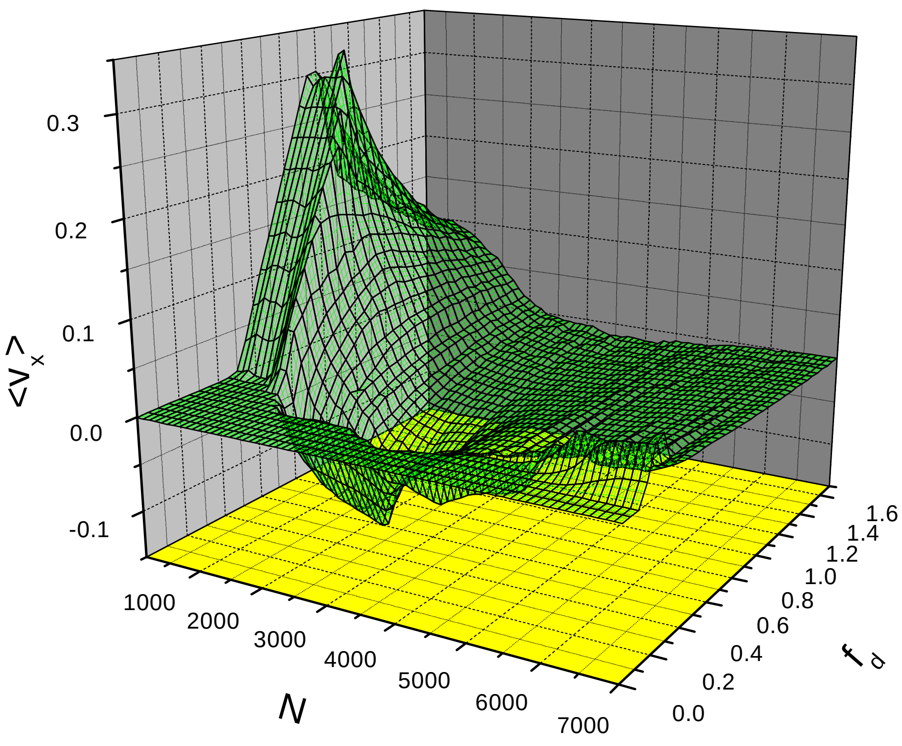


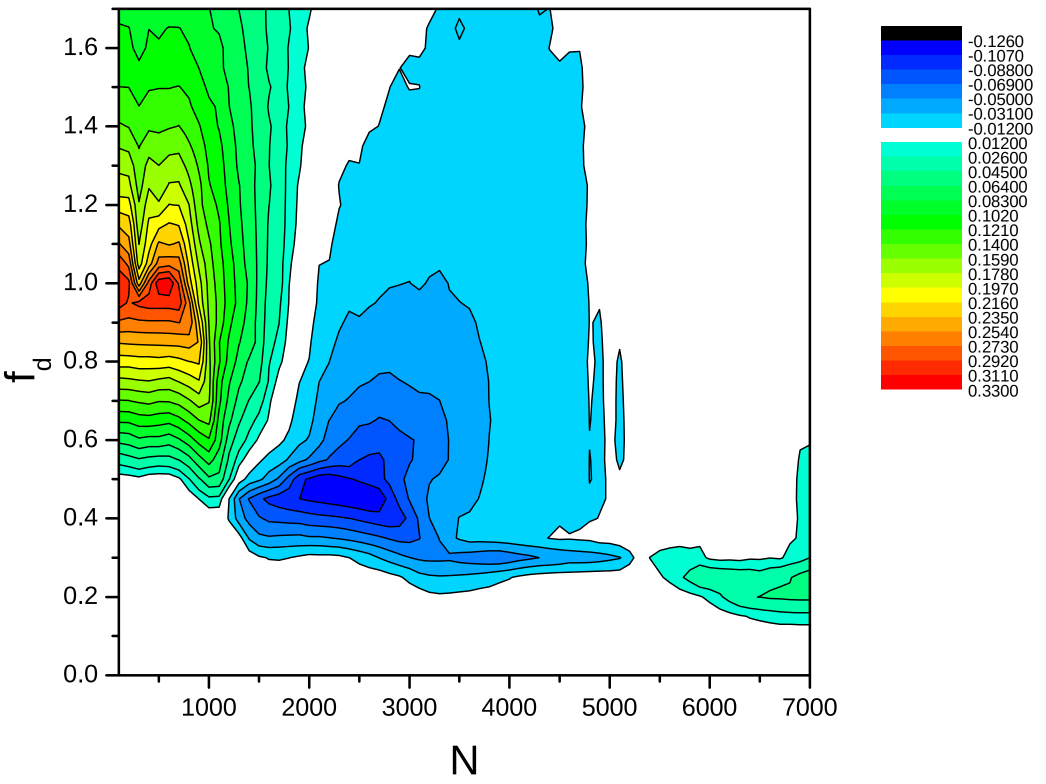


Ratchet Effect

Vortex-vortex interactions and reversed ratchet effect

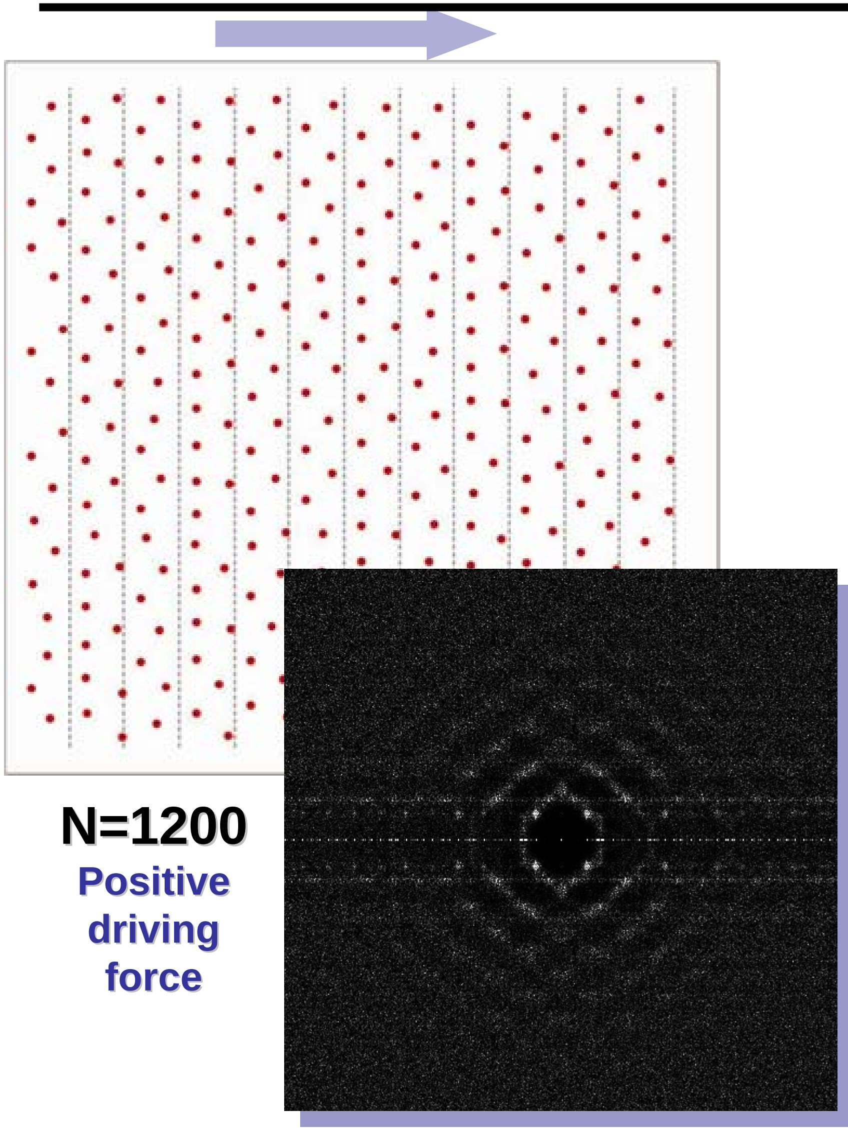
- Ratchet displacement on plane N and f_d (normalized by N)





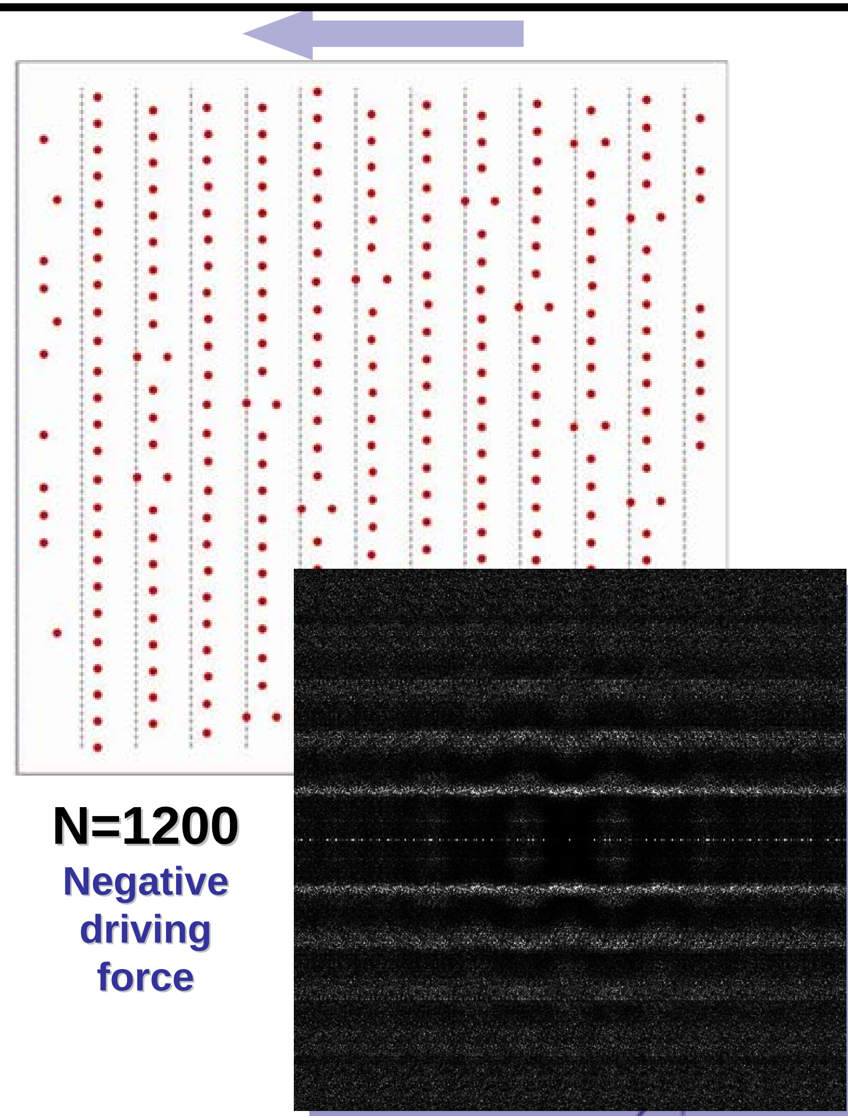
Ratchet Effect

Vortex-vortex interactions and reversed ratchet effect



N=1200

Positive driving force



N=1200

Negative driving force

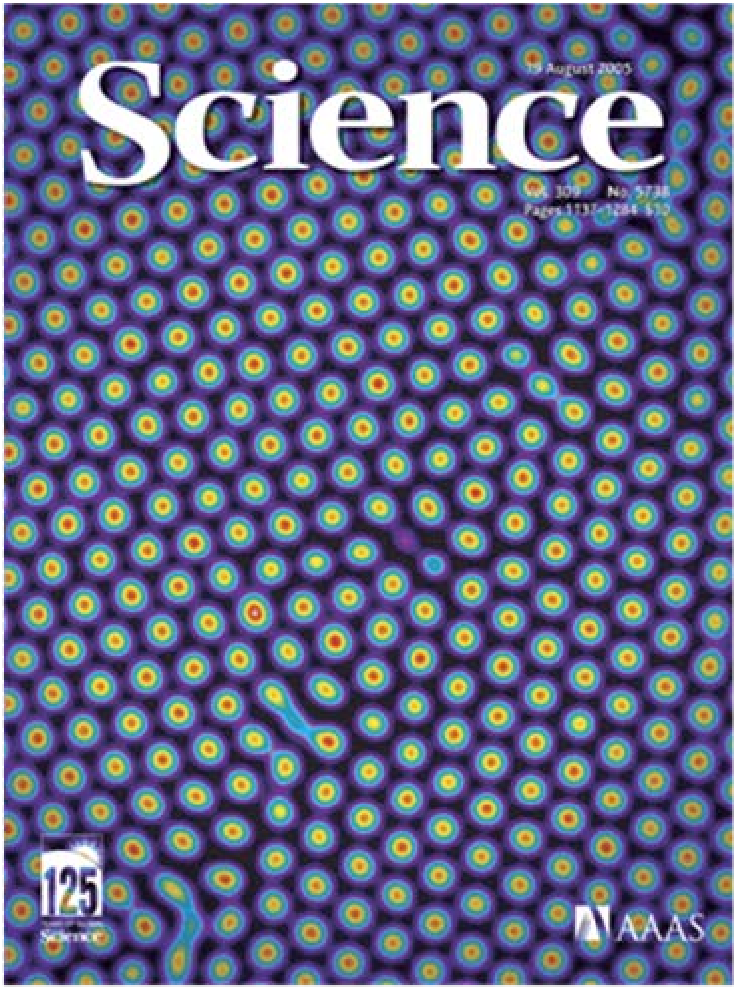
Ratchet example 2: Colloidal logic

Typical example: polystyrene sulfate spheres 0.2 to 1 micron in diameter

2D and 3D systems

Monodisperse and polydisperse
Charged and uncharged
Dynamics with applied
E or B fields

Relevant to industrial applications:
paints, emulsions,
nanostructures,
photonic band gap materials,
biological transport

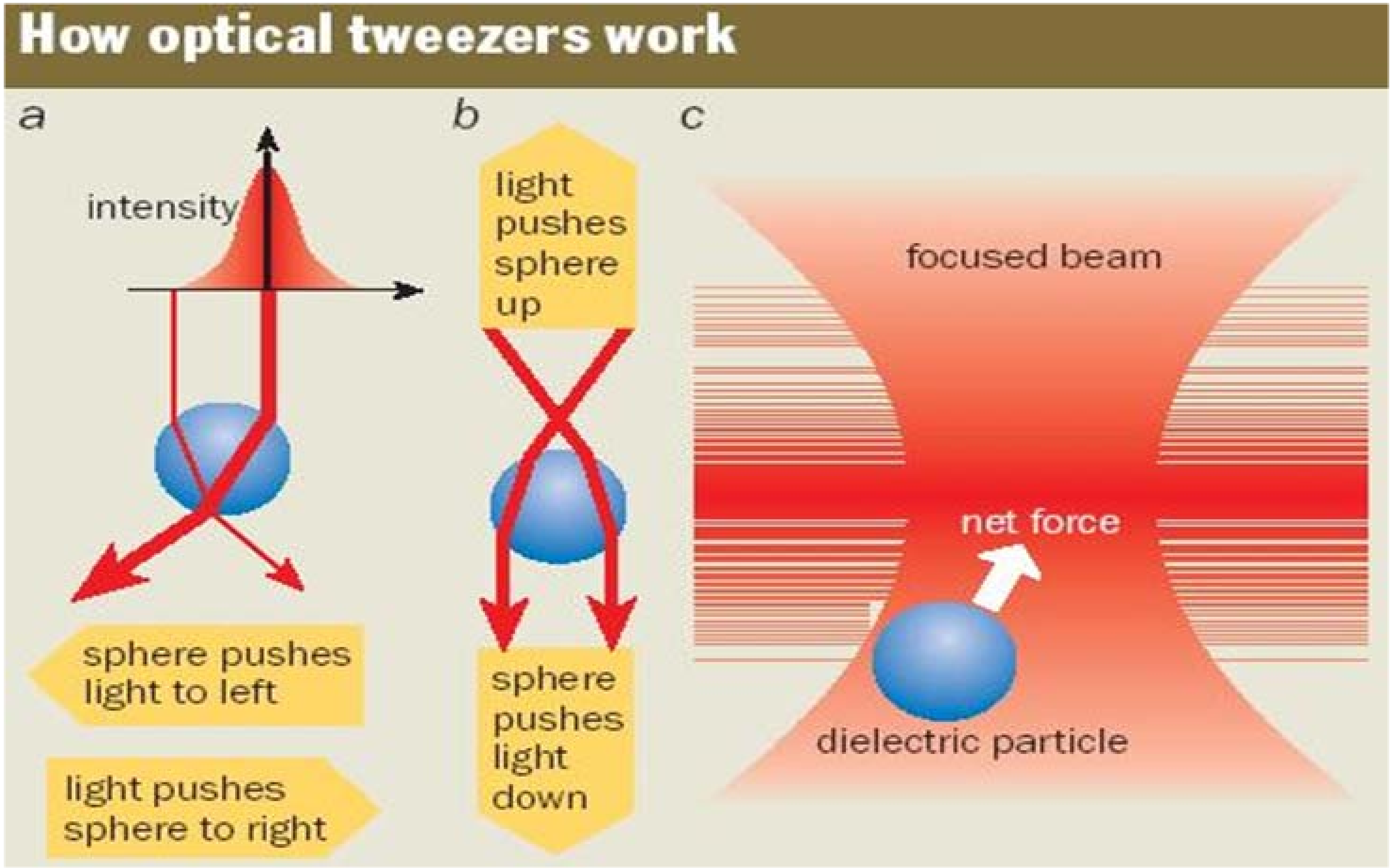


August 2005

Manipulating Colloids with External Fields

Optical Traps

K. Dholakia, G. Spalding, and M. MacDonald, Physics World, Oct 2002



Computational modelling of colloids on periodic substrate

$$\eta \frac{d\mathbf{R}_i}{dt} = \mathbf{F}_i^{cc} + \mathbf{F}_i^{T} + \mathbf{F}_i^{s} + \mathbf{F}_i^{ext}$$

Overdamped Langevin dynamics

$$\mathbf{F}_i^{cc} = q_i \sum_{i \neq j}^{N_i} -\nabla_i V(r_{ij})$$

$$V(r_{ij}) = (q_j/|\mathbf{r}_i - \mathbf{r}_j|)\exp(-\kappa|\mathbf{r}_i - \mathbf{r}_j|)$$

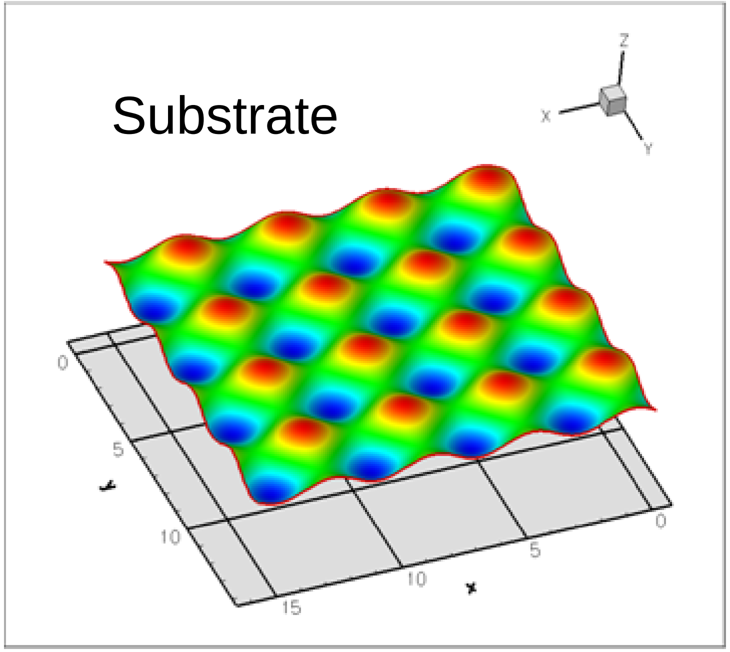
$$\langle \mathbf{F}_i^{T} \rangle = 0$$

$$\langle \mathbf{F}^{T}(t)\mathbf{F}^{T}(t') \rangle = 2\pi\eta k_B T \delta(t - t')$$

$$\mathbf{F}_i^{s} = A\sin(2\pi x/a_x)\hat{\mathbf{x}} + B\sin(2\pi y/a_y)\hat{\mathbf{y}}$$

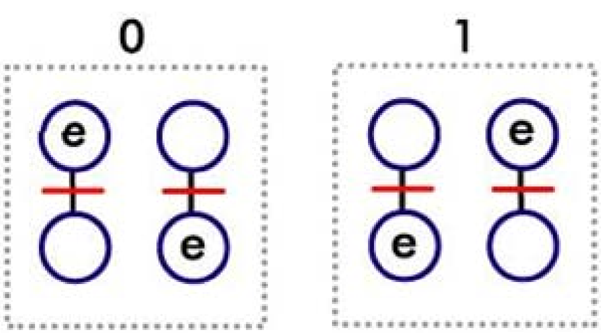
$$\mathbf{F}_i^{ext} = F^{dc}\hat{\mathbf{x}}$$

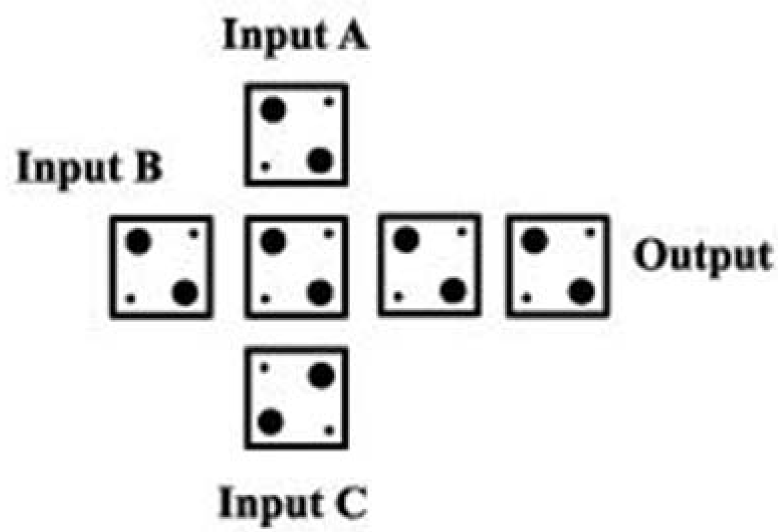
$$\mathbf{F}_i^{ext} = F^{ac}\sin((\omega_d + \phi)t)\hat{\mathbf{x}}$$

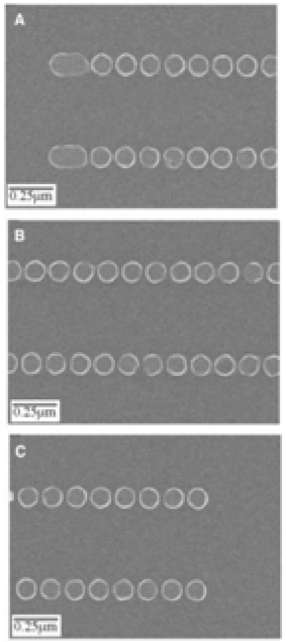


Quantum Cellular Automata

- C.S. Lent, P.D. Tougaw, W. Porod, G.H. Bernstein, Nanotechnol. 4, 49 (1993)
- I Amlani, A.O. Orlov, G. Toth, G.H. Bernstein, C.S. Lent, and G.L. Snider, Science 284, 289 (1999).

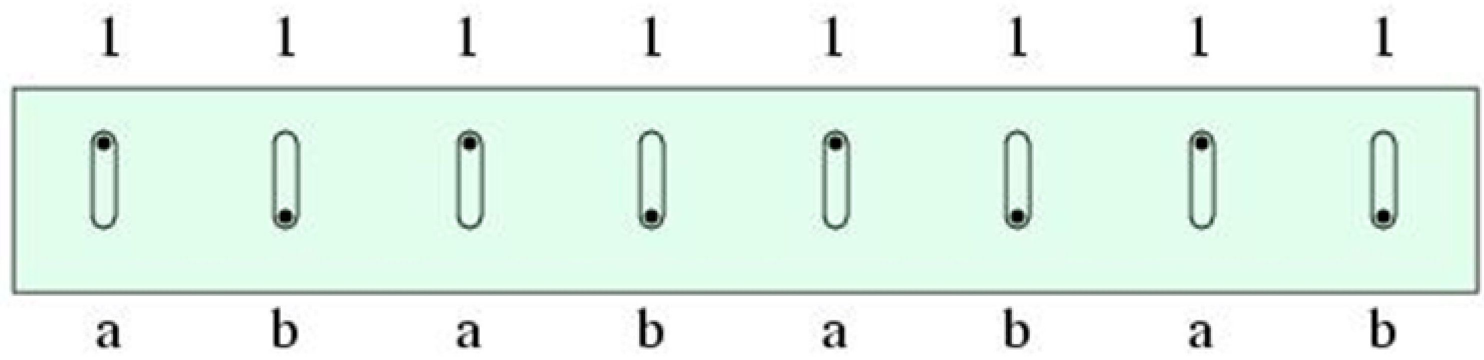






Magnetic QCA: R.P. Cowburn, M.E. Welland, Science 287, 1466 (2000)

Logic states for repulsive particles

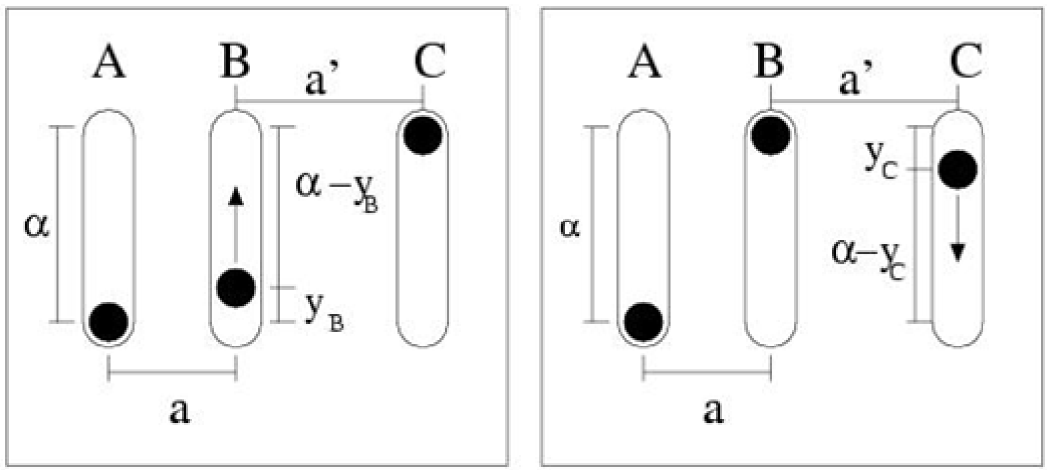


Simulation result.

Particle at top of dot a: Logic state 1
Particle at bottom of dot a: Logic state 0
If leftmost particle is flipped, will the change propagate?

Colloids: screened Coulomb interaction
Vortices: logarithmic interaction
Classical electrons: in quantum dots.

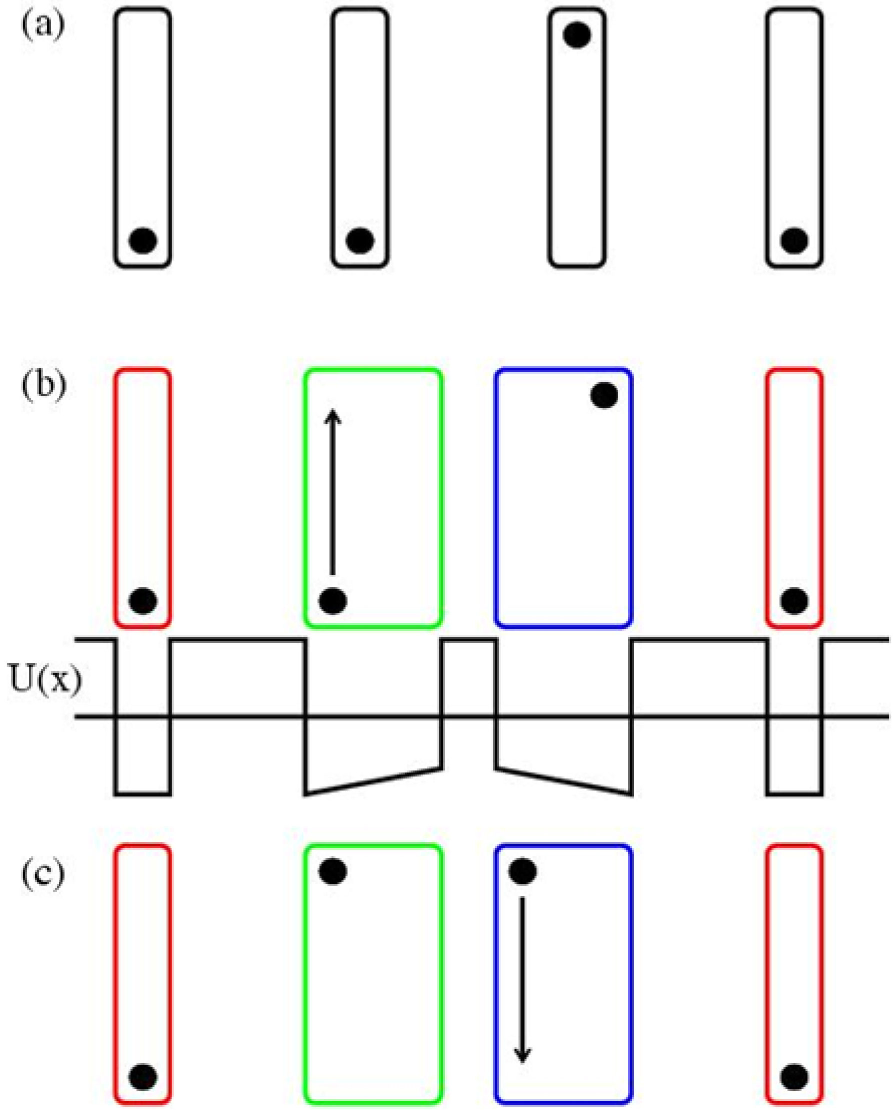
Problem: State indeterminacy



a

b

Ratchet Geometry



Signal cannot propagate
No inertia to carry particle over center barrier created by particle-particle interactions

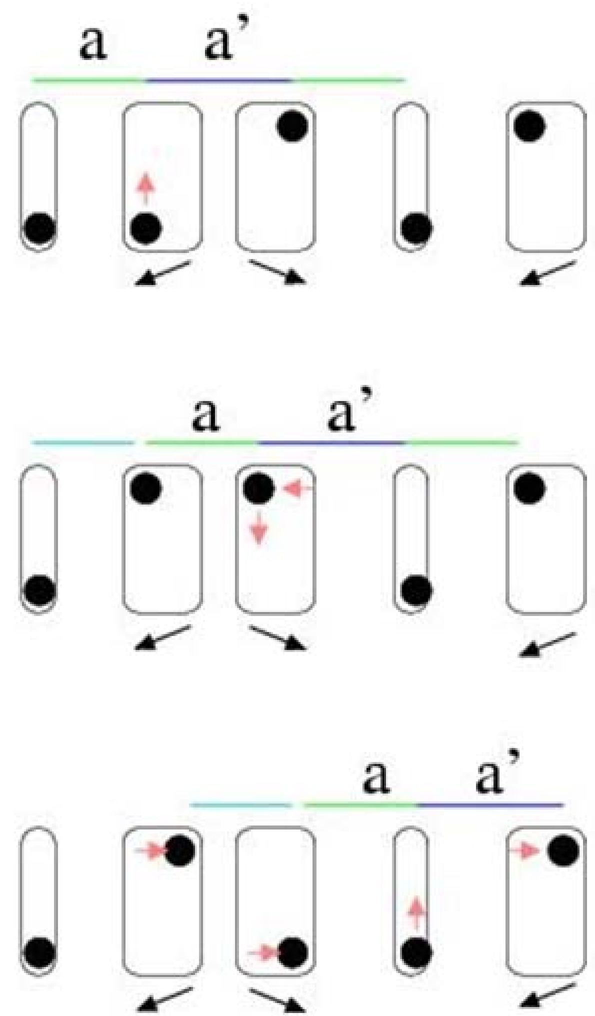
Need to modulate particle spacing to eliminate barrier. Three state ratchet overcomes this

Three shapes breaks spatial symmetry. Additionally we apply a three state AC drive

PRL 90, 247004 (2003)

Ratchet operation

AC external drive cycle



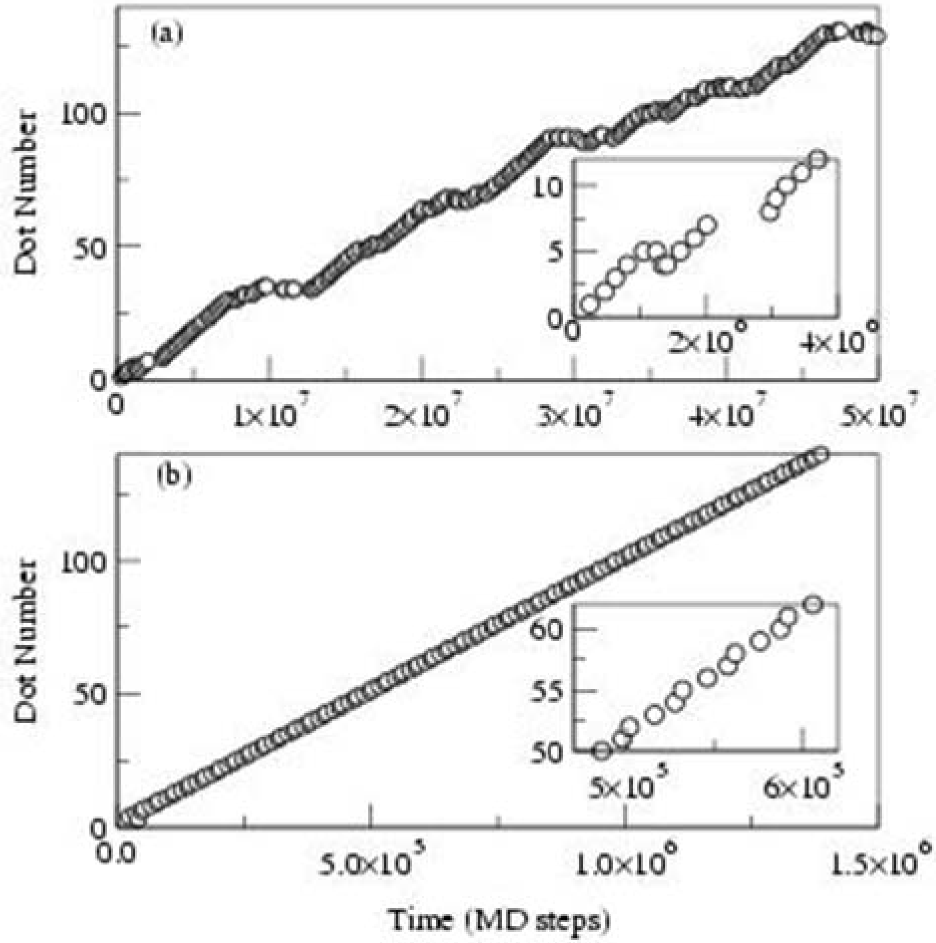
$F_{AC} = 0.0$

$F_{AC} = -x$

$F_{AC} = +x$

Simulation

Signal Propagation

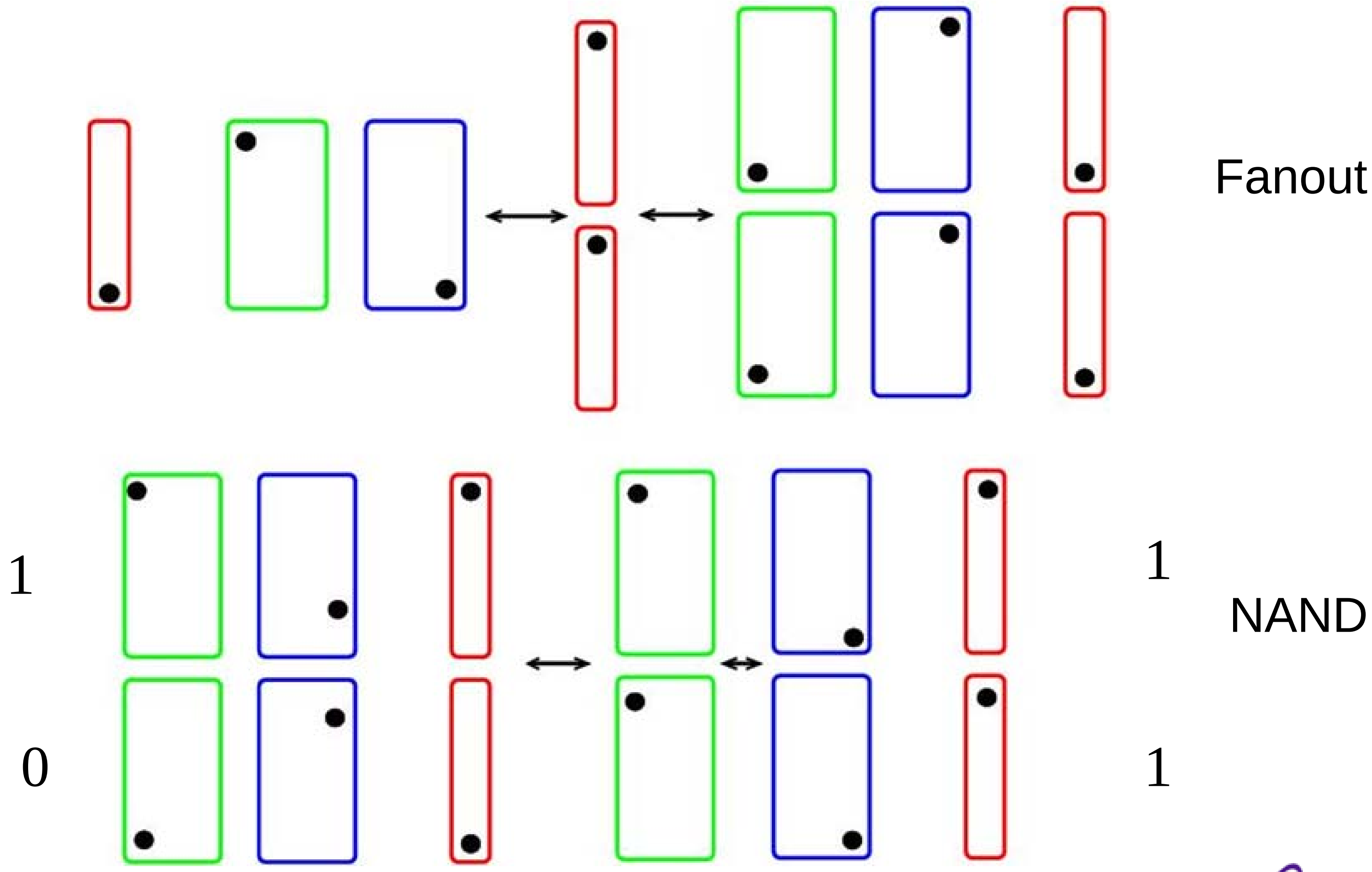


Small barrier in center of pin requires thermal activation.

Increasing depth of the center of the pin removes this barrier completely.

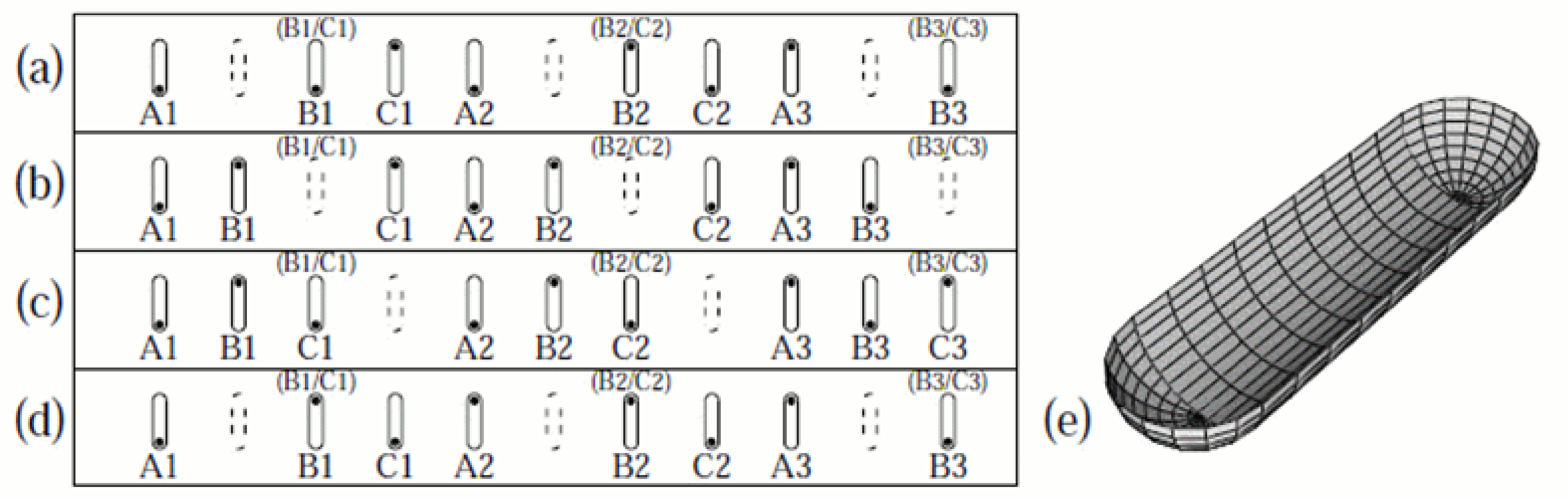
PRL 90, 247004 (2003)

Fanout, NAND gates



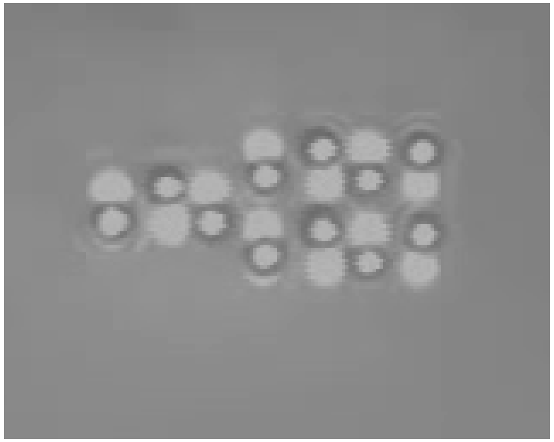
RCA for colloids in optical traps

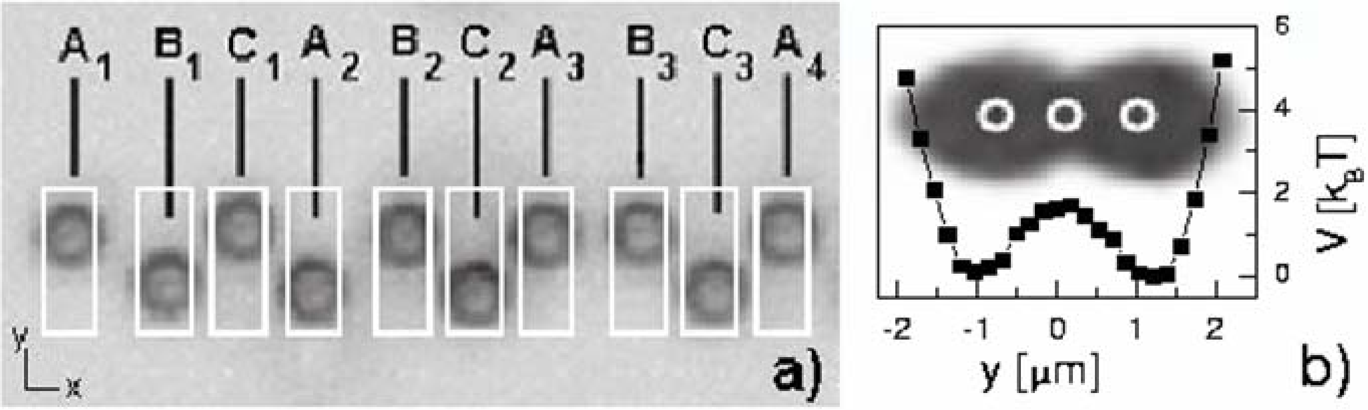
Micron-sized polystyrene sulfate spheres in water
Equally sized traps created using a rastered laser
The traps are shifted back and forth to mimic RCA



Experimental realization of Colloidal Ratchet Cellular Automata

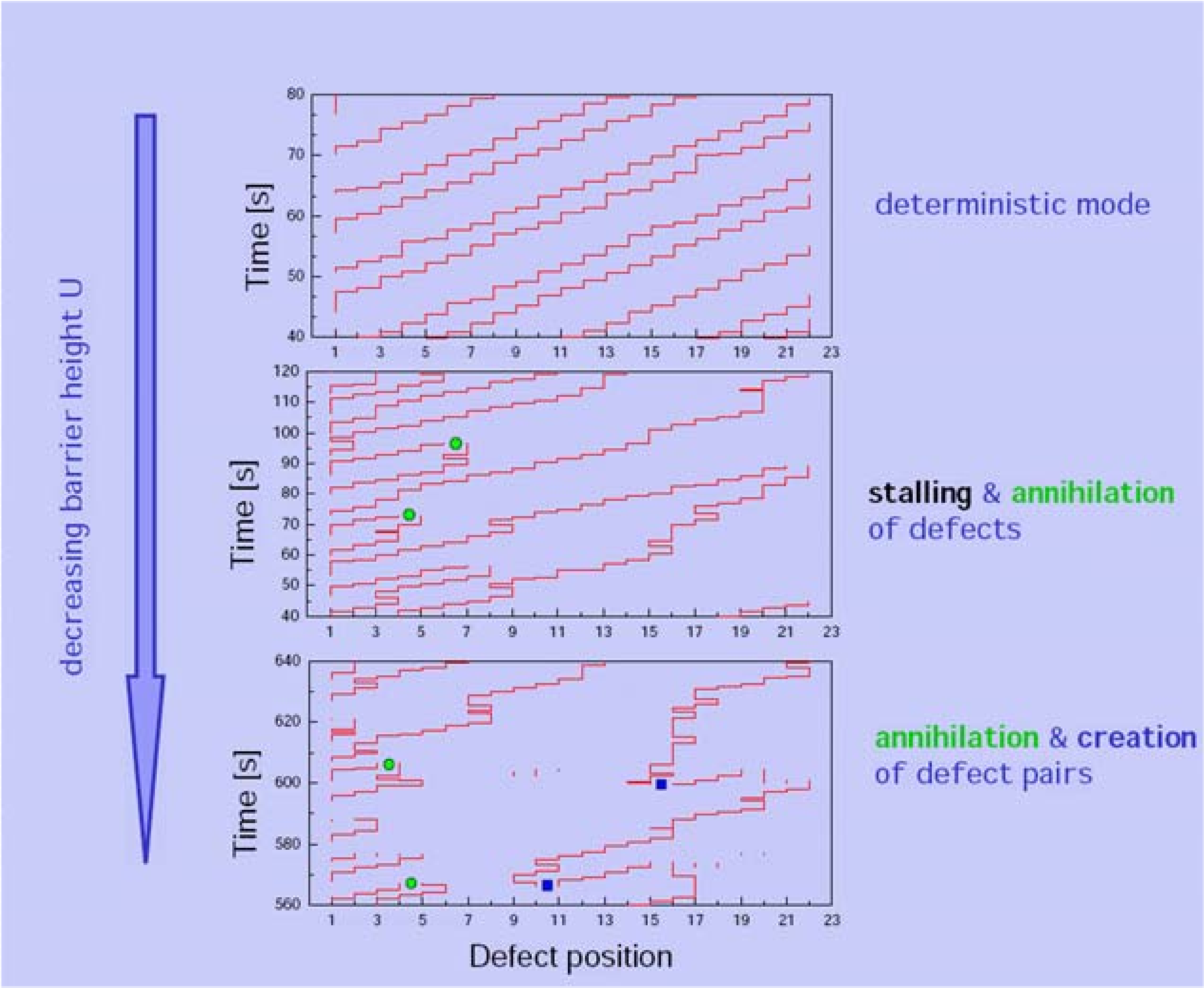
Fanout gate





D. Babic & C. Bechinger, PRL 94, 148303 (2005)

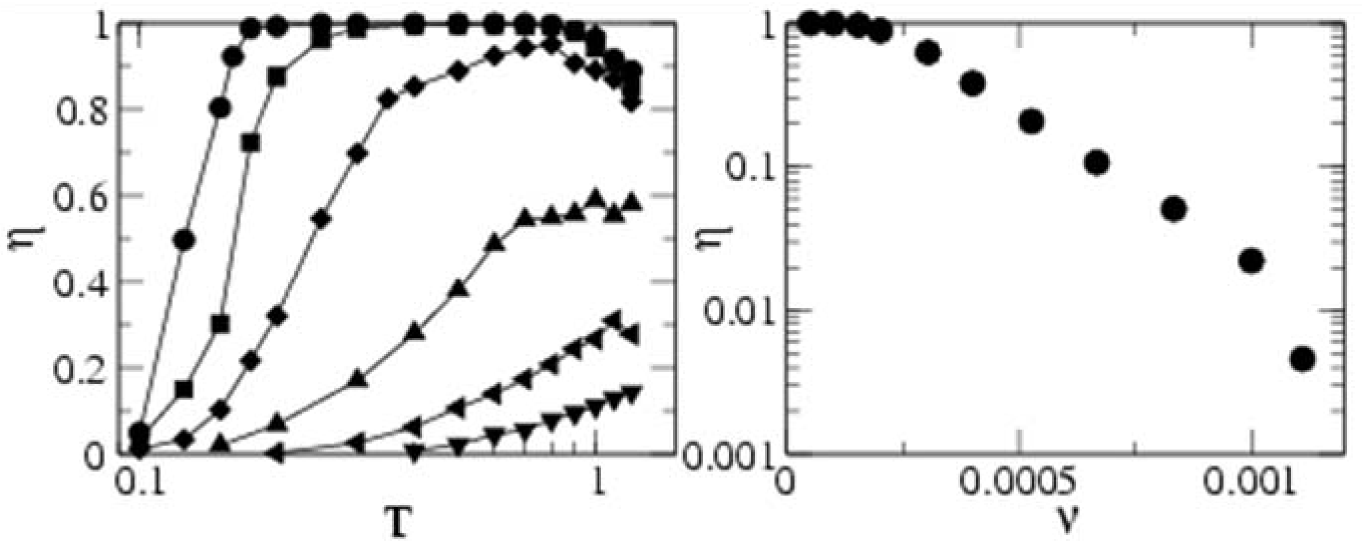
Experimental propagation of logic state



D. Babic & C. Bechinger, PRL 94, 148303 (2005)

Ratchet efficiency Colloidal RCA

Full efficiency can be achieved with the addition of thermal noise!



η=deterministic propagation time/actual propagation time

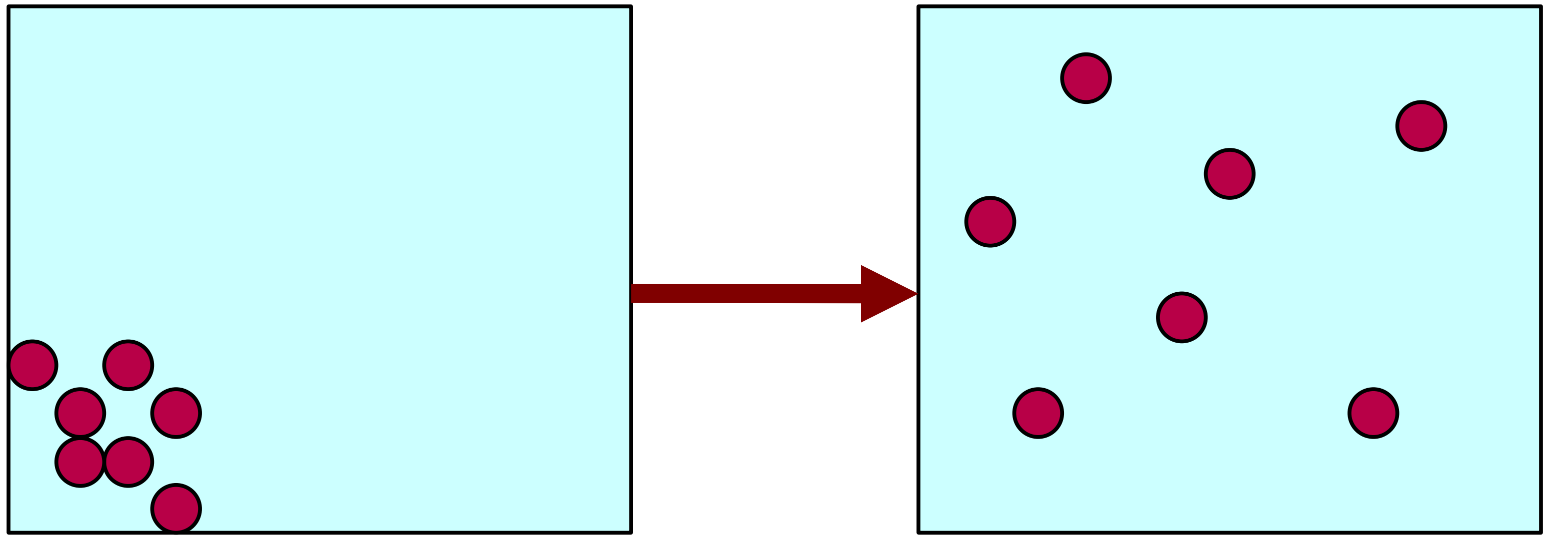
Europhys. Lett. 74, 792 (2006)

Ratchet Example 3: Bacteria Ratchet (Self-driven)

- Inspired by work of R. Austin’s group
- Experimentalists describe their system as a “Maxwell’s demon”
- Can you recognize the broken symmetries that instead make this a realization of a simple Brownian ratchet?

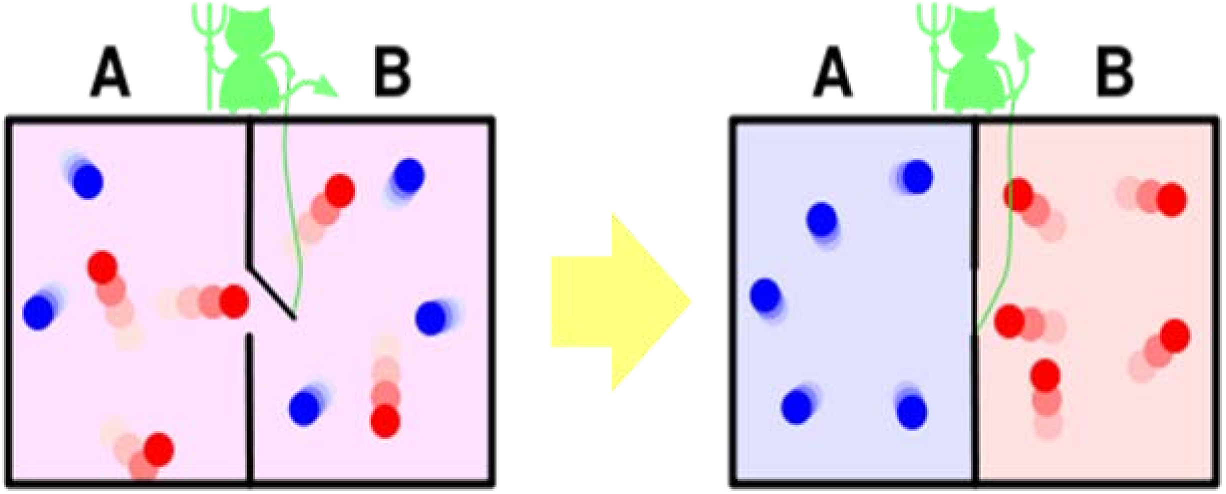
Second Law of Thermodynamics

- The entropy of an isolated system which is not in equilibrium will tend to increase over time, approaching a maximum value at equilibrium.



Maxwell's Demon

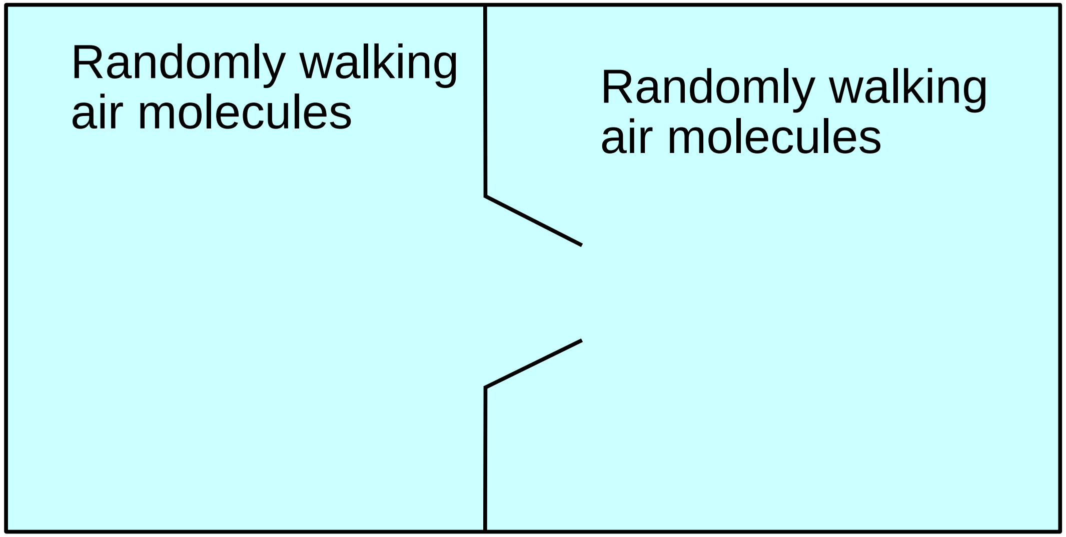
- Maxwell proposed a demon that could allow only one of two particle species to pass through a barrier and allow a thermalized system to demix. Such a system appears to violate the second law.



In reality, the demon itself is a nonthermodynamic entity.

Asymmetry

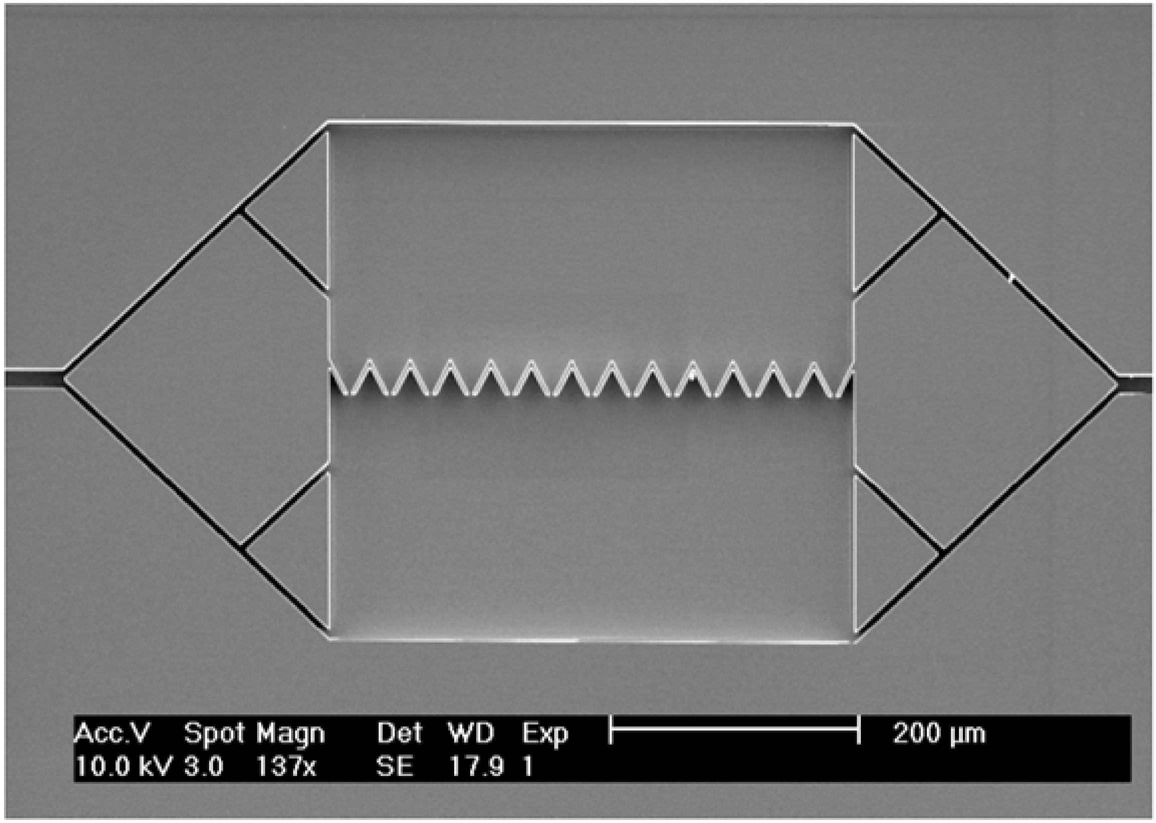
- Imagine two rooms connected by a funnel-shaped door. This door geometry should not be able to cause all of the air to move into only one room.



If it did happen, there would have to be a “demon” present

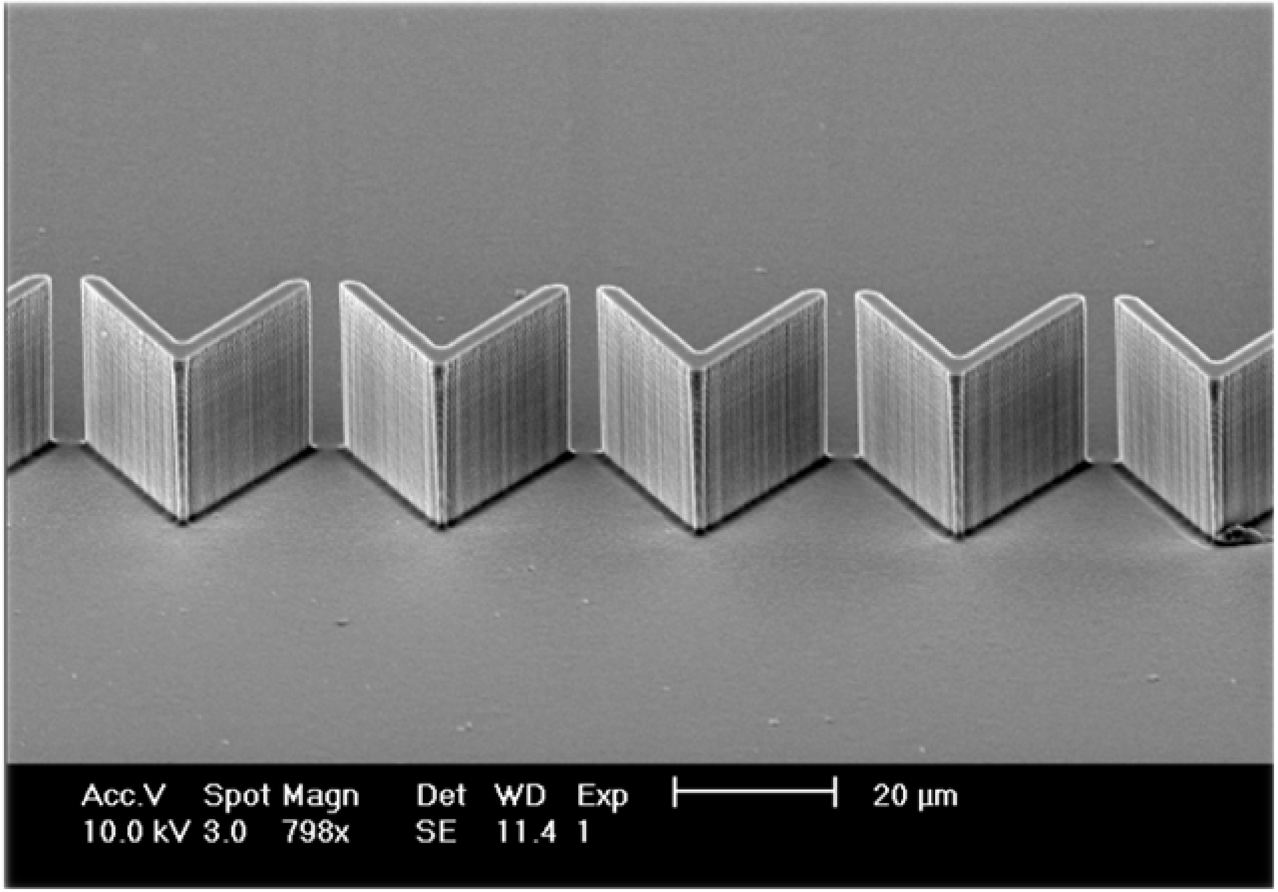
Bacteria instead of air?

- R. Austin (Princeton) nanofabricated an asymmetric array



Bacteria instead of air?

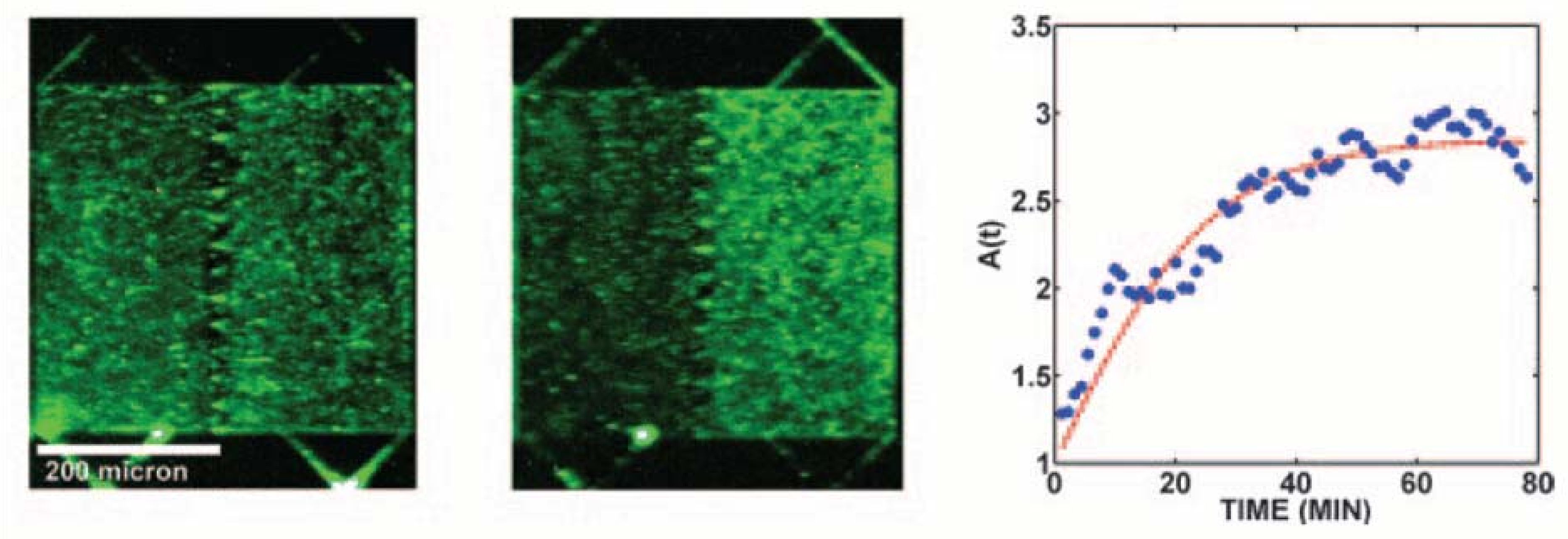
- 3D view of array of asymmetric posts



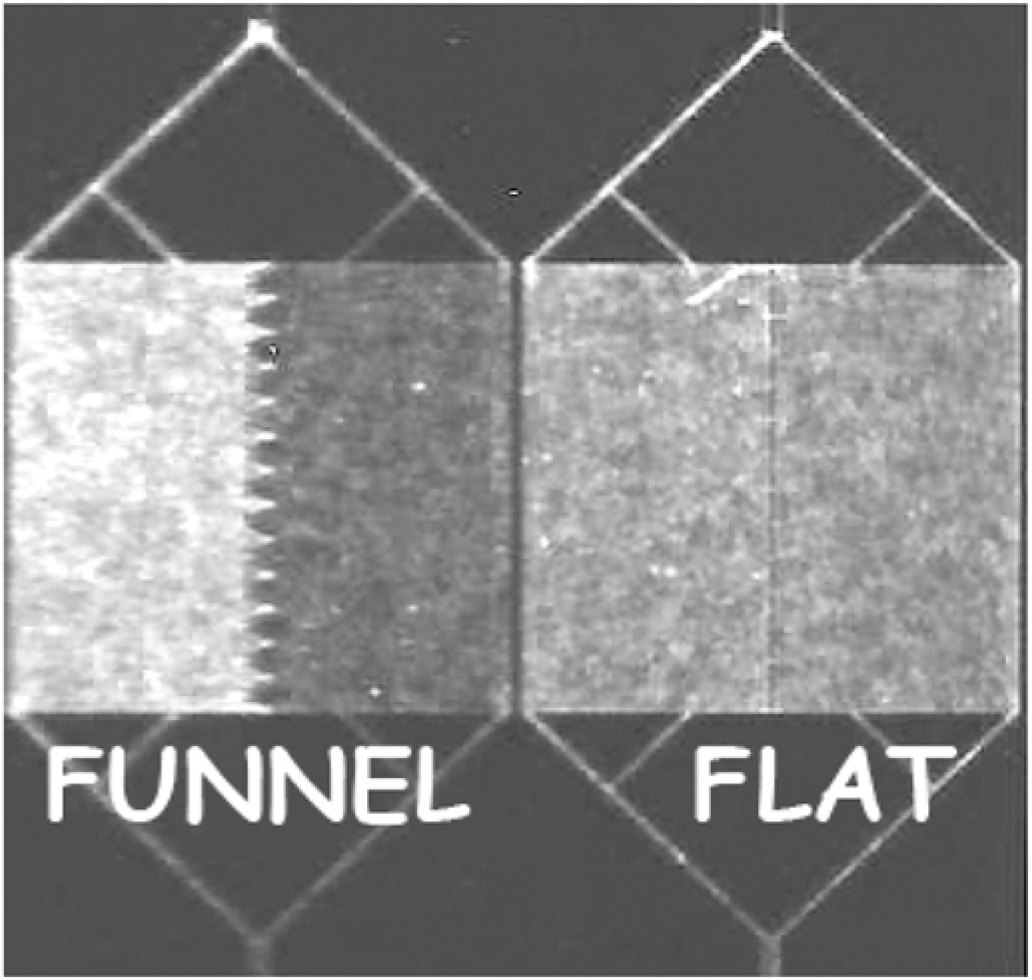
Bacteria concentrate on one side of container

- P. Galajda, J. Keymer, P. Chaikin, R. Austin, J. Bacteriol. 189, 8704 (2007)

Concentration

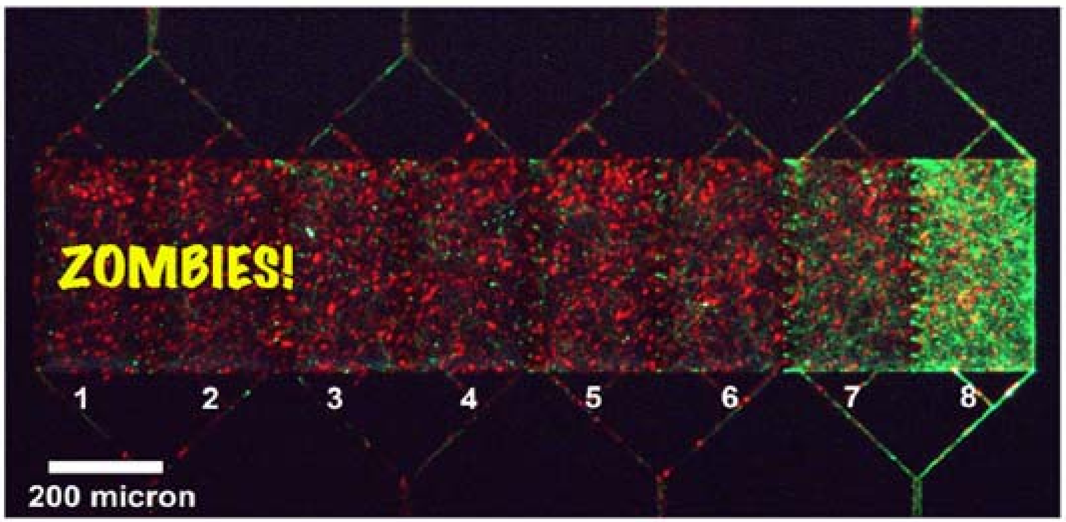


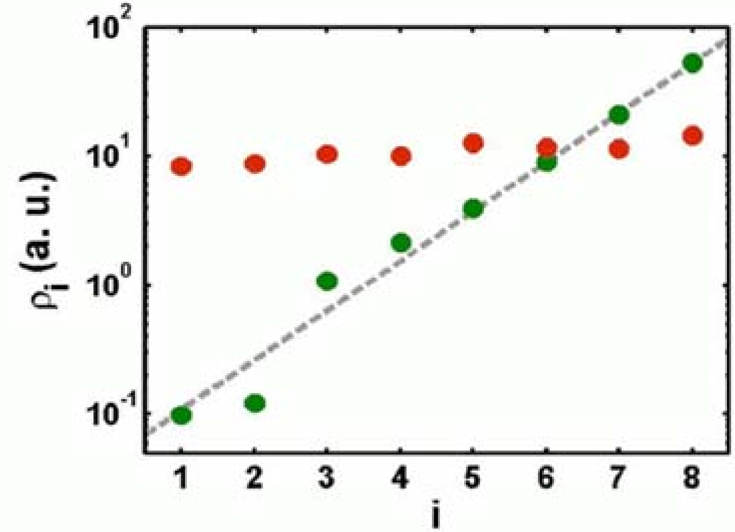
You need funnels: flat openings do nothing.



Importance of swimming

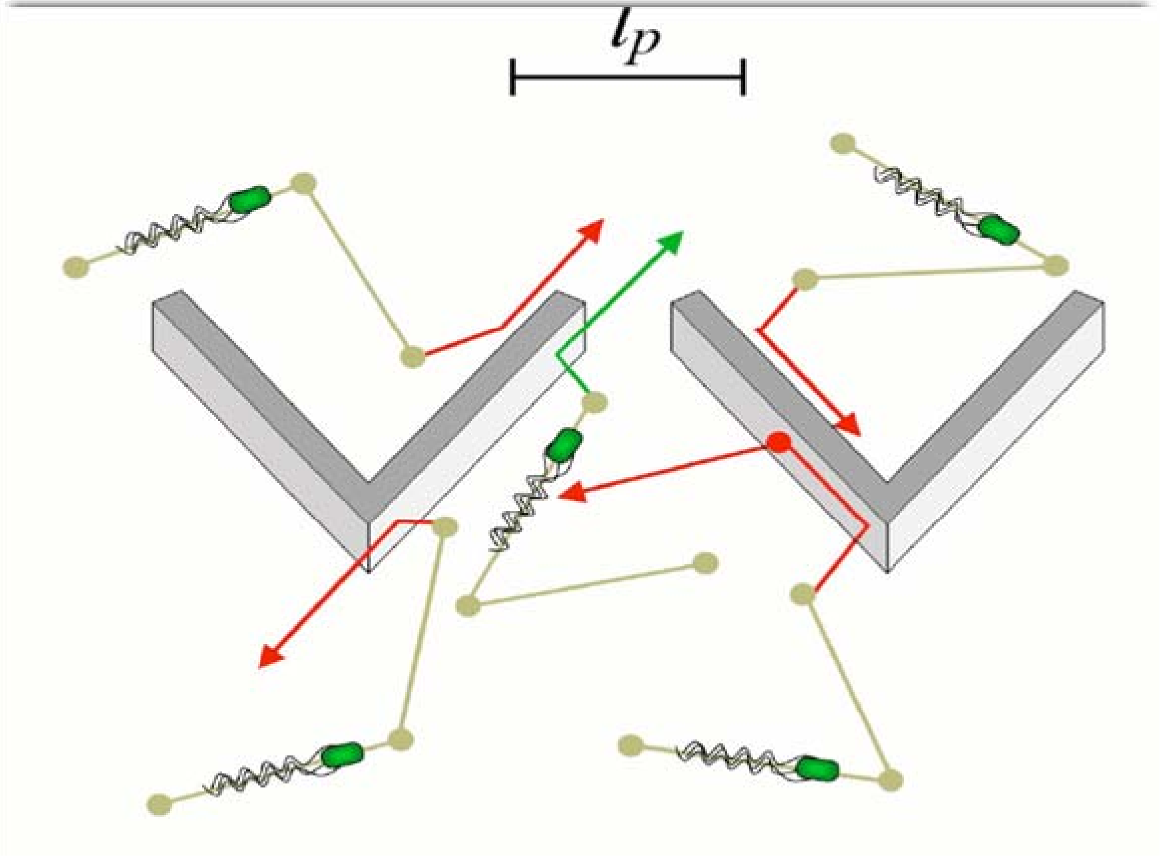
Only swimming bacteria are concentrated by the ratchet geometry. Nonswimming bacteria (whether dead or genetically engineered) undergo Brownian motion.





Cause of rectification?

Bacteria are asymmetric swimmers. Does motor placement matter? Chemotaxis? Hydrodynamic interactions with wall?



Simplest model for swimming bacteria

- Real bacteria move in a roughly straight line of length l_b before tumbling and randomly changing direction.
- On long times, the bacteria acts like a Brownian particle, but on shorter times it acts ballistically.
- We propose that this is all you need to explain the rectification and the phenomena observed in the experiments by the Austin group.
- The “demon” is the nondiffusive nature of the bacteria motion on the length scale of the asymmetric barriers.

Model

- Noninteracting point particles that move via the following overdamped equation of motion

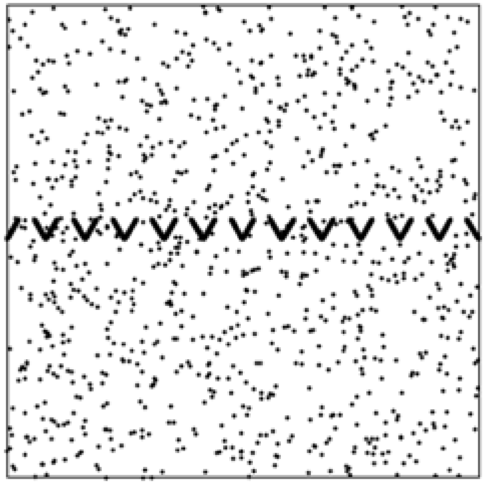
$$\eta \frac{d\mathbf{R}_i}{dt} = \mathbf{F}_i^m(t) + \mathbf{F}_i^T + \mathbf{F}_i^B + \mathbf{F}_i^S$$

$\mathbf{F}_i^m(t)$: Ballistic motion during a time interval τ corresponding to a distance l_b

$\mathbf{F}_i^T$:Thermal force from surrounding fluid with step $l_T << l_b$

$\mathbf{F}_i^B$: Interaction with barriers of length 5

$\mathbf{F}_i^S$: Steric bacteria-bacteria interaction (set to zero for most of study)



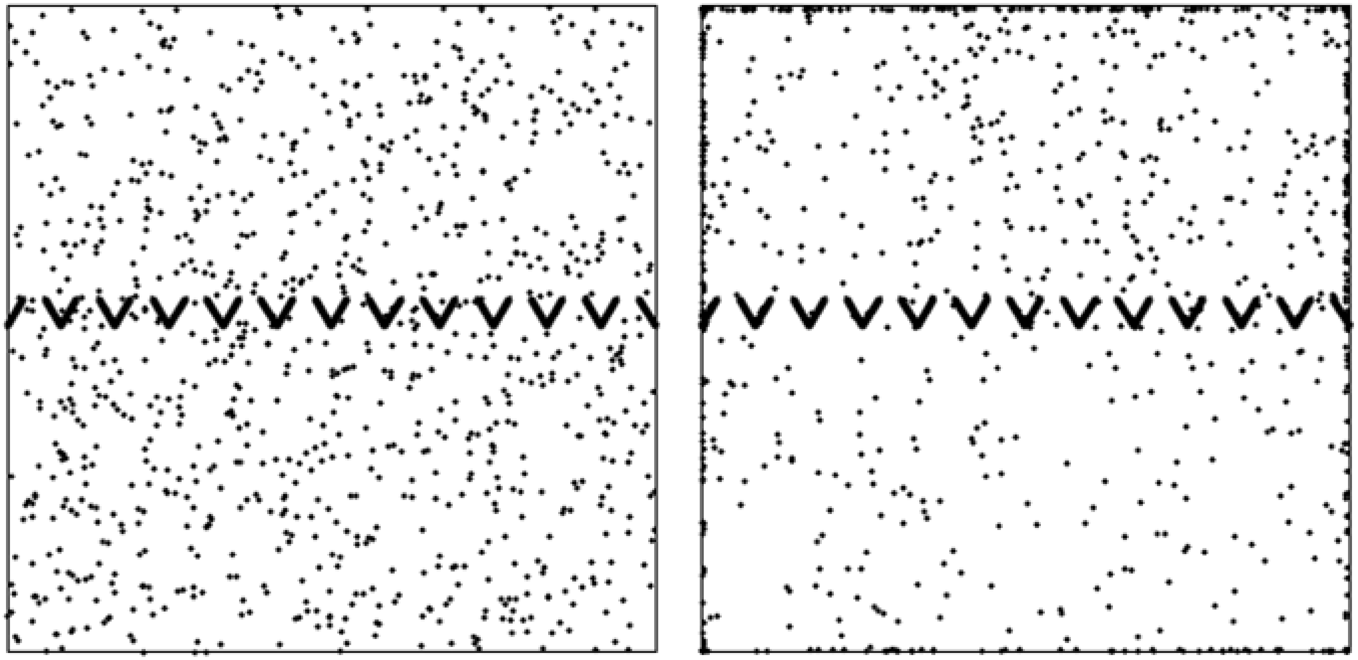
System size: L x L, L=99
Hard walls around edge
Asymmetric barriers in center

Nondiffusive and diffusive behavior

(a) (b) (c)

Ballistic distance l_b= 10 (a), 1 (b), 10 + thermal fluctuations (c)
a: Diffusive on long times, ballistic on short times
b: Always diffusive
c: Persistent random walk

What happens

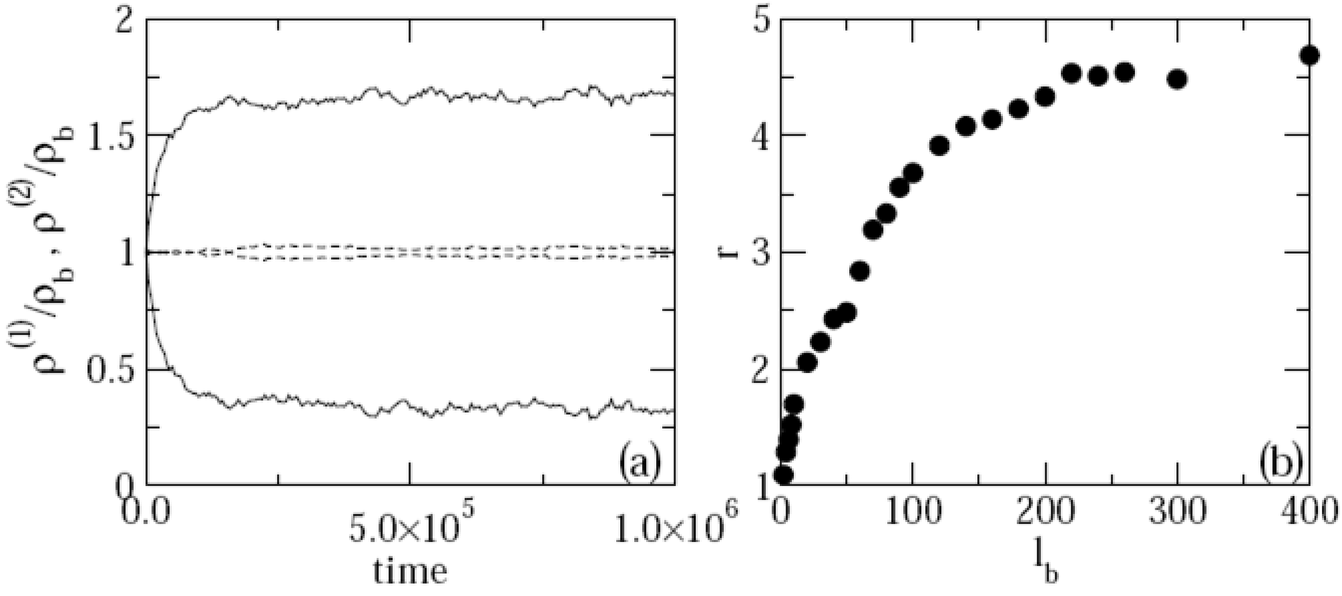


(a) (b)

t=0 t=100τ

l_b=40. Initial and final states

Bacteria density

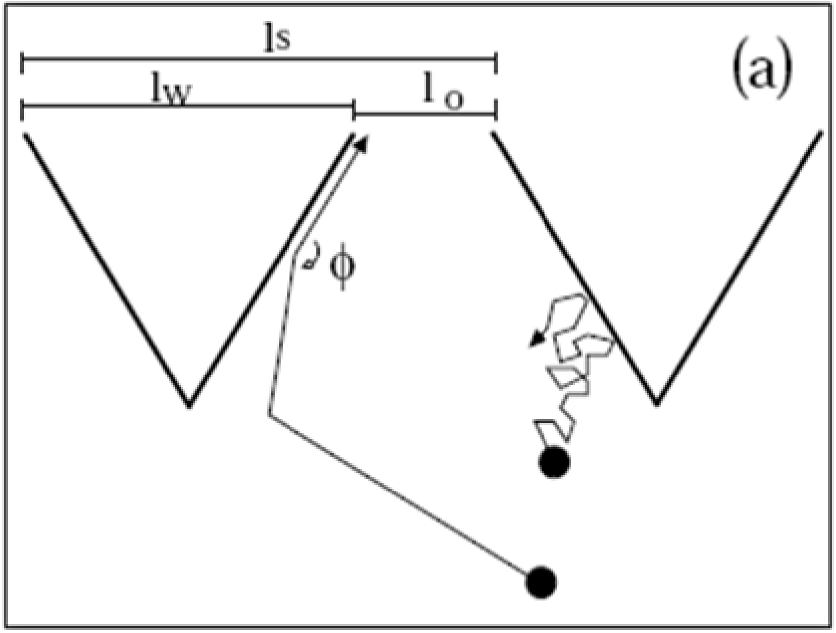


$$r = \rho^{(1)}/\rho^{(2)}$$

l_b=180 (solid line); l_b=0.01 (dashed line)

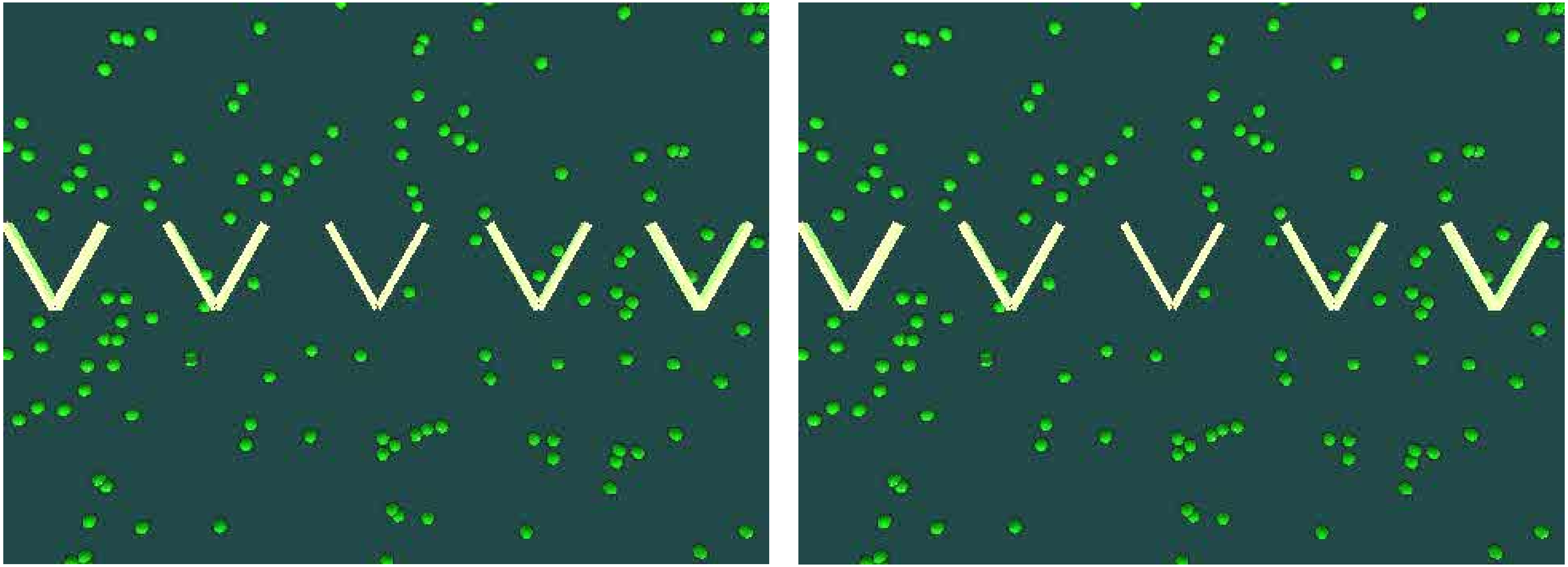
This implies that the ballistic component of the bacteria motion is what produces the rectification effect.

Mechanism leading to rectification



- When the periods of ballistic motion are long, the bacteria glide along the barrier for a time of up to τ.
- Under diffusive motion, the bacteria can instantaneously jump away from the barrier at any time.
- Nondiffusive interactions with the barrier produce the rectification.

Mechanism leading to rectification



- The role of Maxwell's demon is played by the fact that the bacteria motor force generates ballistic motion over length scales similar to the size of the barriers.

Summary

- Ratchet effect – directed transport in a periodic potential – can occur only in nonequilibrium systems and only if enough symmetries are broken

- Quasi-1D ratchet: asymmetric substrate + asymmetric ac drive with zero mean = ratchet effect. Under certain conditions, a reversed ratchet effect occurs. Ratchet reversals are difficult to predict analytically.

- Colloidal logic ratchet: Colloid realization of the “quantum cellular automata” turns out to require imposition of a ratchet effect to work. Resulting “ratchet cellular automata” could be used in an alternative logic device.

- Bacteria ratchet: The bacteria motor breaks time reversal symmetry, and when this is combined with spatial asymmetry, a ratchet effect results.