Phase transitions, metastability and critical slowing down in statistical physics

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Algorithms & Computationally Intensive Inference Seminars

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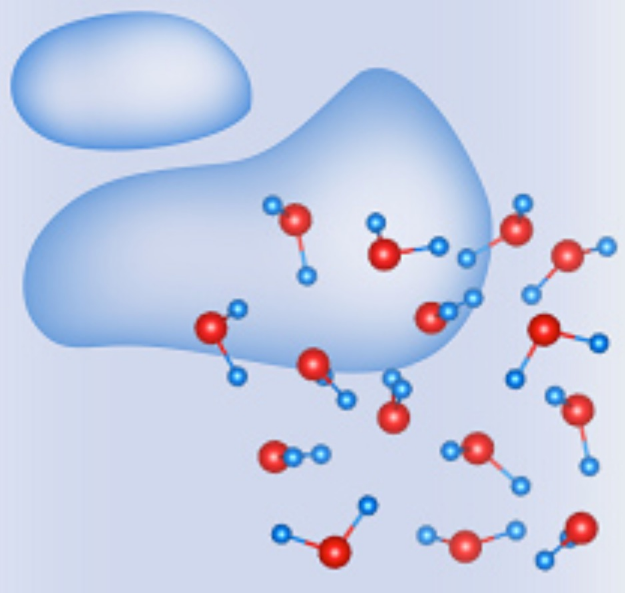
Both research fields estimate expectations wrt some probability distribution $\pi(x; \beta, \theta) \propto e^{-\beta U(x; \theta)}$

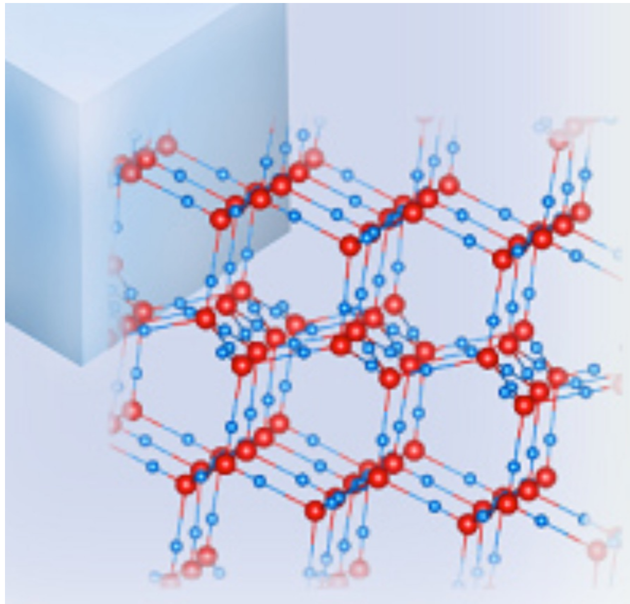
Bayesian inference

- $\pi(x \mid y, \beta, \theta) \propto e^{-\beta U(x \mid y, \theta)}$
- *Fix* hyperparameters β, θ.
- Encode input data y via likelihood…
- …and estimate expectations wrt x.

Statistical physics

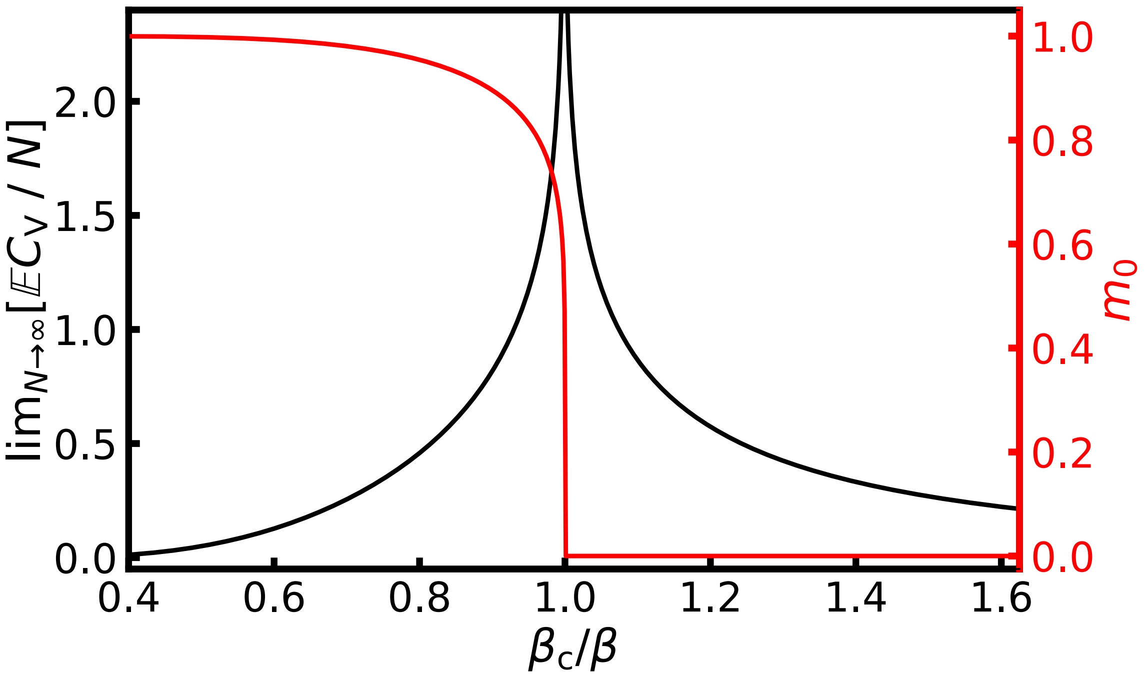
- $\pi(x; \beta, \theta) \propto e^{-\beta U(x; \theta)}$
- Defined *independent of input data*.
- Expectations are *functions* of β and θ.
- β, θ are thermodynamic parameters, eg, system temperature $\equiv 1/\beta$.





Liquid to solid

Expected potential variance per particle (black) is non-analytic at β_c

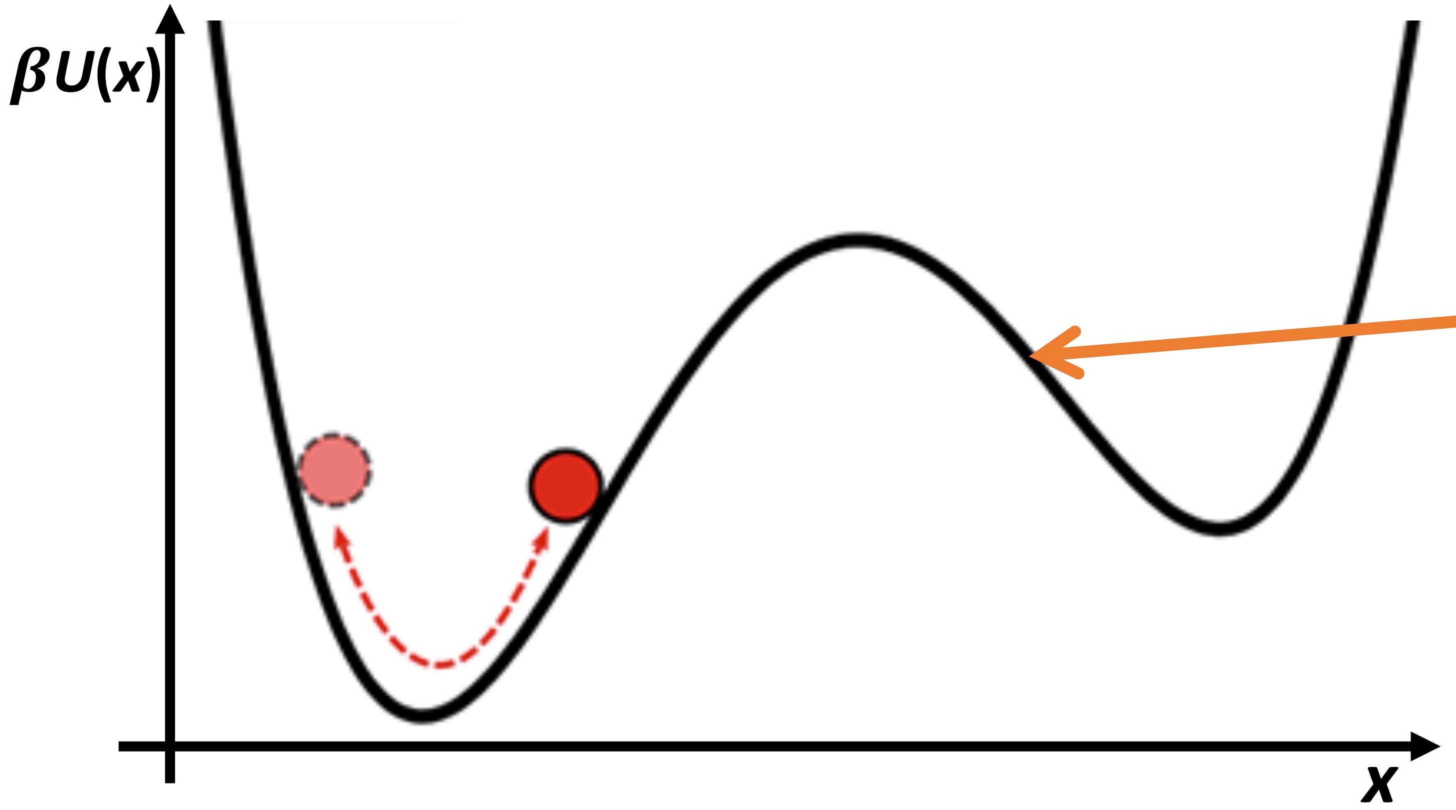


magnetic to non-magnetic

Fig.: Murayama, Kasahara, Matsuda (2020)

Fig.: Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023)

Metastability informs…



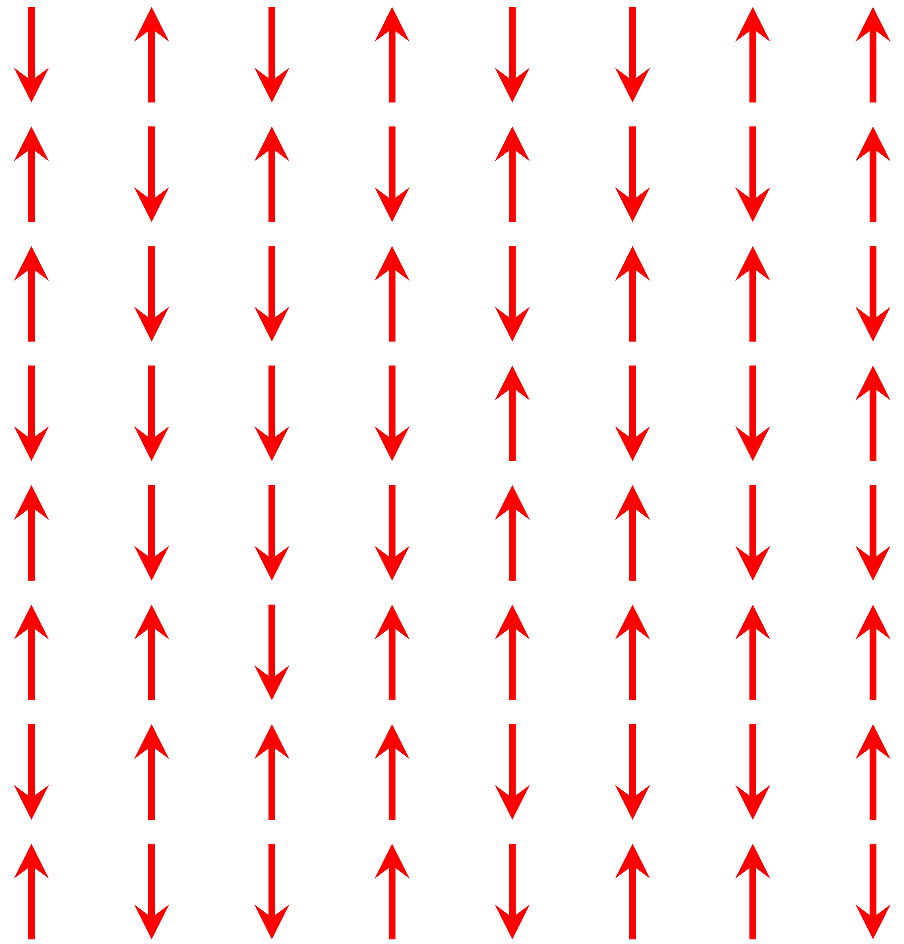
Diverging barrier height blocks access to right-hand well of potential $\beta U(x)$

…Bayesian computation

Fig.: Pampel & Valsson, *J. Chem. Theory Comput.* 18, 4127 (2022)

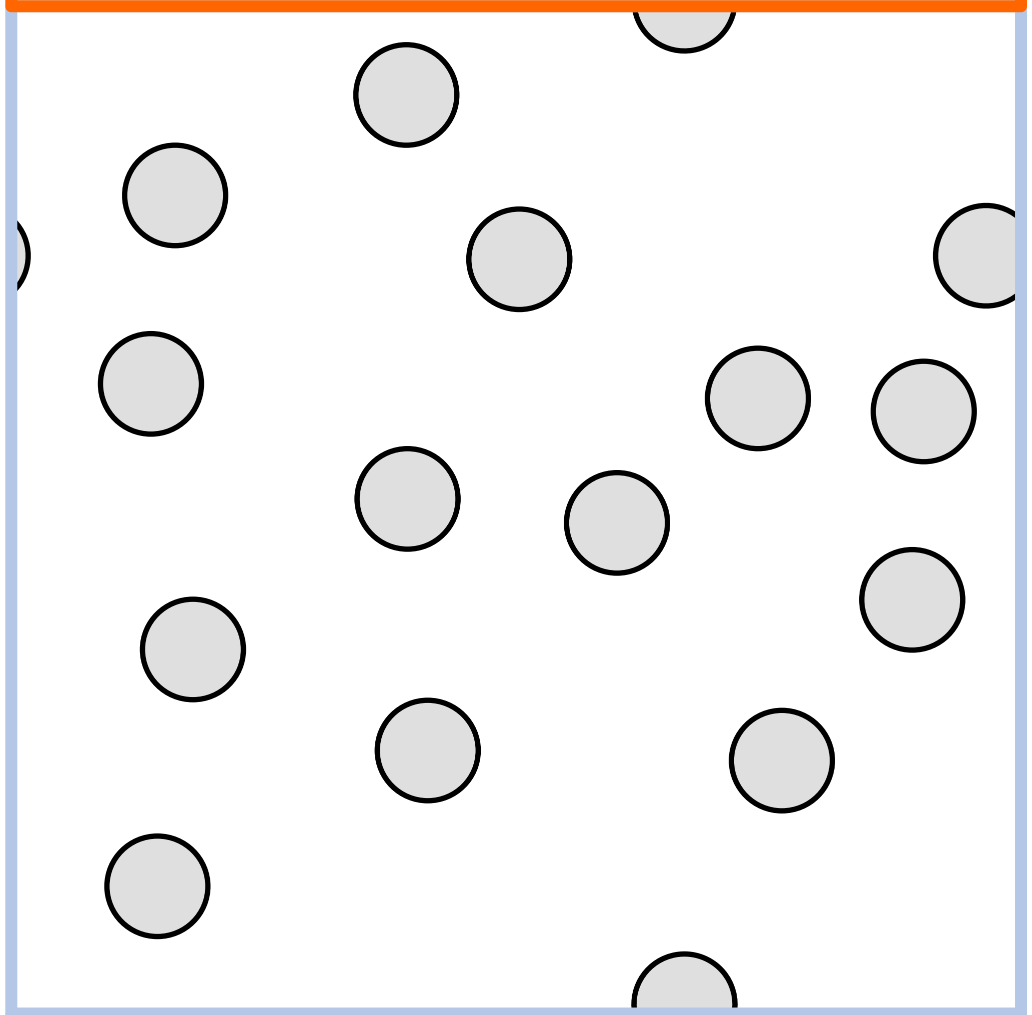
- Statistical physics and phase transitions
- Metastability and Wolff algorithm
- Continuous state spaces and ECMC

2D Ising model

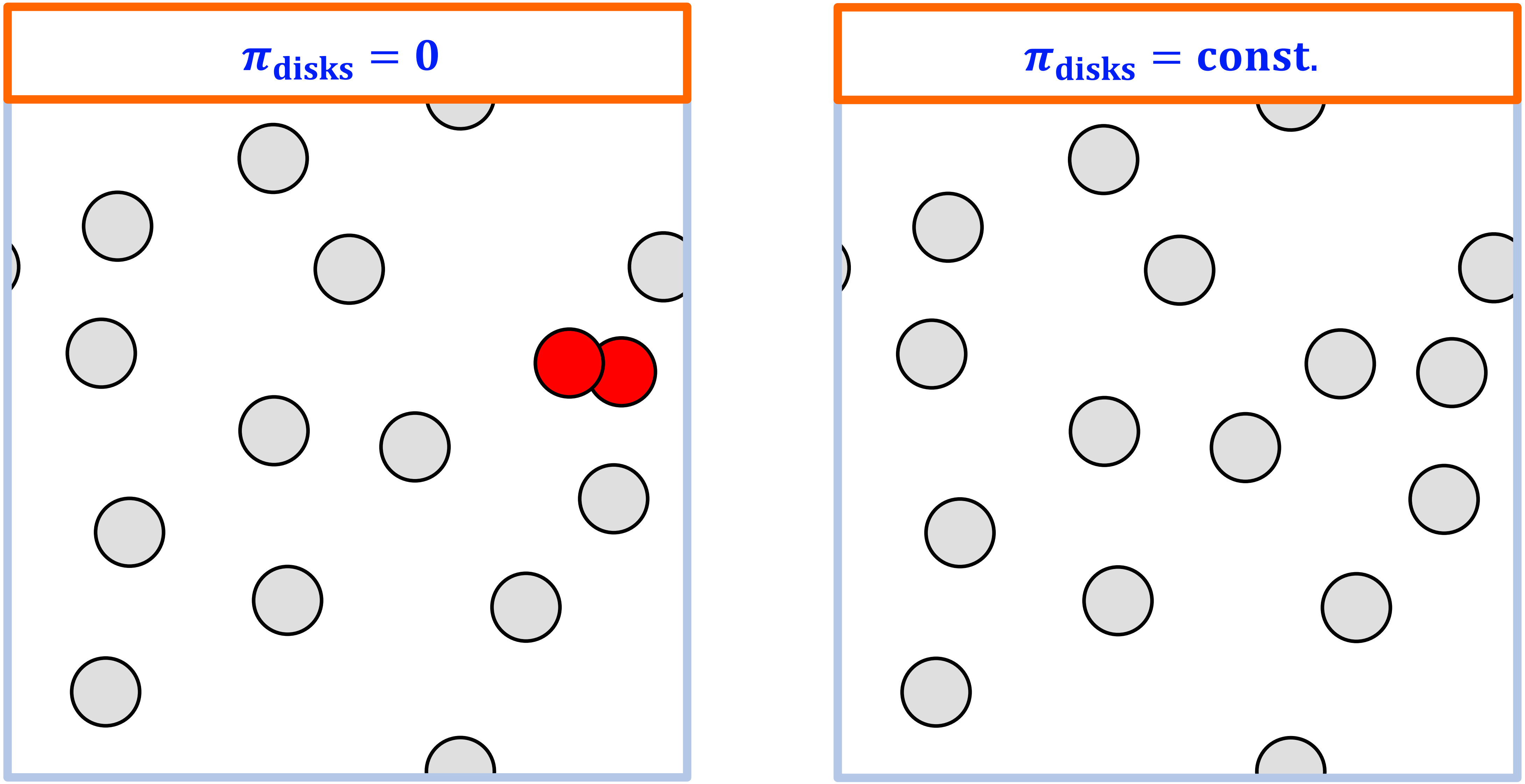


$U_{\text{Ising}} = -\frac{J}{2}\sum_{i=1}^{N}\sum_{j\,\in\, S_i} x_i x_j \,,\, x_i = \pm 1$

2D hard-disk model

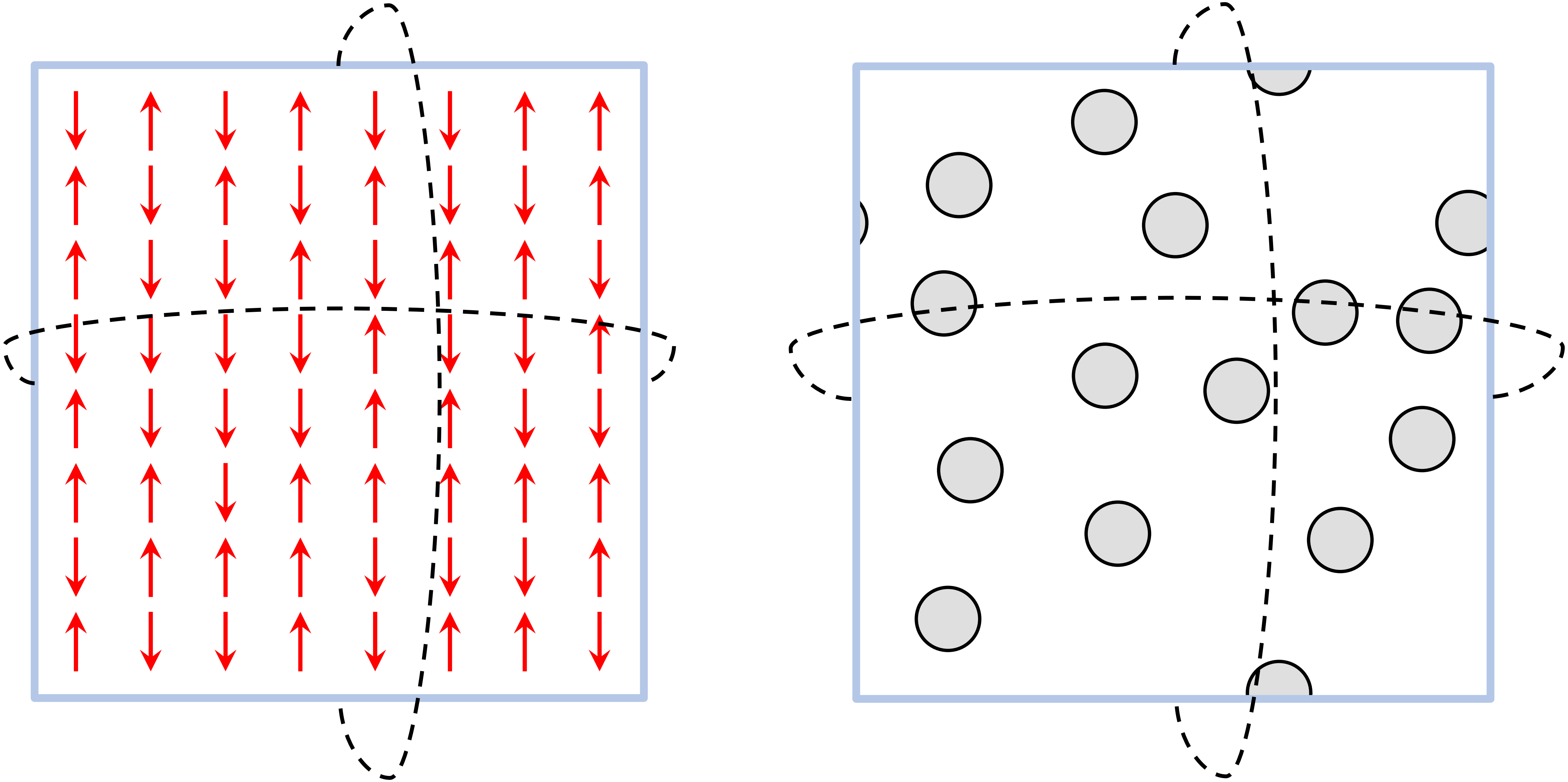


$\pi_{\text{disks}} = 0$ or constant



$\pi_{\text{disks}} = 0$
$\pi_{\text{disks}} = \text{const.}$

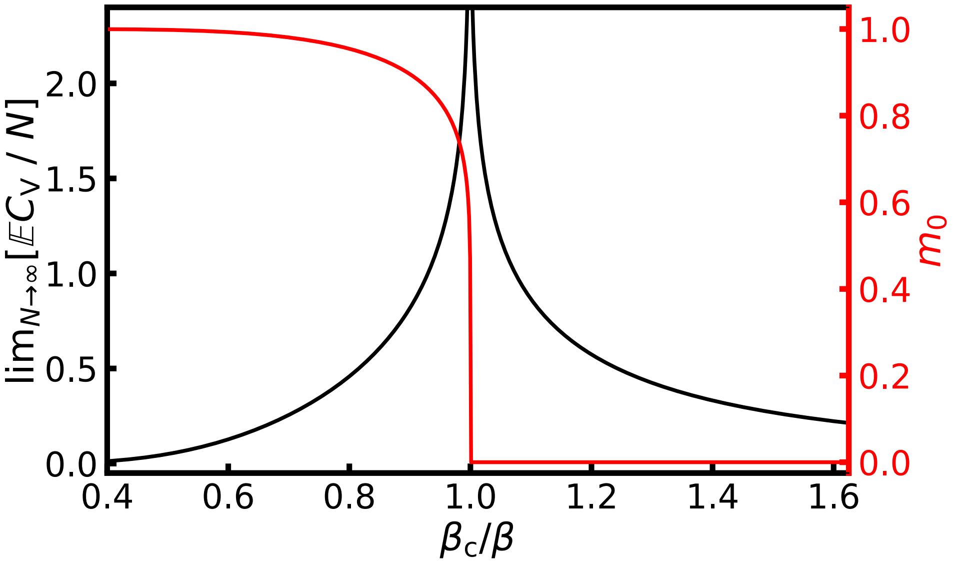
Periodic boundary conditions



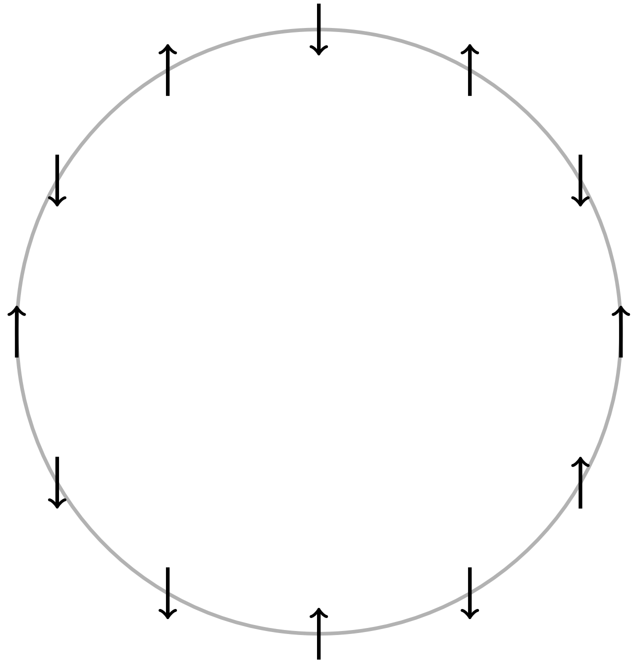
Thermodynamic phase space

- **With $\chi(x; \boldsymbol{\beta}, \boldsymbol{\theta}, N)$ some observable…**
- **<u>Thermodynamic phase space</u> (TPS) of $\chi(x; \boldsymbol{\beta}, \boldsymbol{\theta}, N)$ is $\lim_{N\to\infty} \mathbb{E}[\chi(x; \boldsymbol{\beta}, \boldsymbol{\theta}, N)]$ as a function of $\boldsymbol{\beta}$ and $\boldsymbol{\theta}$.**
- **<u>Thermodynamic phase</u>: any open and connected region of TPS where $\lim_{N\to\infty} \mathbb{E}[\chi(x; \boldsymbol{\beta}, \boldsymbol{\theta}, N)]$ is analytic.**
- **<u>Phase transition</u>: any boundary between any two thermodynamic phases.**

2D Ising model has non-analytic expectations at $\beta = \beta_c$…



…but no phase transition has been detected in 1D case



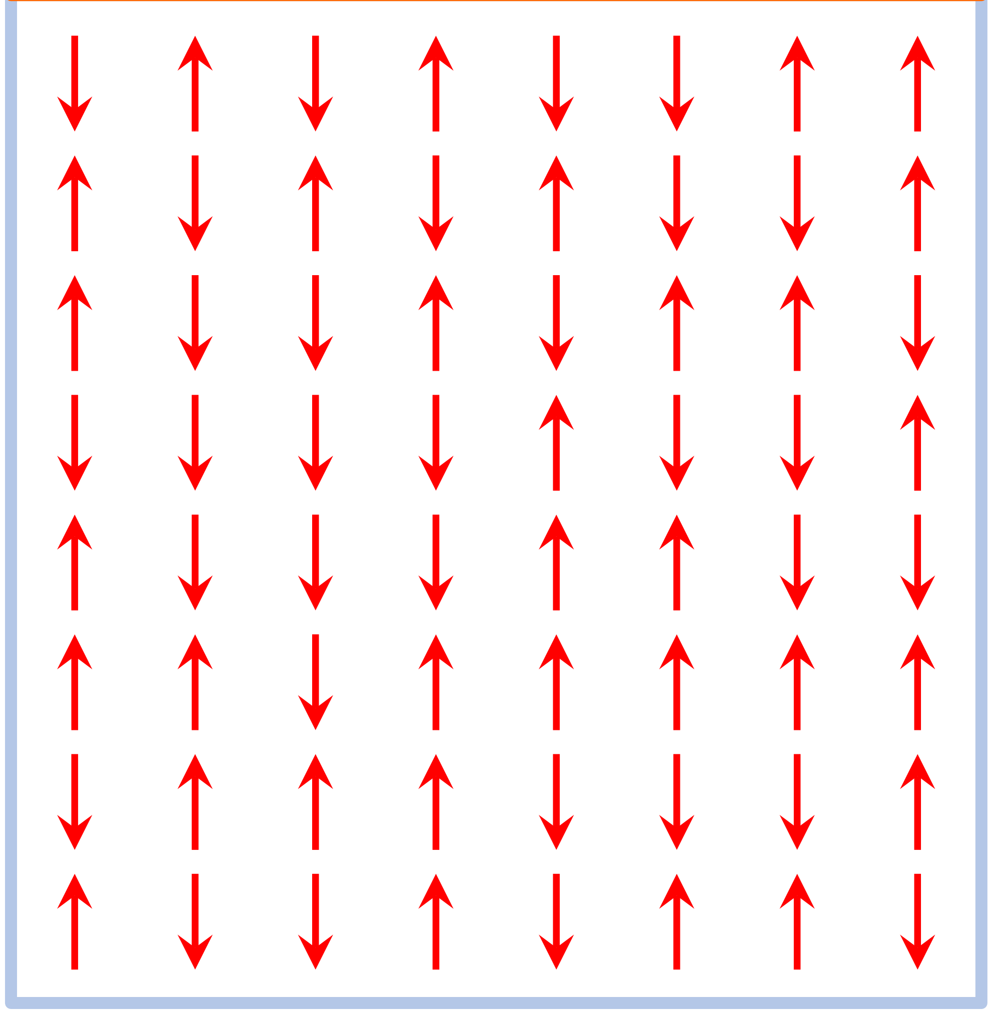
$$U_{\text{Ising}} = -\frac{J}{2}\sum_{i=1}^{N}\sum_{j\in S_i} x_i x_j\,,\, x_i = \pm 1$$

Figs: Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023)

Theory: Onsager, *Phys. Rev.* 65, 117 (1944); Ising, *Z. Physik 31*, 253 (1925)

- Statistical physics and phase transitions
- **Metastability and Wolff algorithm**
- Continuous state spaces and ECMC

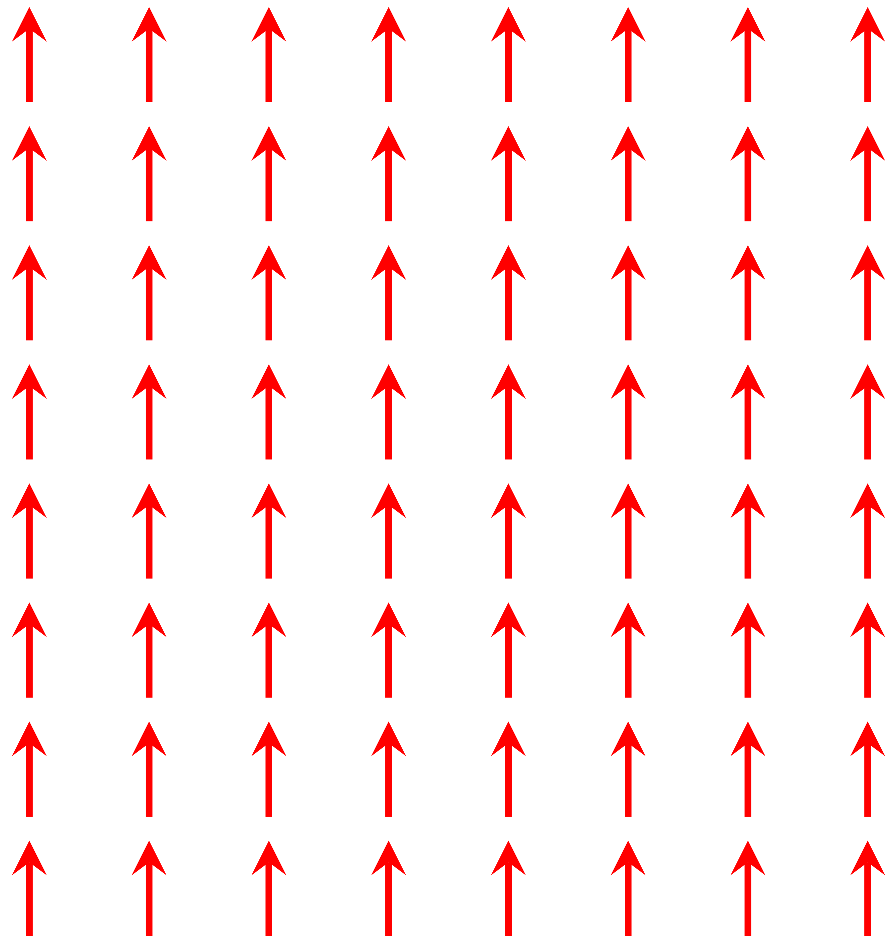
2D Ising model



- Single active particle $a \in \{1, \ldots, N\}$
- $x'_a = -x_a$
- $\Delta U_{\text{Ising}} = J \sum_{j \in S_a} x_a x_j$
- Accept x'_a w/prob $\min[1, \exp(-\beta \Delta U_{\text{Ising}})]$
- NB, one unit of MC time corresponds to *N* attempted particle moves

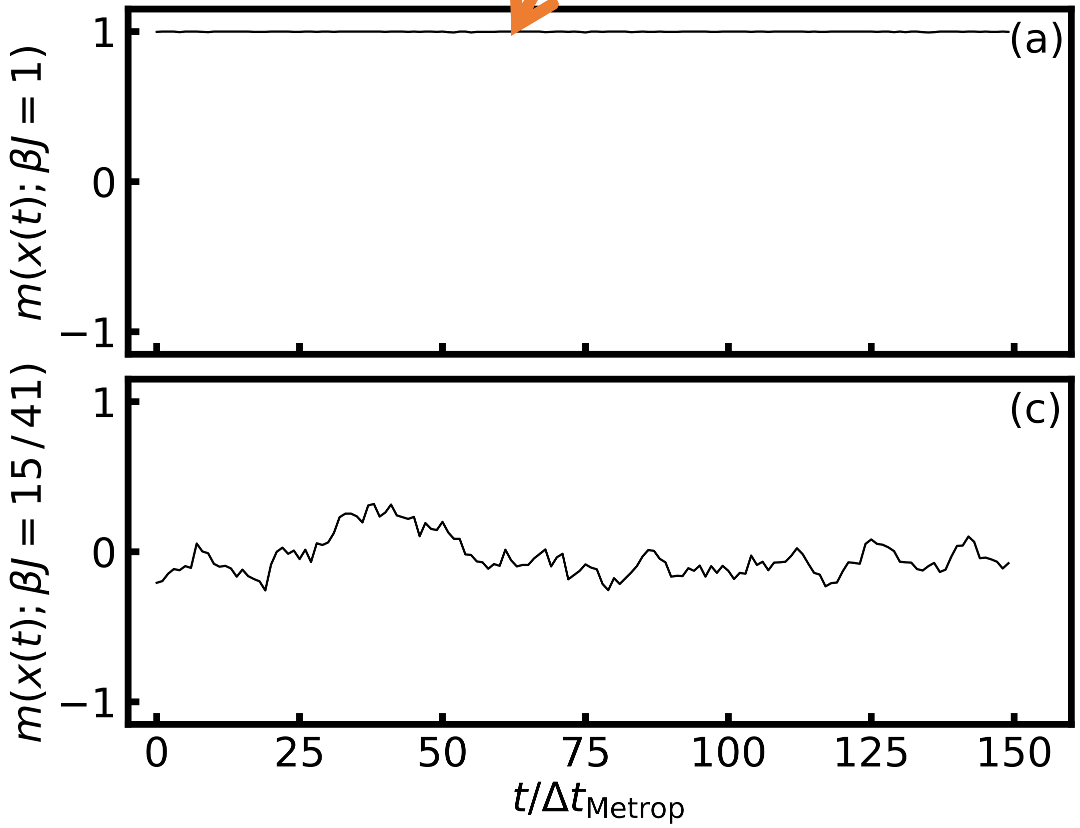
- <u>**Magnetisation:**</u> $\boldsymbol{m(x;\beta,J,h,N) := \frac{1}{N}\sum_{i=1}^{N} x_i}$
- $\boldsymbol{\mathbb{E}[m(x;\beta J,h=0,N)] = 0}$ **for all** $\boldsymbol{\beta < \infty}$ **(spin-flip symmetry)**
- **So** $\boldsymbol{\frac{1}{\tau_n}\sum_{t=\tau_1}^{\tau_n} m(x_t;\beta J,h=0,N) \to 0}$ **on some timescale** $\boldsymbol{\tau_n}$
- **But at low temperature and w/Metropolis dynamics…**
- **…**$\boldsymbol{\tau_n}$ **diverges with system size *N***

Low-temp Metrop dynamics freeze…



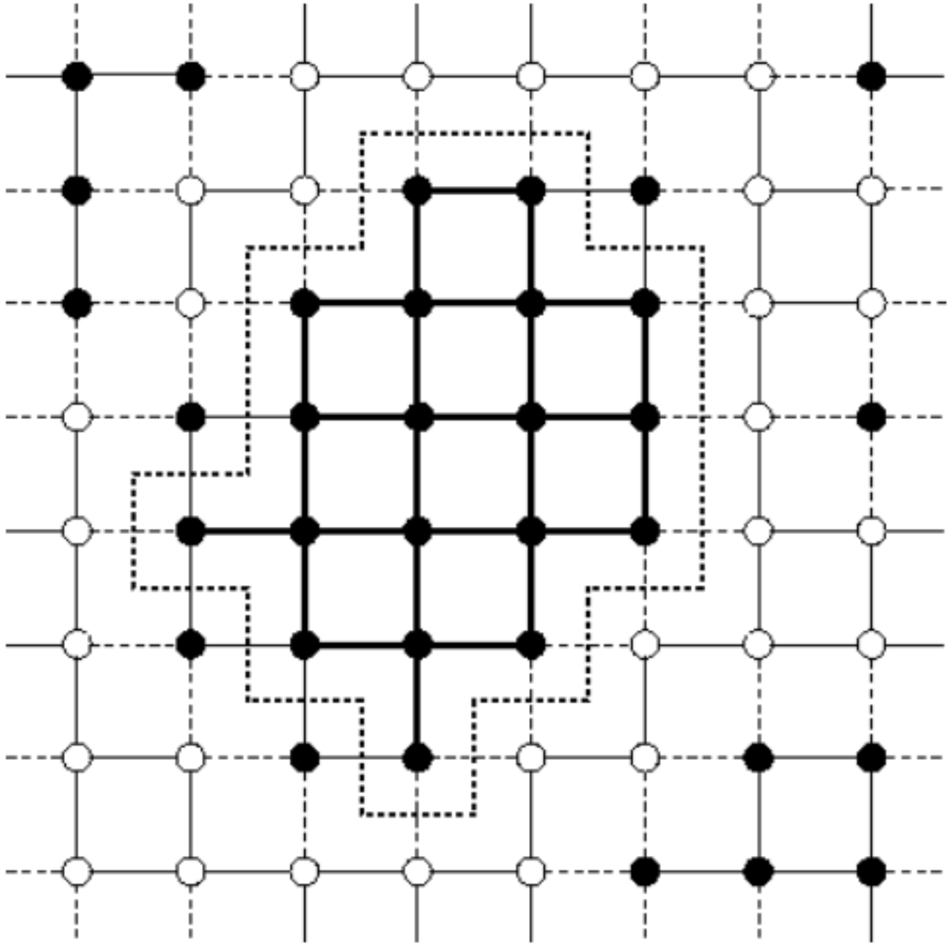
…as neighbours are typically aligned

Metastable dynamics result in
<u>*m*(*t*) close to 1 at low temp.</u>



Right-hand figs: Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023)

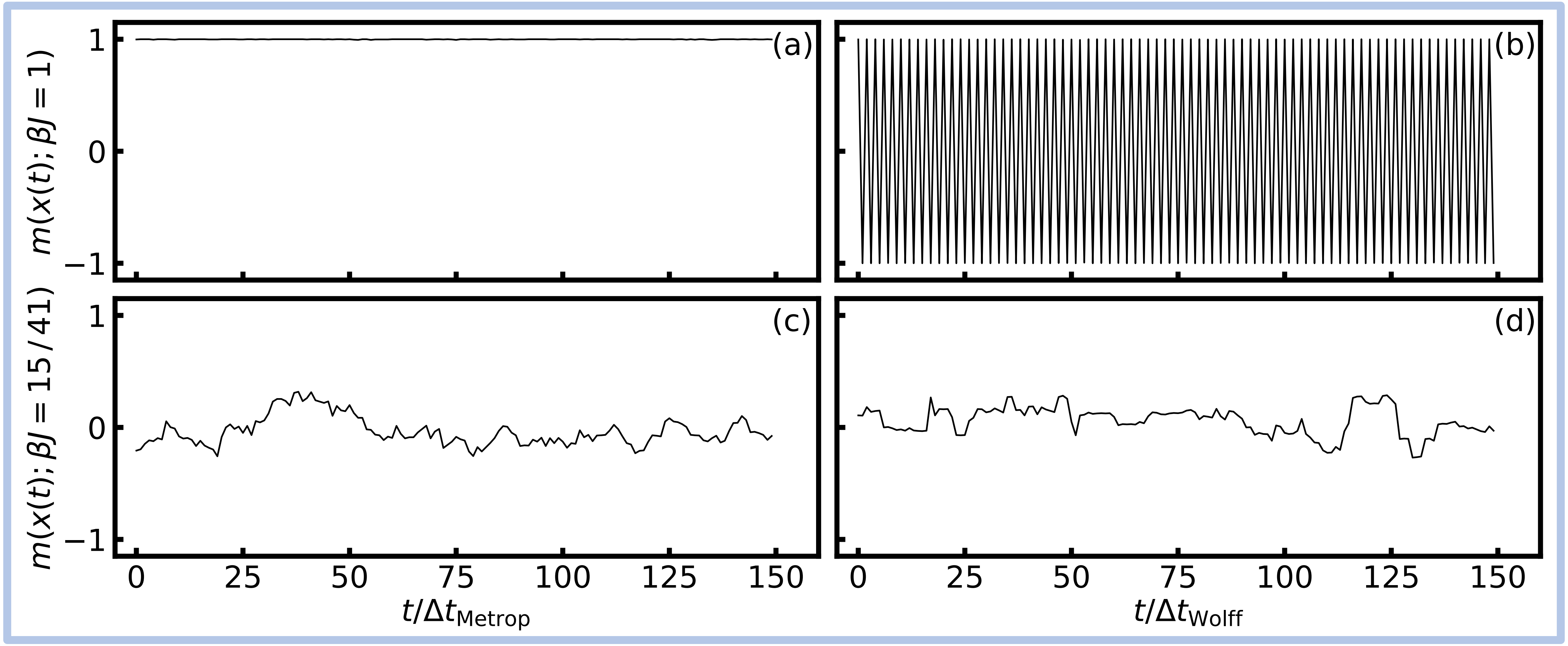
Wolff algorithm



Flips entire clusters of aligned spins in ‘intelligent’ way

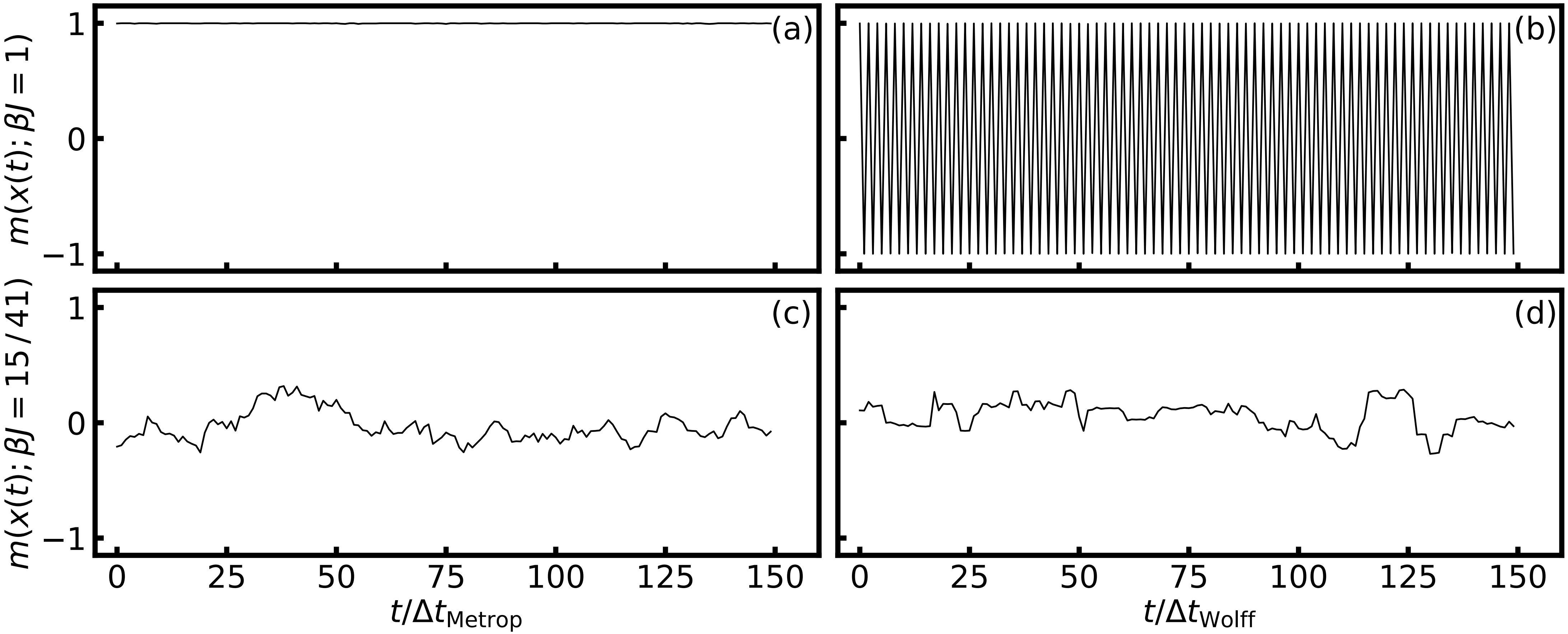
1. Randomly pick base lattice site for new cluster
2. Add aligned neighbours (to cluster) with probability $p := 1 - e^{-2\beta J}$
3. Repeat step 2 for each new spin…
4. …and flip entire cluster with probability one.

Algorithms: Swendsen & Wang, *PRL* 58, 86 (1987); Wolff, *PRL* 62, 361 (1989)
Fig.: Jorge L. deLyra, Sao Paulo Physics
Proof: Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023)



Magnetisation: $m(x;\beta,J,h,N) := \frac{1}{N}\sum_{i=1}^{N} x_i$

Figs: Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023) (*N* = 32x32 spins)



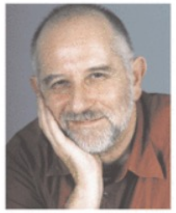
Experimental-theoretical discrepancies are essence of symmetry breaking

Figs: Faulkner & Livingstone, *Stat. Sci., in press* (2023) (*N* = 32x32 spins)

Metropolis convergence: Neal & Roberts, *Ann. Appl. Probab.* 16 475 (2006)

Singular Limits

Michael Berry



Biting into an apple and finding a maggot is unpleasant enough, but finding half a maggot is worse. Discovering one-third of a maggot would be more distressing still: The less you find, the more you might have eaten. Extrapolating to the limit, an encounter with no maggot at all should be the ultimate bad-apple experience. This remorseless logic fails, however, because the limit is singular: A very small maggot fraction ($f \ll 1$) is qualitatively different from no maggot ($f = 0$). Limits in physics can be singular too—indeed they usually are—reflecting deep aspects of our scientific description of the world.

In physics, limits abound and are fundamental in the passage between descriptions of nature at different levels. The classical world is the limit of the quantum world when Planck's constant h is inappreciable; geometrical optics is the limit of wave optics when the wavelength λ is insignificant; thermodynamics is the limit of statistical mechanics when the number of particles N is so large that $1/N$ is negligible; mechanics of a slippery fluid is the limit of mechanics of a viscous fluid when the inverse Reynolds number $1/R$ can be disregarded. These limits have a common feature: They are all singular—they must be, because the theories they connect involve concepts that are qualitatively very different. As I explain here, there are both reassuring and creative aspects to singular limits. And by regarding them as a general feature of physical science, we get insight into two related philosophical problems: how a more general theory can reduce to a less general theory and how higher-level phenomena can emerge from lower-level ones.

The coherence of our physical worldview requires the reassurance that, singularities notwithstanding, quantum mechanics does reduce to classical mechanics, statistical mechanics does reduce to thermodynamics, and so on, in the appropriate limits. We know that when calculating the orbit of a spacecraft (and indeed knowing that it has an orbit) we can safely use classical mechanics, rather than having to solve the Schrödinger equation. An engineer designing a bridge can rely on continuum elasticity theory, without needing to know the atomic arrangements underlying the equation of state of the materials used in the construction. However, getting these reassurances from fundamental theory can involve subtle and unexpected concepts.

Perhaps the simplest example is two flashlights shining on a wall. Their combined light is twice as bright as when each shines separately: This is the optical embodiment of the equation $1 + 1 = 2$. But we learned from Thomas Young almost exactly two centuries ago that this mathematics does not describe the intensity of superposed light beams: To account for wave interference, *amplitudes* must be added, and the sum then squared to give the intensity. This involves the phases of the two waves, $\pm\phi$ say, and gives the intensity as $|\exp(i\phi) + \exp(-i\phi)|^2 = 2 + 2\cos 2\phi$, which can take any value between 0 and 4. So, what becomes of $1 + 1 = 2$? Young himself, responding to a critic who claimed that the wall should be covered with interference fringes, agreed, but pointed out that "the fringes will demonstrably be invisible . . . a hundred . . . would not cover the point of a needle." Underlying this explanation is a singular limit: The unwanted $\cos 2\phi$ does not vanish but oscillates rapidly. If the beams make an angle θ, the fringe spacing is $\lambda/2\theta$, vanishing in the geometrical limit of small λ. The limit is singular because the cosine oscillates infinitely fast as λ vanishes. Mathematically, this is an essential singularity of a type dismissed as pathological to students learning mathematics, yet here it appears naturally in the geometrical limit of the simplest wave pattern.

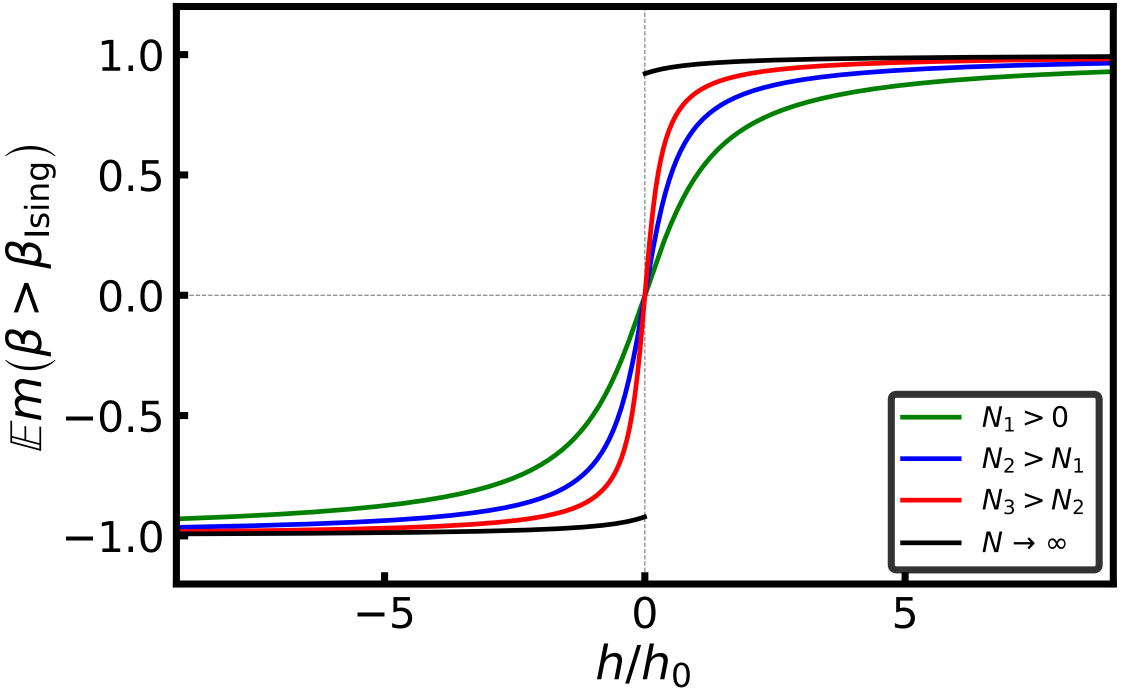
Young's "demonstrable" invisibility requires an additional concept, later made precise by Augustin Jean Fresnel and Lord Rayleigh: The rapidly varying $\cos 2\phi$ must be replaced by its average value, namely zero, reflecting the finite resolution of the detectors, the fact that the light beam is not monochromatic, and the rapid phase variations in the uncoordinated light from the two flashlights. Only then does $1 + 1 = 2$ apply—a relation thus reinterpreted as a singular limit.

Nowadays this application of the idea that the average of a cosine is zero, elaborated and reincarnated, is called decoherence. This might seem a bombastic redescription of the commonplace, but the applications of decoherence are far from trivial. Decoherence quantifies the uncontrolled extraneous influences that could upset the delicate superpositions in quantum computers. And, as we have learned from the work of Wojciech Zurek and others, the same concept governs the emergence of the classical from the quantum world in situations more sophisticated than Young's, where chaos is involved. For example, the chaotic tumbling of Saturn's satellite Hyperion, regarded as a quantum rotator with about 10^{60} quanta of angular momentum, would, according to an unpublished calculation by Ronald Fox, be suppressed in a few decades by the discrete nature of the energy spectrum. However, nobody expects to witness this suppression, because Hyperion is not isolated: Just one photon arriving from the Sun (whose reemission enables our observations) destroys the coherence responsible for quantization in a time of the order of 10^{-50} seconds, and reinstates classicality.[1] Alternatively stated, decoherence suppresses the quantum suppression of chaos.

Other reassurances are equally hard to come by. For example, for-

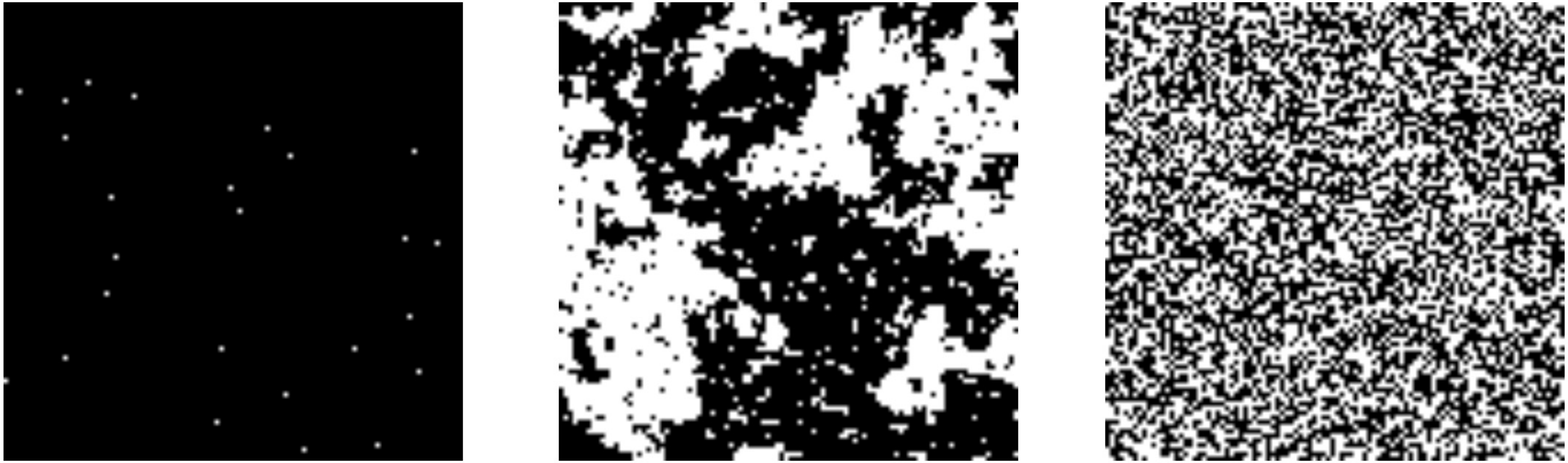
Michael Berry *(http://www.phy.bris.ac.uk/uk/staff/berry_mv.html) is Royal Society Research Professor in the physics department of Bristol University, in the UK.*

Thermodynamic limit of expected magnetisation is <u>singular</u> for all $\beta > \beta_{\mathrm{Ising}}$



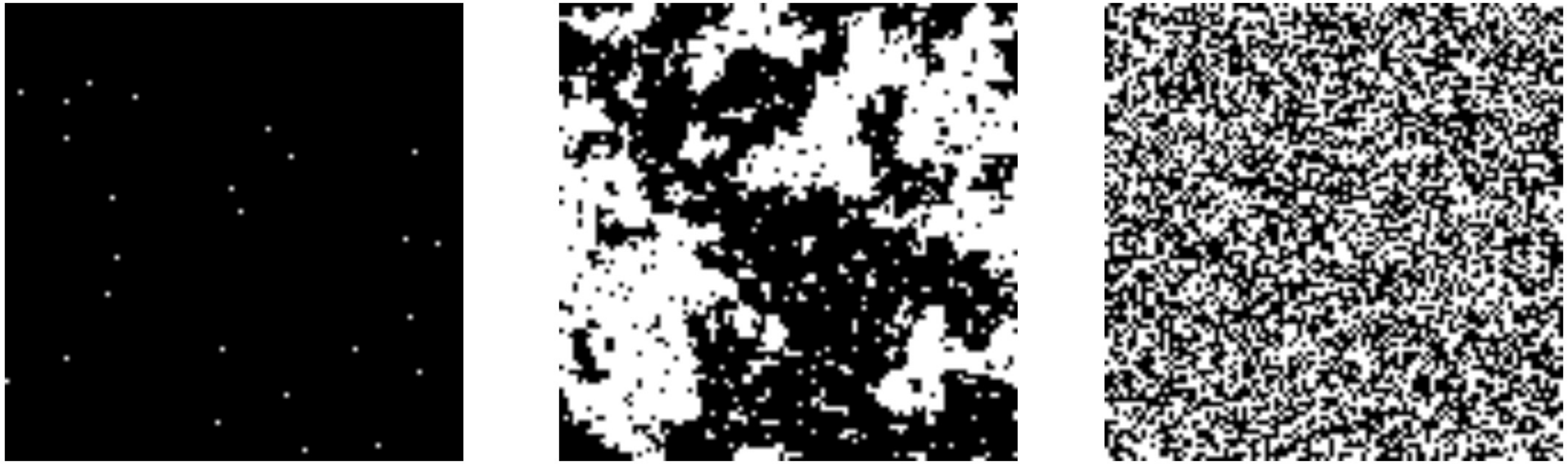
$$\lim_{h\downarrow 0}\lim_{N\to\infty} \mathbb{E}\boldsymbol{m}(\boldsymbol{x};\boldsymbol{\beta J},\boldsymbol{h},\boldsymbol{N}) \neq \boldsymbol{0} = \lim_{N\to\infty}\lim_{h\downarrow 0} \mathbb{E}\boldsymbol{m}(\boldsymbol{x};\boldsymbol{\beta J},\boldsymbol{h},\boldsymbol{N})$$

Berry, *Physics Today 55*, 10 (2002)

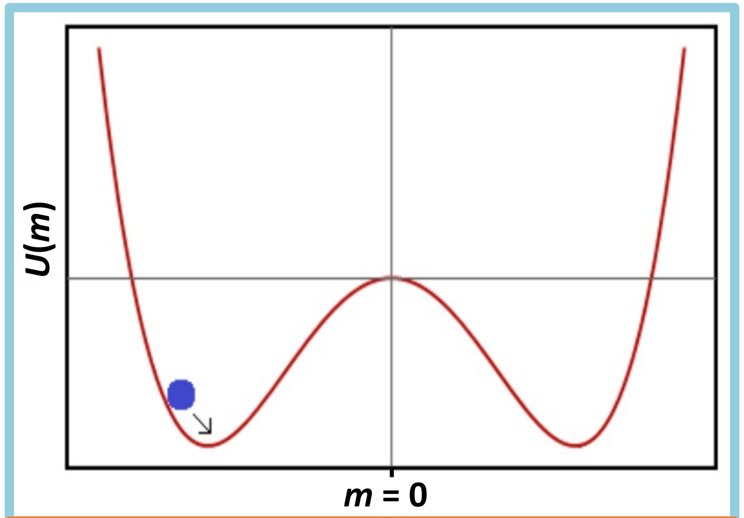


$\boldsymbol{\beta \gg \beta_c}$	$\boldsymbol{\beta \approx \beta_c}$	$\boldsymbol{\beta \ll \beta_c}$

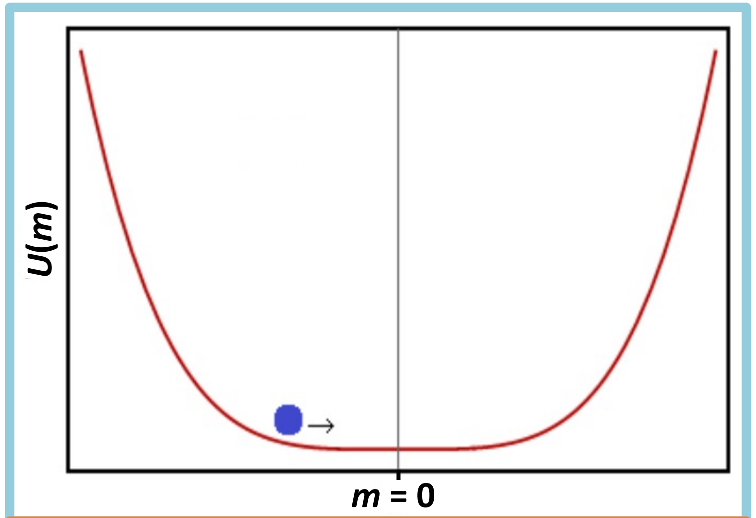
Figs: Walter & Barkema, *Physica A* 418, 78 (2015)



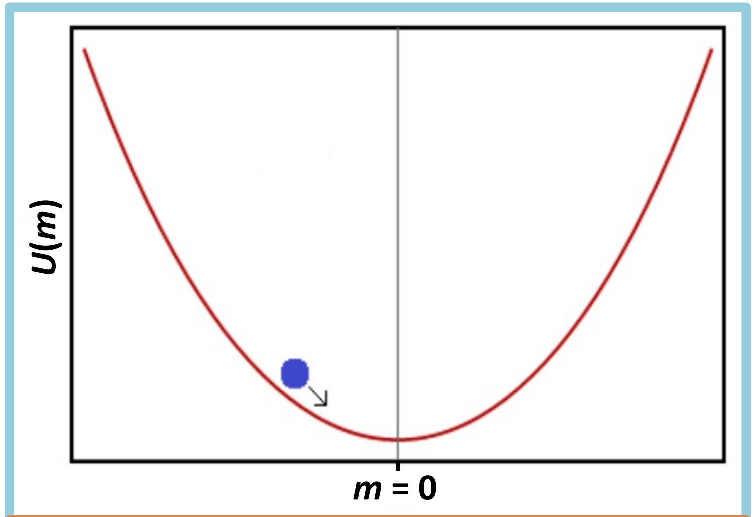
$\beta \gg \beta_c$	$\beta \approx \beta_c$	$\beta \ll \beta_c$



Low-temperature bimodal



Critical flattening



High-temperature unimodal

Top figs: Walter & Barkema, *Physica A* 418, 78 (2015); bottom figs: Anshul Kogar

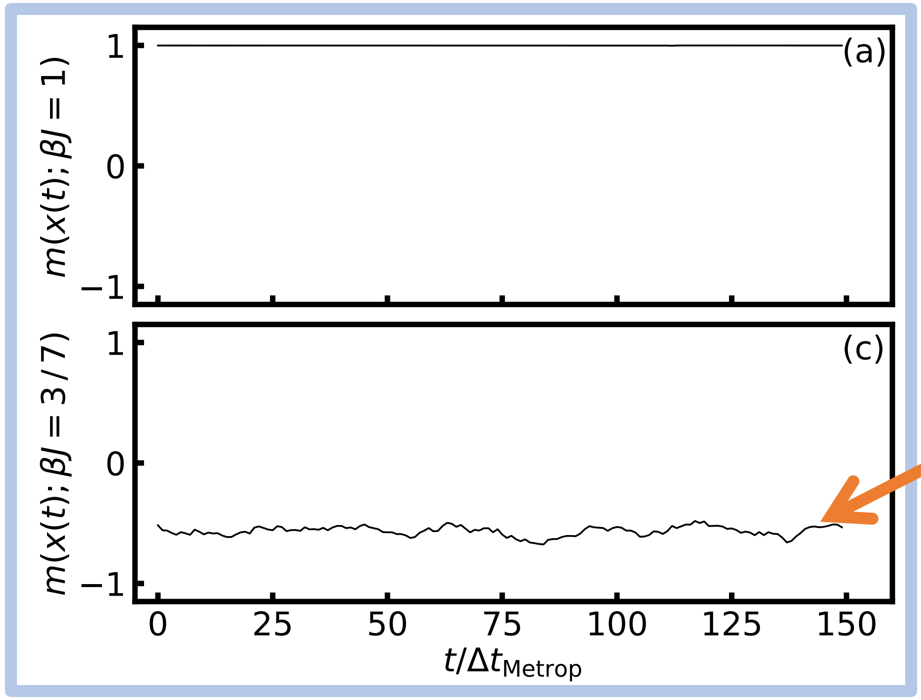
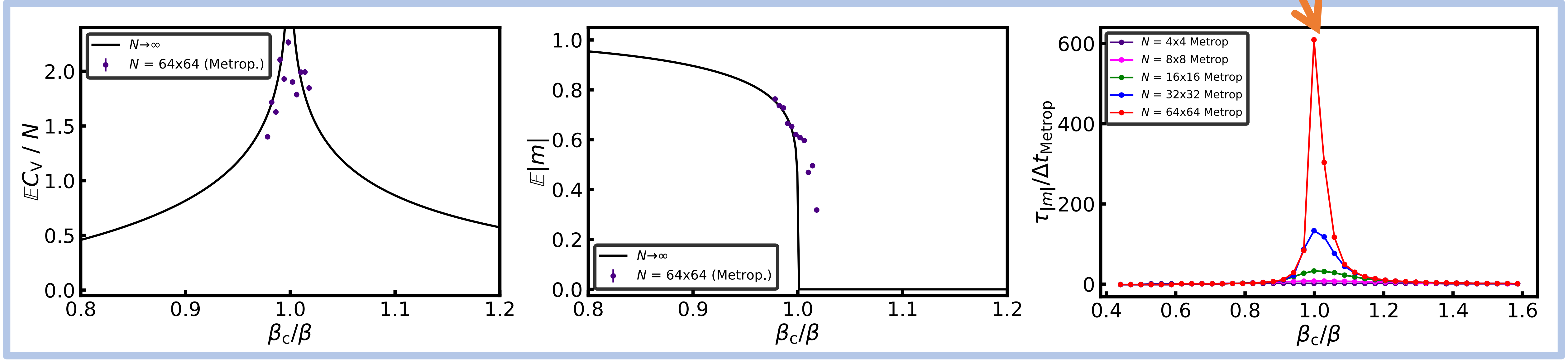
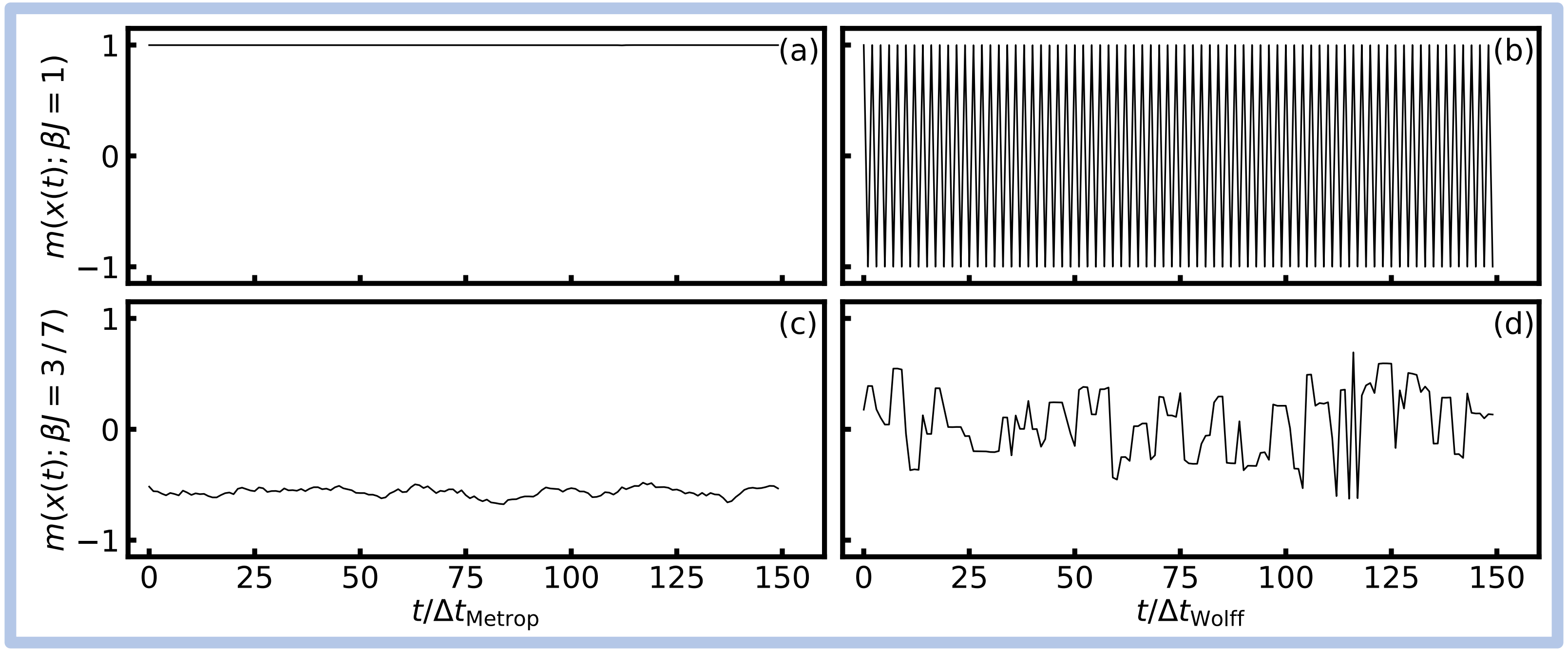
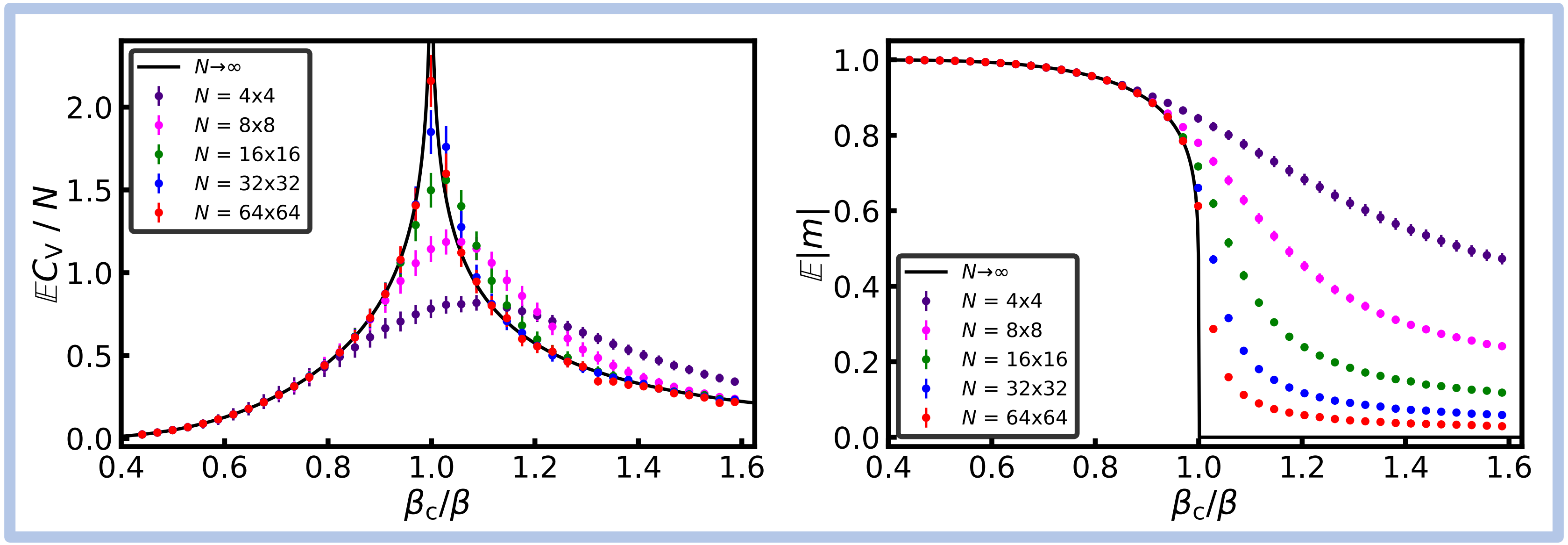


Fig. (c) is now *near the transition* where growing correlated clusters induce strong autocorrelations



Figs: Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023) (*N* = 64x64 spins in top panel)





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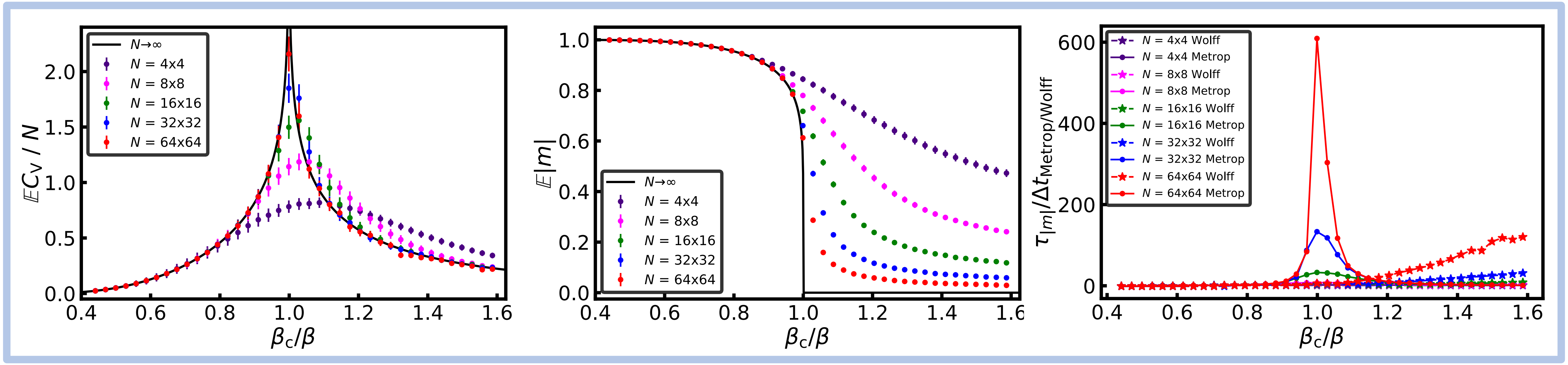
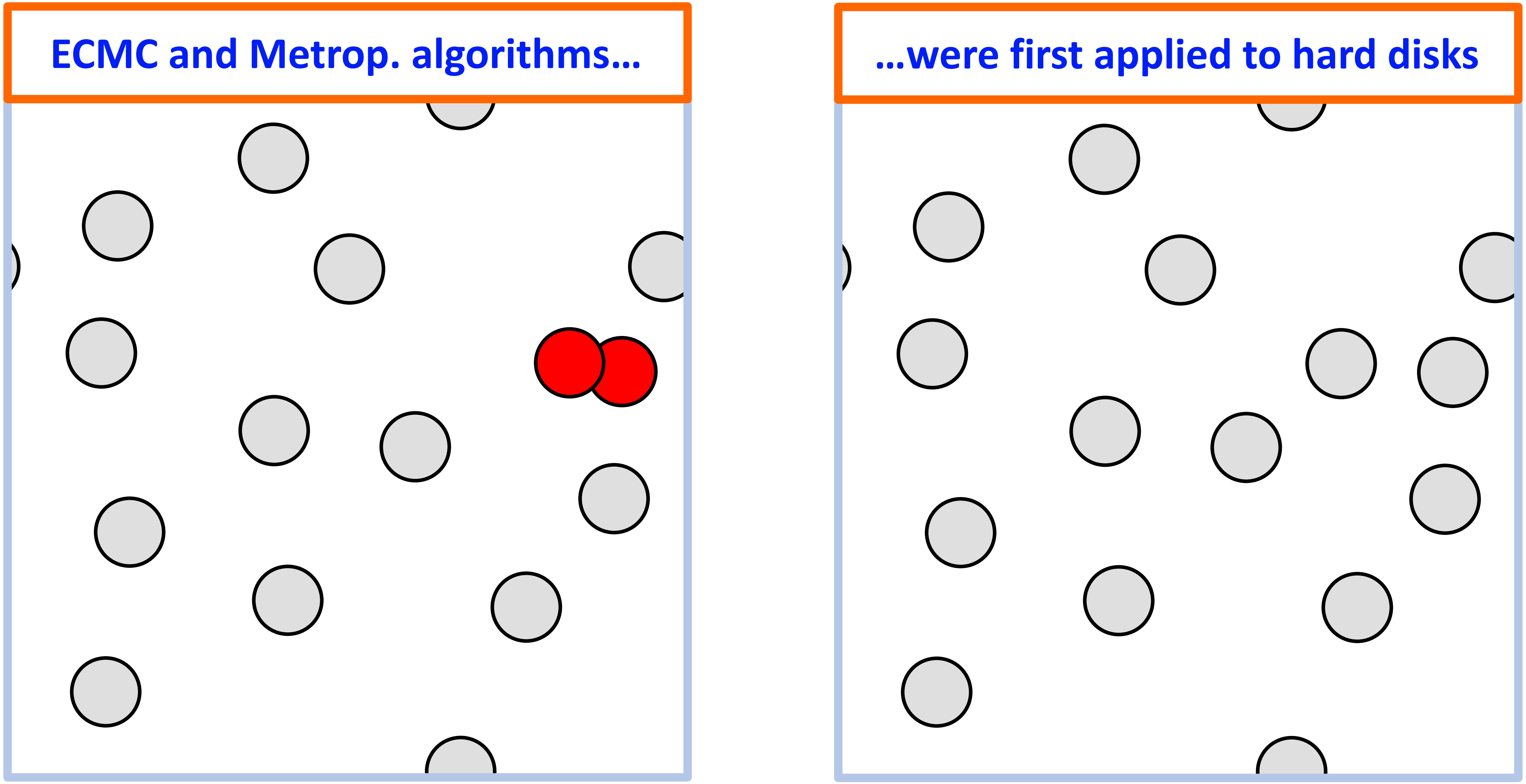


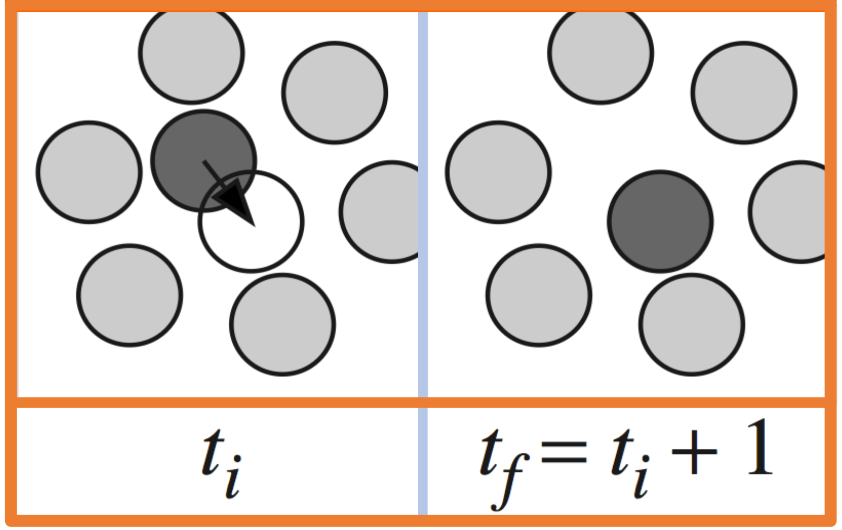
Figs: Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023)

- Statistical physics and phase transitions
- Metastability and Wolff algorithm
- **Continuous state spaces and ECMC**

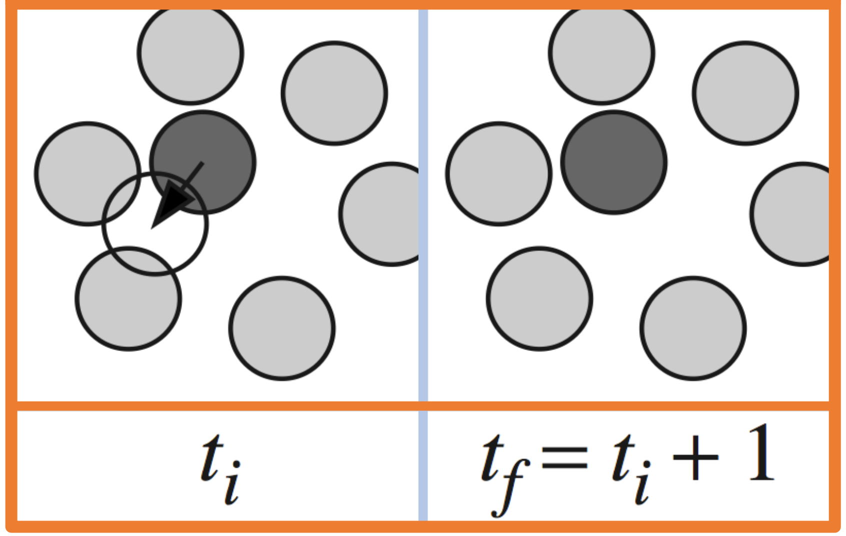

ECMC and Metrop. algorithms...
...were first applied to hard disks

- **Evolve single particle at each iteration**
- $x'_a = x_a \oplus u$, **where…**
- $u_j \sim \mathcal{U}(-\varepsilon, \varepsilon)$ **for** $j \in \{1, \ldots, d\}, \varepsilon > 0$
- **…and $\oplus$ indicates addition on torus**
- **Accept/reject configs without/with overlaps**

Metropolis move accepted

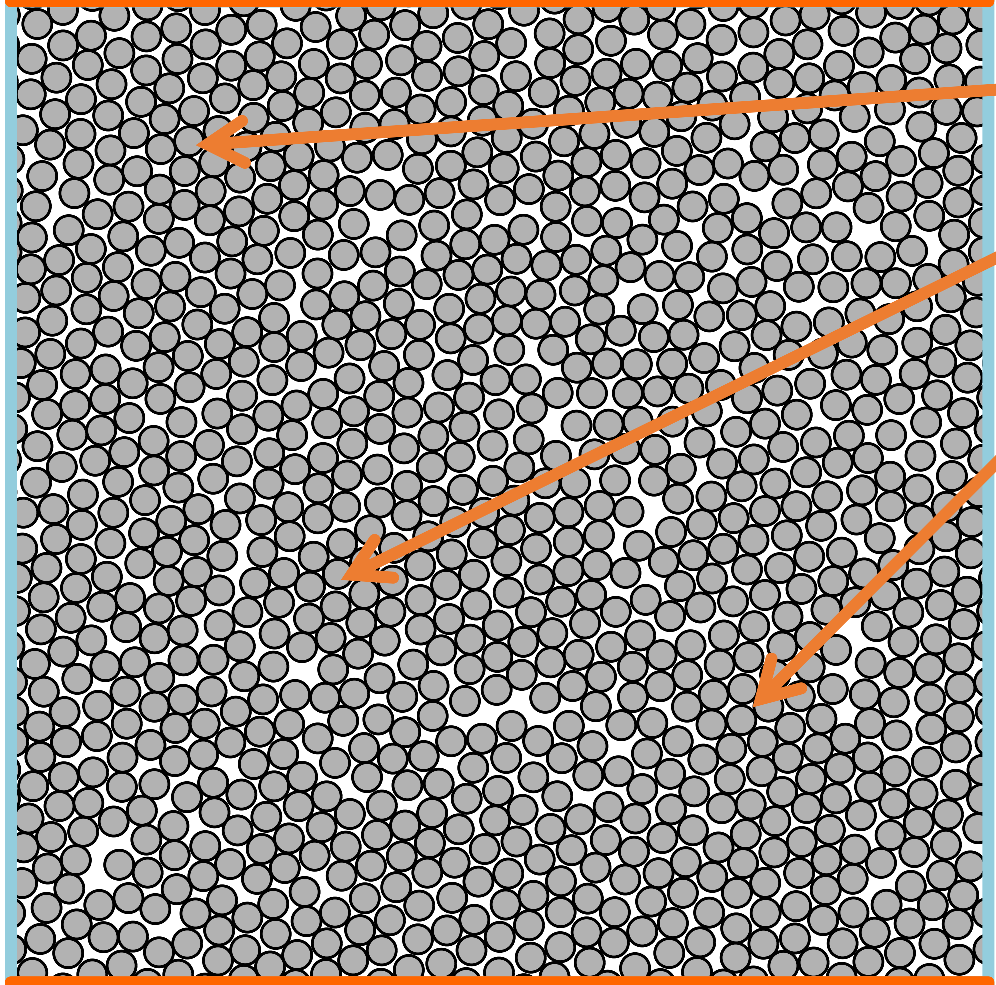


Discrete moves → rejections



Algorithm: Metropolis *et al.*, *J. Chem. Phys.* 21, 1087 (1953)
Fig.: Bernard, Krauth & Wilson, *Phys. Rev. E* 80, 056704 (2009)

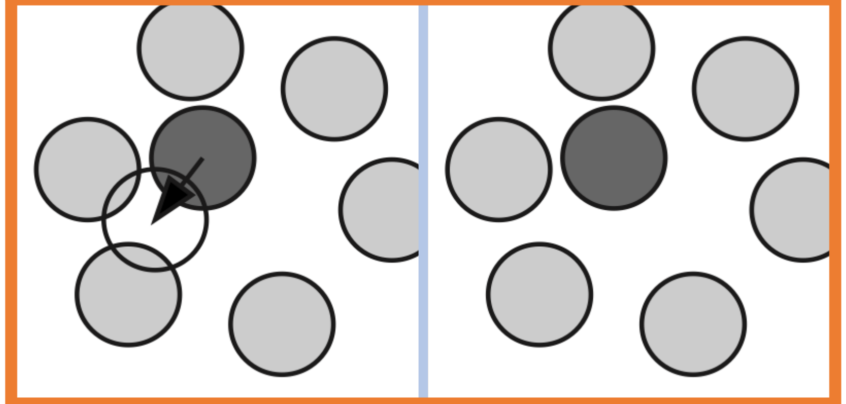
Hard-disk model



π(overlaps / no overlaps) = 0 / Unif.

Tightly packed clusters $\Longrightarrow$ high rejection rates

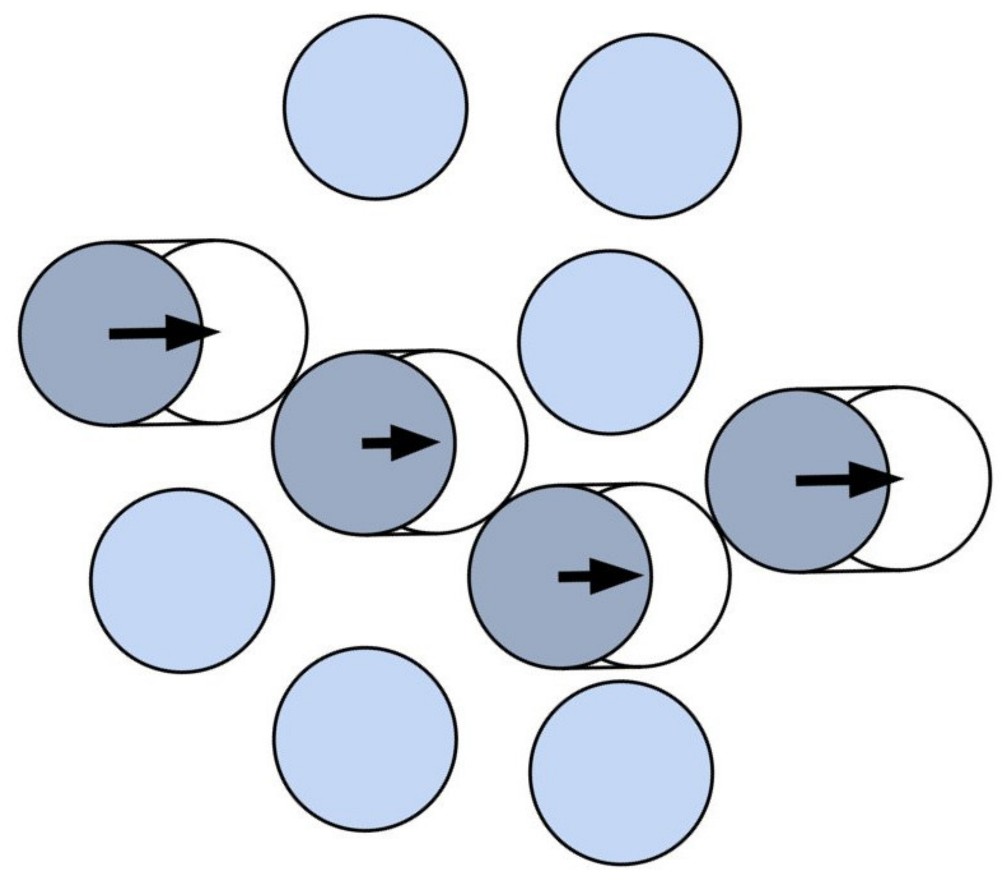
Discrete moves $\Longrightarrow$ rejections



t_i | $t_f = t_i + 1$

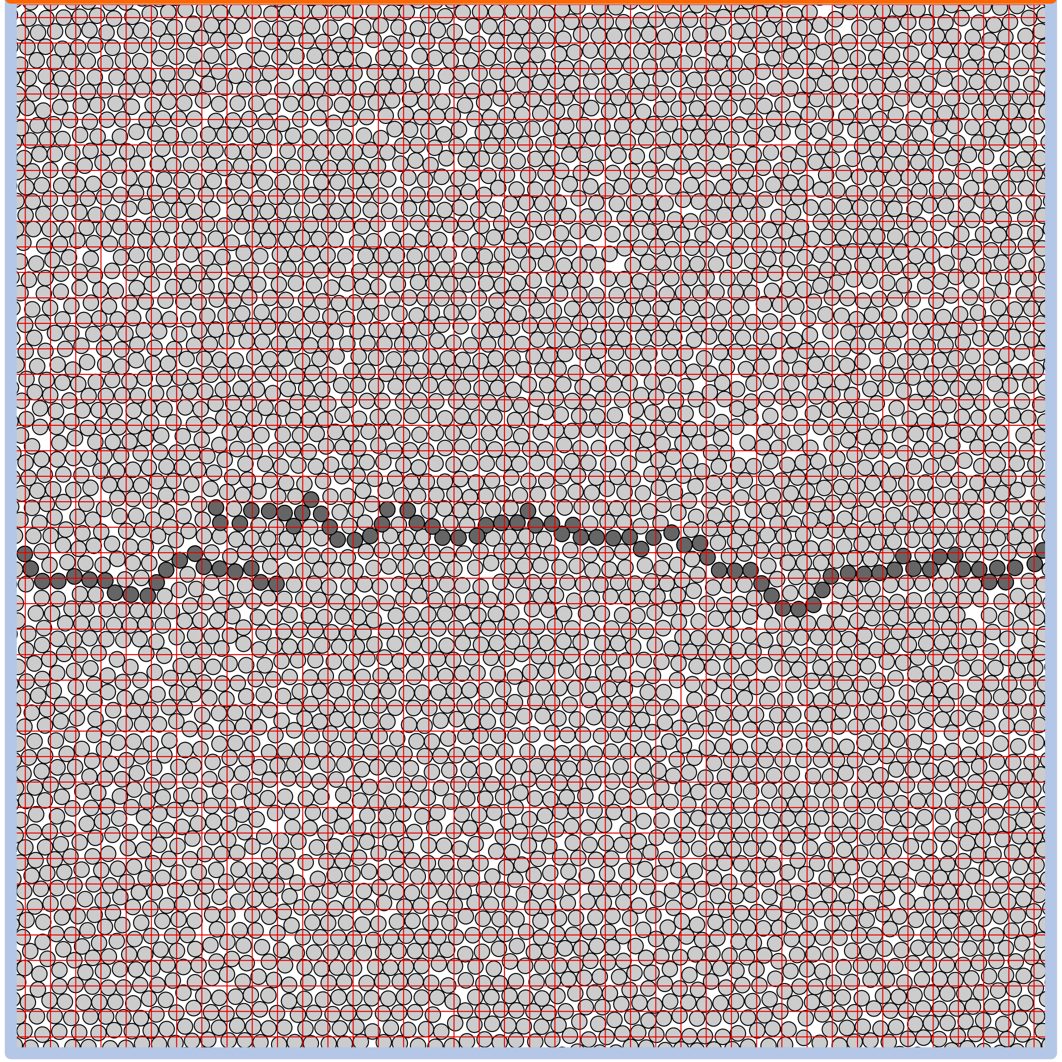
Left-hand fig.: Bernard, PhD thesis, ENS (2011)
Right-hand fig.: Bernard, Krauth & Wilson, *Phys. Rev. E* 80, 056704 (2009)

Event-chain Monte Carlo



Nonreversible, continuous moves ➔ events replace rejections

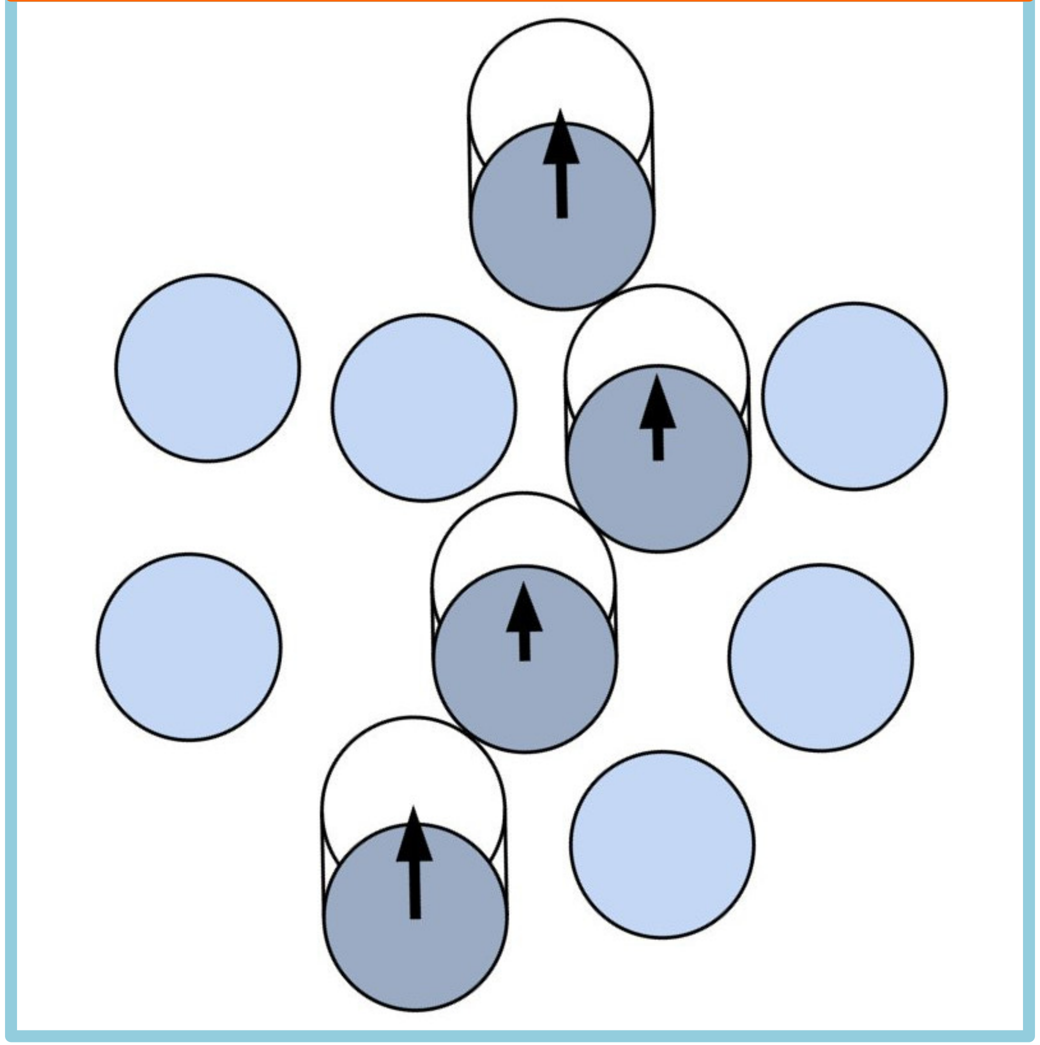
Chain of events traverses system



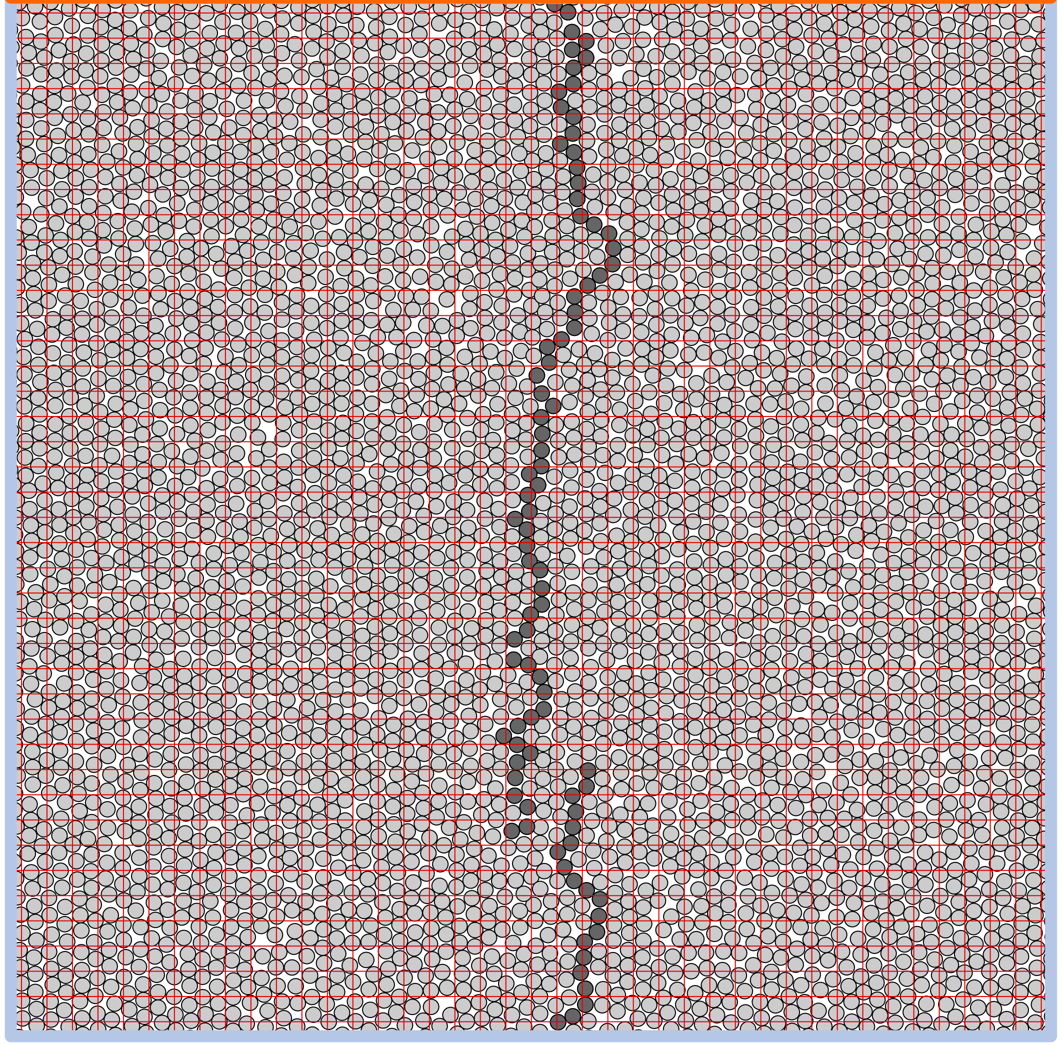
Left-hand fig.: Krauth, unpublished

Right-hand fig.: Bernard, PhD thesis, ENS (2011)

Random coordinate switches…



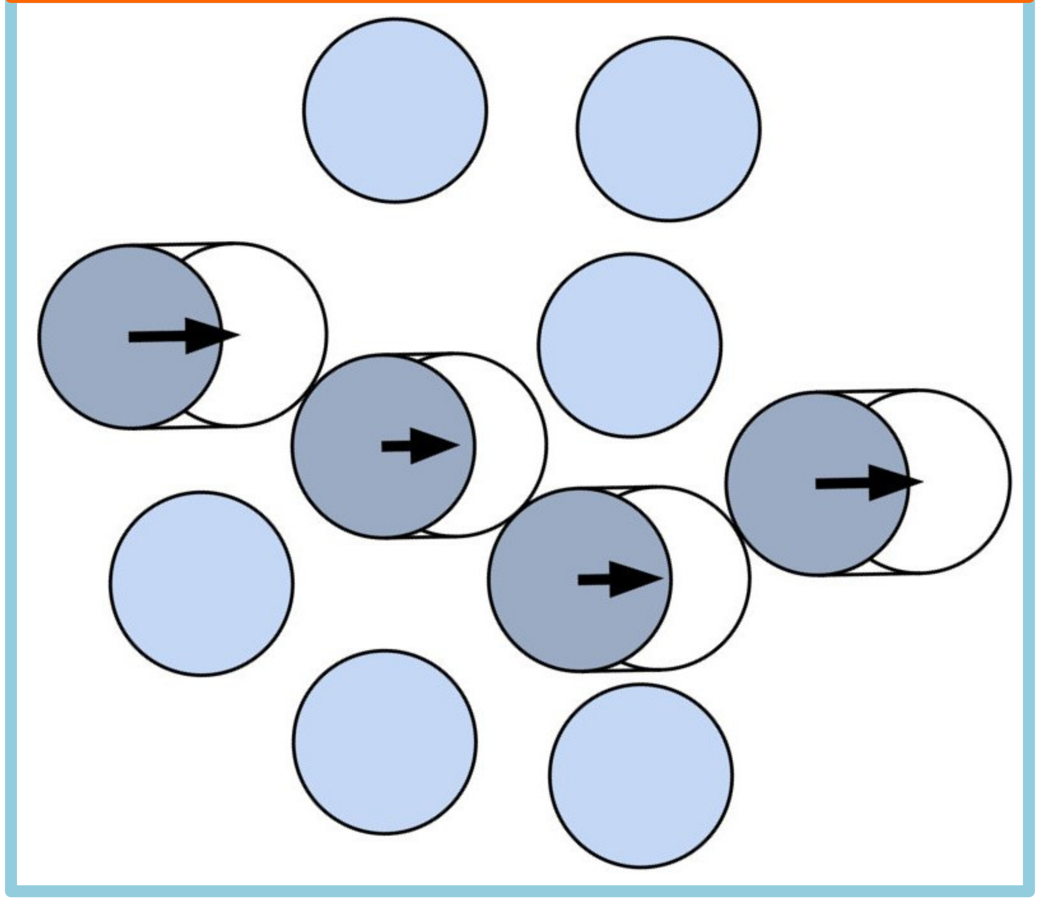
…to sample along both dimensions



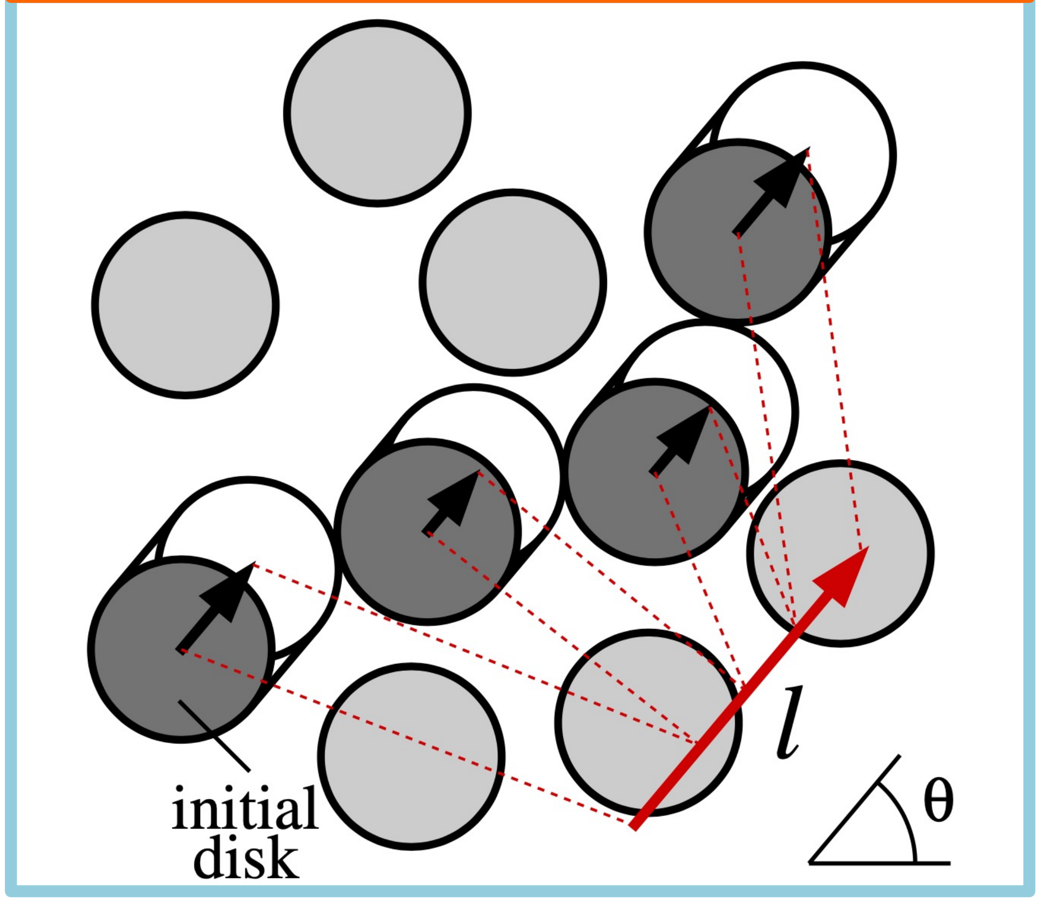
Left-hand fig.: Krauth, unpublished

Right-hand fig.: Bernard, PhD thesis, ENS (2011)

xy refreshment…



…vs uniform refreshment

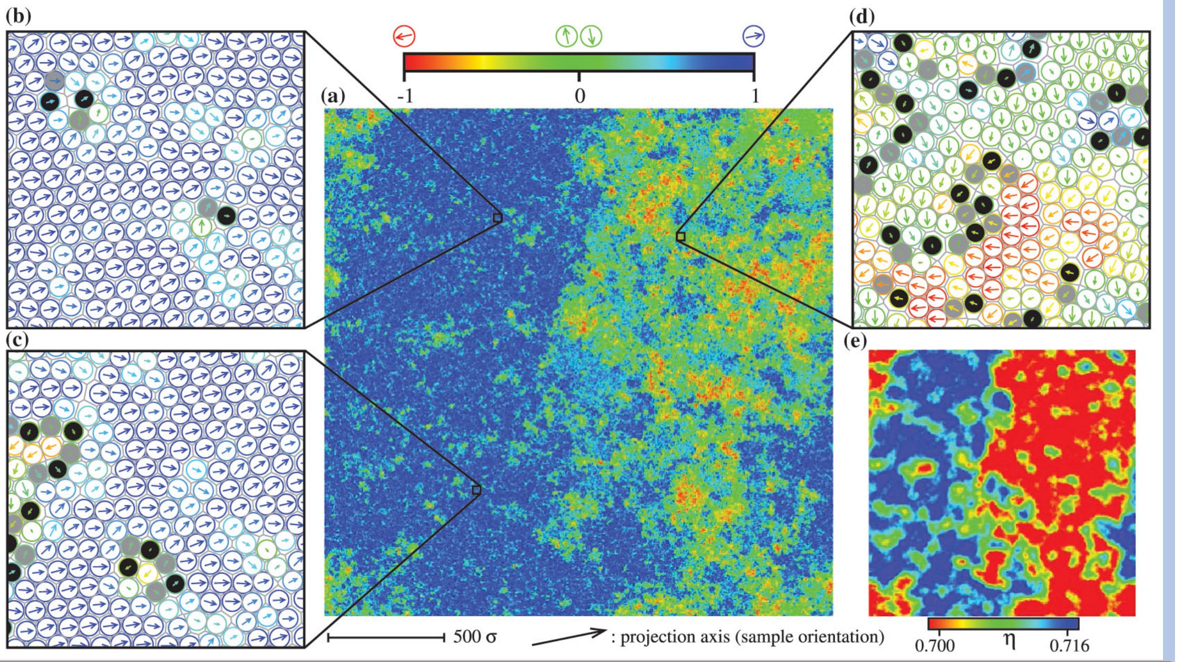


Left-hand fig.: Krauth, unpublished

Right-hand fig.: Bernard, PhD thesis, ENS (2011)

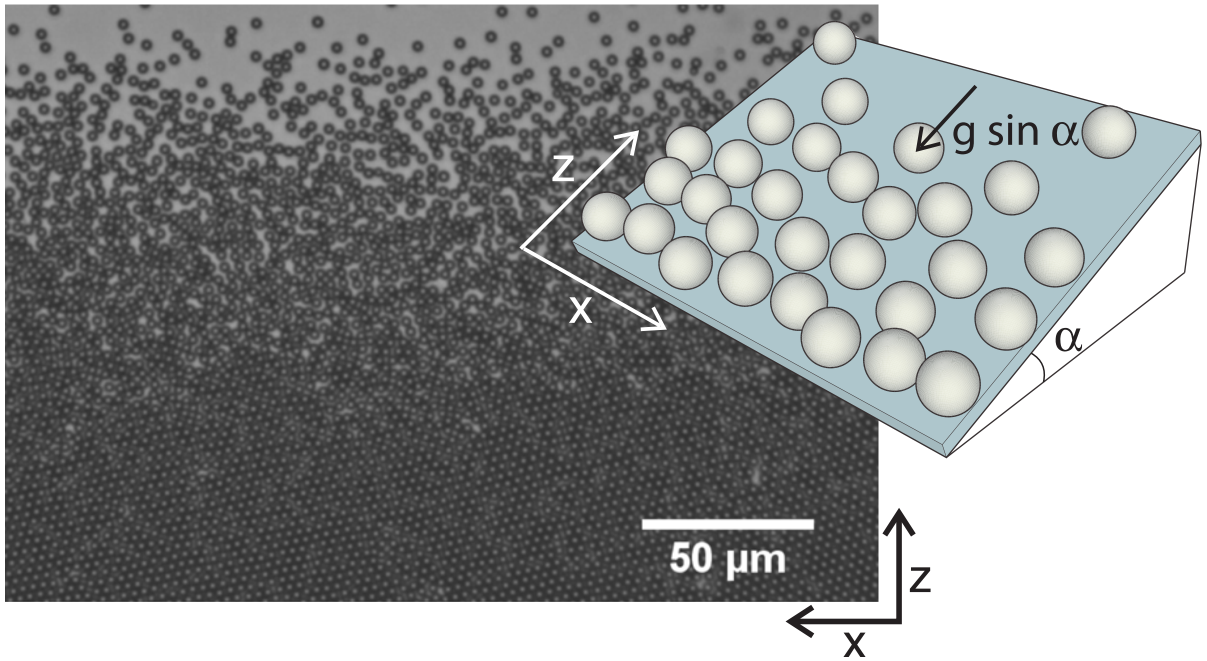
π-invariance: Andrieu & Livingstone, *Ann. Stat.* 49, 1958 (2021)

ECMC solved 2D melting



Disputed for 50 years

Colloidal hard-disk experiment



Confirms ECMC numerics

Left-hand fig.: Bernard & Krauth, *Phys. Rev. Lett.* 107, 155704 (2011)

Right-hand fig.: Thorneywork *et al.*, *Phys. Rev. Lett.* 118, 158001 (2017)

Continuous potentials[1]

- $\pi_{\mathrm{hard}}(x)$ = 0 or const. $\Longleftrightarrow$ $U_{\mathrm{hard}}(x) = \infty$ or finite…
- …so ECMC freely advances hard disks until $\mathrm{d}U/\mathrm{d}x_a = \infty$…
- …but particles never collide in the case of continuous potentials $U(x)$
- ➔ somehow account for continuous increases in $U(x)$?

1 Peters & de With, *Phys. Rev. E* 85, 026703 (2012); Michel, Kapfer & Krauth, *J. Chem. Phys.* 140, 054116 (2014)

- Consider *m* Metropolis translations of length Δ in a fixed direction.
- Probability of translating active particle *a* through distance η := *m*Δ is…
- $$\begin{aligned} p(x_a \to x_a + \eta) &= \prod_{i=1}^{m} \min\left[1, \exp\left(-\beta\left[U(x_a + \Delta i) - U\left(x_a + \Delta(i-1)\right)\right]\right)\right] \\ &= \exp\left[-\beta \sum_{i=1}^{m} \max\left(0, U(x_a + \Delta i) - U\left(x_a + \Delta(i-1)\right)\right)\right] \\ &\to \exp\left[-\beta \int_0^{\eta} \max(0, \nabla_a U(x)) \mathrm{d}x_a\right] \text{ as } \Delta \to 0 \end{aligned}$$
- ➔ Advance active particle at constant velocity v from time $t_0 \geq 0$ and solve:

  $$-\log \Upsilon = \beta \int_{t_0}^{t_\eta} \max(0, v \cdot \nabla_a U(x)) \mathrm{dt} \text{ where } \Upsilon \sim \mathcal{U}[0,1)\ldots$$
- …to find the next *event time* $t_\eta \coloneqq t_0 + \eta / v$ (assuming no 'boundary' collisions).
- Particle *i* then becomes active w/prob. $\propto \max\left(0, -v \cdot \nabla_i U\left[x\left(t_\eta\right)\right]\right)$ at $t = t_\eta$.

Peters & de With, *Phys. Rev. E* 85, 026703 (2012); Michel, Kapfer & Krauth, *J. Chem. Phys.* 140, 054116 (2014)

- Need to integrate $v \cdot \nabla_a U(x)$ over *only* positive contributions…

- …but this is non-trivial for multiple particles

- So we have two options for Poisson process (PP):
  1. Thinned PP: choose $\widetilde{q_a}$ to overestimate event rate $q_a(x) \coloneqq \beta \max(0, v \cdot \nabla_a U(x))$, then confirm events with probability $q_a(x)/\widetilde{q_a}(x)$

  2. 2-particle blocking: Sample Poisson process of each two-particle interaction and take shortest displacement (superposition of PPs)

2-particle sampling

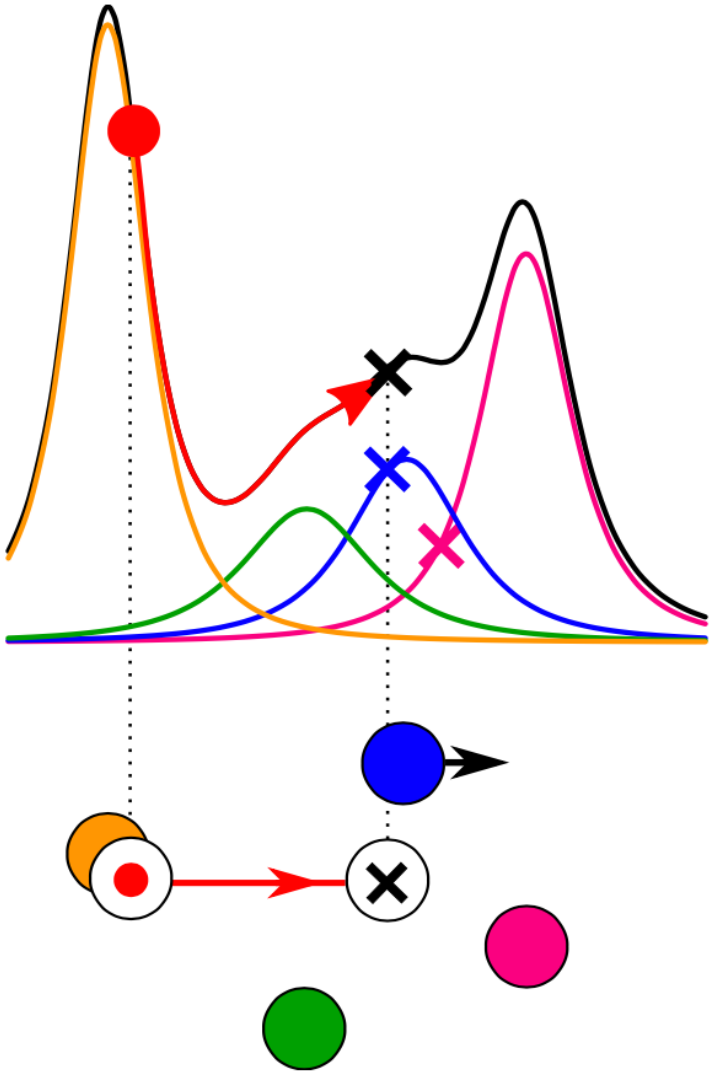
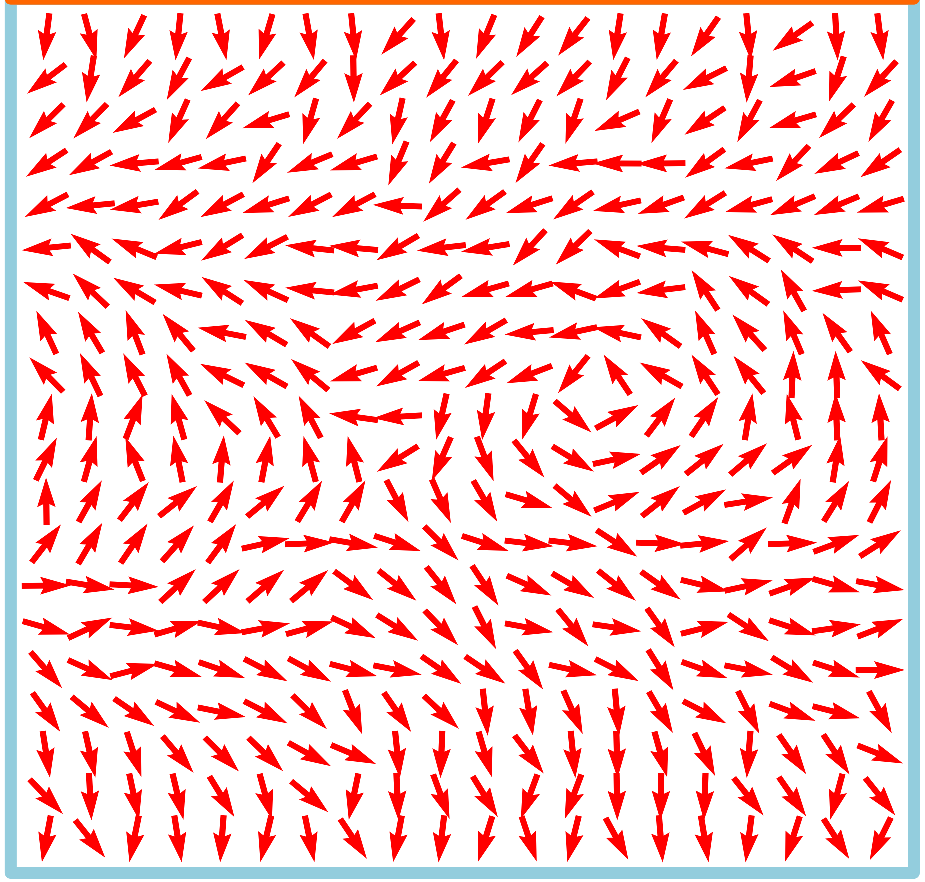


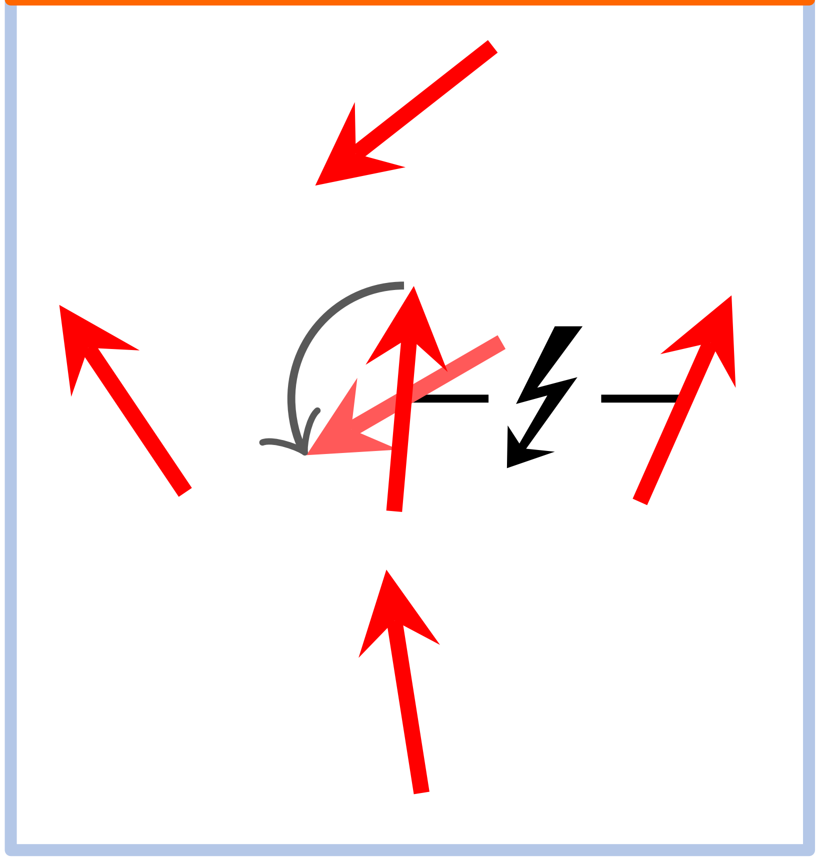
Fig.: Manon Michel, PhD thesis, ENS (2015)

2DXY model

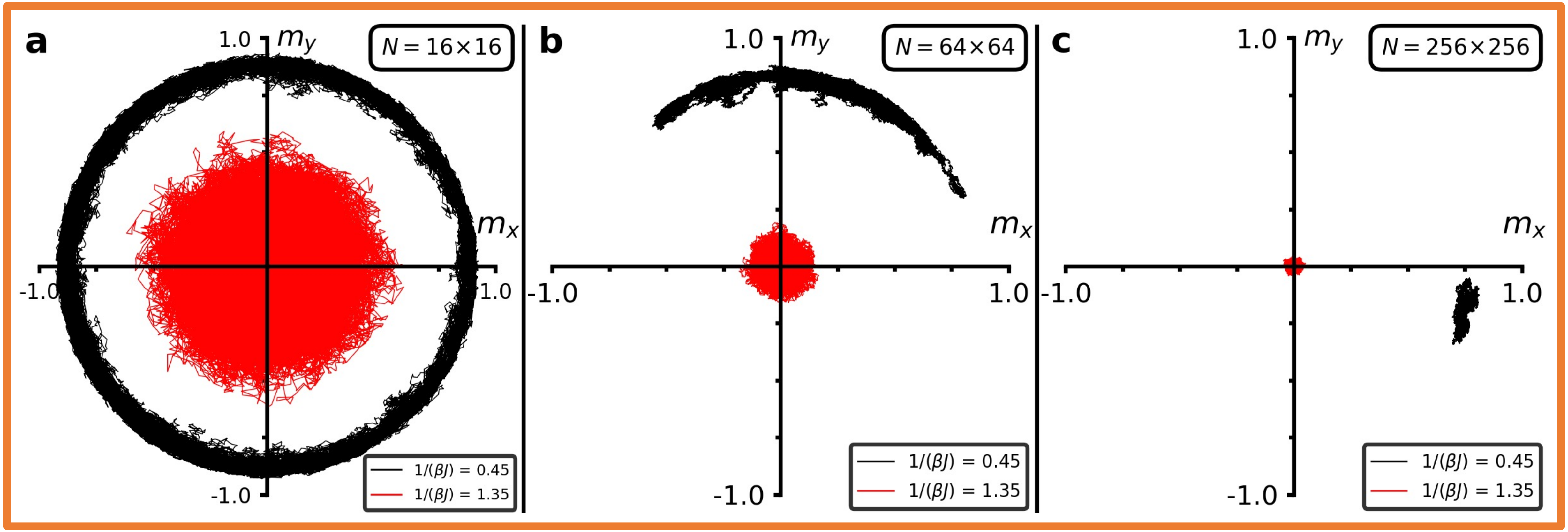


$$U_{XY} = -J \sum_{i=1}^{N} \sum_{j \in S_i} \cos(x_i - x_j) \text{ with } x_i \in (-\pi, \pi], J > 0$$

ECMC rotates active spin until neighbouring veto

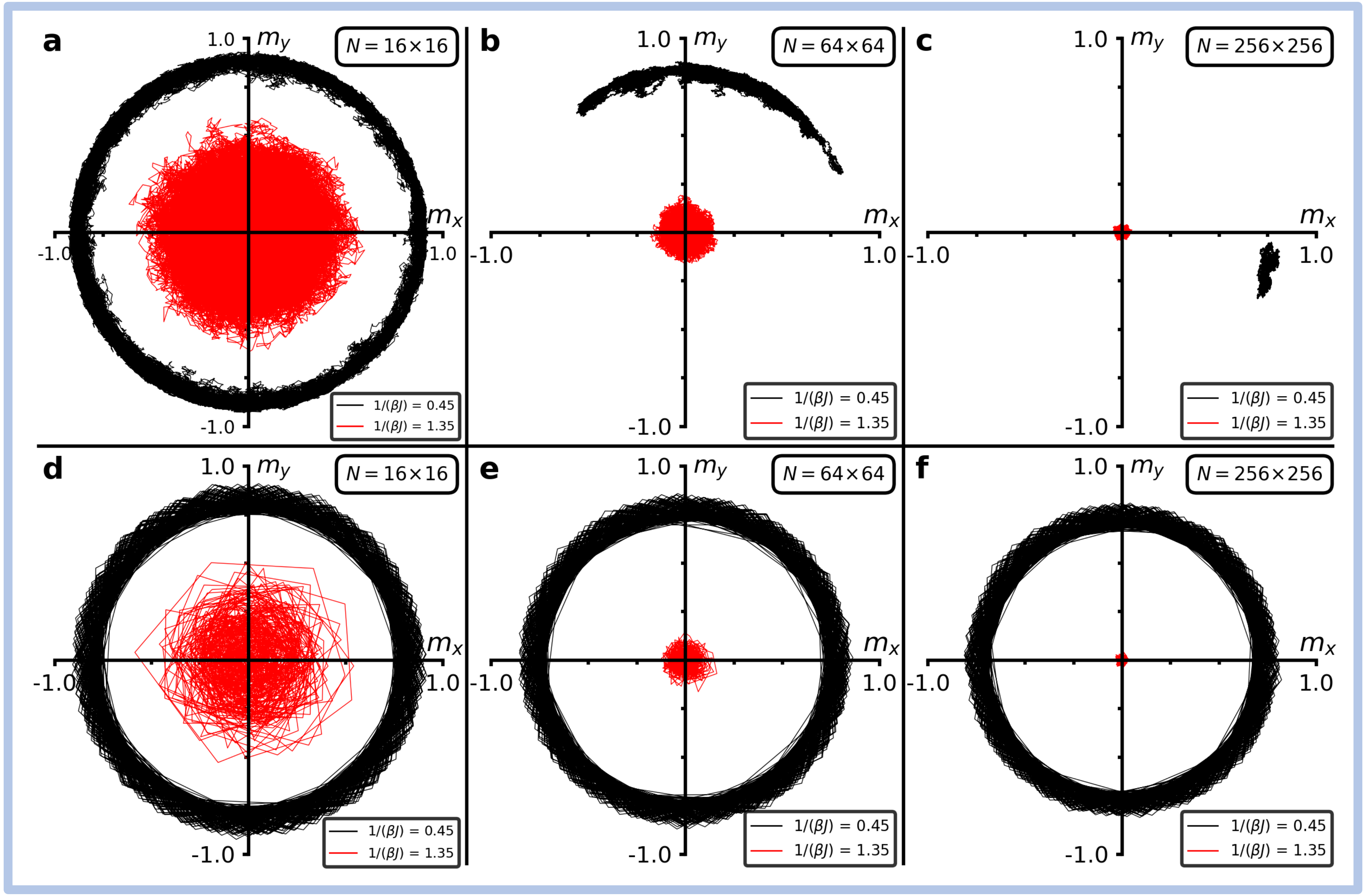


$$U_{XY} = -J\sum_{i=1}^{N}\sum_{j\in S_i}\cos(x_i - x_j) \text{ with } x_i \in (-\pi, \pi], J > 0$$

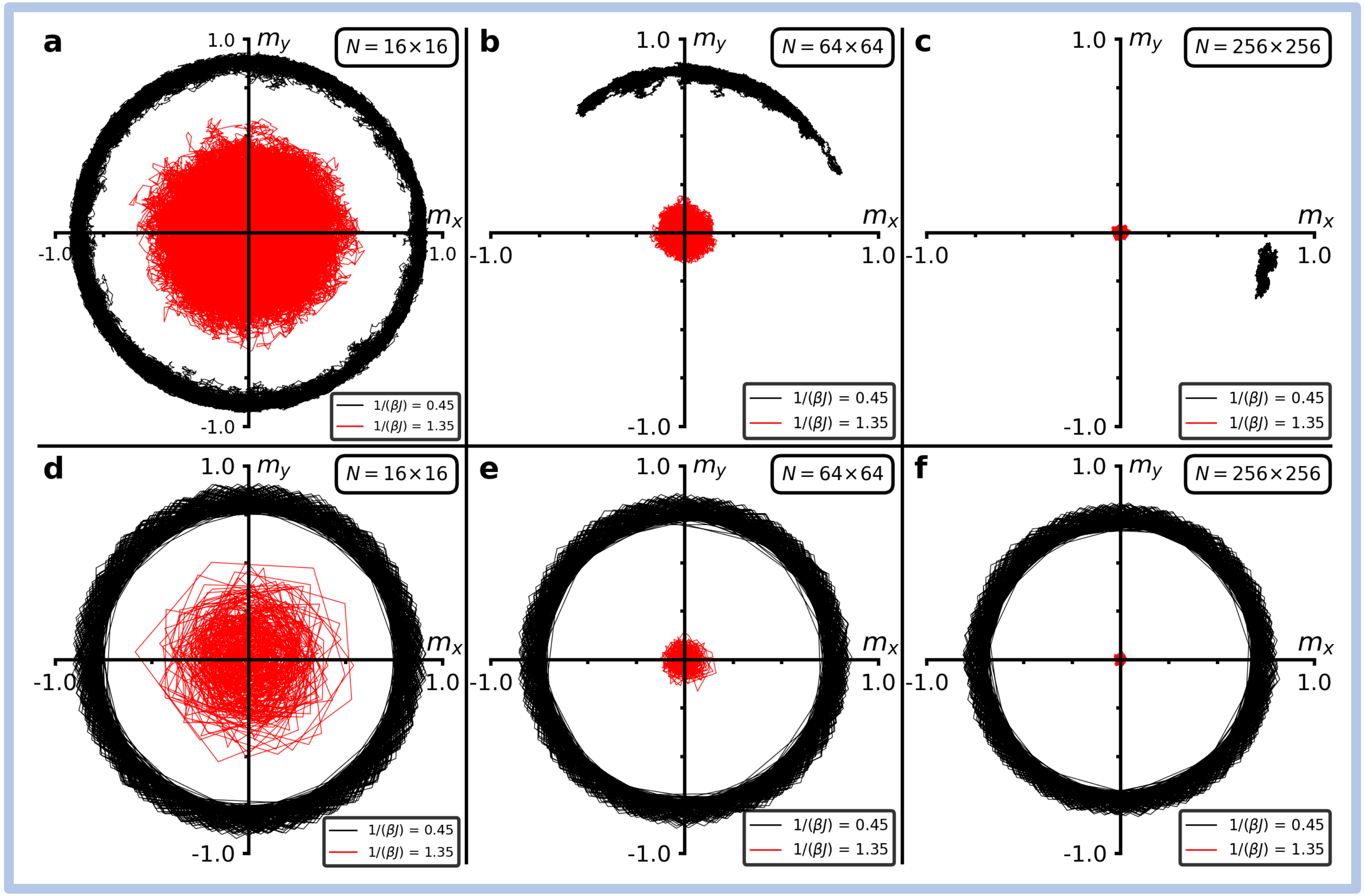


$$\boldsymbol{m}(\boldsymbol{x};\beta,J,h,N) \coloneqq \frac{1}{N}\sum_{i=1}^{N}(\cos x_i, \sin x_i)^t,\ x_i \in (-\pi,\pi]$$

Faulkner, arXiv:2209.03699 (2022); Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023)



Faulkner, arXiv:2209.03699 (2022); Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023)



ECMC’s constant-speed dynamics circumvent critical slowing down?

Faulkner, arXiv:2209.03699 (2022); Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023)

Summary and outlook

- Bayesians ***fix*** hyperparameters, whereas physicists ***vary*** them.
- Varying hyperparameters can induce metastability and critical slowing down.
- Physicists combat these phenomena w/sophisticated sampling algorithms.
- **Future plans:** use ECMC to characterise CSD in 2DXY model; explore Bayesian analogues.
- Also interested in π-invariance of canonical ECMC if anyone has any ideas!
- Thanks to Sam Livingstone[1], EPSRC and Advanced Computing Research Centre (Bristol).

1 Faulkner & Livingstone, *Stat. Sci.*, *in press* (2023)

Example 2D Ising configuration

↑	↓	↓	↑	↓	↑
↓	↓	↓	↓	↑	↓
↑	↓	↓	↓	↑	↑
↑	↑	↓	↑	↑	↑
↓	↑	↑	↑	↓	↓
↑	↓	↓	↑	↑	↑

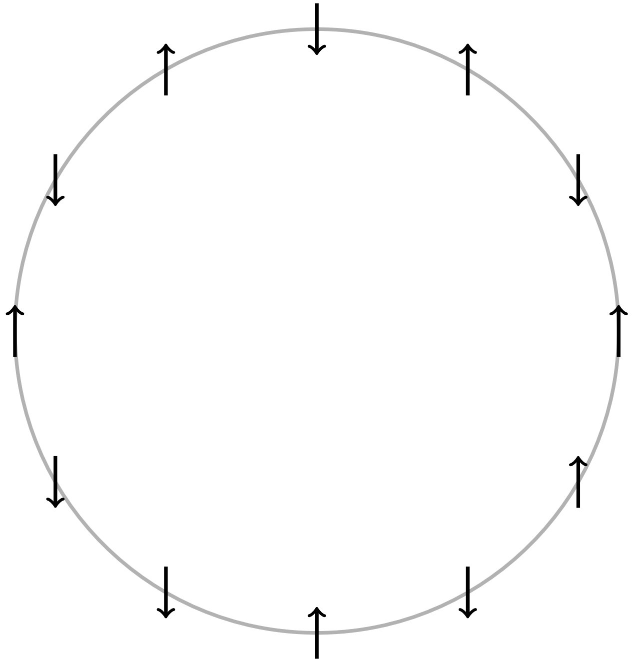
- $U_{\text{Ising}} = -\frac{J}{2}\sum_{i=1}^{N}\sum_{j \in S_i} x_i x_j \,, x_i = \pm 1$
- **Spin—spin correlation length increases as temperature decreases**
- **➔ nonergodic Metropolis dynamics**
- **Wolff combats this by flipping clusters**

Swendsen & Wang, *PRL* 58, 86 (1987); Wolff, *PRL* 62, 361 (1989)

Fundamental axiom

- If some scalar observable $\chi(x; \beta, \theta, N)$ is sum of $O(N)$ random numbers…
- …and $\frac{\sigma_\chi}{\mathbb{E}[\chi]}$ can be made arbitrarily small as $N \to \infty$ (with $\lim_{N\to\infty} \mathbb{E}[\chi(x; \beta, \theta, N)] \neq 0$)…
- …then $\exists\, N_0 \in \mathbb{N}$ s.t. $\left| \frac{\mathbb{E}[\chi(x;\beta,\theta,N=N_0)]}{\lim_{N\to\infty} \mathbb{E}[\chi(x;\beta,\theta,N)]} - 1 \right| < \varepsilon$ (with $\varepsilon > 0$ immeasurably small)
- $\Rightarrow$ thermodynamic limit (usually!) reflects macroscopic physics

1D Ising model



No phase transition wrt free energy, *F*

- $U_{\text{Ising}} = -\frac{J}{2}\sum_{i=1}^{N}\sum_{j\in S_i} x_i x_j \; - h\sum_{i=1}^{N} x_i \,, h \in \mathbb{R}$
- $F_{\text{Ising}}^{d=1}\,(\beta, J, h, N) = -\beta^{-1}\log[\lambda_+^N(\beta, J, h) + \lambda_-^N(\beta, J, h)]$
- $\lambda_\pm^N(\beta, J, h) := e^{\beta J}[\cosh(\beta h) \pm \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}]$

Fig.: Faulkner & Livingstone, arXiv:2208.04751 (2022)
Theory: Ising, *Z. Physik 31*, 253 (1925)

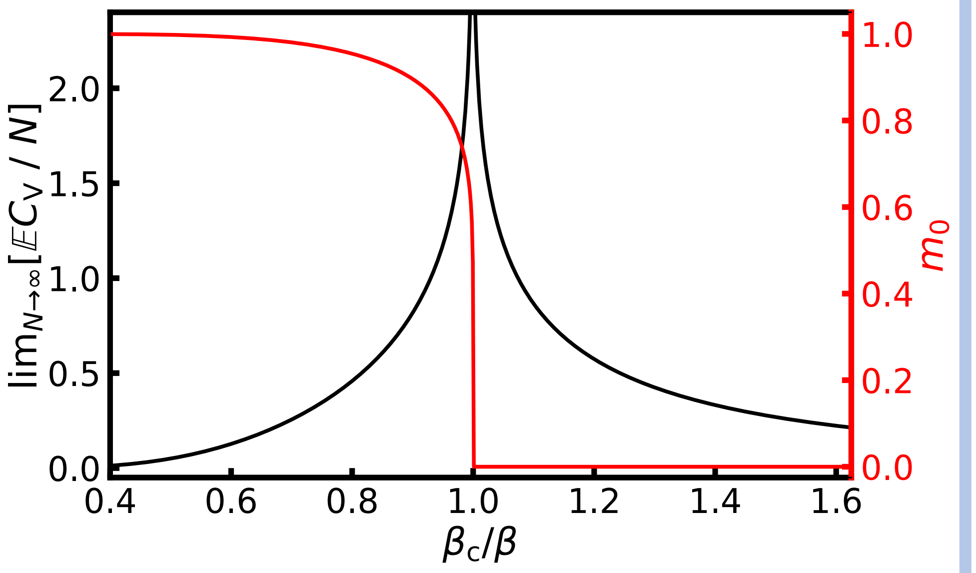
2D Ising model

- **Expected specific heat ($\mathbb{E}C_{\mathrm{V}} = \beta^2 \mathrm{Var}[U]$) is non-analytic as $N \to \infty$ at $\beta = \beta_{\mathrm{c}}, h = 0$ (black curve)**

- $$\lim_{N\to\infty} \frac{\mathbb{E}C_{\mathrm{V}}(x;\beta,J,h=0,N)}{N} = \beta^2 \partial_\beta^2 \gamma(\beta J)$$

- $$\gamma(\beta J) \coloneqq \ln[2\cosh(2\beta J)] + \frac{1}{\pi}\int_0^{\pi/2} \ln\left[\frac{1}{2}\left(1 + \sqrt{1 - \frac{4\sinh^2(2\beta J)\sin^2(w)}{\cosh^4(2\beta J)}}\right)\right] \mathrm{d}w$$

Thermodynamic specific heat per particle (black curve) diverges at $\beta = \beta_{\mathrm{c}}, h = 0$

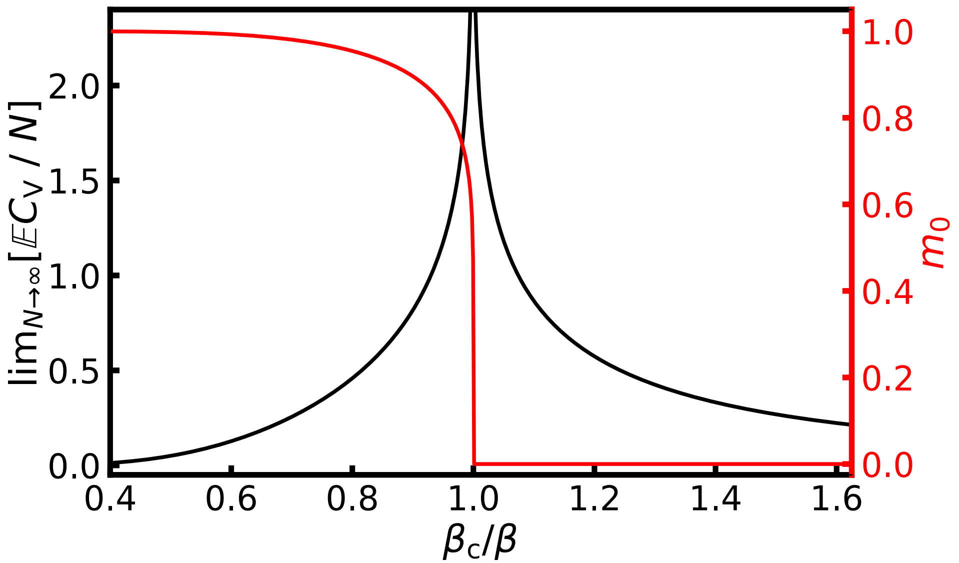


Theory: Onsager, *Phys. Rev.* 65, 117 (1944)
Fig.: Faulkner & Livingstone, arXiv:2208.04751 (2022)

What about order and magnetisation?

- $m(x;\beta,J,h,N) := \frac{1}{N}\sum_{i=1}^{N} x_i$
- $m_0(\beta,J) := \lim_{h\downarrow 0}\lim_{N\to\infty} \mathbb{E}m(x;\beta,J,h,N)$ is…
- …also non-analytic at $\beta = \beta_c$ (below & red curve)
- $m_0(\beta,J) = \begin{cases}(1-(\sinh(2\beta J))^{-4})^{1/8} & \text{for } \beta > \beta_c \\ 0 & \text{for } \beta < \beta_c\end{cases}$

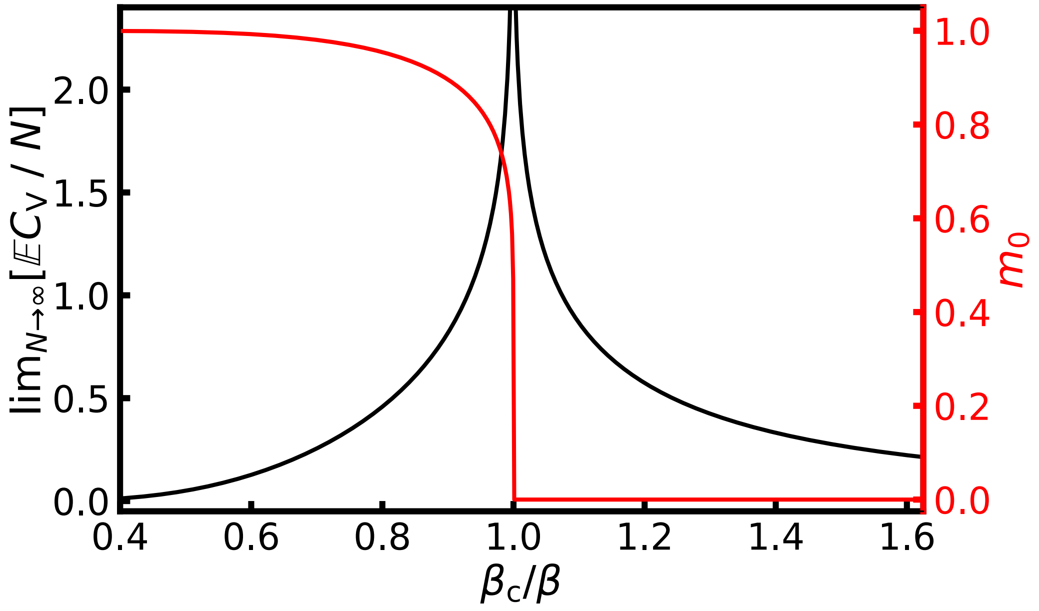
Spontaneous magnetisation (m_0 in red) is also non-analytic…



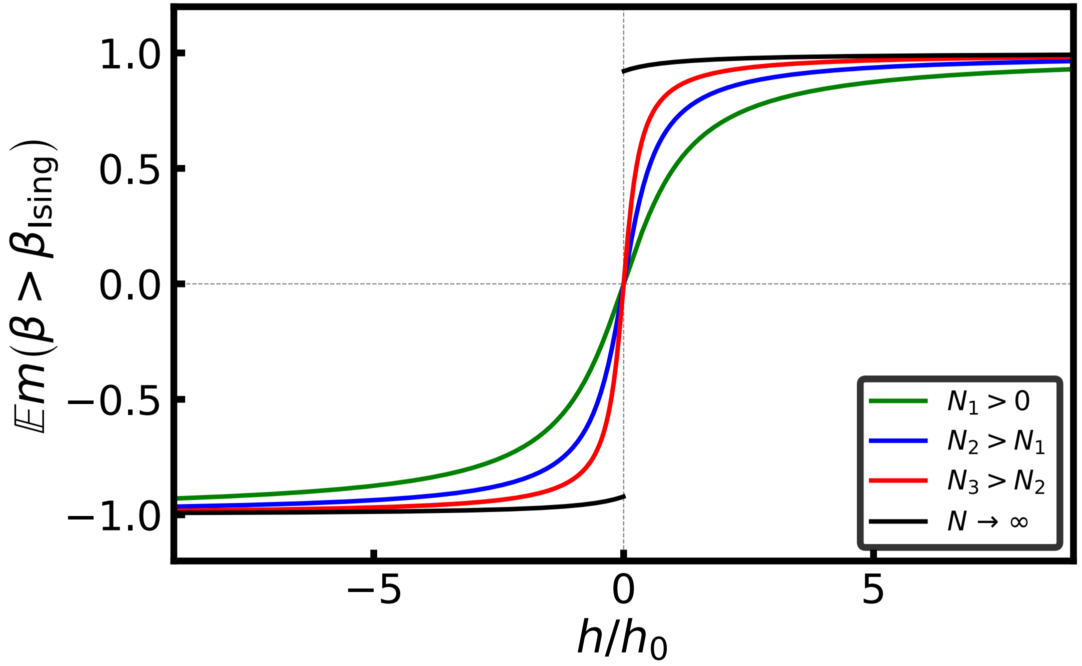
…indicating an order—disorder transition at $\beta = \beta_c$

Theory: Onsager, *Nuovo Cimento* 6, 261 (1949); Yang, *Phys. Rev.* 85, 808 (1952)
Fig.: Faulkner & Livingstone, arXiv:2208.04751 (2022)

Spontaneous magnetisation (m_0 in red) reflects experimental reality…



…as symmetry breaking induces $N \to \infty$ discontinuity in $\mathbb{E}m$ at $h = 0$



$$\boldsymbol{m_0(\beta, J) \coloneqq \lim_{h\downarrow 0}\lim_{N\to\infty} \mathbb{E}m(x; \beta, J, h, N)}$$

Singular Limits

Michael Berry

Biting into an apple and finding a maggot is unpleasant enough, but finding half a maggot is worse. Discovering one-third of a maggot would be more distressing still: The less you find, the more you might have eaten. Extrapolating to the limit, an encounter with no maggot at all should be the ultimate bad-apple experience. This remorseless logic fails, however, because the limit is singular: A very small maggot fraction ($f \ll 1$) is qualitatively different from no maggot ($f = 0$). Limits in physics can be singular too—indeed they usually are—reflecting deep aspects of our scientific description of the world.

In physics, limits abound and are fundamental in the passage between descriptions of nature at different levels. The classical world is the limit of the quantum world when Planck's constant h is inappreciable; geometrical optics is the limit of wave optics when the wavelength λ is insignificant; thermodynamics is the limit of statistical mechanics when the number of particles N is so large that $1/N$ is negligible; mechanics of a slippery fluid is the limit of mechanics of a viscous fluid when the inverse Reynolds number $1/R$ can be disregarded. These limits have a common feature: They are all singular—they must be, because the theories they connect involve concepts that are qualitatively very different. As I explain here, there are both reassuring and creative aspects to singular limits. And by regarding them as a general feature of physical science, we get insight into two related philosophical problems: how a more general theory can reduce to a less general theory and how higher-level phenomena can emerge from lower-level ones.

The coherence of our physical worldview requires the reassurance that, singularities notwithstanding, quantum mechanics does reduce to classical mechanics, statistical mechanics does reduce to thermodynamics, and so on, in the appropriate limits. We know that when calculating the orbit of a spacecraft (and indeed knowing that it has an orbit) we can safely use classical mechanics, rather than having to solve the Schrödinger equation. An engineer designing a bridge can rely on continuum elasticity theory, without needing to know the atomic arrangements underlying the equation of state of the materials used in the construction. However, getting these reassurances from fundamental theory can involve subtle and unexpected concepts.

Perhaps the simplest example is two flashlights shining on a wall. Their combined light is twice as bright as when each shines separately: This is the optical embodiment of the equation $1 + 1 = 2$. But we learned from Thomas Young almost exactly two centuries ago that this mathematics does not describe the intensity of superposed light beams: To account for wave interference, *amplitudes* must be added, and the sum then squared to give the intensity. This involves the phases of the two waves, $\pm\phi$ say, and gives the intensity as $|\exp(i\phi) + \exp(-i\phi)|^2 = 2 + 2\cos 2\phi$, which can take any value between 0 and 4. So, what becomes of $1 + 1 = 2$? Young himself, responding to a critic who claimed that the wall should be covered with interference fringes, agreed, but pointed out that "the fringes will demonstrably be invisible . . . a hundred . . . would not cover the point of a needle." Underlying this explanation is a singular limit: The unwanted $\cos 2\phi$ does not vanish but oscillates rapidly. If the beams make an angle θ, the fringe spacing is $\lambda/2\theta$, vanishing in the geometrical limit of small λ. The limit is singular because the cosine oscillates infinitely fast as λ vanishes. Mathematically, this is an essential singularity of a type dismissed as pathological to students learning mathematics, yet here it appears naturally in the geometrical limit of the simplest wave pattern.

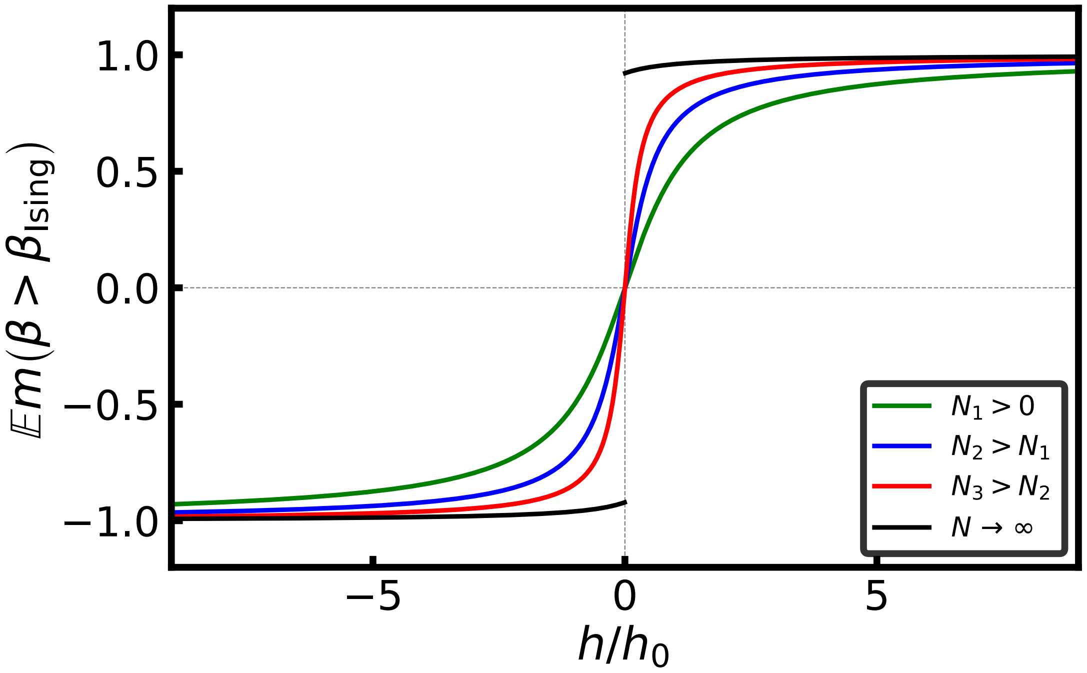
Young's "demonstrable" invisibility requires an additional concept, later made precise by Augustin Jean Fresnel and Lord Rayleigh: The rapidly varying $\cos 2\phi$ must be replaced by its average value, namely zero, reflecting the finite resolution of the detectors, the fact that the light beam is not monochromatic, and the rapid phase variations in the uncoordinated light from the two flashlights. Only then does $1 + 1 = 2$ apply—a relation thus reinterpreted as a singular limit.

Nowadays this application of the idea that the average of a cosine is zero, elaborated and reincarnated, is called decoherence. This might seem a bombastic redescription of the commonplace, but the applications of decoherence are far from trivial. Decoherence quantifies the uncontrolled extraneous influences that could upset the delicate superpositions in quantum computers. And, as we have learned from the work of Wojciech Zurek and others, the same concept governs the emergence of the classical from the quantum world in situations more sophisticated than Young's, where chaos is involved. For example, the chaotic tumbling of Saturn's satellite Hyperion, regarded as a quantum rotator with about 10^{60} quanta of angular momentum, would, according to an unpublished calculation by Ronald Fox, be suppressed in a few decades by the discrete nature of the energy spectrum. However, nobody expects to witness this suppression, because Hyperion is not isolated: Just one photon arriving from the Sun (whose reemission enables our observations) destroys the coherence responsible for quantization in a time of the order of 10^{-50} seconds, and reinstates classicality.[1] Alternatively stated, decoherence suppresses the quantum suppression of chaos.

Other reassurances are equally hard to come by. For example, for-

MICHAEL BERRY (*http://www.phy.bris.ac.uk/uk/staff/berry_mv.html*) *is Royal Society Research Professor in the physics department of Bristol University, in the UK.*

Thermodynamic limit is singular as swapping limits in equation returns zero



$$\boldsymbol{m_0(\beta, J) := \lim_{h\downarrow 0}\lim_{N\to\infty} \mathbb{E}m(x; \beta, J, h, N)}$$

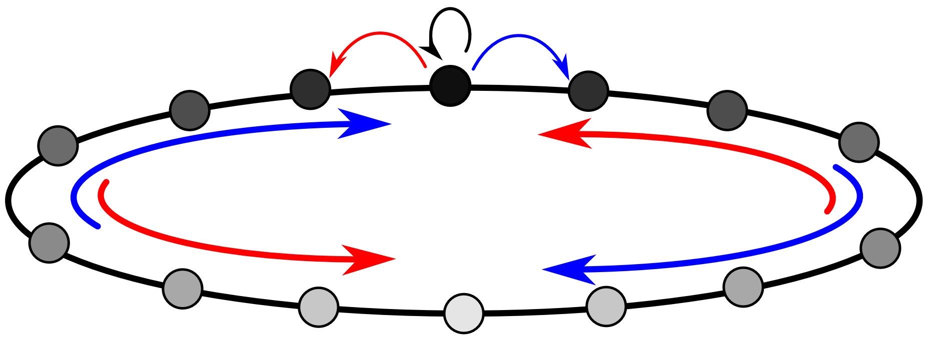
Berry, *Physics Today 55*, 10 (2002)

Translational symmetry

- ECMC potentials: symmetric to simultaneous translation of both particles;
- $U(x_i, x_j) = f(x)$;
- $x := (x_i - x_j + L / 2) \bmod (L) - L / 2$ is shortest separation with PBCs.

1D, two-particle model

Time-driven, reversible algorithm



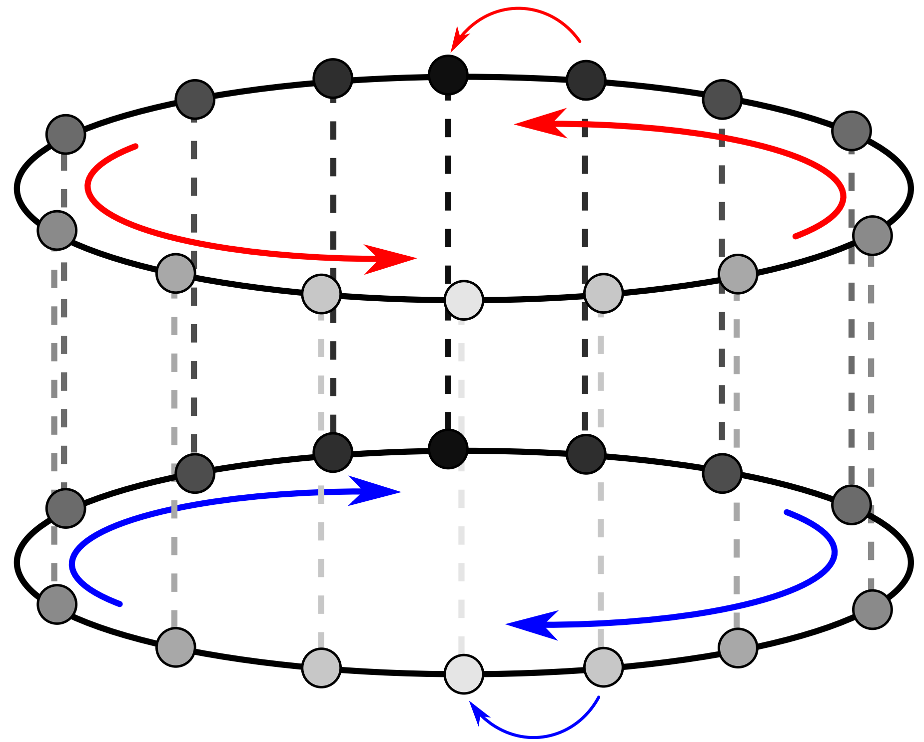
Red / blue: +ve / -ve *x* evolution

Fig.: Michel, PhD thesis, ENS Paris (2015)

Lifted Markov process

- Can explore x via positive particle motion;
- Active particles augment the configuration space: $x \rightarrow (x, \xi = \pm 1)$;
- Lifting variable $\xi = \pm 1$ describes two copies of the original config. space (x);
- $\pi(x, \xi = 1) = \frac{1}{2}\pi(x) = \pi(x, \xi = -1)$;
- <u>Red:</u> particle i active ➔ $\xi = +1$; system on positive copy of config. space;
- <u>Blue:</u> particle j active ➔ $\xi = -1$; system on negative copy of config. space;

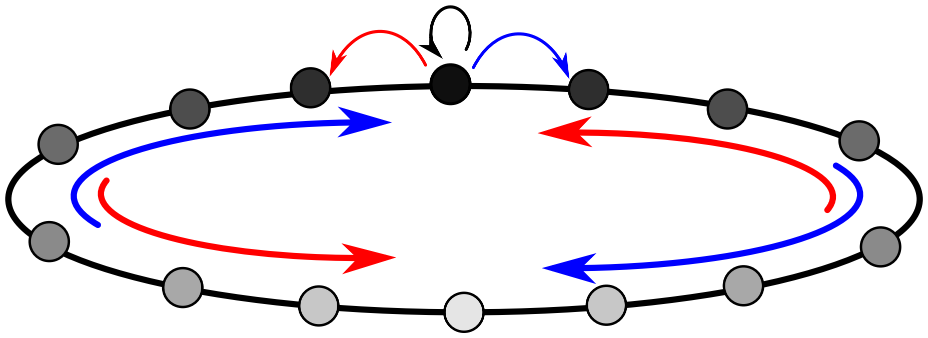
Two copies of space



Red / blue: +ve / -ve x evolution

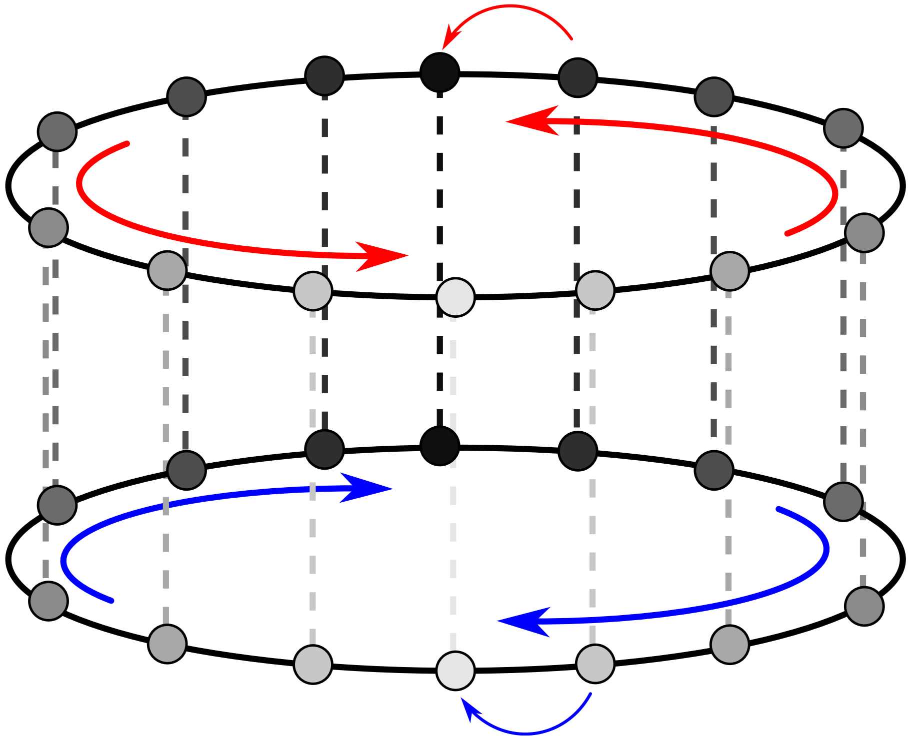
Fig.: Michel, PhD thesis, ENS Paris (2015)

Reversible process



Detailed balance ➔ π-invariant

Nonreversible process

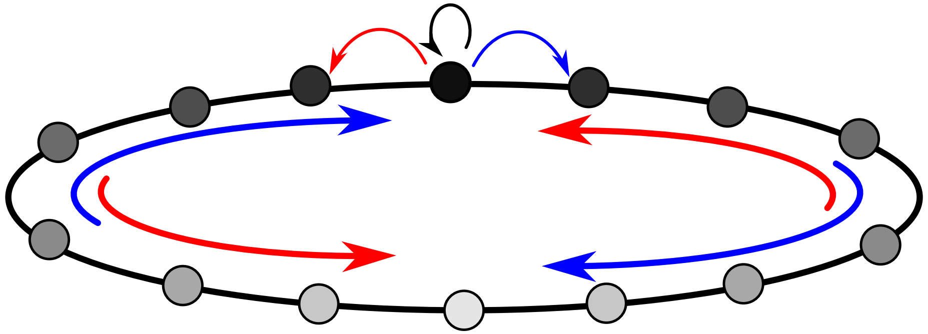


π-invariant?

Figs: Michel, PhD thesis, ENS Paris (2015)

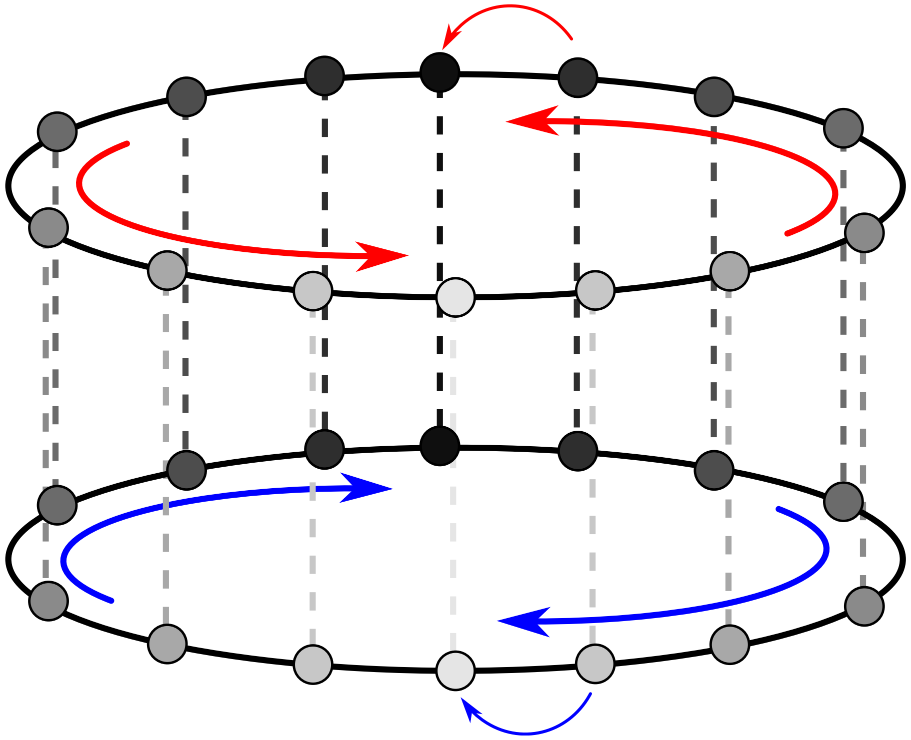
Faulkner & Livingstone, in preparation

At x: $p(x \rightarrow x \pm 1) = \min\{1, \pi(x \pm 1) / \pi(x)\}$



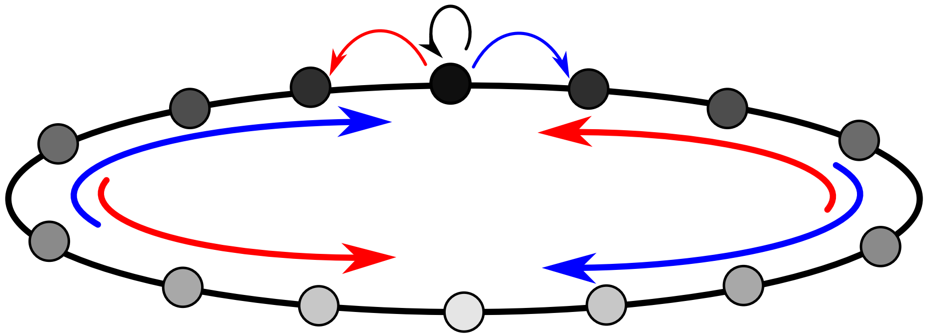
$$\pi(x)p(x \rightarrow x + 1) = \pi(x + 1)p(x + 1 \rightarrow x)$$

At $(x, \xi = \pm 1)$: $p(x \rightarrow x + \xi) = \min\{1, \pi(x + \xi, \xi) / \pi(x, \xi)\}$



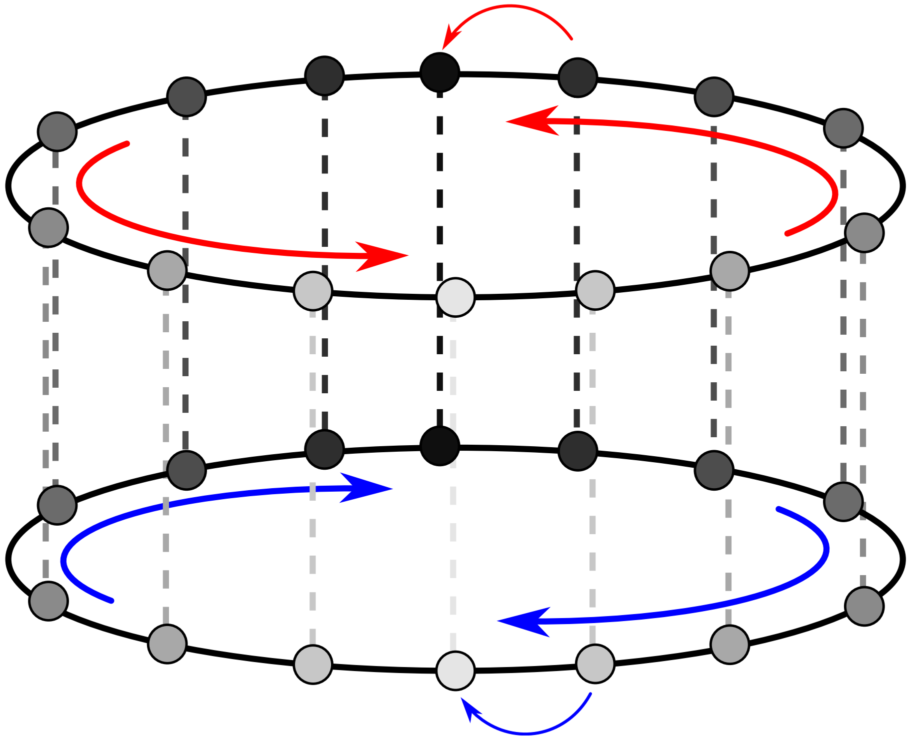
$$\pi(x, \xi = 1)\, p(x \rightarrow x + 1) = \pi(x + 1, \xi = -1)\, p(x + 1 \rightarrow x)$$

Detailed balance



π-invariant

Skew detailed balance



π-invariant

Figs: Michel, PhD thesis, ENS Paris (2015)

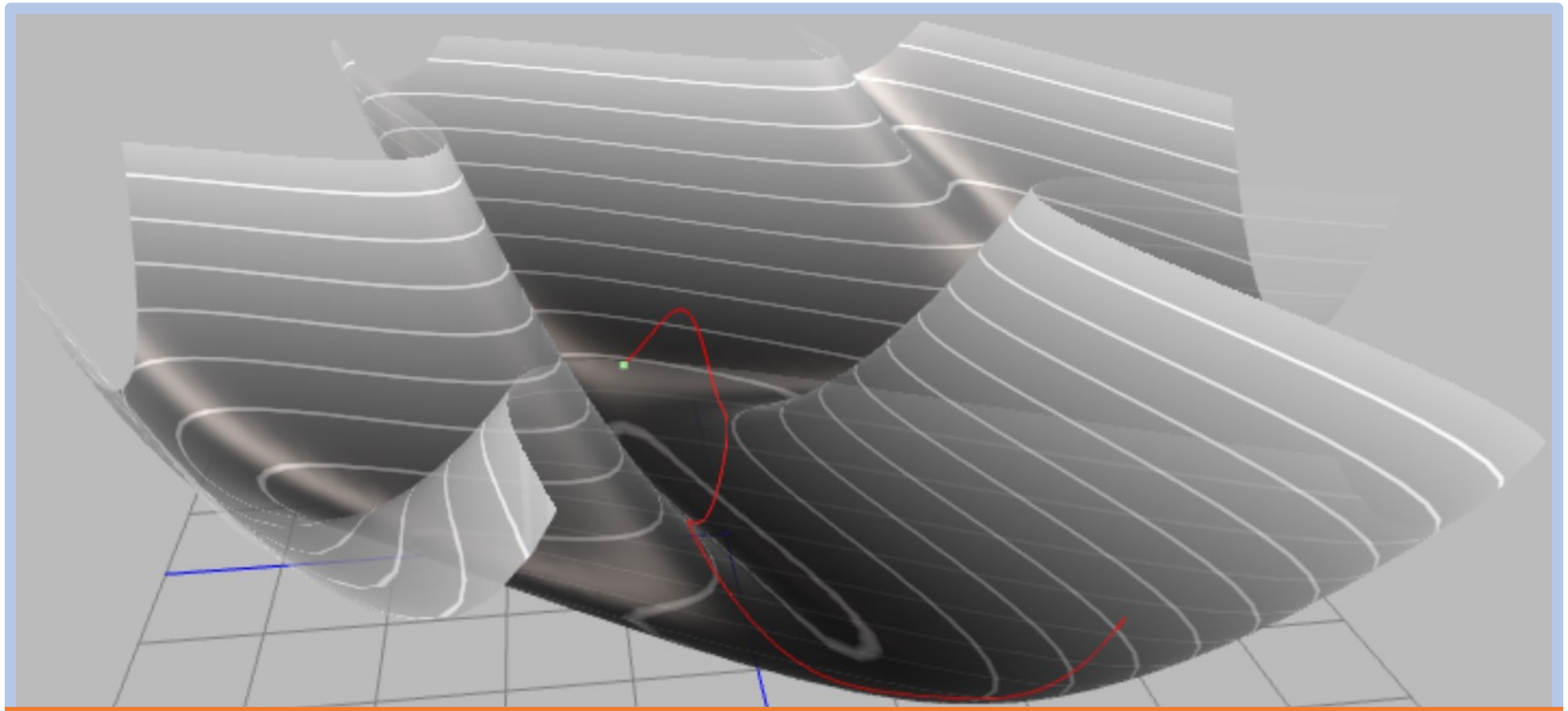
Faulkner & Livingstone, in preparation

Metropolis is very successful

- Easy to implement.
- Converges quickly enough in many settings.
- Recreates physical Brownian dynamics – useful for experiment.

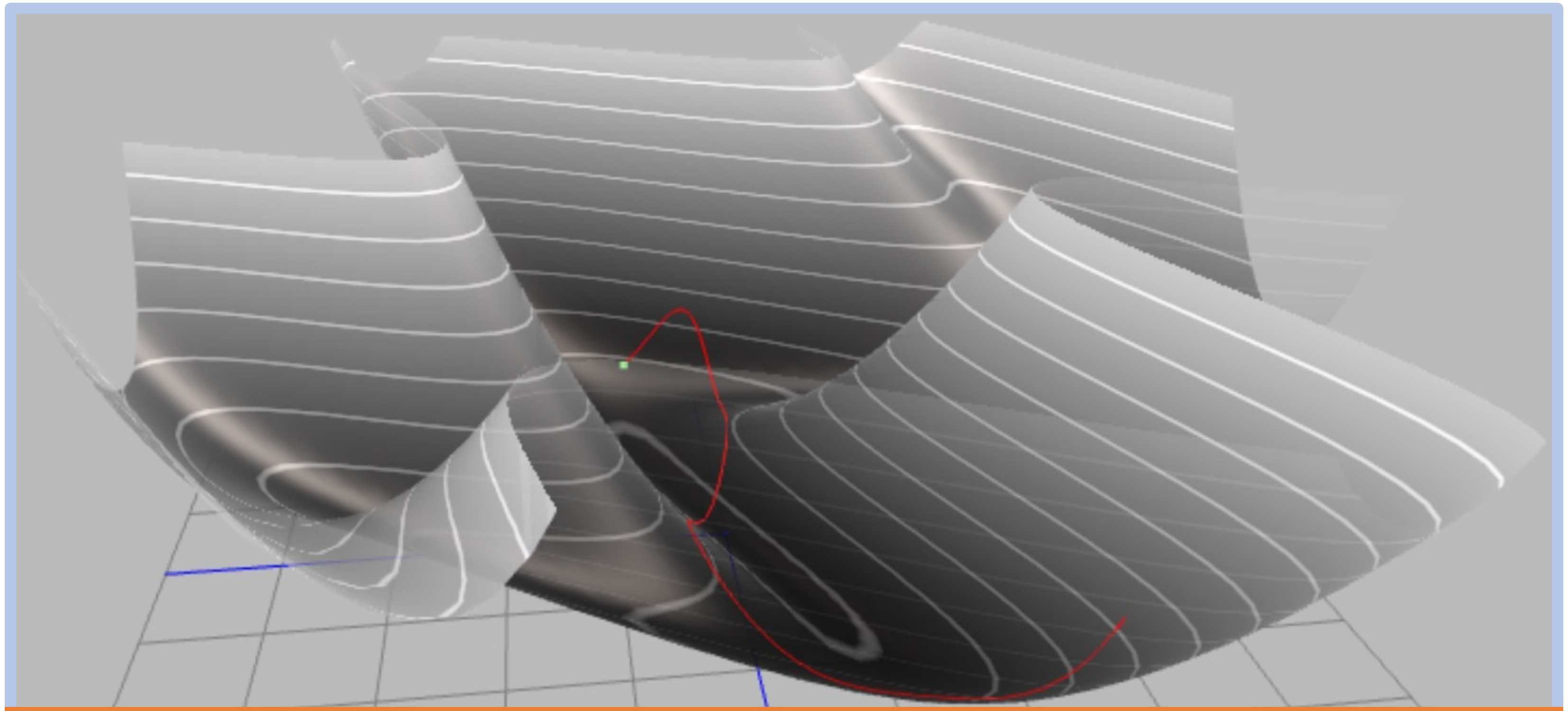
However…

- Convergence slow at high particle density with long-range interactions.
- Suffers from symmetry breaking.
- And critical slowing down – inducing strongly non-convergent estimates.



- Molecular dynamics (MD) follows numerical Newtonian trajectories (eg, red curve on potential landscape)
- It sets random initial particle positions and velocities…
- …then solves $\ddot{x}_i = -\nabla_i U(x)\ \forall i$ at each time step.
- Approximately converges on π w/resampled velocities.

Fig.: arogozhnikov.github.io (2016)



- **MD is typically much more efficient than Metropolis…**
- **…and captures physical Newtonian dynamics.**
- **<u>BUT</u> it's unstable – especially at high particle density with long-range interactions…**
- **…and it also suffers from energy drifts.**

Fig.: arogozhnikov.github.io (2016)