Dynamical behaviour of Brownian particles coupled to a critical field

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LIPh Winter Workshop 2023 - 21 February 2023

References

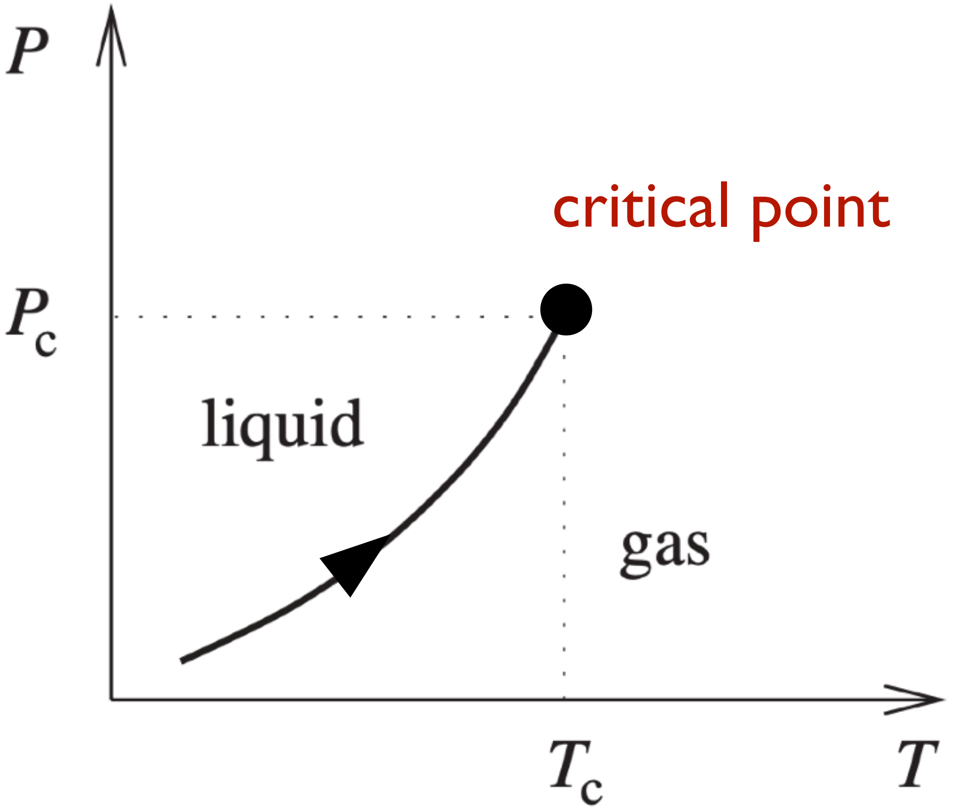
- D. Venturelli, F. Ferraro, A. Gambassi
  Nonequilibrium relaxation of a trapped particle in a near-critical Gaussian field
  Physical Review E 105 (5), 054125 (2022)

- U. Basu, V. Démery, A. Gambassi
  Dynamics of a colloidal particle coupled to a Gaussian field: from a confinement-dependent to a non-linear memory
  SciPost Physics 13 (4), 078 (2022)

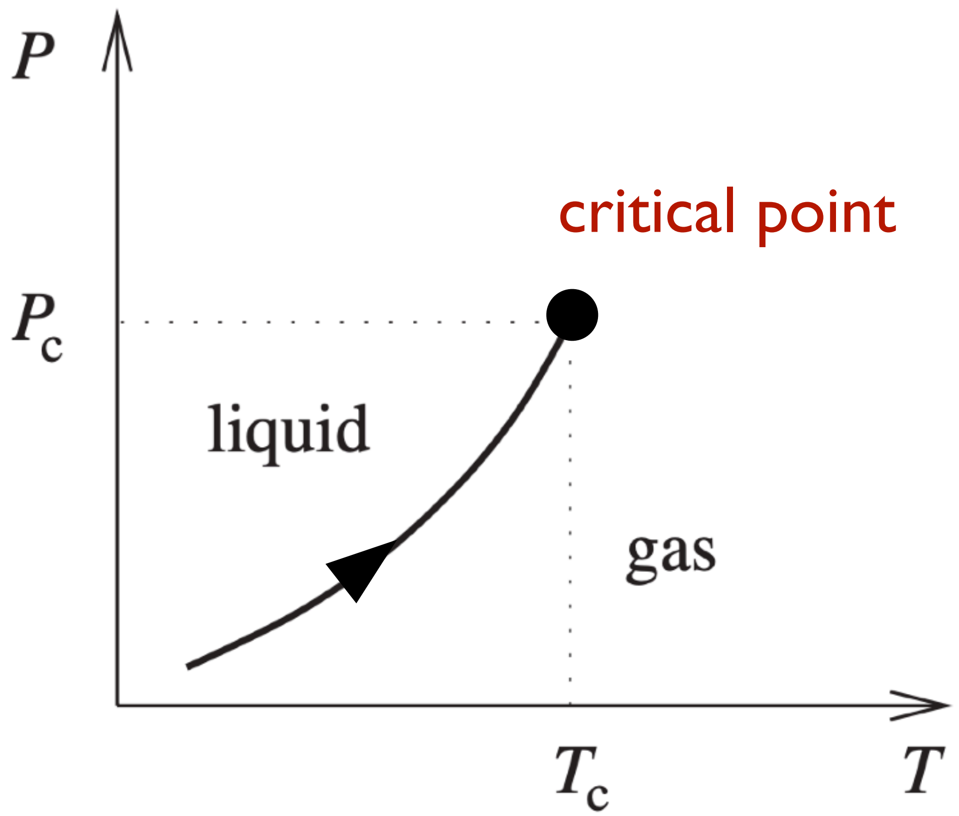
- D. Venturelli, A. Gambassi
  Inducing oscillations of trapped particles in a near-critical Gaussian field
  Physical Review E 106 (4), 044112 (2022)

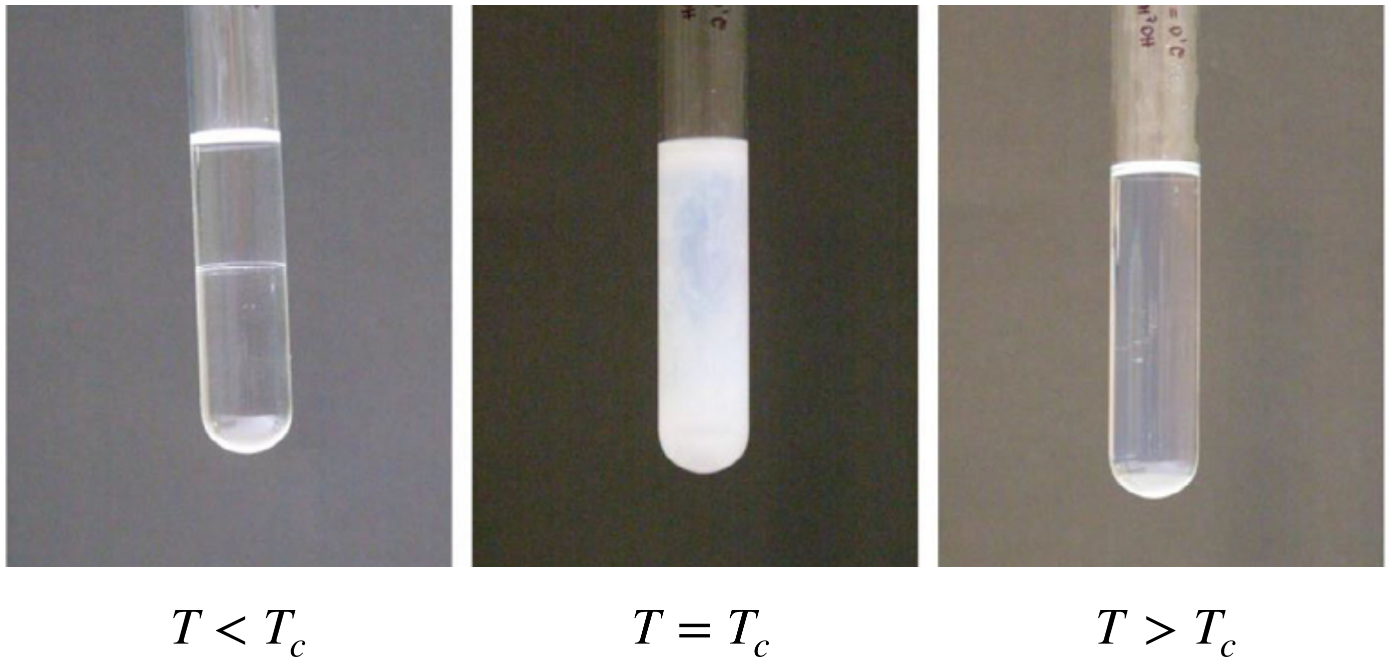
- D. Venturelli, M. Gross,
  Tracer particle in a confined correlated medium: an adiabatic elimination method
  Journal of Statistical Mechanics: Theory and Experiment (12), 123210, (2022)

Phases of matter and critical points



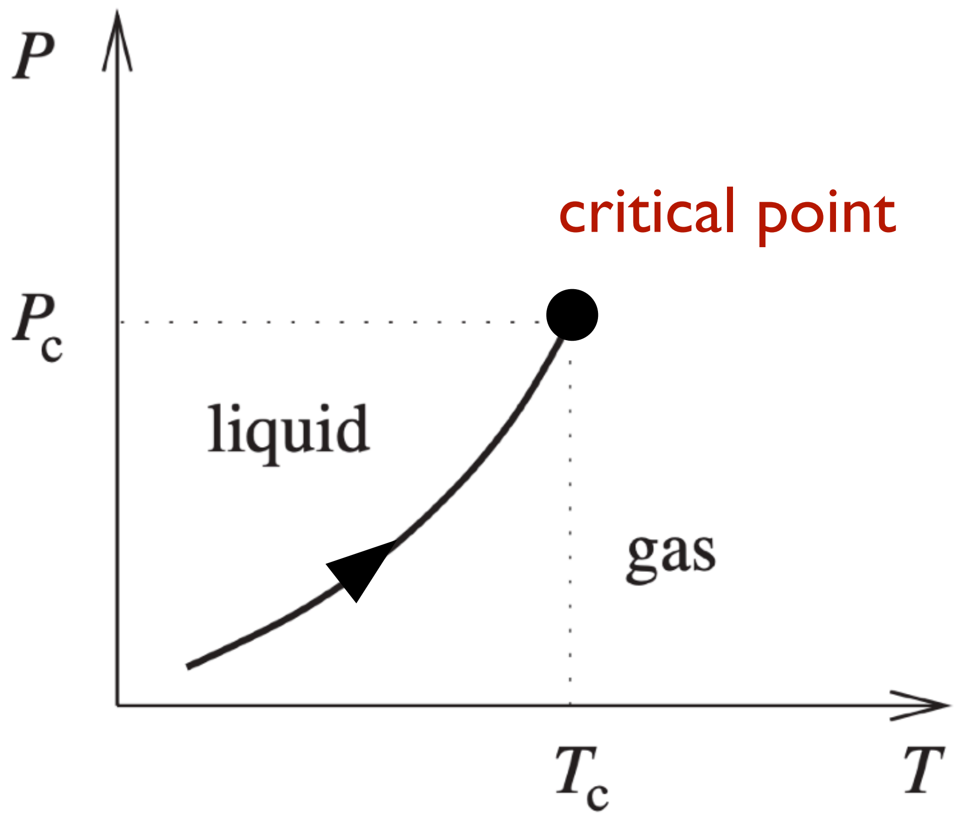
Phases of matter and critical points

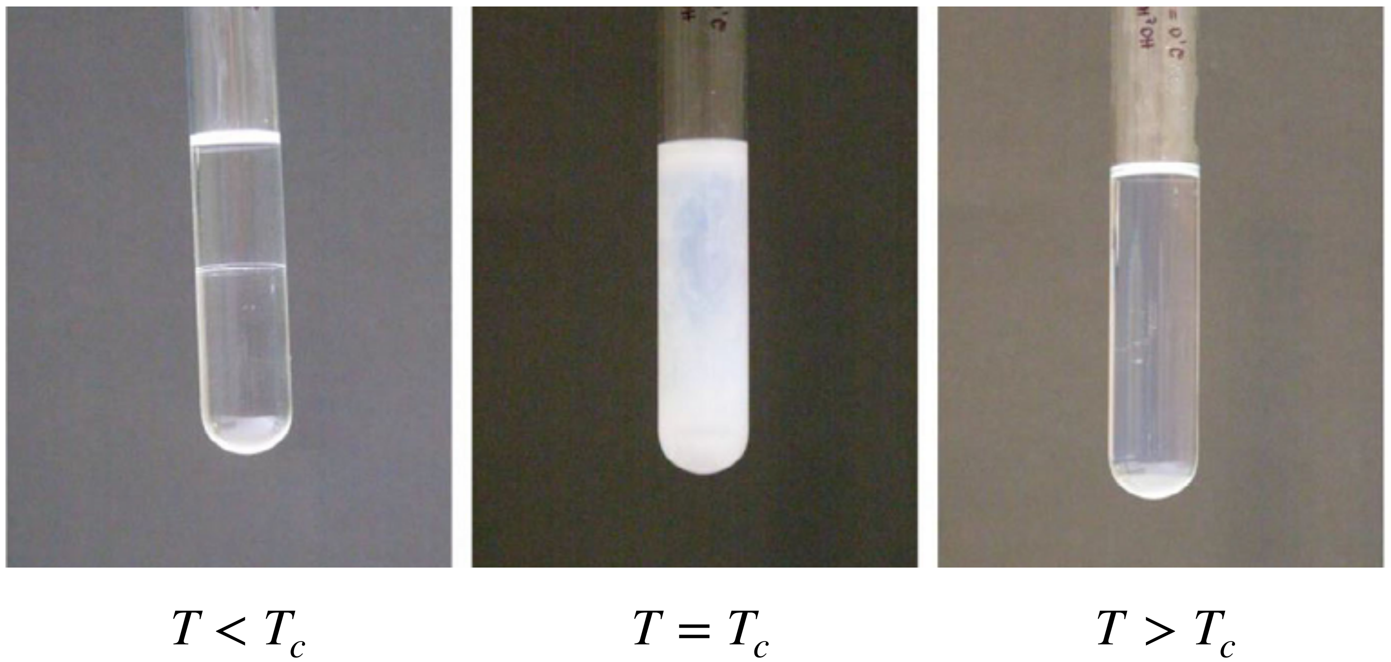




characteristic length: $\xi \sim (T - T_c)^{-\nu}$

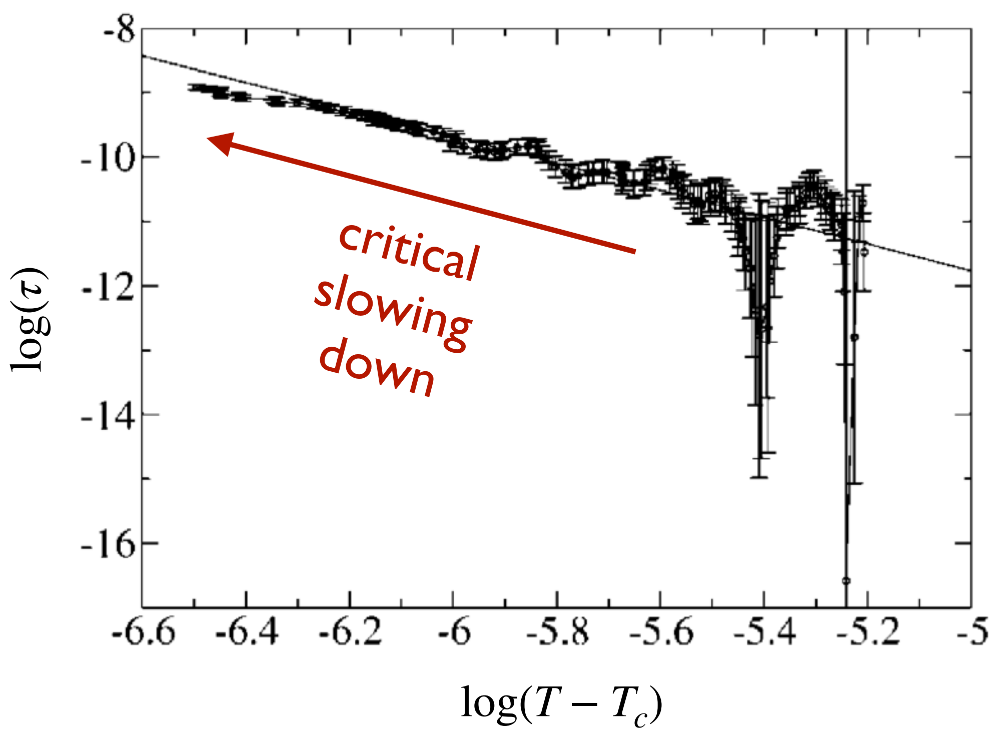
Phases of matter and critical points





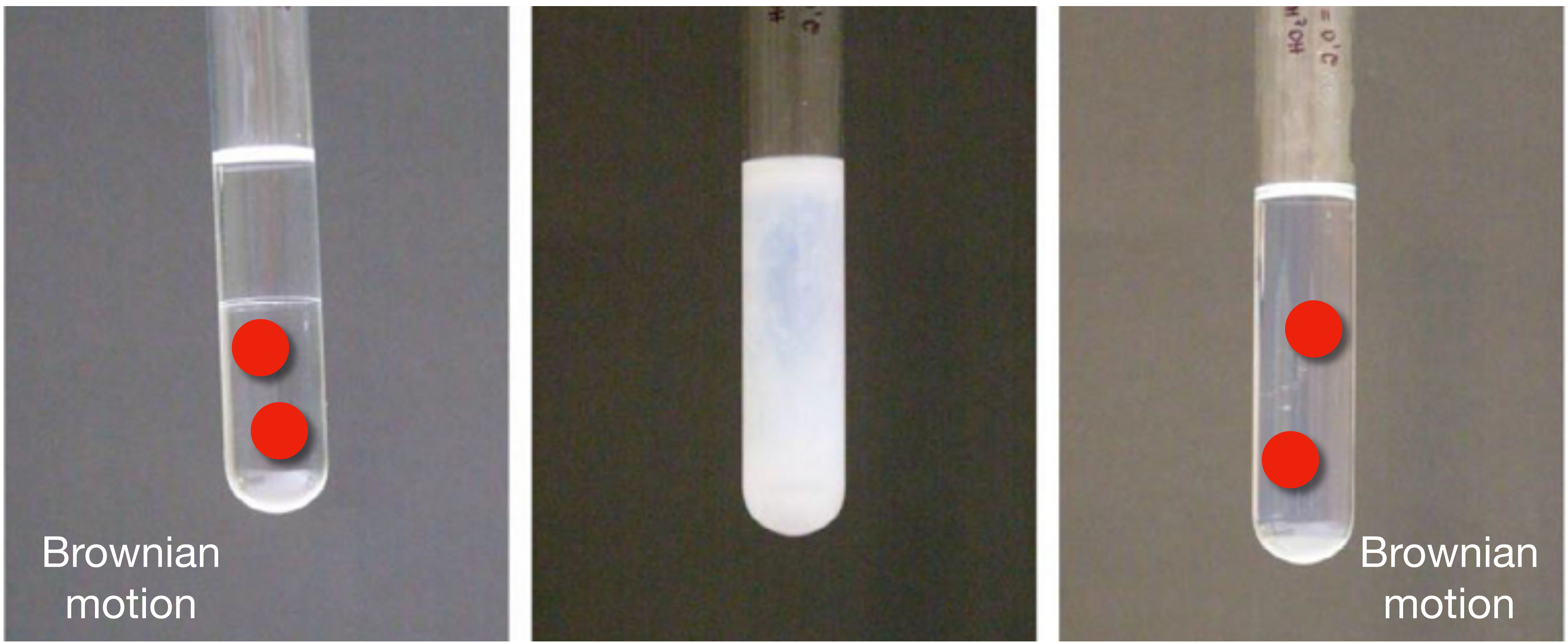
characteristic length: $\xi \sim (T - T_c)^{-\nu}$

characteristic time: $\tau \sim \xi^z$



Phases of matter and critical points

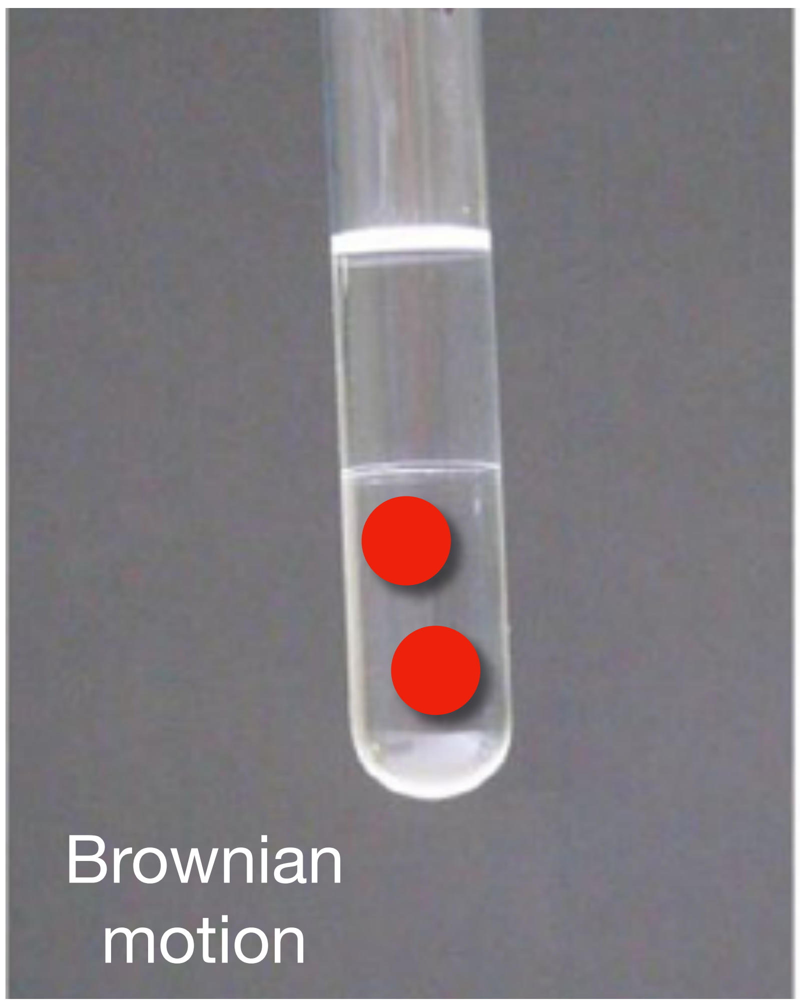
What happens to the dynamics of mesoscopic particles in a critical fluid?



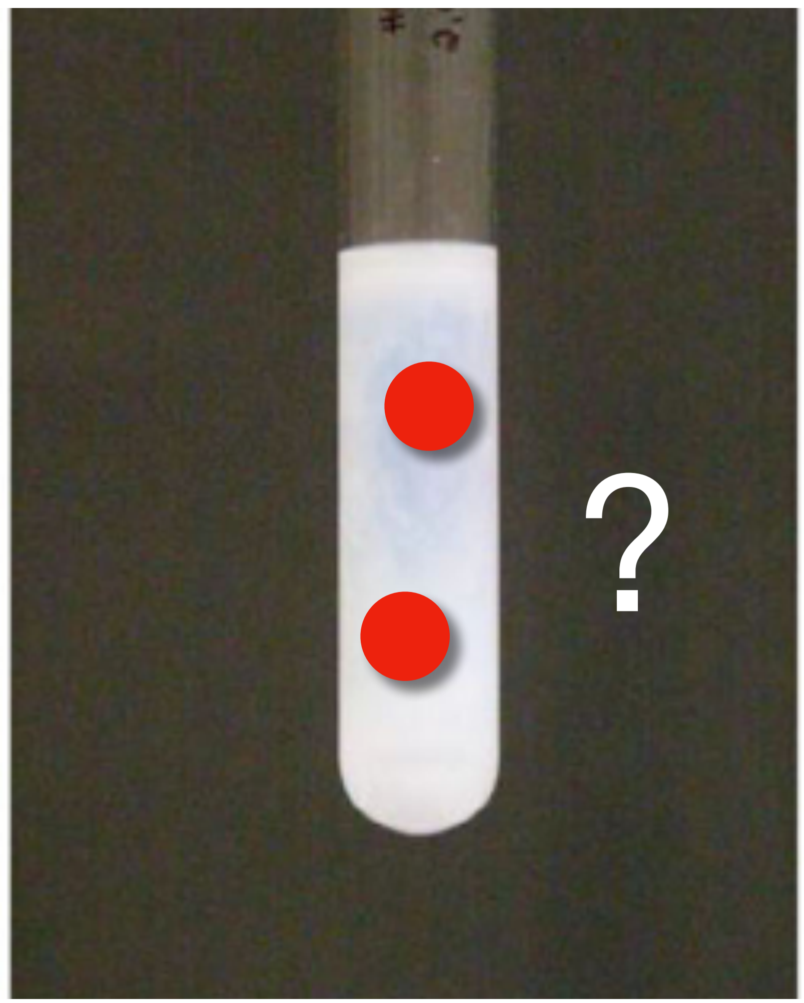
$T < T_c$ $T = T_c$ $T > T_c$

Phases of matter and critical points

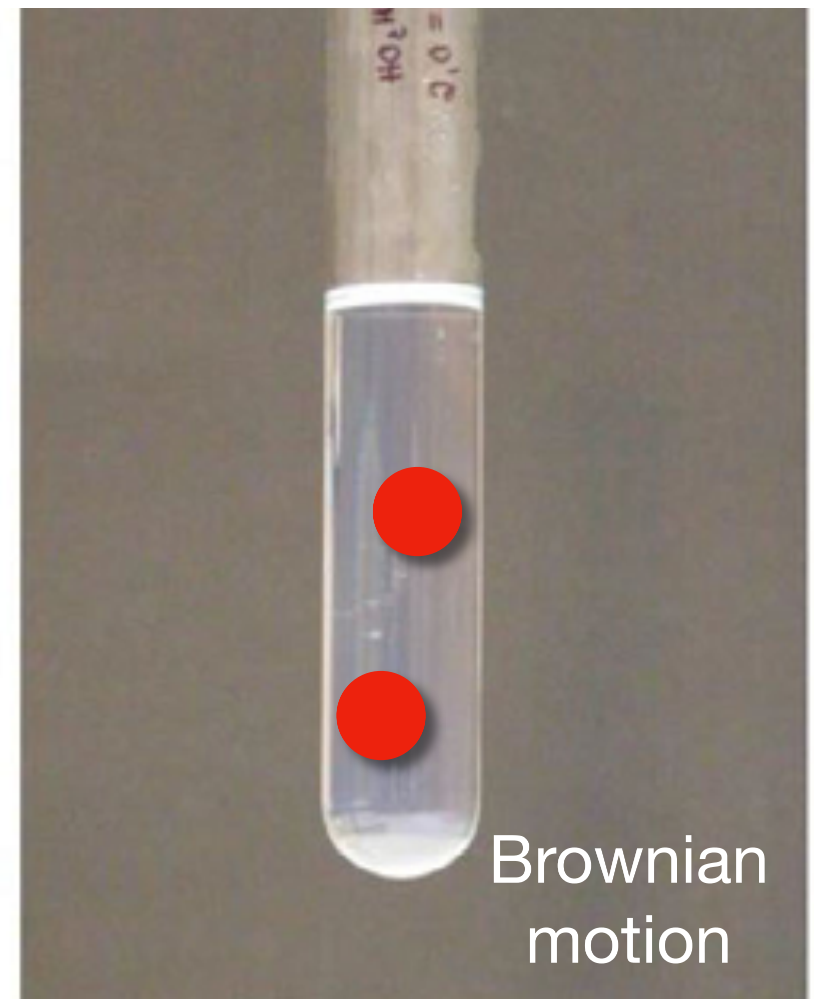
What happens to the dynamics of mesoscopic particles in a critical fluid?



$T < T_c$



$T = T_c$



$T > T_c$

Modeling of a colloid

- Motion in a thermal bath

$$\dot{X} = -\nu \frac{\partial H}{\partial X} + \xi(t)$$

external potential

stochastic forcing due to collisions with fluid molecules

Modeling of a colloid

- Motion in a thermal bath

$$\dot{X} = -\nu \frac{\partial H}{\partial X} + \xi(t)$$

- In a harmonic trap $H = kx^2/2$

$$\tau_X = \frac{1}{\nu k}$$

$$\langle X(t) \rangle = X(0) \ \exp\left(-\frac{t}{\tau_X}\right)$$

$$\langle X(t)X(t') \rangle = \frac{T}{k} \exp\left(-\frac{|t-t'|}{\tau_X}\right)$$

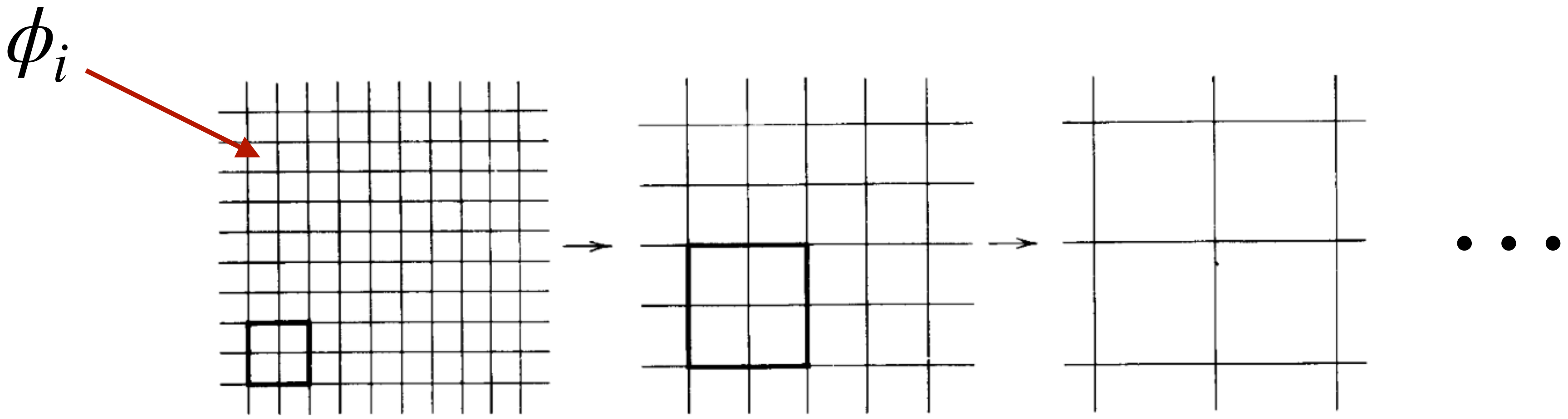
$$\ldots$$

Modeling of critical media

- Exploit scale invariance near critical point

Modeling of critical media

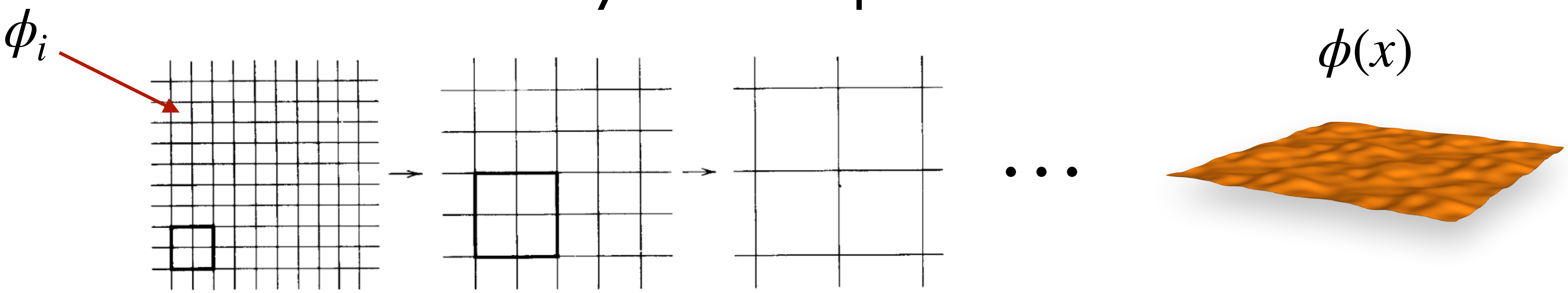
- Exploit scale invariance near critical point
  ⇨ coarse-grain



$$H[\{\phi_i\}] = \sum_{\langle ij \rangle} \phi_i \phi_j + \ldots$$

Modeling of critical media

- Exploit scale invariance near critical point
  - ⇨ coarse-grain
  - ⇨ obtain field theory of order parameter



$$H[\{\phi_i\}] = \sum_{\langle ij \rangle} \phi_i \phi_j + \dots$$

$$H[\phi] = \int d^d x \left[\frac{1}{2}(\nabla \phi)^2 + \frac{1}{2} r \phi^2 + \frac{1}{4!} u \phi^4 + \dots \right]$$

Modeling of critical media

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  - ➯ coarse-grain
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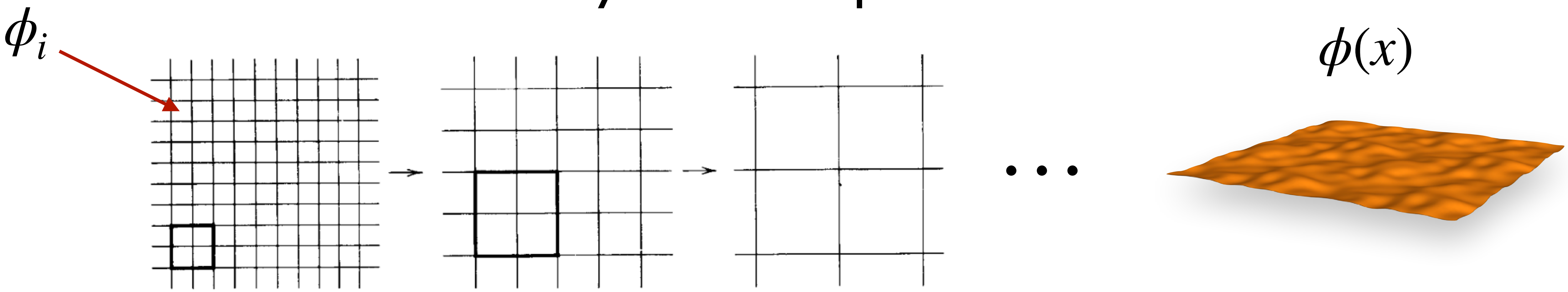

$$H[\{\phi_i\}] = \sum_{\langle ij \rangle} \phi_i \phi_j + \dots$$

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- ➯ $\phi(x)$ evolves slower than microscopic d.o.f.

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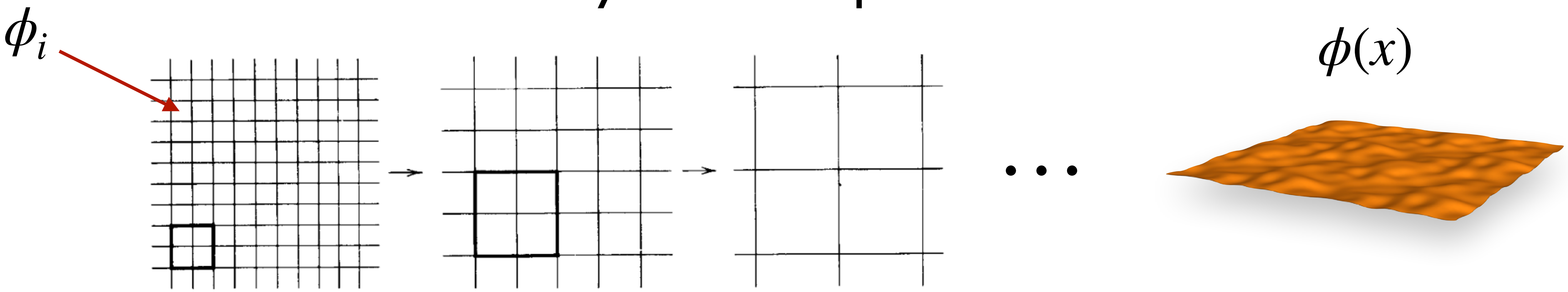

$$H[\{\phi_i\}] = \sum_{\langle ij \rangle} \phi_i \phi_j + \dots$$

$$H[\phi] = \int d^d x \left[\frac{1}{2}(\nabla \phi)^2 + \frac{1}{2} r \phi^2 + \frac{1}{4!} u \phi^4 + \dots \right]$$

- ➩ $\phi(x)$ evolves slower than microscopic d.o.f.
- ➩ any* dynamics collapses to

$$\partial_t \phi(x) = -D \frac{\delta H}{\delta \phi(x)} + \zeta(x,t)$$

relaxation to eq.

stochastic forcing

Modeling of critical media

- …any dynamics up to conservation laws

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- No conservation laws

$$\partial_t \phi(x) = -D \frac{\delta H}{\delta \phi(x)} + \zeta(x, t)$$

Modeling of critical media

- …any dynamics up to conservation laws
- No conservation laws

$$\partial_t \phi(x) = -D\frac{\delta H}{\delta \phi(x)} + \zeta(x,t)$$

- Conserved field → $\frac{d}{dt}\int d^d x\, \phi(x,t) = 0$

$$\partial_t \phi(x) = D\,\nabla^2 \frac{\delta H}{\delta \phi(x)} + \zeta(x,t)$$

Modeling of critical media

- …any dynamics up to conservation laws
- No conservation laws

Model A

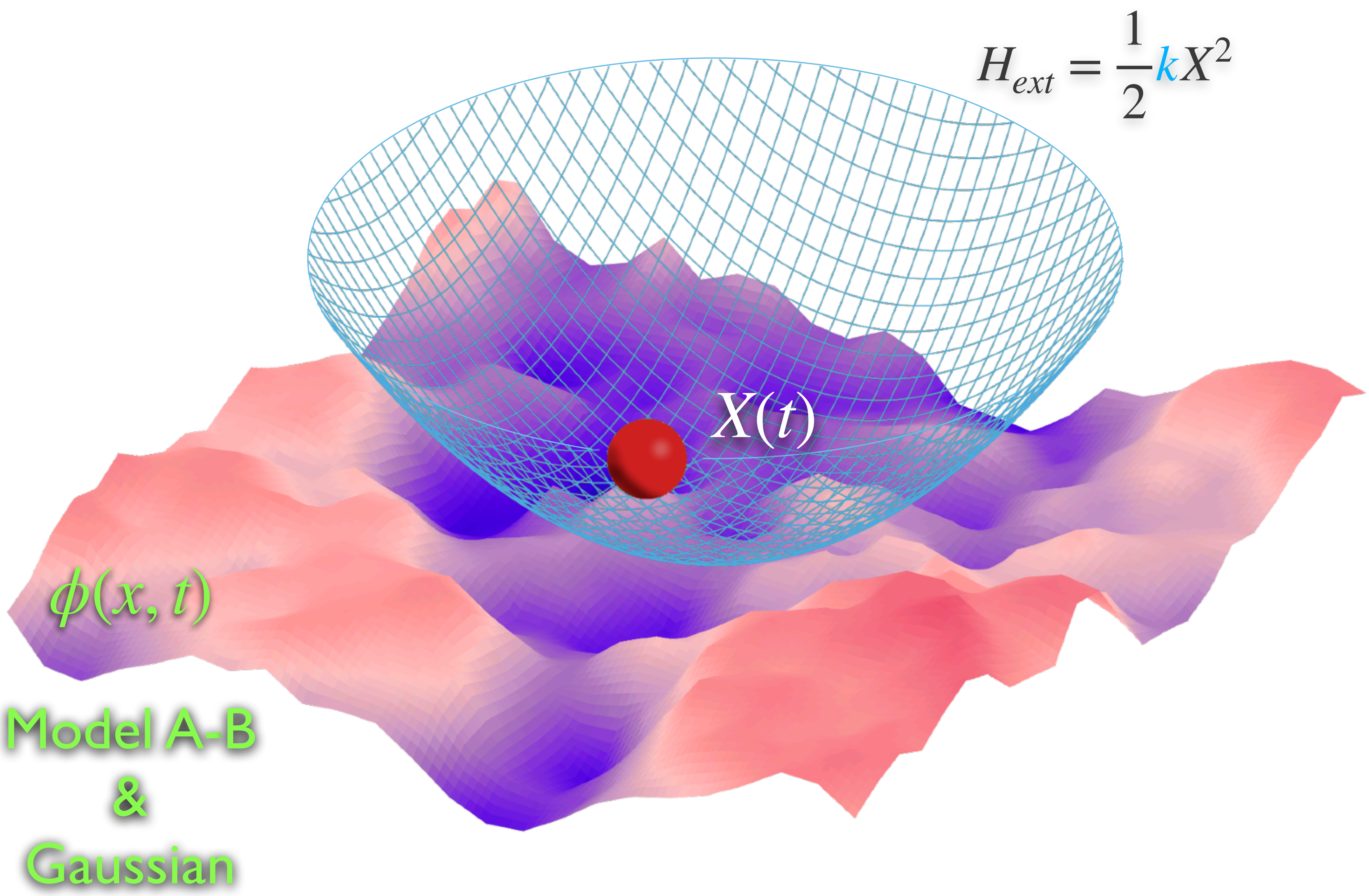
$$\partial_t \phi(x) = -D \frac{\delta H}{\delta \phi(x)} + \zeta(x, t)$$

- Conserved field

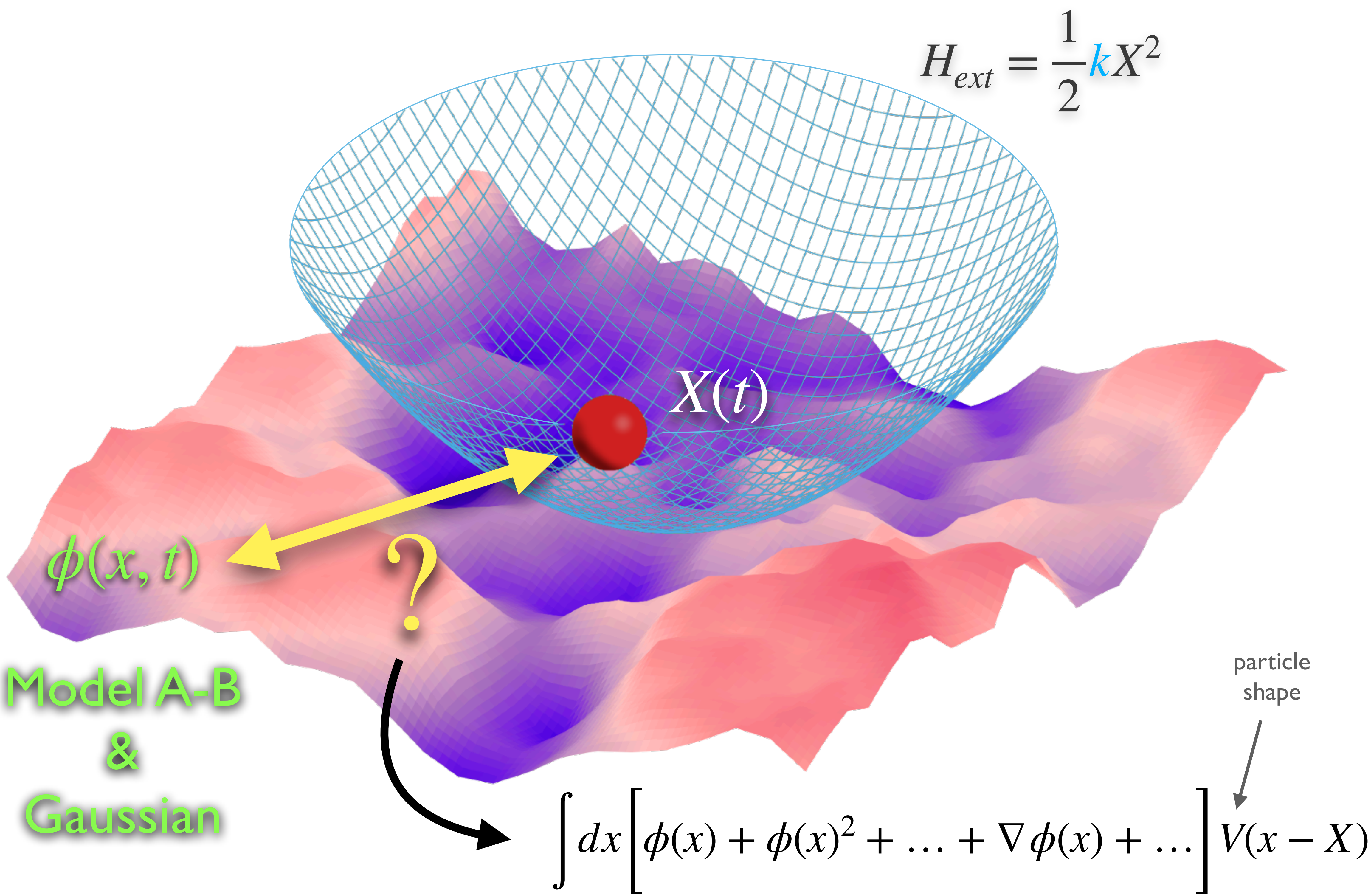
Model B

$$\partial_t \phi(x) = D \nabla^2 \frac{\delta H}{\delta \phi(x)} + \zeta(x, t)$$

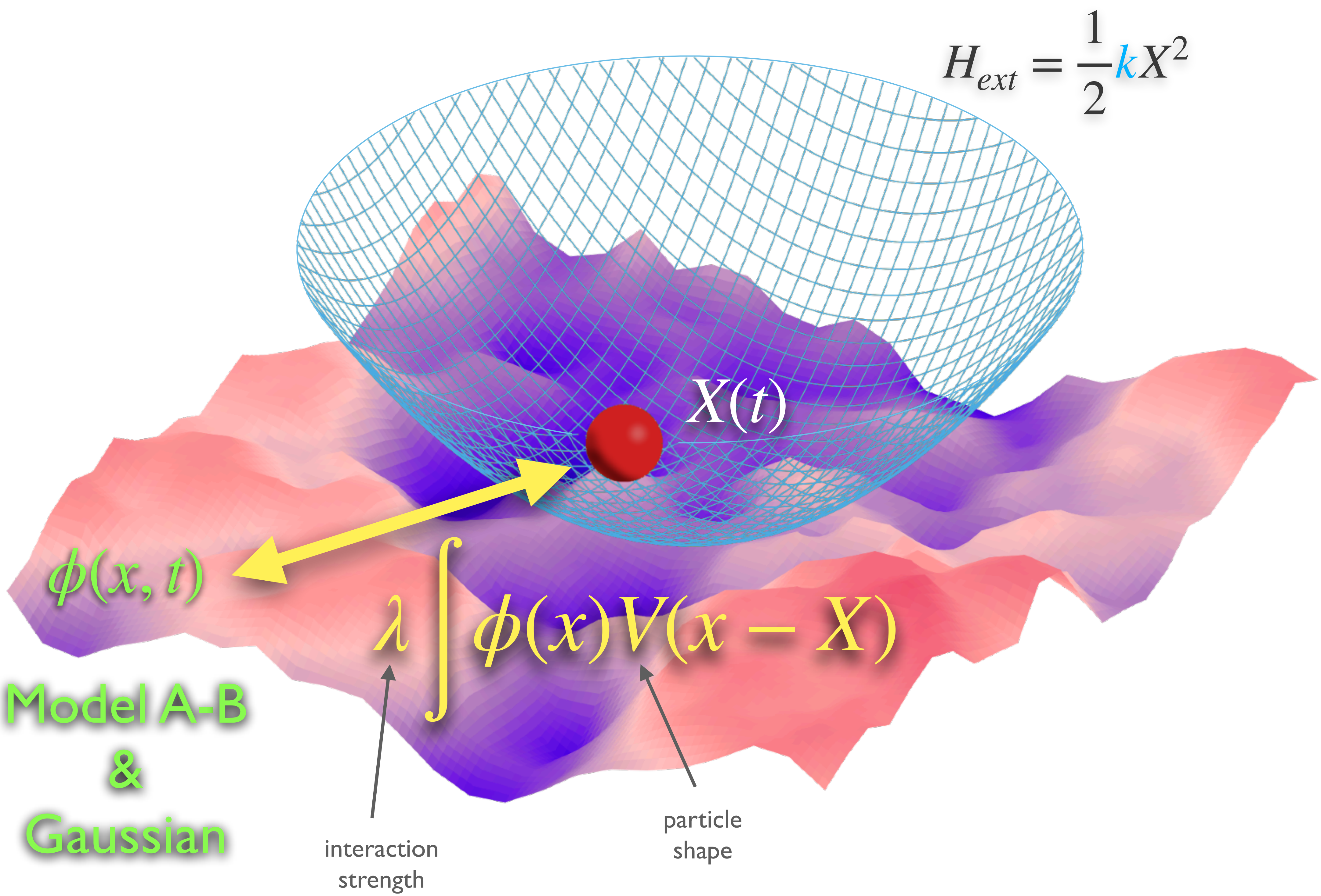
The model



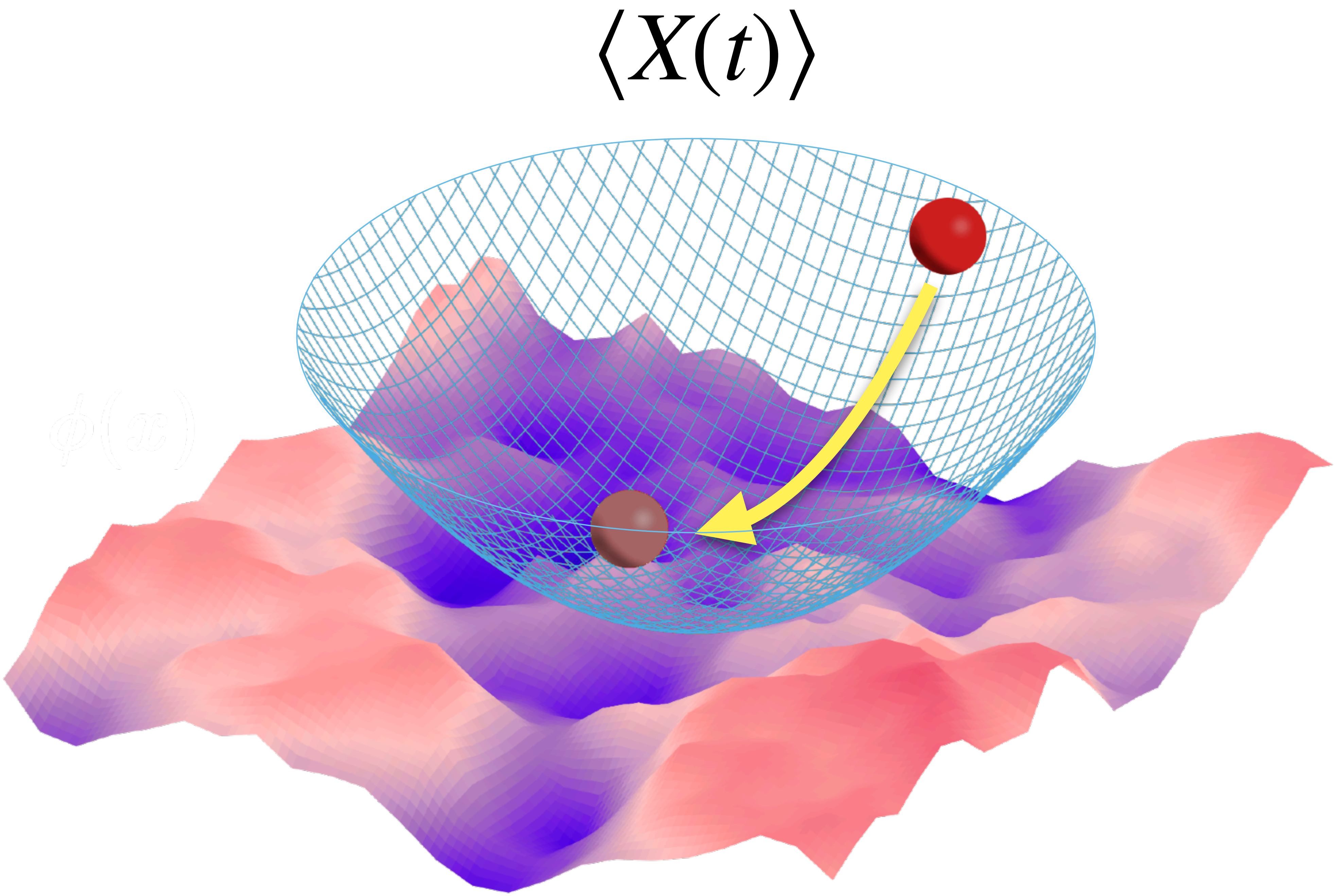
The model: which interaction?



The model: which interaction?



Relaxation to equilibrium: model A



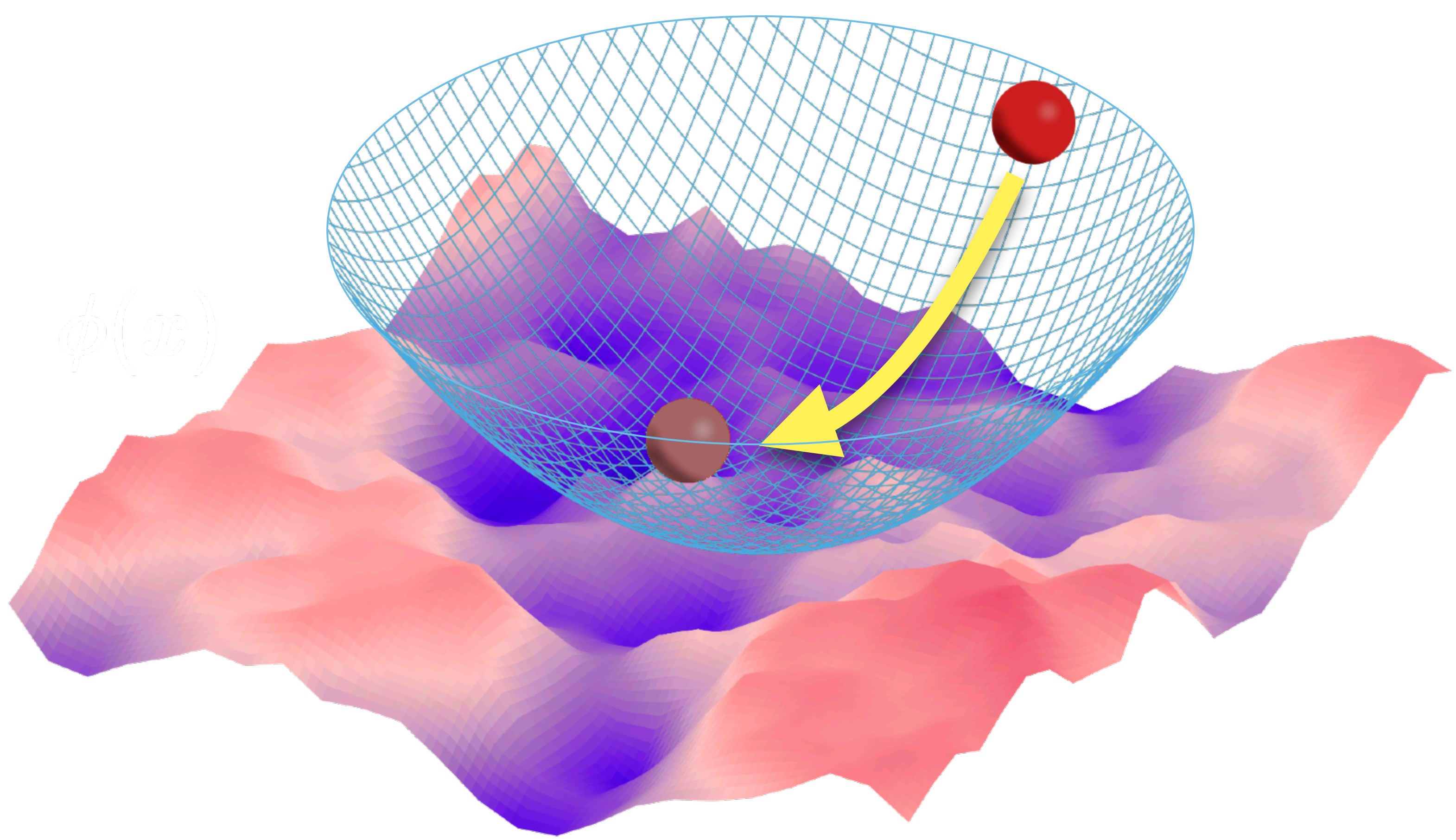
Relaxation to equilibrium: model A

$$\langle X(t) \rangle \sim \lambda^2 \begin{cases} e^{-t/\tau_X} & \tau_X > \tau_\phi \\ & \\ & \end{cases} + o(\lambda^4)$$

with:

$$\tau_x = 1/\nu k$$

$$\tau_\phi = 1/Dr$$



Relaxation to equilibrium: model A

$$\langle X(t) \rangle \sim \lambda^2 \begin{cases} e^{-t/\tau_X} & \tau_X > \tau_\phi \\ e^{-t/\tau_\phi} & \tau_\phi > \tau_X \end{cases} + o(\lambda^4)$$

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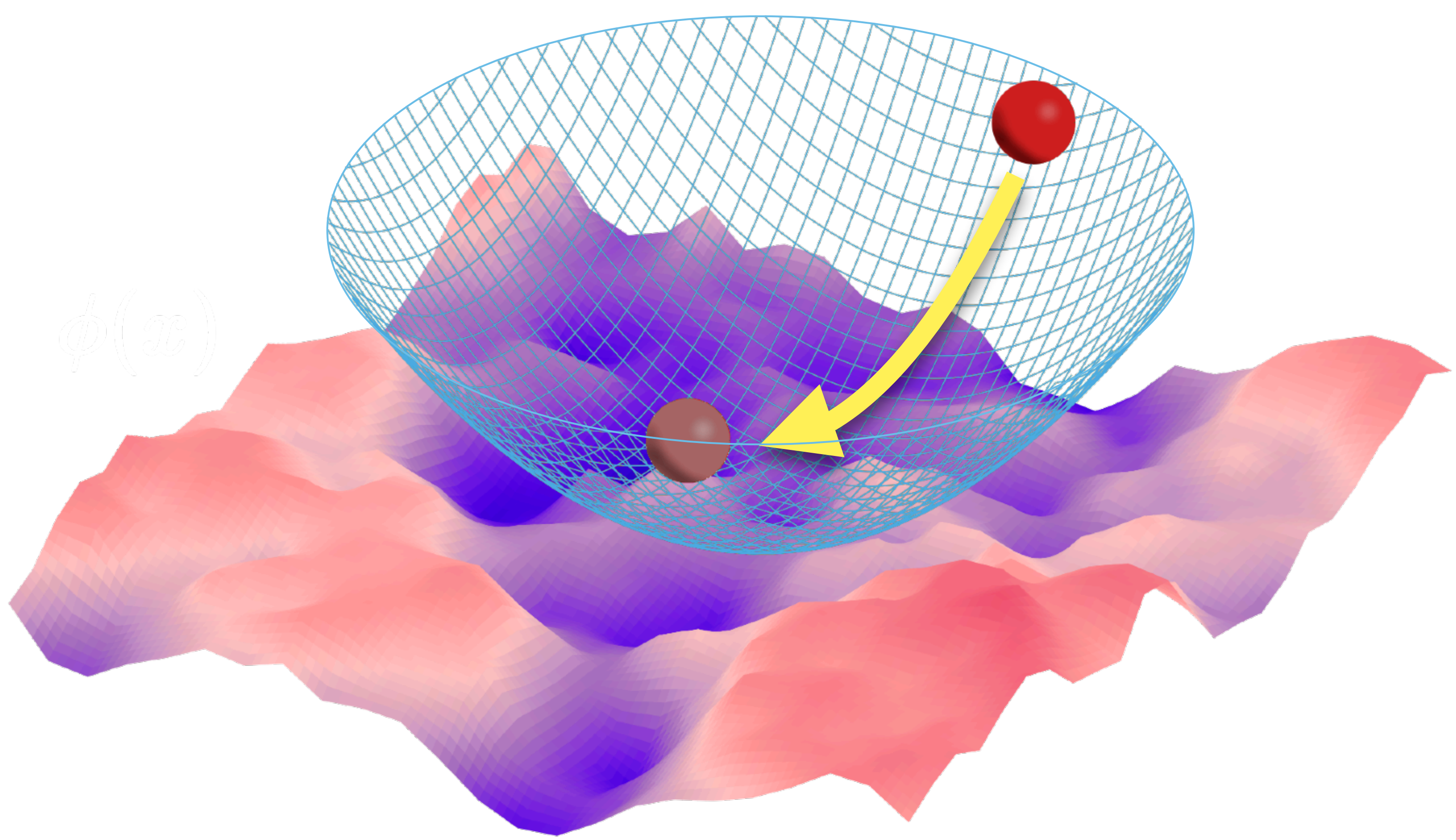


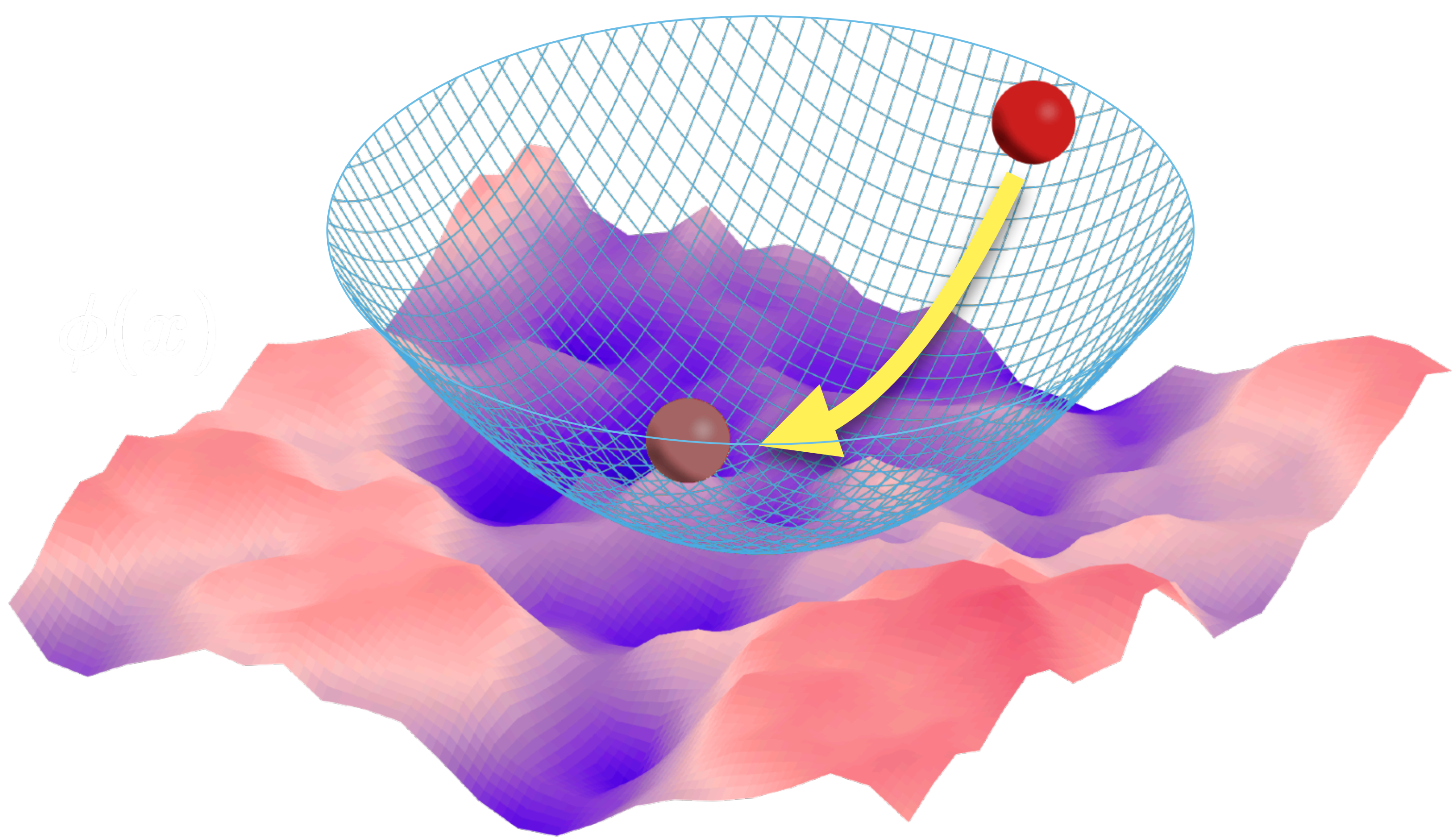
Relaxation to equilibrium: model A

$$\langle X(t) \rangle \sim \lambda^2 \begin{cases} e^{-t/\tau_X} & \tau_X > \tau_\phi \\ e^{-t/\tau_\phi} & \tau_\phi > \tau_X \\ t^{-(d/2+1)} & r = 0 \end{cases} + o(\lambda^4)$$

with:

$$\tau_x = 1/\nu k$$

$$\tau_\phi = 1/Dr$$



Autocorrelation: model A

- Same behaviour as relaxation

$$\langle X(t) \cdot X(0) \rangle \quad \sim \quad \lambda^2 \begin{cases} e^{-t/\tau_X} & \tau_X > \tau_\phi \\ e^{-t/\tau_\phi} & \tau_\phi > \tau_X \\ t^{-d/2} & r = 0 \end{cases}$$

Dynamics in model B conserved field

$$\langle X(t) \rangle \sim \lambda^2 \begin{cases} t^{-(d/2+2)} & r > 0 \\ t^{-(d/4+1)} & r = 0 \end{cases}$$

$$\langle X(t) \cdot X(0) \rangle \sim \lambda^2 \begin{cases} t^{-(d/2+1)} & r > 0 \\ t^{-d/4} & r = 0 \end{cases}$$

Critical behaviour of dynamical quantities

Model A

$$\langle X(t)\rangle \sim \lambda^2 \begin{cases} e^{-t/\tau_x} & \tau_X > \tau_\phi \\ e^{-t/\tau_\phi} & \tau_\phi > \tau_X \\ t^{-(d/2+1)} & r = 0 \end{cases}$$

$$\langle X(t)\cdot X(0)\rangle \sim \lambda^2 \begin{cases} e^{-t/\tau_X} & \tau_X > \tau_\phi \\ e^{-t/\tau_\phi} & \tau_\phi > \tau_X \\ t^{-d/2} & r = 0 \end{cases}$$

Model B

$$\langle X(t)\rangle \sim \lambda^2 \begin{cases} t^{-(d/2+2)} & r > 0 \\ t^{-(d/4+1)} & r = 0 \end{cases}$$

$$\langle X(t)\cdot X(0)\rangle \sim \lambda^2 \begin{cases} t^{-(d/2+1)} & r > 0 \\ t^{-d/4} & r = 0 \end{cases}$$

- Relaxation and correlation behaviour is related
- Relation between particle crit exp and field crit exp?

Non-perturbative fluctuation dissipation relation

- If system is slightly perturbed from equilibrium

$$\dot{X} = \ldots + f(t)$$

then response of an observable

$$\langle O(t) \rangle = \int dt' R(t - t') f(t')$$

is related to its equilibrium correlations as

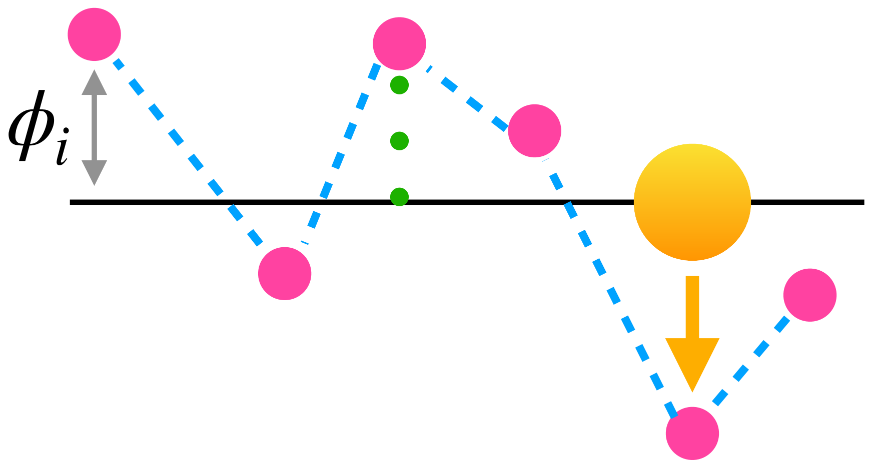
$$R(t) \propto \frac{d}{dt} \langle O(t) O(0) \rangle_{eq}$$

- Setting $X(0) = X_0$ is equivalent to $f(t) = X_0 \delta(t)$
- Taking $O(t) = X(t)$

$$\langle X(t) \rangle \propto \frac{d}{dt} \langle X(t) X(0) \rangle_{eq} \longrightarrow \langle X(t) \rangle \propto t^{-1} \langle X(t) X(0) \rangle_{eq}$$

Simulation algorithm and lattice polymer mapping

- Field: discretized equation



$$\partial_t \phi_i = \frac{D}{\Delta x^2}\left(\phi_{i+1} + \phi_{i-1} - 2\phi_i\right) + \zeta_i \quad - Dr\phi_i \quad + \quad \frac{D\lambda}{\Delta x}\delta_{i,X_t}$$

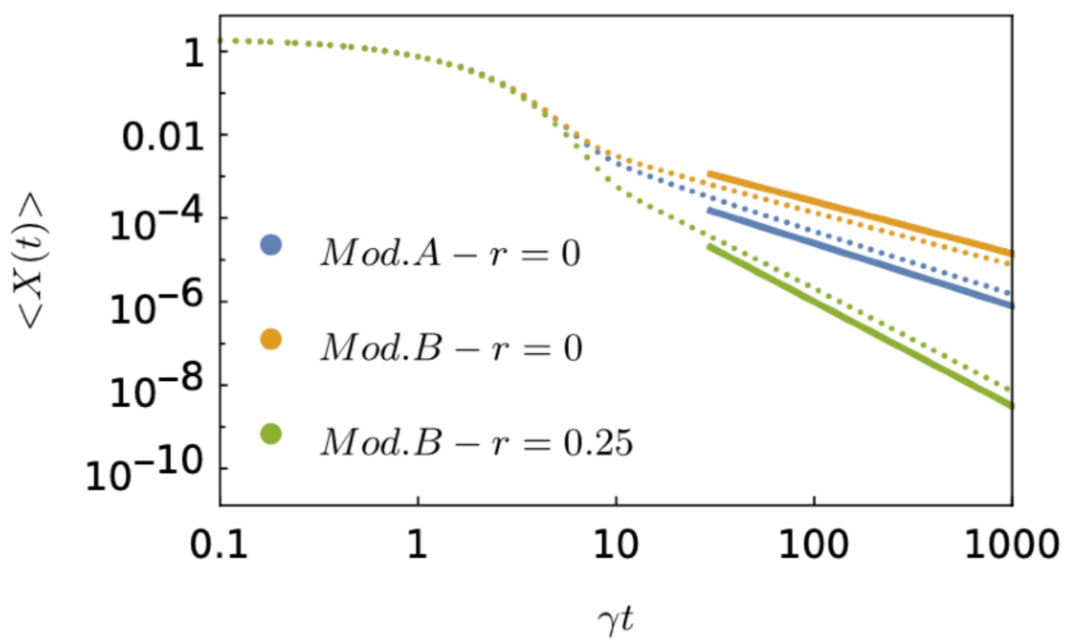
Rouse model

- Particle: random walker

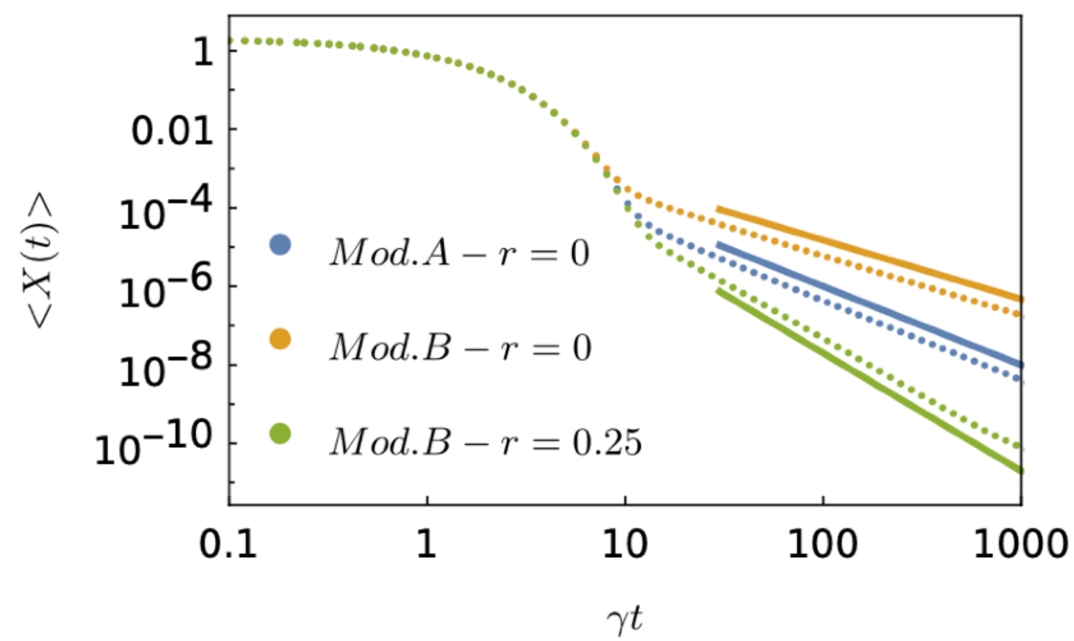
$$W(i \to i \pm +1) \propto \min\left\{1, \exp\left[-\frac{H(i \pm 1) - H(i)}{T}\right]\right\}$$

Simulation algorithm and lattice polymer mapping

Low T, $\lambda = 2$

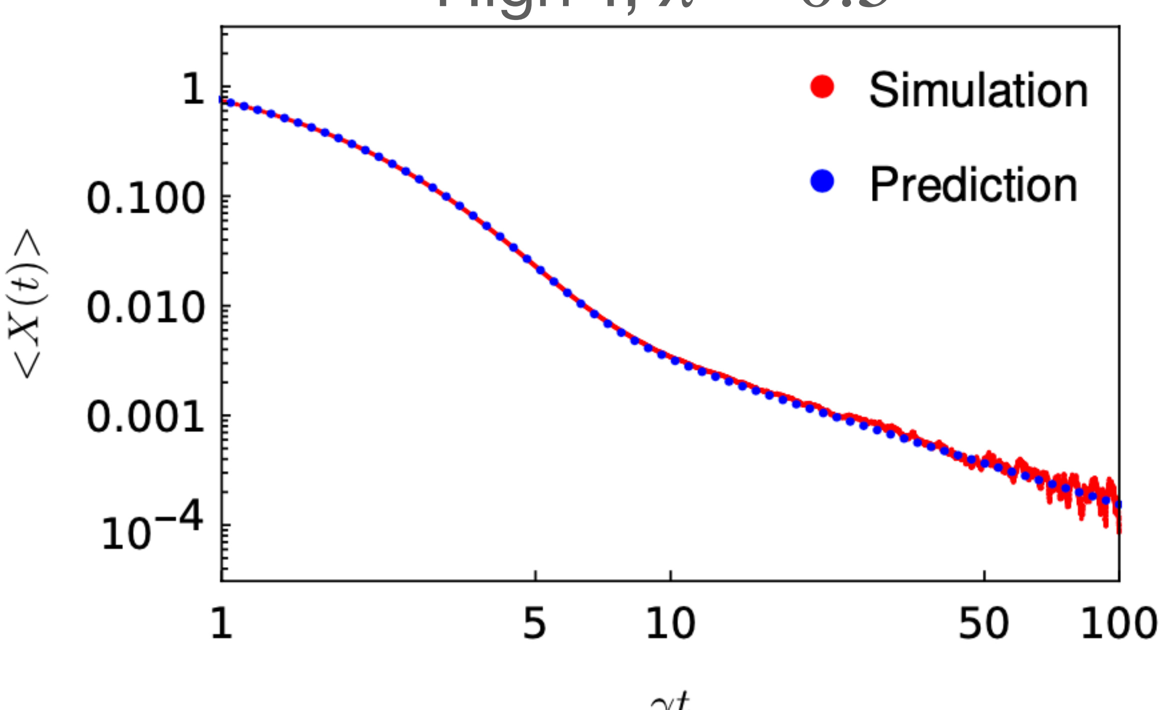


(a) $d = 1$

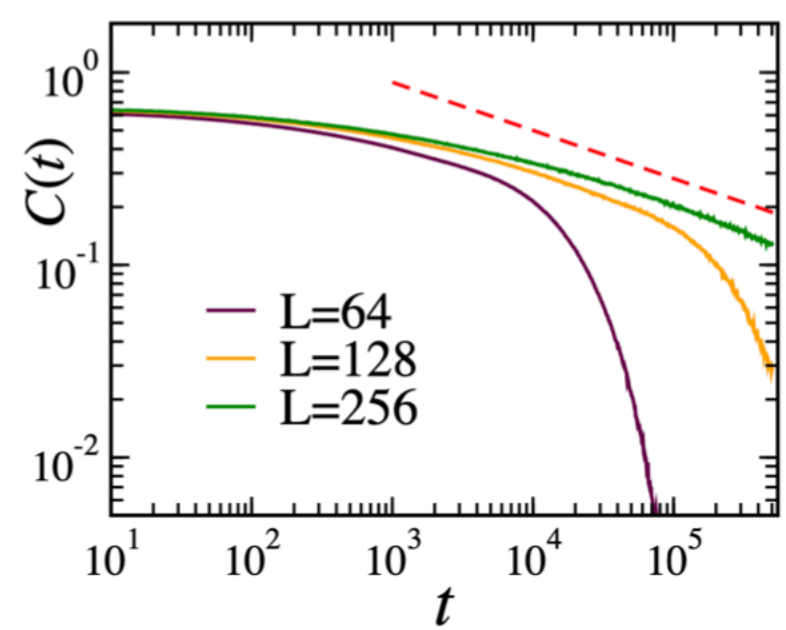


(b) $d = 2$

High T, $\lambda = 0.5$



Finite-size scaling



Summary of results

- Equilibrium behaviour [see article]
- Critical exponents and universality [article] of relaxation, autocorrelation, cross-correlation
- Connection to field scaling exponent z, e.g. [article]

$$\langle X(t)\rangle \sim t^{-(d/z+1)}$$

- Fluctuation-dissipation relation

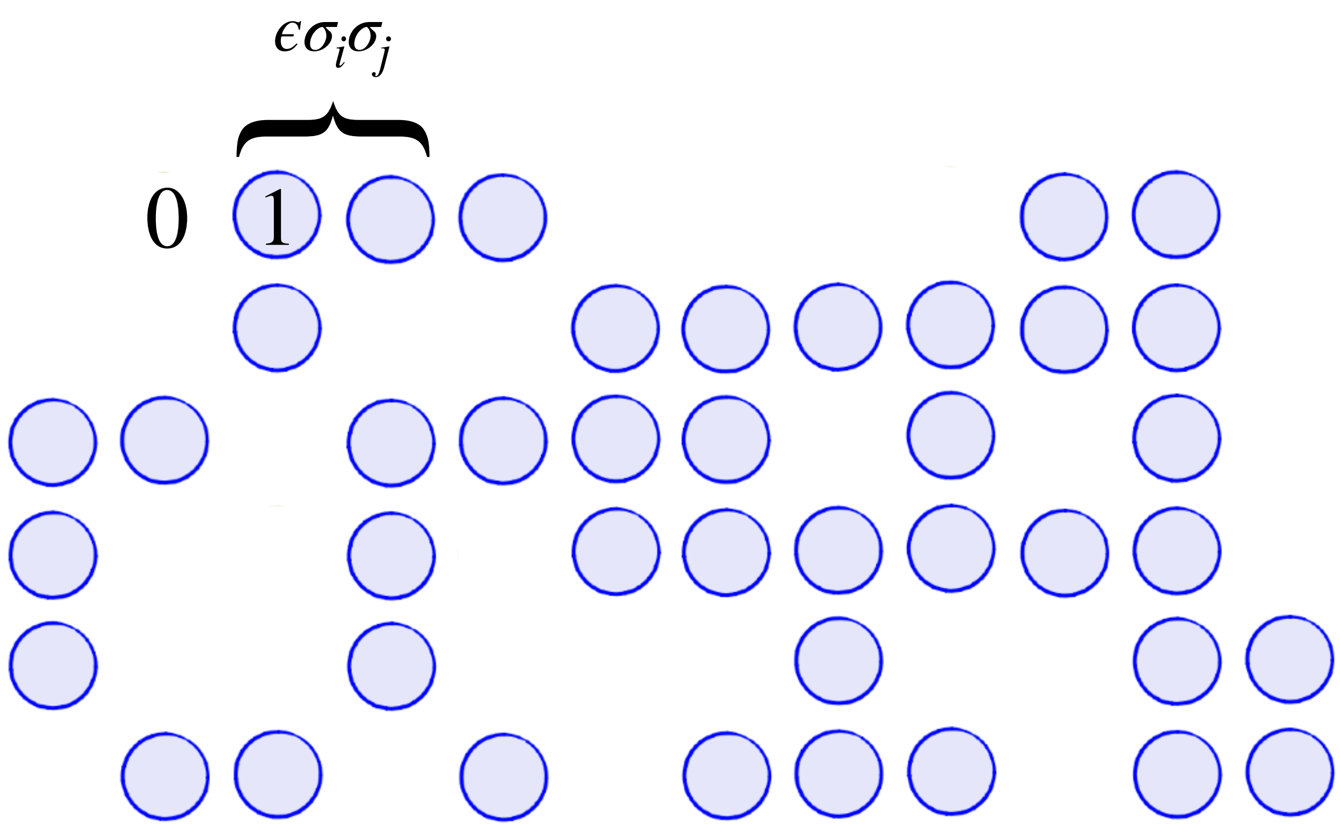
$$\langle X(t)\rangle \sim \frac{d}{dt}\langle X(t)X(0)\rangle$$

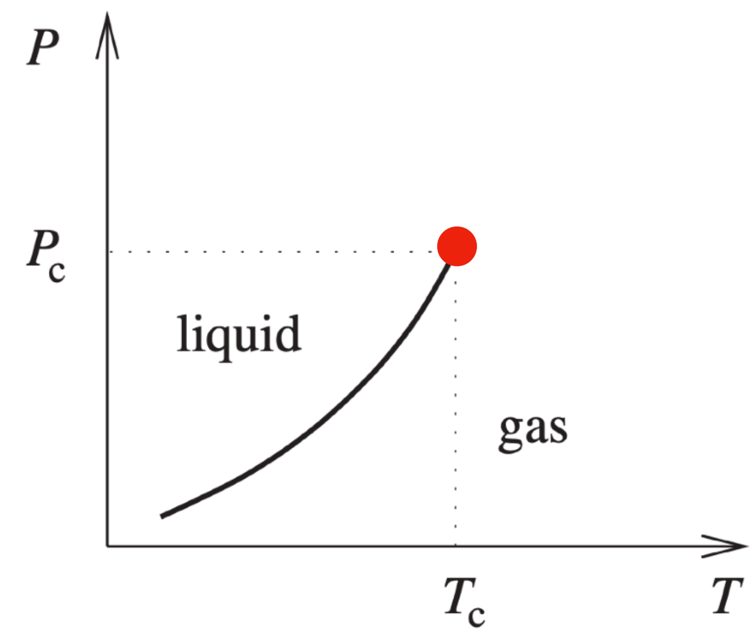
- Non-perturbative numerical validation

Thank you for your attention!

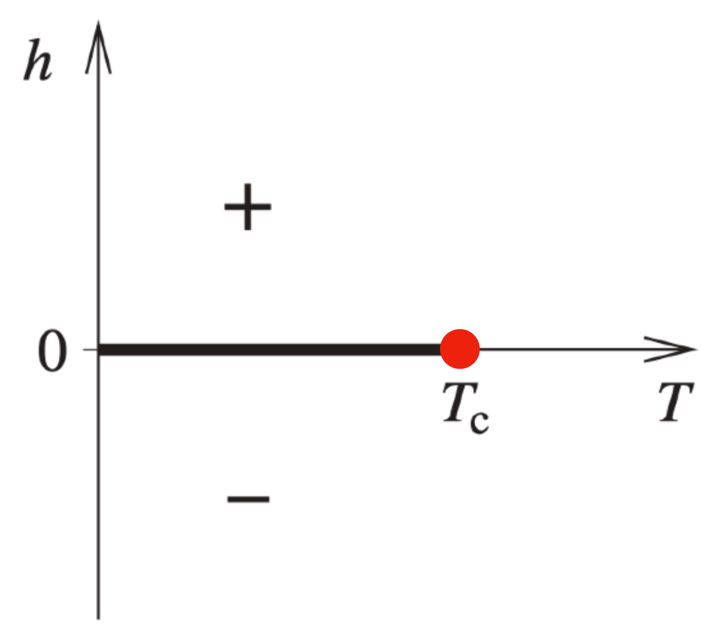
Extra slides

Mapping of single-component fluid to Ising





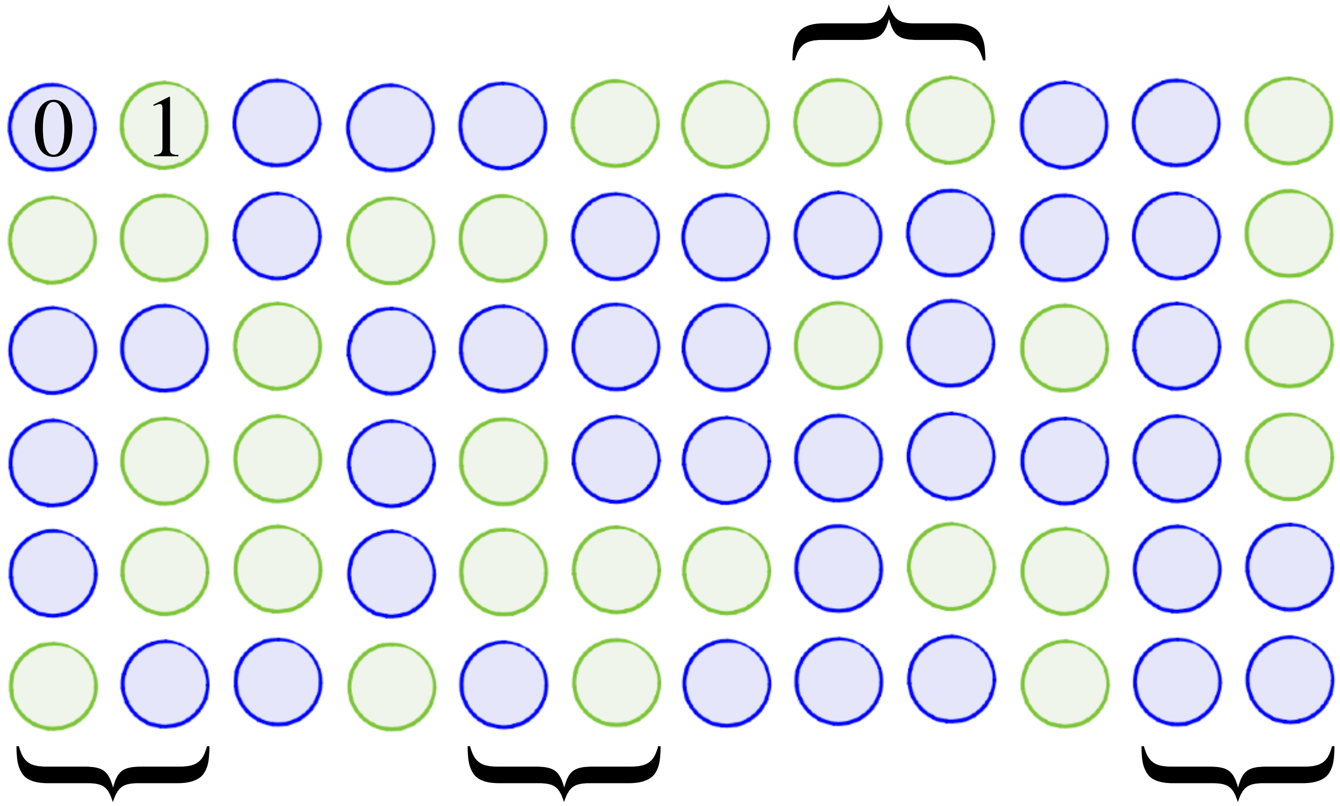
$$H[\{\sigma\}] = \sum_{\langle i,j \rangle} \epsilon \sigma_i \sigma_j$$



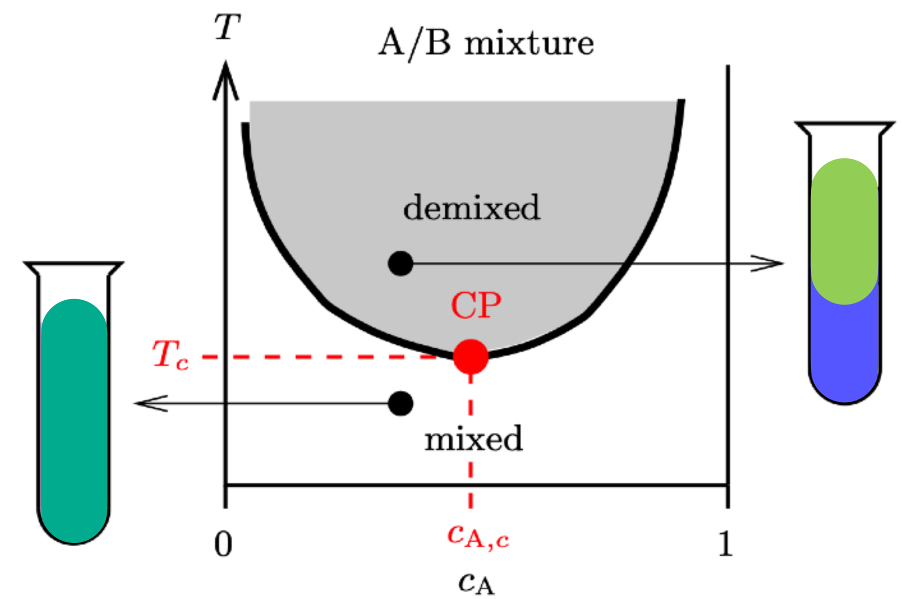
Extra

Mapping of binary mixture to Ising

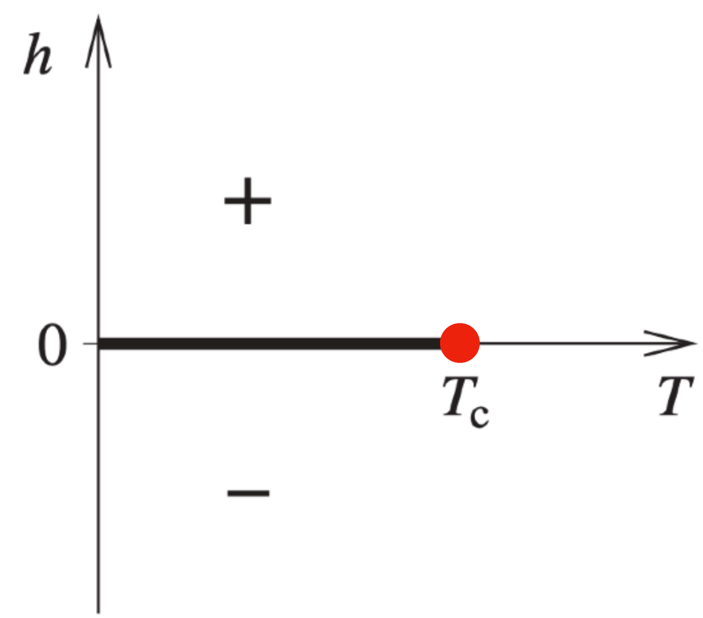
$\epsilon_{AA}\sigma_i\sigma_j$



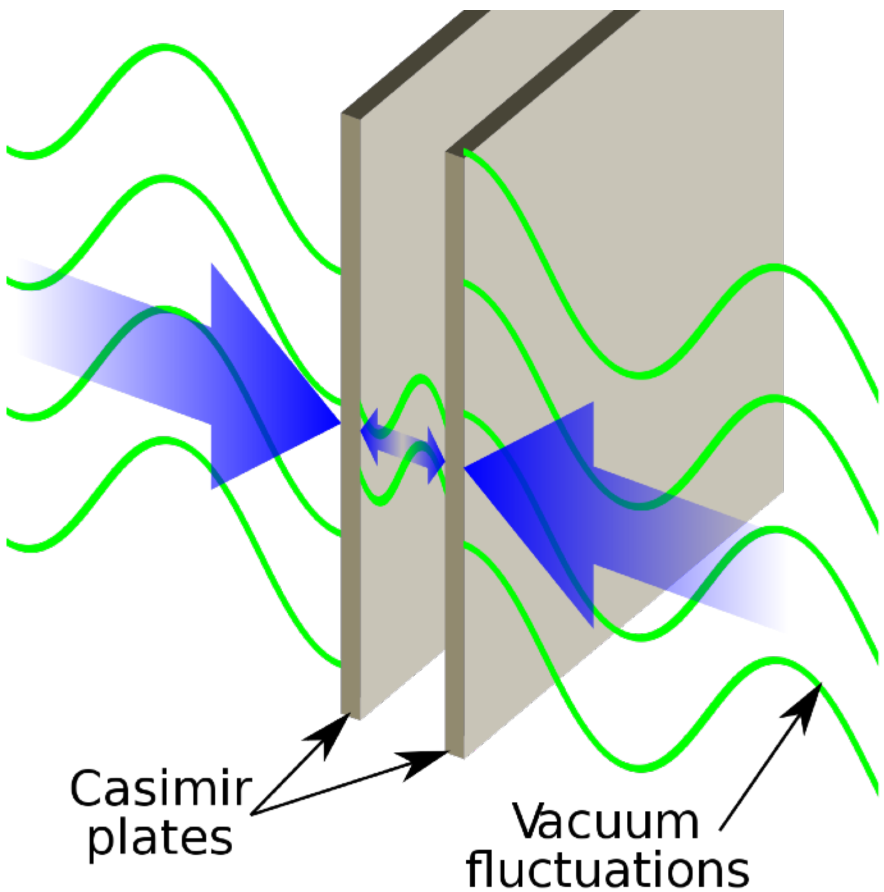
$\epsilon_{AB}\sigma_i(1-\sigma_j)$ $\epsilon_{AB}(1-\sigma_i)\sigma_j$ $\epsilon_{BB}(1-\sigma_i)(1-\sigma_j)$



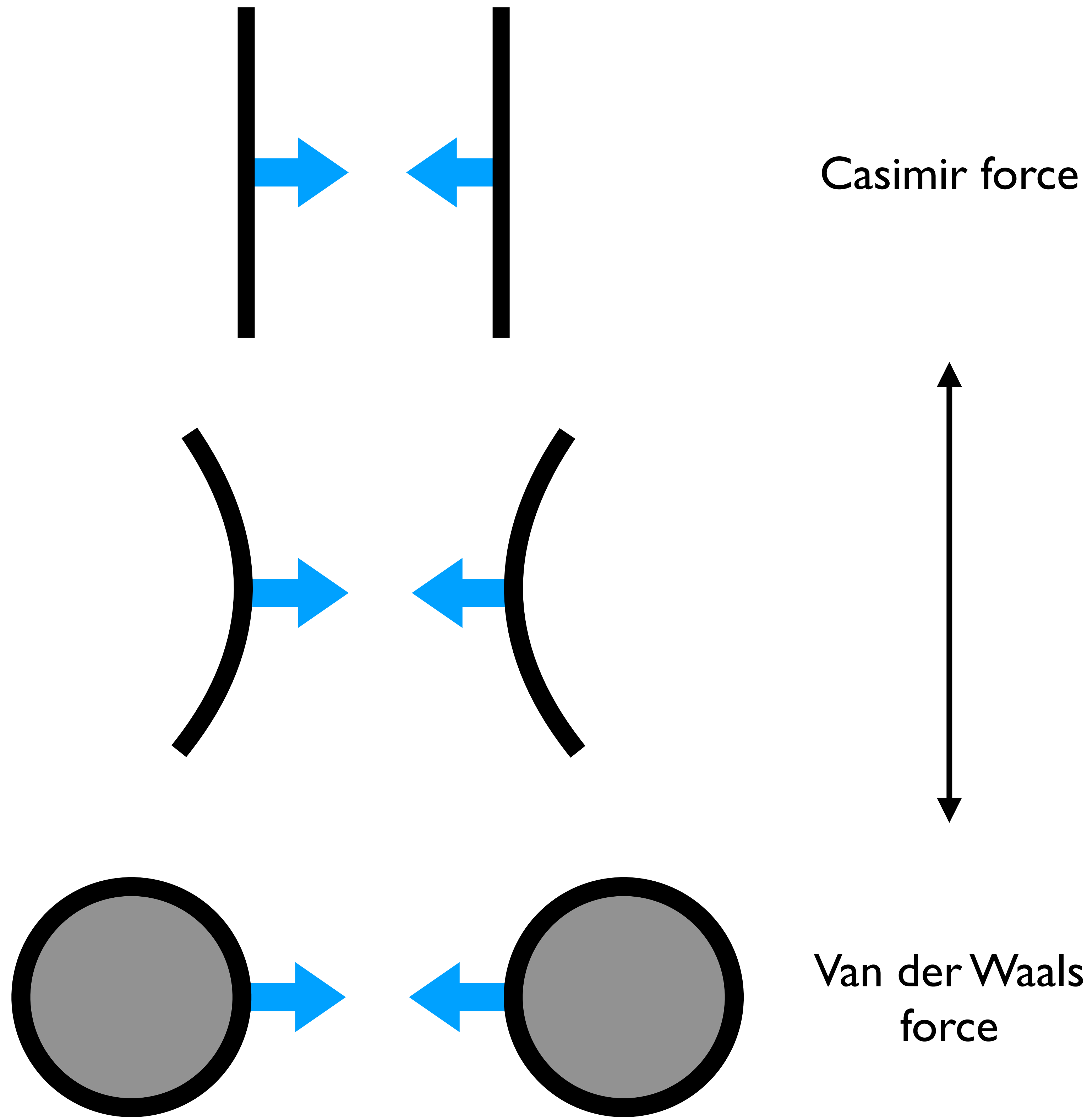
$$
\begin{aligned}
H[\{\sigma\}] &= \sum_{\langle i,j\rangle}\left[\epsilon_{AA}\sigma_i\sigma_j + \epsilon_{AB}\sigma_i(1-\sigma_j) + \ldots\right] \\
&= A\sum_{\langle i,j\rangle}\sigma_i\sigma_j + B\sum_i \sigma_i
\end{aligned}
$$



Why colloids in critical fluids? Casimir force in QED



$$E \propto -\frac{\hbar c}{L^3}$$

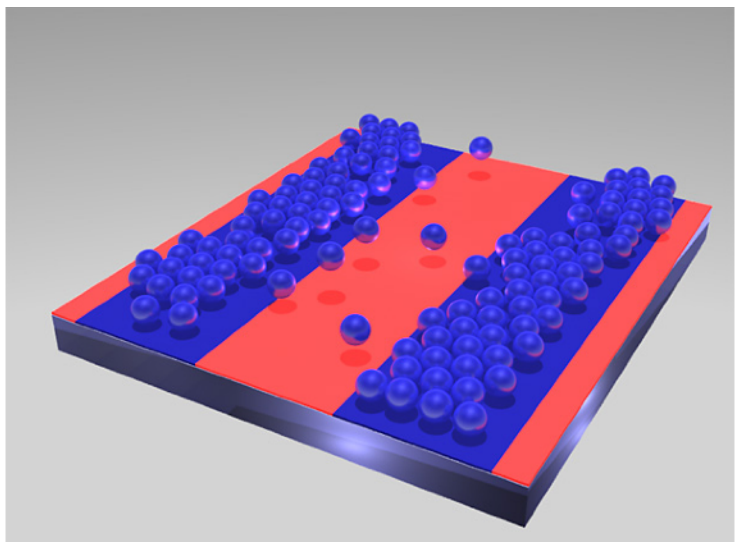


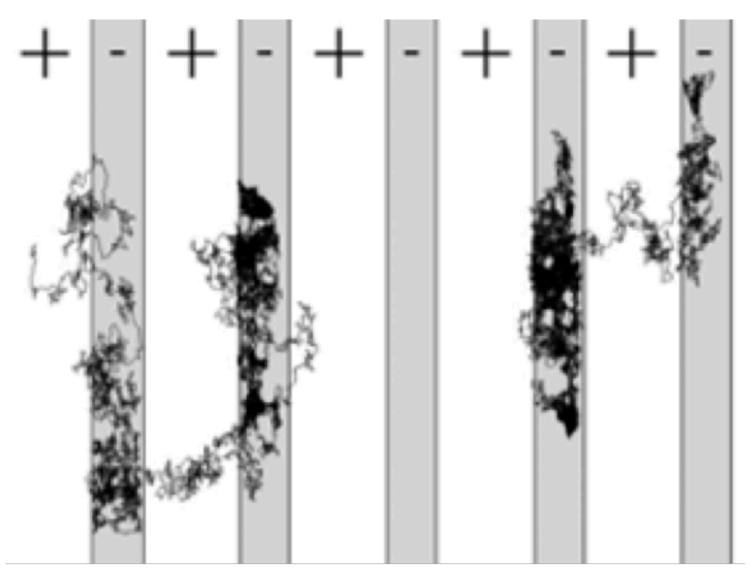
Casimir force in QED and StatPhys

	QED	**StatPhys**
Fluctuating quantity	E, B	Order parameter ϕ
Source of fluctuations	Quantum $\hbar > 0$	Thermal $kT > 0$
Range of fluctuations	∞ $(m_\gamma = 0)$	Correlation length ξ ∞ at CP
Resulting force after confinement	Long-range	**Variable range ξ** Long range at CP

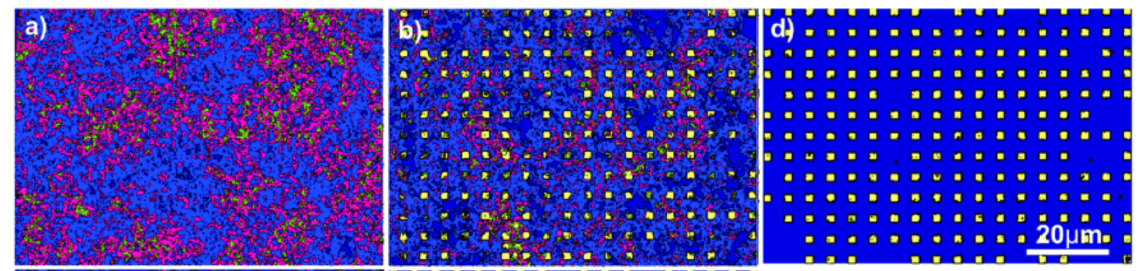
[Review: Gambassi - JPCS '09]

Critical Casimir force and patterned surfaces





Aggregation and assembly

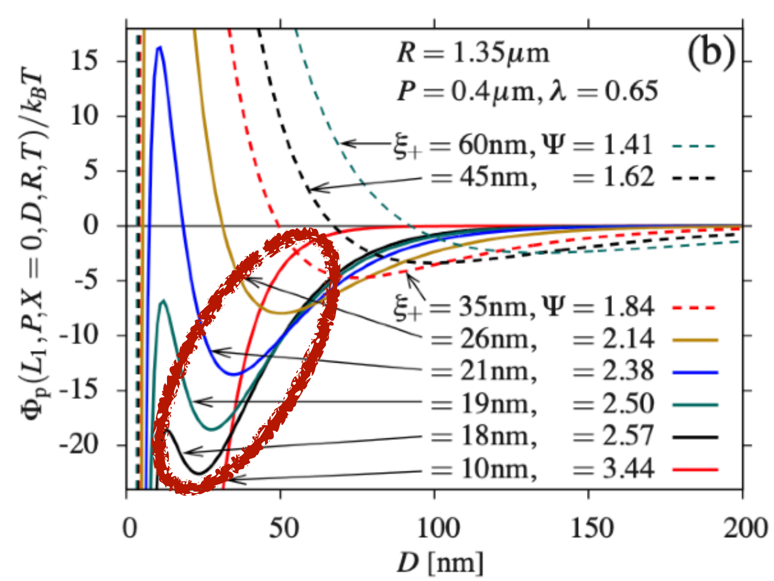


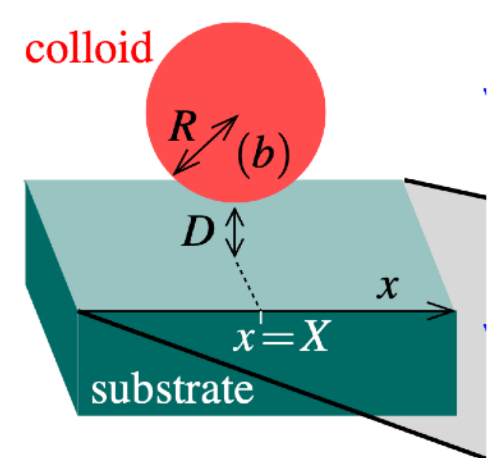
$T \longrightarrow T_c$

(19) **United States**
(12) **Patent Application Publication**
MARINO et al.

(54) METHOD FOR ASSEMBLING SEMICONDUCTOR NANOCRYSTALS

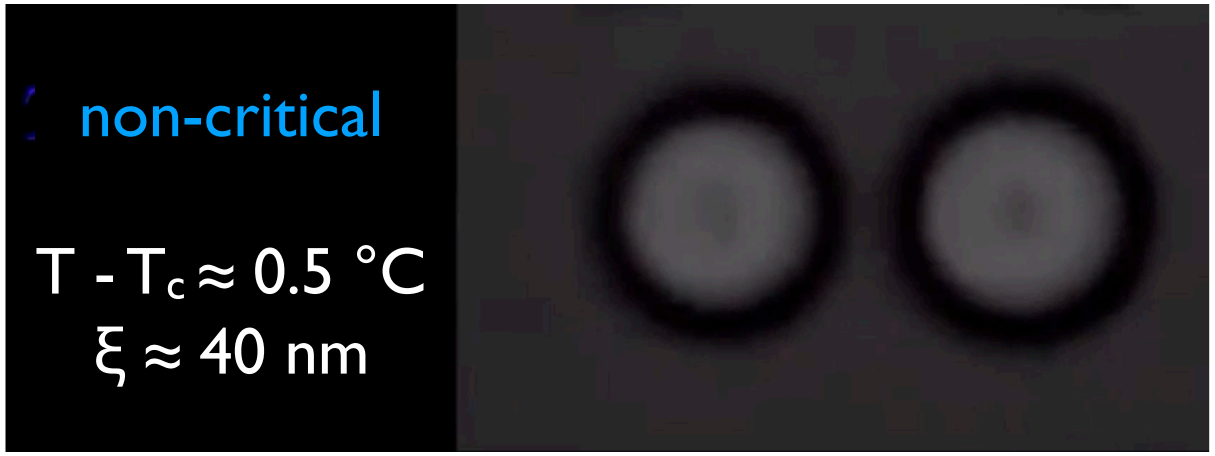
Levitation

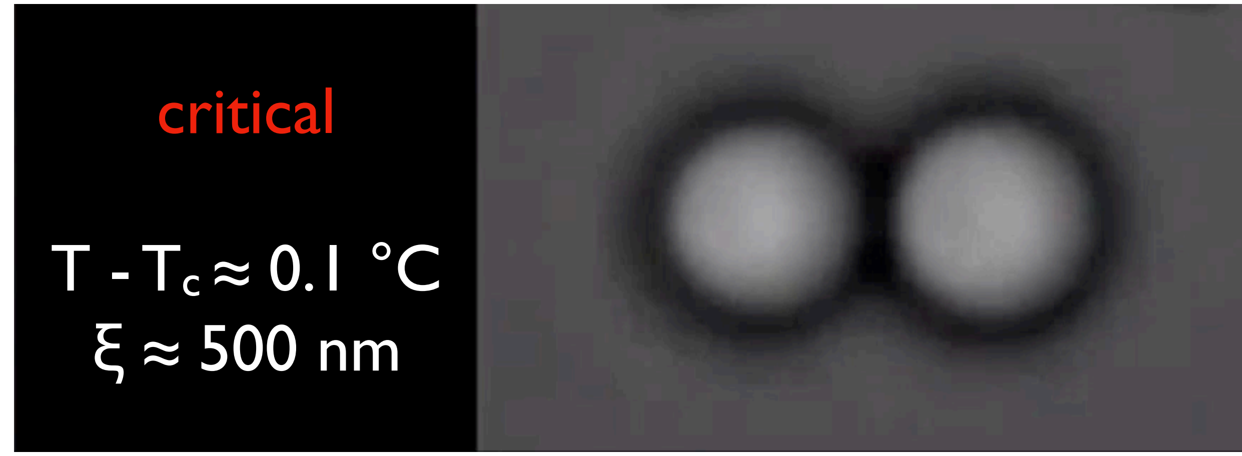


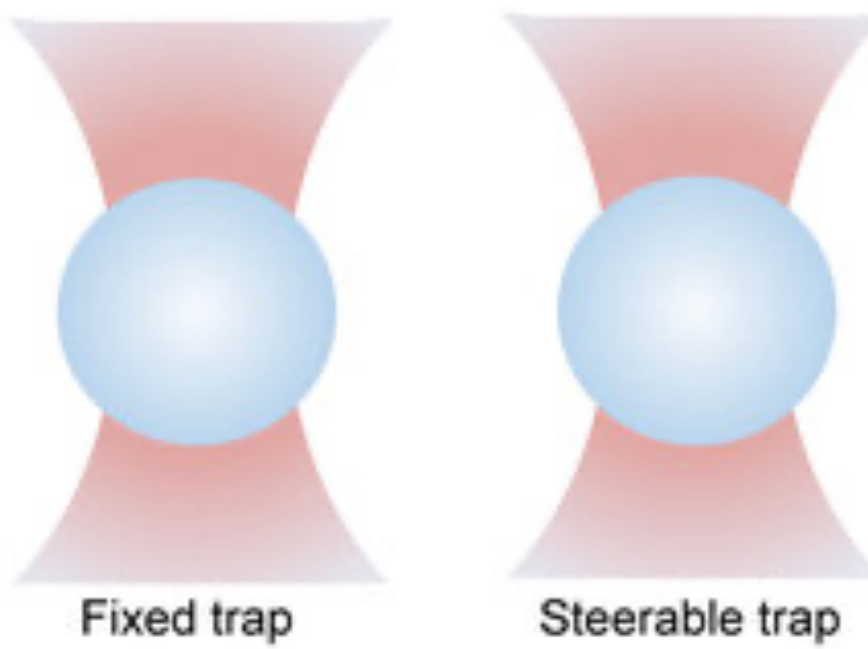


[Review: Gambassi, Dietrich - Soft Matter '10]

Why colloids in critical fluids? Critical Casimir force





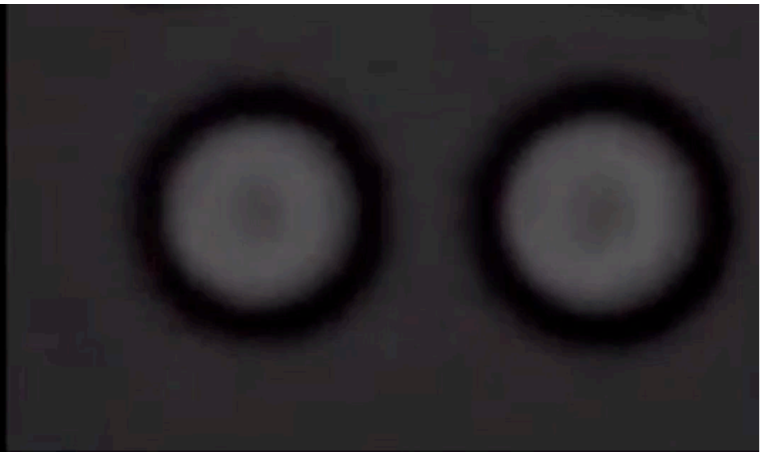


[Martinez, Devailly, Petrosyan, Ciliberto - Entropy MDPI '19]
[Martinez youtu.be/-jWnQdMqipM]

Why colloids in critical fluids? Critical Casimir force

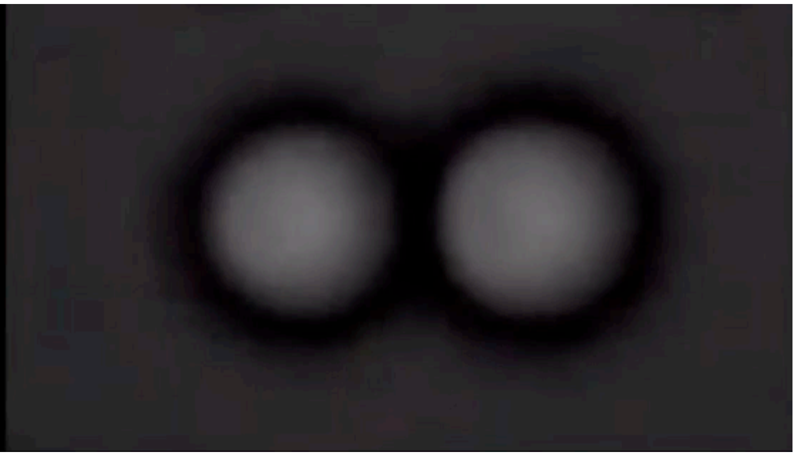
non-critical

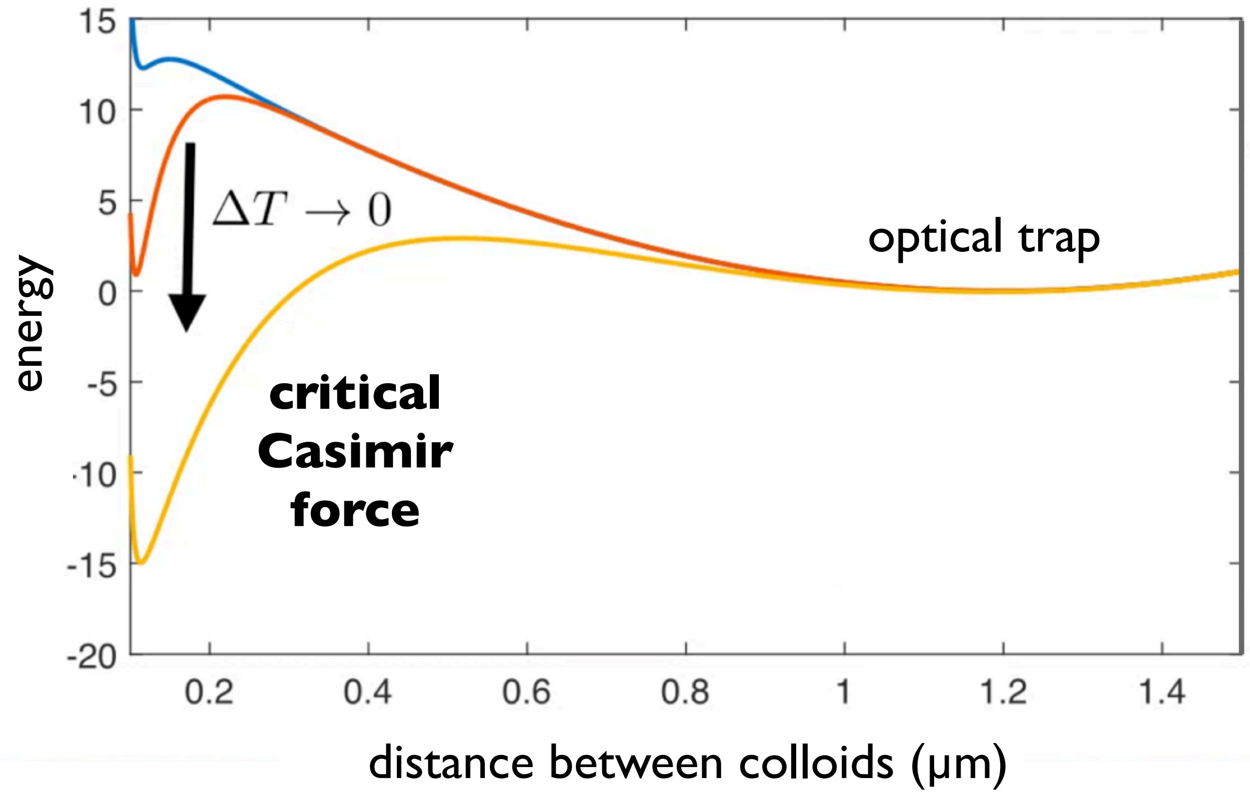
$T - T_c \approx 0.5$ °C
$\xi \approx 40$ nm



critical

$T - T_c \approx 0.1$ °C
$\xi \approx 500$ nm





[Martinez, Devailly, Petrosyan, Ciliberto - Entropy MDPI '19]
[Martinez youtu.be/-jWnQdMqipM]

Equilibrium distribution of the particle

$$P_{eq}(X) \propto \int [d\phi] e^{-\beta H[\phi,X]}$$

$$= e^{-\beta H_X} \cdot \int [d\phi] e^{-\beta(H_\phi + H_{int})}$$

$$\propto e^{-\beta H_X}$$

$$\psi(x) = \phi(x + X)$$

$$[d\phi] = [d\psi]$$

$$H_\phi[\phi] = H_\phi[\psi]$$

$$H_{int}[\phi, X] = H_{int}[\psi, 0]$$

Any field theory
Any field-particle coupling
Any external potential