Phase coexisting heat conduction in the Hamilton Potts model

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Mar. 16 2023,Japan-France joint seminar "Physics of dense and active disordered materials"

MK, N. Nakagawa, and S. Sasa, arXiv:2212.12289

Collaborators

- Shin-ichi Sasa (Kyoto University)

- Naoko Nakagawa (Ibaraki University)

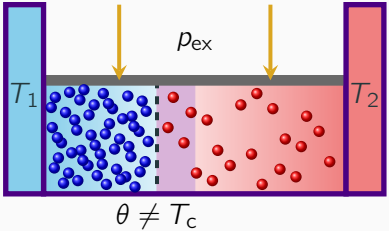
What we want to show

Phase coexistence under heat conduction (previous talk by N. Nakagawa)

N. Nakagawa and S. Sasa, PRL **119** 260602 (2017); JSP **177** 825 (2019); PRR **4** 033155 (2022)

Phase coexistence separated by the interface

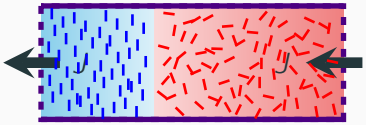
Non-equilibrium (with current)



- Temperature gradient appears
- Interface temperature θ differs from T_{c}
- $\Rightarrow$ Supercooled (or heated) is stabilized
- $\theta \neq T_{\mathrm{c}}$: Violation of local equilibrium thermodynamics.

What we show in this talk

Order-disorder coexistence separated by an interface



$\theta \neq T_c$

- Order-disorder coexistence (1st ordered transition) separated by an interface.
- Energy conserving system with equal heat injection and release.

We try to numerically show the violation of the local equilibrium thermodynamics by confirming $\theta \neq T_c$ with the dynamical field model.

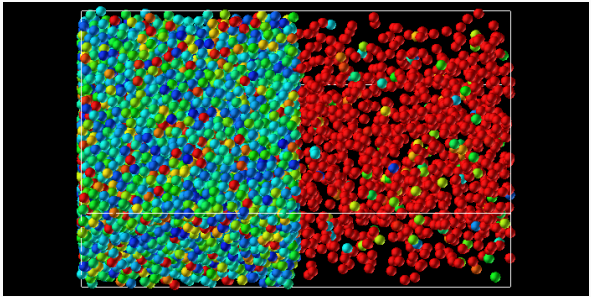
Global thermodynamics prediction

$$\theta - T_c = |J| \left(\frac{1}{\kappa^o} - \frac{1}{\kappa^d} \right) \frac{X(L_x - X)}{2L_x} + O(\varepsilon^2)$$

This work

Experimental and numerical confirmation are challenging

- Experiment: controlling adiabaticity is difficult
- MD simulation : detection of interface temperature is difficult due to discreteness



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Experimental and numerical confirmation are challenging

- Experiment: controlling adiabaticity is difficult
- MD simulation : detection of interface temperature is difficult due to discreteness

$$\Downarrow$$

We try to numerically detect global thermodynamic prediction
by using the continuous and dynamical field theory : "*Hamilton-Potts model*"

Hamilton-Potts model

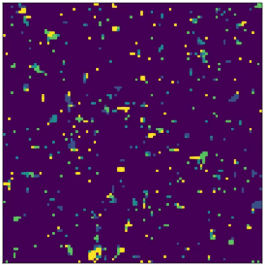
Potts model

q-state Potts model as statistical model showing phase transition

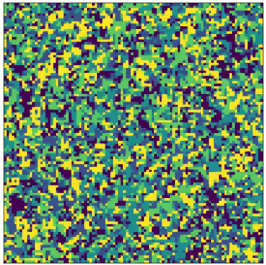
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{a_i, a_j} \qquad a_i = 1, \cdots, q$$

$q = 5$ Potts model

$T = 0.9T_c$



$T = 1.2T_c$



We can obtain 1st ordered phase transition in 2-dimensional system for $q \geq 5$

Extension to dynamical model

q-state Potts model is not dynamical model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{a_i, a_j} \qquad a_i = 1, \cdots, q$$

$\Downarrow$ Extension to dynamical model as continuous-field theory

q-state Hamilton Potts model

$$\mathcal{H}(\phi, \pi) = \int_D d^2 r \left[\frac{1}{2} \sum_{a=1}^{q-1} \left\{ \pi^a(\boldsymbol{r})^2 + |\nabla \phi^a(\boldsymbol{r})|^2 \right\} + V(\phi) \right]$$

$(\phi^1(\boldsymbol{r}), \phi^2(\boldsymbol{r}), \cdots, \phi^{q-1}(\boldsymbol{r}))$: $(q-1)$-dimensional real field

$(\pi^1(\boldsymbol{r}), \pi^2(\boldsymbol{r}), \cdots, \pi^{q-1}(\boldsymbol{r}))$: Momentum field conjugate to ϕ

Hamilton Potts model

q-state Hamilton Potts model

$$\mathcal{H}(\phi,\pi) = \int_D d^2r \left[\frac{1}{2} \sum_{a=1}^{q-1} \left\{ \pi^a(\boldsymbol{r})^2 + |\nabla\phi^a(\boldsymbol{r})|^2 \right\} + V(\phi) \right]$$

Potential $V(\phi)$ has q symmetric minima

$$V(\phi) = \frac{1}{2} \prod_{k=1}^{q} \sum_{a=1}^{q-1} (\phi^a - \mu_k^a)^2 \qquad \mu^a_{1\leq k\leq q} : \ q\text{-vertices of } (q-1)\text{-regular simplex}$$

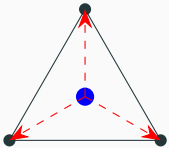
$(q-1)$ regular simplex

Potential $V(\phi)$ has q symmetric minima

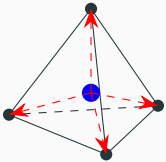
$$V(\phi) = \frac{1}{2}\prod_{k=1}^{q}\sum_{a=1}^{q-1}(\phi^a - \mu_k^a)^2 \qquad \mu^a_{1\le k\le q} : q\text{-vertices of } (q-1) \text{ regular simplex}$$

Example of regular simplex

$q = 2$
line segment
on a 1D line



$q = 3$
regular triangle
on a 2D plane



$q = 4$
regular tetrahedron
in 3D space

$q = 2$ case : Continuous extension of Ising model

1-simplex : line segment on a 1D line

Real Ginzburg-Landau model

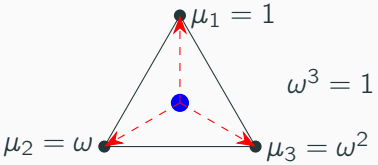
$$\mathcal{H}(\phi, \pi) = \int_D d^2r \left[\frac{1}{2} \sum_{a=1}^{q-1} \left\{ (\pi^a)^2 + |\nabla \phi^a|^2 \right\} + \frac{1}{2} \prod_{k=1}^{q} \sum_{a=1}^{q-1} (\phi^a - \mu_k^a)^2 \right]$$

$$\xrightarrow{q=2} \int_D d^2r \left[\frac{1}{2} \left(\pi^2 + |\nabla \phi|^2 \right) + \frac{1}{2} (\phi^2 - 1)^2 \right]$$

$q = 3$ case : Continuous extension of 3-state Potts (or 3-state clock) model

2-dimensional real field $(\phi^1, \phi^2) \Rightarrow$ complex field $\phi = \phi^1 + i\phi^2$

2-simplex : regular triangle on a complex plane



Complex Ginzburg-Landau model with 6-ordered nonlinearity

$$\mathcal{H}(\phi, \pi) \xrightarrow{q=3} \int_D d^2r \left[\frac{1}{2}\{\pi\pi^* + |\nabla\phi||\nabla\phi^*|\} + \frac{1}{2}|\phi^3 - 1|^2\right] \qquad \phi^3 = 1 \to \phi = 1, \frac{-1 \pm \sqrt{3}}{2}$$

Characteristics of Hamilton Potts model

- Model shows the 1st ordered phase transition in 2-dimensional space with $q \geqq 5$
- We can consider the natural dynamics with the Hamilton's equation:

$$\frac{\partial \phi^a}{\partial t} = \frac{\delta \mathcal{H}}{\delta \pi^a} \qquad \frac{\partial \pi^a}{\partial t} = -\frac{\delta \mathcal{H}}{\delta \phi^a}$$

- Energy injection and release can be easily introduced by the energy flux:

$$\frac{\partial \mathcal{H}}{\partial t} = \int_D d^2 r \sum_{a=1}^{q-1} \nabla \cdot (\pi^a \nabla \phi^a) \;\Rightarrow\; \boldsymbol{j} = \sum_{a=1}^{q-1} \pi^a \nabla \phi^a$$

Numerical simulation
– Fixing phase diagram with isothermal system –

Numerical parameters

Number of state	$q = 11$: Strong 1st ordered transition
System size	$L_x = L_y = 64$
Grid spacing	$\Delta x = 1/8$
$\Rightarrow$ Number of grids	$(64 \times 8) \times (64 \times 8) = 512 \times 512$
Boundary condition	Periodic
Treatment of spatial differential	Spectral decomposition

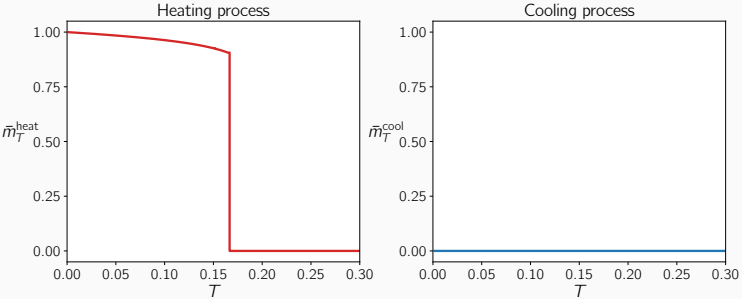
Langevin equation for isothermal system

Langevin equation with temperature T

$$\frac{\partial \phi^a}{\partial t} = \frac{\delta \mathcal{H}}{\delta \pi^a} \qquad \frac{\partial \pi^a}{\partial t} = -\frac{\delta \mathcal{H}}{\delta \phi^a} - \gamma \pi^a + \sqrt{2\gamma T}\xi^a$$

$$\langle \xi^a(\boldsymbol{x}, t)\xi^b(\boldsymbol{x}', t')\rangle = \delta^{ab}\delta(\boldsymbol{x}-\boldsymbol{x}')\delta(t-t')$$

Temperature dependence of order parameter



$$\bar{m}_T = \left\langle \int \frac{d^2\boldsymbol{r}}{L_x L_y} \sum_{a=1}^{q-1} \phi^a(\boldsymbol{r})\mu_1^a \right\rangle_T$$

Transition temperature is ambiguous due to hysteresis (metastability)

Accelerated Langevin equation with duplicated systems

M. Ohzeki and A. Ichiki, PRE 92, 012105 (2015)

Duplicated Langevin equations

$$\frac{\partial \phi_1^a}{\partial t} = \frac{\delta \mathcal{H}(\phi_1, \pi_1)}{\delta \pi_1^a} - \frac{\delta \mathcal{H}(\phi_2, \pi_2)}{\delta \pi_2^a} \qquad \frac{\partial \pi_1^a}{\partial t} = -\frac{\delta \mathcal{H}(\phi_1, \pi_1)}{\delta \phi_1^a} - \frac{\delta \mathcal{H}(\phi_2, \pi_2)}{\delta \phi_2^a} - \pi_1^a + \xi_1^a$$

$$\frac{\partial \phi_2^a}{\partial t} = \frac{\delta \mathcal{H}(\phi_2, \pi_2)}{\delta \pi_2^a} + \frac{\delta \mathcal{H}(\phi_1, \pi_1)}{\delta \pi_1^a} \qquad \frac{\partial \pi_2^a}{\partial t} = -\frac{\delta \mathcal{H}(\phi_2, \pi_2)}{\delta \phi_2^a} + \frac{\delta \mathcal{H}(\phi_1, \pi_1)}{\delta \phi_1^a} - \pi_2^a + \xi_2^a$$

Duplication is originally introduced to accelerate canonical ensemble averaging

$$\rho_T(\phi, \pi) = \frac{1}{\mathcal{Z}} e^{-\mathcal{H}(\phi,\pi)/T}$$

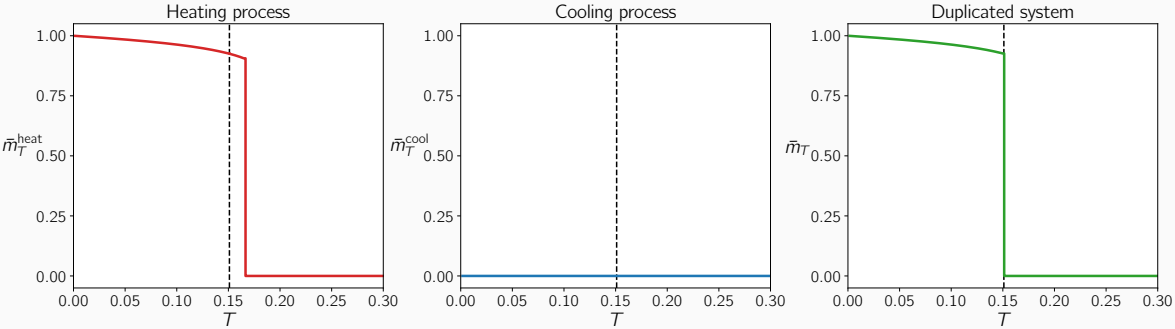
Case of XY model: $z \sim 2$ (simple Langevin) $\Rightarrow z \lesssim 1.2$ (duplicated Langevin)

Accelerated Langevin equation with duplicated systems

M. Ohzeki and A. Ichiki, PRE 92, 012105 (2015)

Initial condition

- (ϕ_1, π_1) : Snapshot for heating process (maybe superheated)
- (ϕ_2, π_2) : Snapshot for cooling process (maybe supercooled)



Equilibrium in isolated system

Numerical parameters

Number of state	$q = 11$: Strong 1st ordered transition
System size	$L_x = 6 \times 64 = 384$ and $L_y = 64$
Grid spacing	$\Delta x = 1/8$
$\Rightarrow$ Number of grids	$(384 \times 8) \times (64 \times 8) = 3072 \times 512$
Boundary condition (y)	Periodic
Boundary condition (x)	Neumann (differential controlled)
Treatment of spatial differential	Spectral decomposition

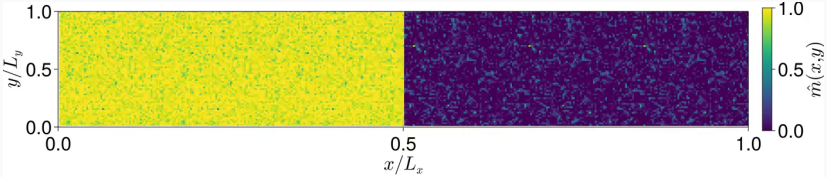
Interface dynamics: interface in equilibrium

Initial state : connecting isothermal snapshots

Left : Ordered equilibrium snapshot Right : Disordered equilibrium snapshot

Energy conserving Hamiltonian equation

$$\frac{\partial \phi^a}{\partial t} = \frac{\delta \mathcal{H}}{\delta \pi^a} \qquad \frac{\partial \pi^a}{\partial t} = -\frac{\delta \mathcal{H}}{\delta \phi^a} \qquad \partial_x \phi^a|_{x=0,L_x} = 0$$



Local OP

$$\hat{m}(x,y) = \sum_{a=1}^{q-1} \phi^a \mu_1^a$$

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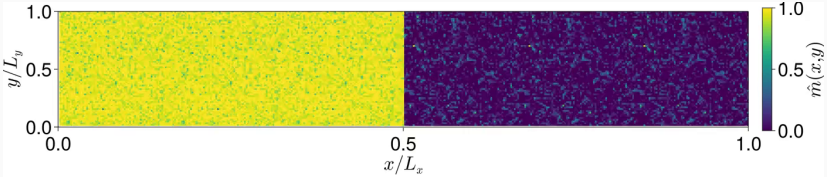

Local OP

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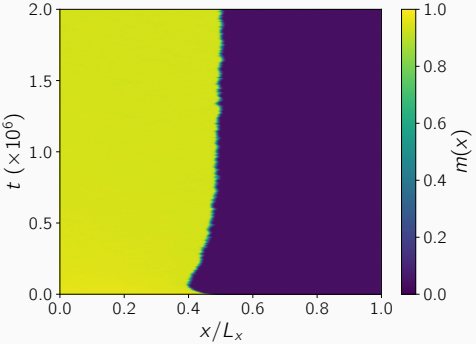
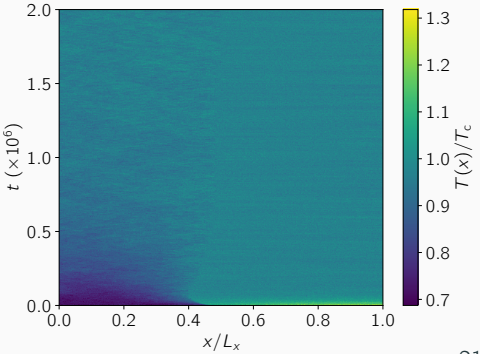
Dynamics of interface and temperature

One-dimensional local order parameter and local temperature

$$m(x) = \int \frac{dy}{L_y} \sum_{a=1}^{q-1} \phi^a \mu_1^a \qquad T(x) = \int \frac{dy}{L_y} \frac{\sum_a \pi^a(\boldsymbol{r})\pi^a(\boldsymbol{r})}{2(q-1)}$$





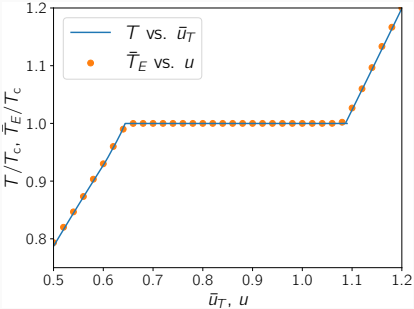
Checking for equivalence of ensembles

Isothermal system

Energy density $\bar{u}_T = \int \frac{d^2\boldsymbol{r}}{L_x L_y} \langle \mathcal{H} \rangle_T$ as a function of T

Isolated system

Temperature $\bar{T}_E = \int \frac{d^2\boldsymbol{r}}{L_x L_y} \left\langle \frac{\sum_a \pi^a(\boldsymbol{r})\pi^a(\boldsymbol{r})}{2(q-1)} \right\rangle_E$ as a function of $u = \mathcal{H}/L_x L_y$



- Isothermal system : $\bar{u}_T$ jumps at $T = T_c$
- Isolated system : $\bar{T}_E$ shows plateau at $u_{\min} \leq u \leq u_{\max}$

Non-equilibrium steady state under heat conduction

Heat conduction

J is set to be $J = -0.00002$
(linear-response region)

Inducing current J as boundary condition

Energy flux

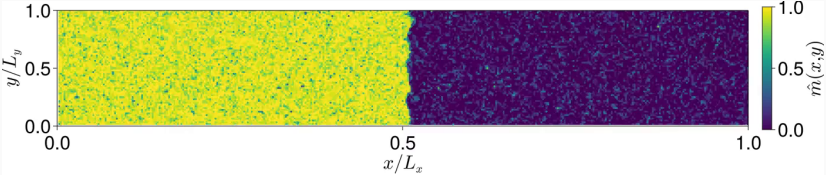
$$\dot{\mathcal{H}} = \int_D d^2r \sum_{a=1}^{q-1} \nabla \cdot (\pi^a \nabla \phi^a) \;\Rightarrow\; \boldsymbol{j} = \sum_{a=1}^{q-1} \pi^a \nabla \phi^a$$

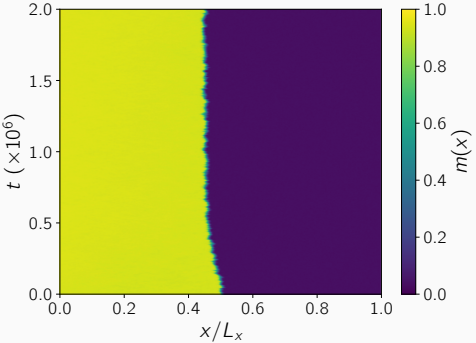
$$\Downarrow$$

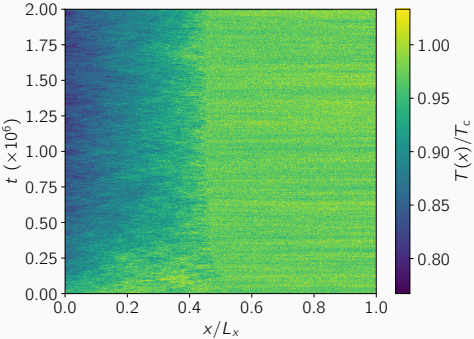
Boundary condition

$$\partial_x \phi^a|_{x=0,L_x} = -\frac{J L_y \pi^a|_{x=0,L_x}}{\displaystyle\int_0^{L_y} dy \sum_{b=1}^{q-1} (\pi^b)^2|_{x=0,L_x}}$$

Interface dynamics: interface under current







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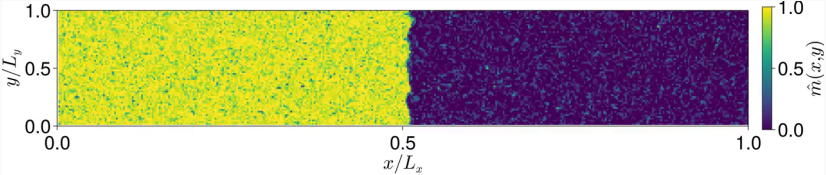
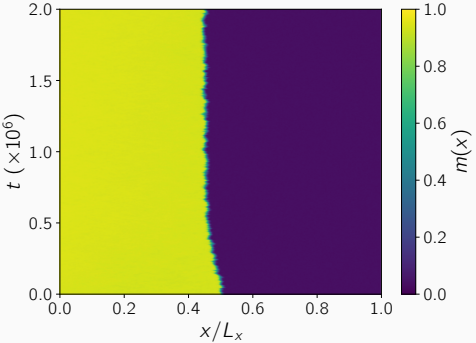
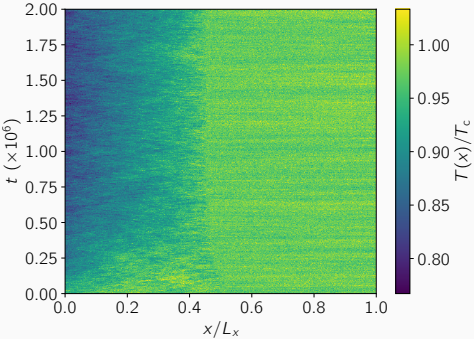




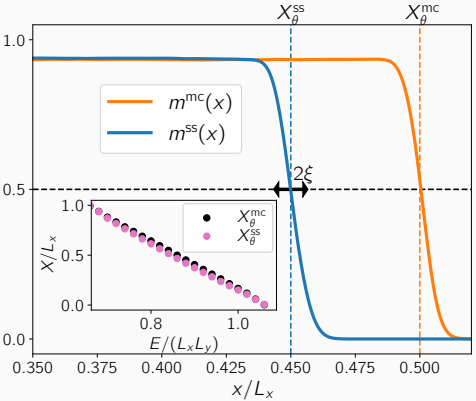


Thermodynamic average

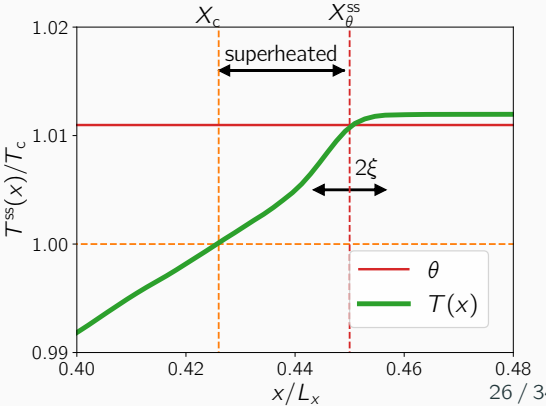
Average

$A^{\mathrm{mc}} \equiv \langle A \rangle_E$: equilibrium with $J = 0$ $\qquad$ $A^{\mathrm{ss}} \equiv \langle A \rangle_{E,J}$: steady state with $J \neq 0$

Local order parameter



Local temperature $T^{\mathrm{ss}}(x)$



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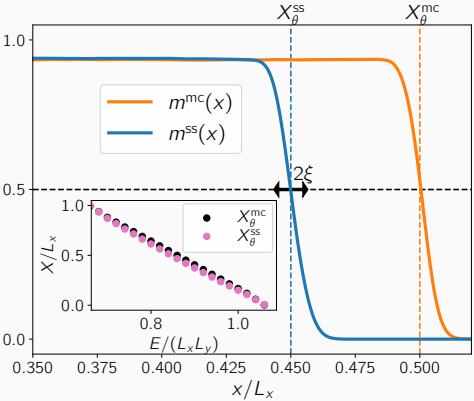


Interface position X_θ is defined as $m(X_\theta) = 0.5$

(Half of the value at $T = 0$)

Thermodynamic average

Average

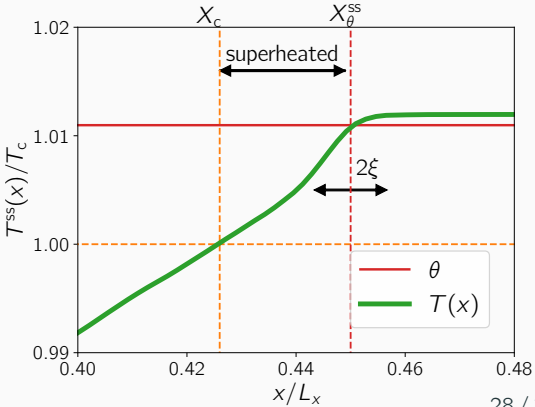
$A^{\mathrm{mc}} \equiv \langle A \rangle_E$: equilibrium with $J = 0$ $\qquad$ $A^{\mathrm{ss}} \equiv \langle A \rangle_{E,J}$: steady state with $J \neq 0$

- $T^{ss}(x) = \dfrac{1}{L_y} \displaystyle\int_0^{L_y} dy \left\langle \sum_{a=1}^{q-1} \frac{(\pi^a)^2}{2(q-1)} \right\rangle_{E,J}$

- Interface position X_θ^{ss} deviates from the position for $T_{\mathrm{c}} = T^{ss}(x = X_{\mathrm{c}})$

  $\Rightarrow$ Stable superheated region appears (Violation of local equilibrium)

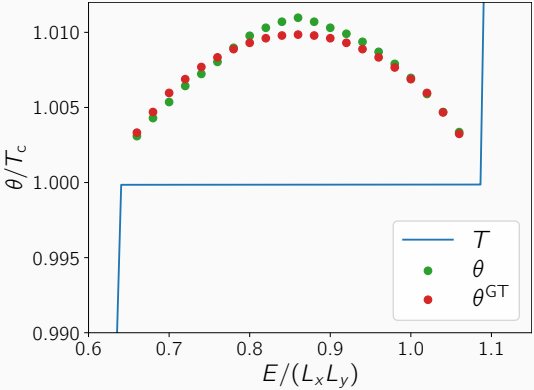
Local temperature $T^{\mathrm{ss}}(x)$



Comparison with global thermodynamics prediction

Global thermodynamics

$$\theta^{\mathrm{Th}} = T_{\mathrm{c}} - \frac{X(L_x - X)}{2L_x} J \left(\frac{1}{\kappa^{\mathrm{o}}} - \frac{1}{\kappa^{\mathrm{d}}} \right) + O(\varepsilon^2) \; (> T_{\mathrm{c}} \text{ for Potts model with } \kappa^{\mathrm{o}} < \kappa^{\mathrm{d}})$$

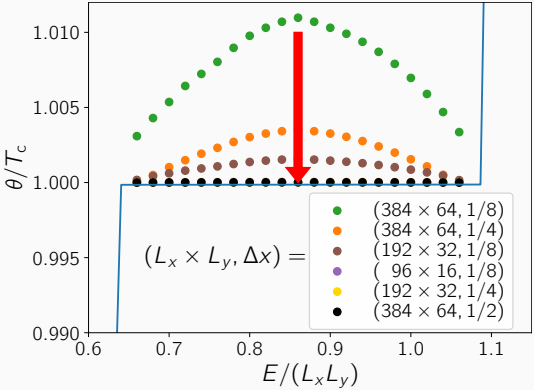


Quantitative agreement between theory and numerical simulation

Finite-size and finite-"smoothness" effects

Global thermodynamics

$$\theta_{\mathrm{Th}} = T_{\mathrm{c}} - \frac{X(L_x - X)}{2L_x} J \left(\frac{1}{\kappa^{\mathrm{o}}} - \frac{1}{\kappa^{\mathrm{d}}} \right) + O(\varepsilon^2) \; (> T_{\mathrm{c}} \text{ for Potts model with } \kappa^{\mathrm{o}} < \kappa^{\mathrm{d}})$$



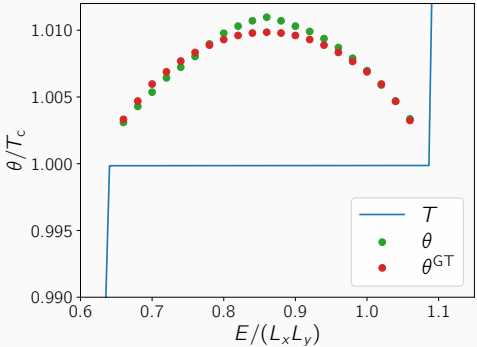
Local equilibrium recovers with not only decreasing the system size $L_x \times L_y$ but also increasing the grid spacing Δx.

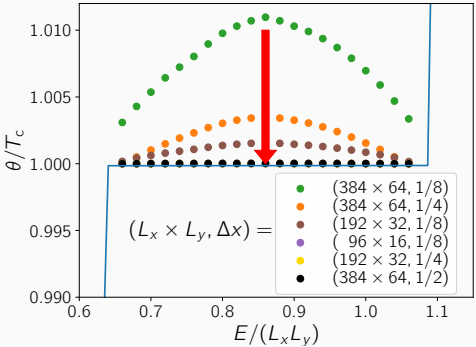
$\Rightarrow$ Smoothness of fields is also needed for the violation of local equilibrium.

Summary

Summary

- We have obtained violation of local equilibrium thermodynamics and the confirmation with theoretical prediction by global thermodynamics by the Hamilton Potts model.
- Violation of local equilibrium strongly depends on not only the finite-size effect but also finite-smoothness effect of fields.





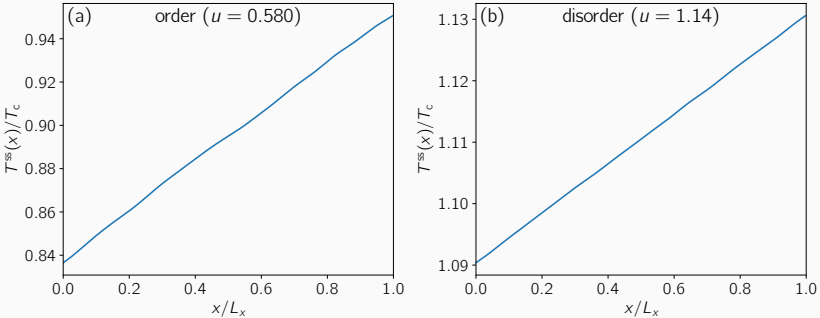
MK, N. Nakagawa, and S. Sasa, arXiv:2212.12289

Is $J = -0.00002$ small enough for linear-response theory to be established?

Global thermodynamics

$$\theta_{\mathrm{Th}} = T_{\mathrm{c}} - \frac{X(L_x - X)}{2L_x} J \left(\frac{1}{\kappa^{\mathrm{o}}} - \frac{1}{\kappa^{\mathrm{d}}} \right) + O(\varepsilon^2)$$

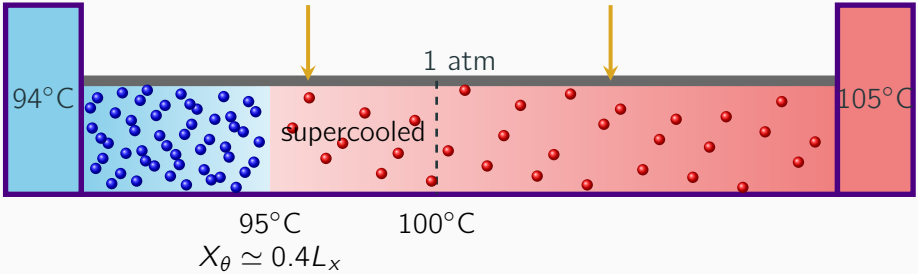
Heat conductivity κ should be obtained



Experimental confirmation is expected now

N. Nakagawa and S. Sasa, PRL **119** 260602 (2017); JSP **177** 825 (2019); PRR **4** 033155 (2022)

Global thermodynamics prediction for water with heat bathes at 94°C and 105°C
(Liquid-gas interface)



Comparison with global thermodynamics prediction

Global thermodynamics

$$\theta_{\mathrm{Th}} = T_{\mathrm{c}} - \frac{X(L_x - X)}{2L_x} J \left(\frac{1}{\kappa^{\mathrm{o}}} - \frac{1}{\kappa^{\mathrm{d}}} \right) + O(\varepsilon^2) \; (> T_{\mathrm{c}} \text{ for Potts model with } \kappa^{\mathrm{o}} < \kappa^{\mathrm{d}})$$