Thermodynamics of Coherent Structures near Phase Transitions

Julia M. Meyer
Purdue University, meyer222@purdue.edu

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Julia Meyer and Ivan Christov
OUR Scholarship 2018-2019, TMNT Laboratory
Mechanical Engineering, Purdue University

Introduction

- Phase transitions within large-scale dynamical systems may be modeled by using stochastic partial differential equations
- System dynamics are captured by an appropriate potential equation $V(\phi)$
- Likelihood of phases being present within the system is reflected in probability density function (PDF) of ϕ values across system
- Realization of this equation is a configuration of coherent structures, distributed along a lattice:

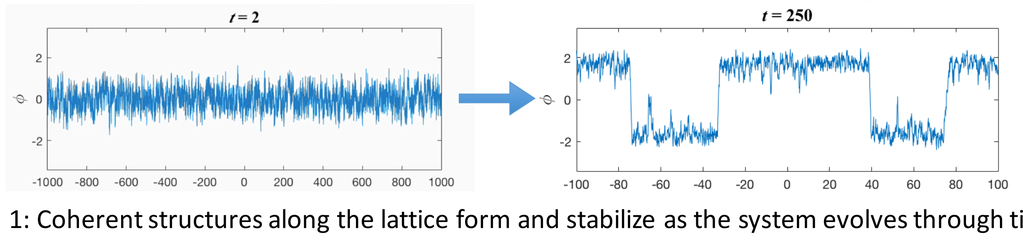


Fig. 1: Coherent structures along the lattice form and stabilize as the system evolves through time.

Applications

- Order of potential (4th, 6th, 10th, etc) determines type of phase transition: first-order, second-order, or multiple [1]
- Applications include modeling:
  - Crystallographic phase transformations
  - Traffic congestion [2]
  - Coherent movement of granular materials [3]

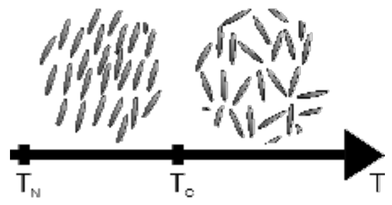


Fig. 2, above: Length between cars in traffic may be modeled by lattice similar to Fig. 1.
Below: Nematic and isotropic phases of liquid crystals differ by particle orientation. [4]

Objectives

- Determine detail of simulation necessary for accurate results
- Derive and verify theoretical solutions of two higher-order potentials (ϕ^6, ϕ^{10})
- Investigate effect of system temperature on system behavior

Methods

Simulation Details

- Utilized first-order Euler discretization methods in large-scale MATLAB simulations
- Time evolution of field modeled with the Langevin equation [4]:

$$\phi_{tt} = \phi_{xx} - \eta\phi_t - V'(\phi) + \hat{F}(x,t)$$

- V: system potential
- η: system viscosity (set to equal 1 during all simulations)
- $\hat{F}$: Gaussian white noise (temperature dependent)

Probability Density Functions

- Probability Density Function (PDF) of ϕ values across lattice computed from simulation
- Results of 100 runs were averaged to obtain final PDF
- PDF equivalent to the square of the system ground-state wave function (Ψ)
  - Obtained from an eigenvalue problem for the Schrödinger equation with the given system potential V [5]:

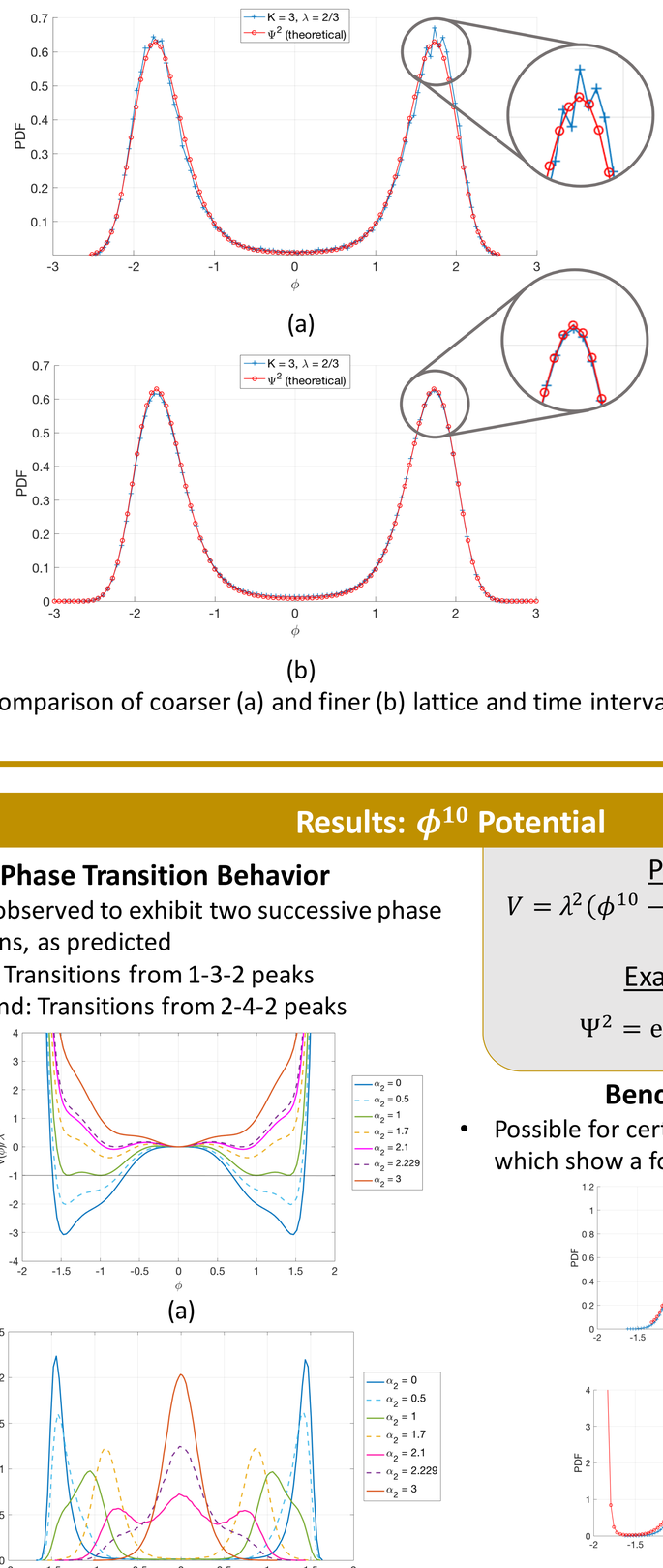
$$-\frac{1}{2\beta^2}\frac{d^2}{d\phi^2}\Psi + V(\phi)\Psi = E\Psi$$

- β: a constant related to external driving force (set to equal 1 during all simulations)
- E: corresponding system energy level (constant)

Results: ϕ^6 Potential

Benchmark Comparison

- Lattice spacing and time interval for accurate results determined by comparing MATLAB simulations to theoretical prediction
  - $\Delta x = 0.01, \Delta t = 0.001, T_{final} = 2000, N_{runs} = 100$
- These values have significant effect on simulation accuracy:



(a)

(b)

Fig. 3: Comparison of coarser (a) and finer (b) lattice and time intervals.

Potential equation:

$$V = \lambda^2\phi^2(\phi^4 - 6\phi^2 + \alpha_2)$$

Exact PDF solution:

$$\Psi^2 = \exp\left[-\frac{1}{3\sqrt{2}}(\phi^2 - 3)^2\right]$$

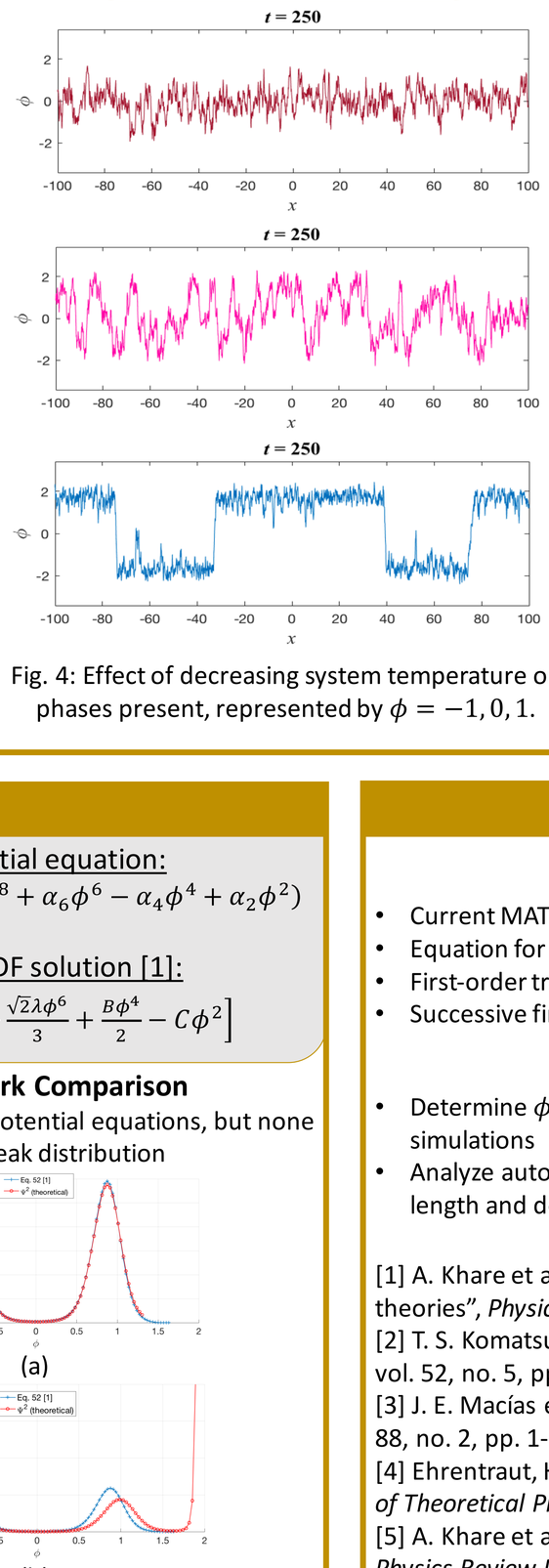
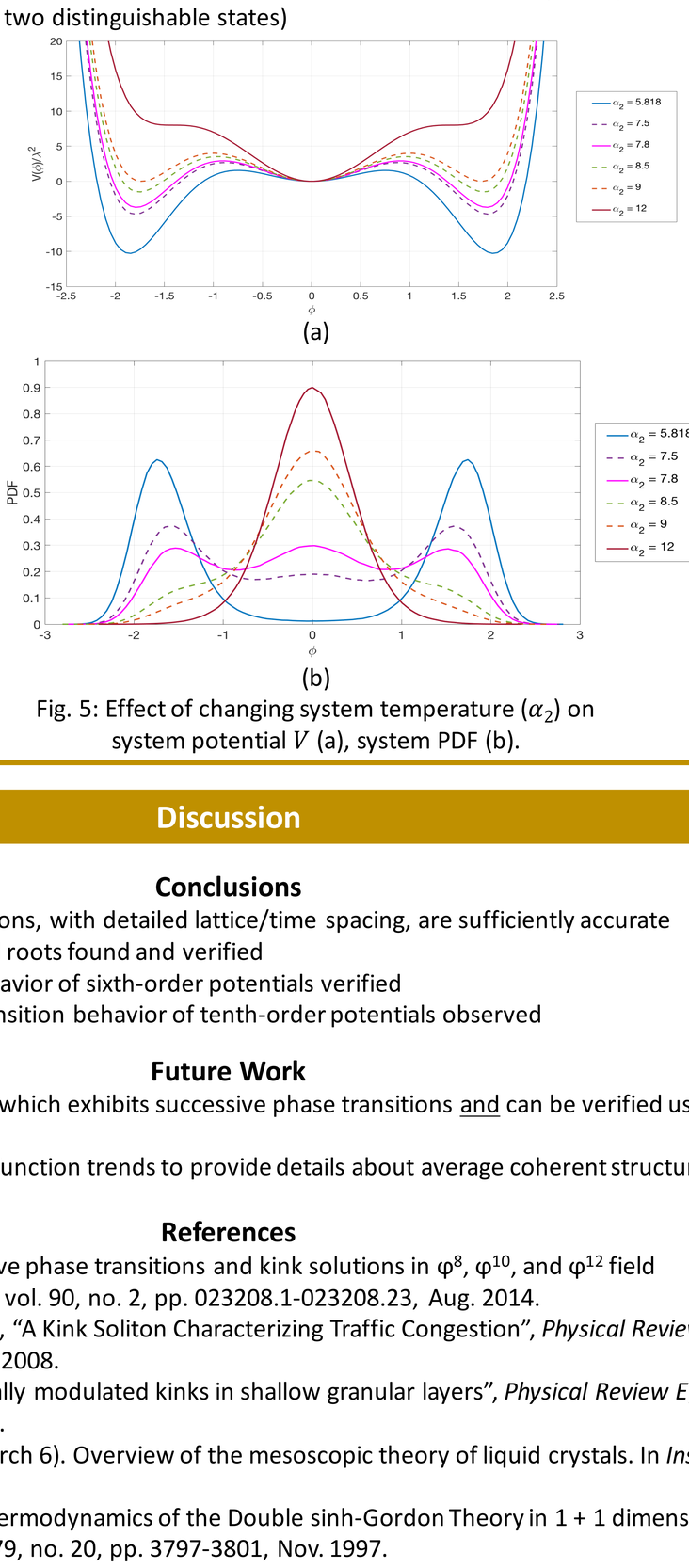


Fig. 4: Effect of decreasing system temperature on phases present, represented by $\phi = -1, 0, 1$.

Phase Transition Behavior

- Sample, verifiable system was investigated
- Temperature of system varied by changing α_2
  - As α_2 increases, temperature (and thus system noise) decreases
  - As temperature decreases, PDF transitions from 1 to 3 to 2 peaks (one excited state to two distinguishable states)



(a)

(b)

Fig. 5: Effect of changing system temperature (α_2) on system potential V (a), system PDF (b).

Results: ϕ^{10} Potential

Phase Transition Behavior

- System observed to exhibit two successive phase transitions, as predicted
  - First: Transitions from 1-3-2 peaks
  - Second: Transitions from 2-4-2 peaks

(a)

(b)

Fig. 6: Effect of changing system temperature on V (a), PDF (b).

Potential equation:

$$V = \lambda^2(\phi^{10} - \alpha_8\phi^8 + \alpha_6\phi^6 - \alpha_4\phi^4 + \alpha_2\phi^2)$$

Exact PDF solution [1]:

$$\Psi^2 = \exp\left[-\frac{\sqrt{2}\lambda\phi^6}{3} + \frac{B\phi^4}{2} - C\phi^2\right]$$

Benchmark Comparison

- Possible for certain potential equations, but none which show a four-peak distribution

(a)

(b)

Fig. 7: Some Ψ^2 representations (a) cannot be properly normalized, as they approach infinity for large values of ϕ (b).

Discussion

Conclusions

- Current MATLAB simulations, with detailed lattice/time spacing, are sufficiently accurate
- Equation for ϕ^6 potential roots found and verified
- First-order transition behavior of sixth-order potentials verified
- Successive first-order transition behavior of tenth-order potentials observed

Future Work

- Determine ϕ^{10} potential which exhibits successive phase transitions and can be verified using simulations
- Analyze autocorrelation function trends to provide details about average coherent structure length and density

References

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[4] Ehrentraut, H. (1997, March 6). Overview of the mesoscopic theory of liquid crystals. In *Institute of Theoretical Physics*.
[5] A. Khare et al., "Exact Thermodynamics of the Double sinh-Gordon Theory in 1 + 1 dimensions", *Physics Review Letters*, vol. 79, no. 20, pp. 3797-3801, Nov. 1997.

Acknowledgements

OUR 2018-2019, SURF 2017