

Analysis on Phases in the Gross-Neveu Model on the Lattice with Shape-based Clustering Method

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- ◆ Motivation & Goal
- ◆ Method : Shape-based Clustering Method
- ◆ Results : 1. Configuration Centroid
2. Analysis on GN model: inhomogeneous phase
- ◆ Summary

Motivation: QCD Phase Diagram at Finite Density

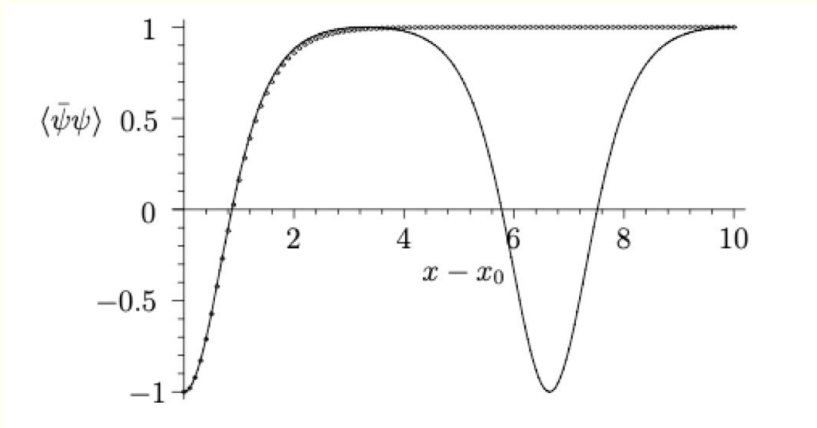
❖ Possible interesting phases at high density



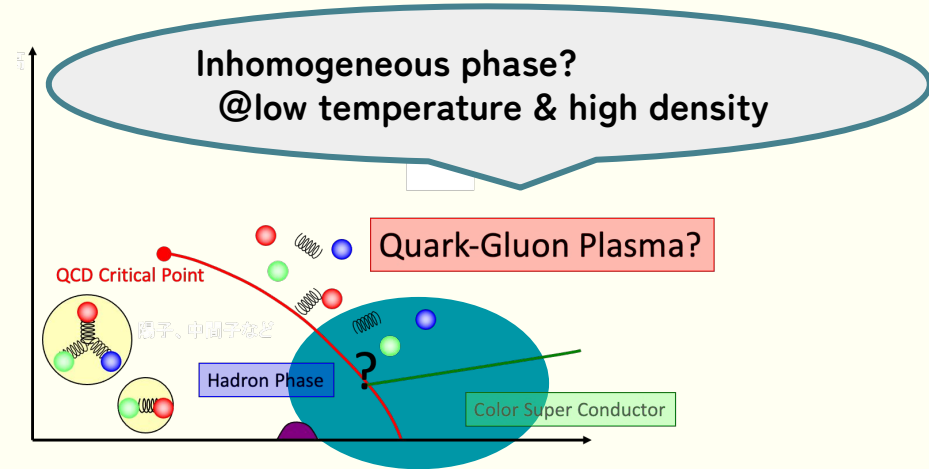
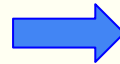
Effective field theory

Inhomogeneous chiral condensation

✧ spatial dependence of chiral condensate $\sigma(x)$



V. Schon and M. Thies, Phys. Rev. D 62, 096002 (2000)



Specific Ansatz @continuous theory
ex) constant, Chiral density wave

A. Heinz et. al., Phys. Rev D 93, no.1 014007 (2016)

Motivation: (1+1)-dimensional Gross-Neveu Model

❖ Lagrangian density

$$\mathcal{L} = \bar{\psi} i \gamma^\nu \partial_\nu \psi + \frac{g^2}{2N} (\bar{\psi} \psi)^2 \quad \sigma \sim \langle \bar{\psi} \psi \rangle$$

D. J. Gross and A. Neveu, Phys. Rev. D 10, 3235 (1974)

Important features from comparison with QCD

- ❑ Asymptotic freedom
- ❑ Spontaneous symmetry breaking of **discrete chiral symmetry**

$$\psi \rightarrow \gamma_5 \psi, \quad \bar{\psi} \rightarrow -\bar{\psi} \gamma_5$$

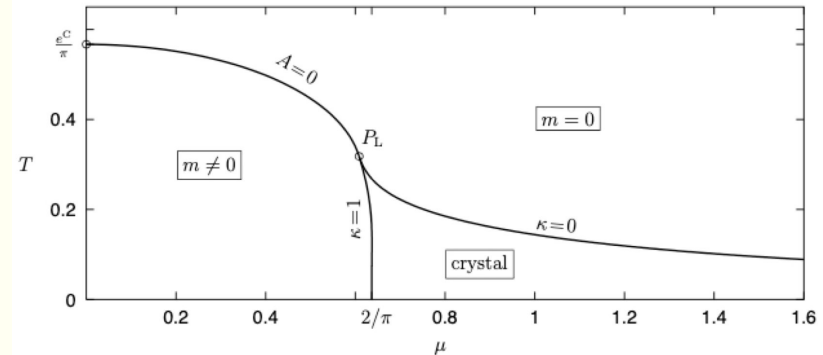
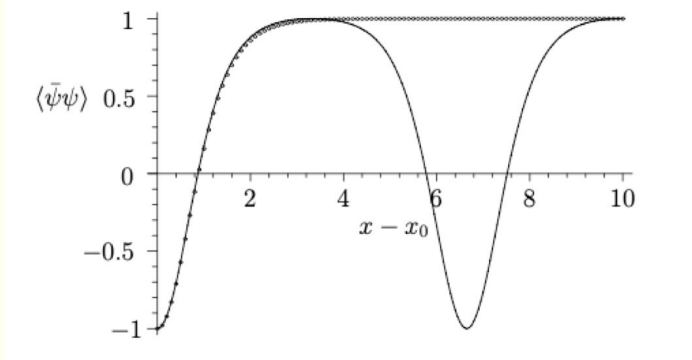
- ❑ **No sign problem** : Monte Carlo simulation
- ❑ Inhomogeneous chiral condensate in large N_f limit

Motivation: (1+1)-dimensional GN Model @ Continuous Theory

- ❖ Lagrangian density in the continuous theory

$$\mathcal{L} = \bar{\psi} i \gamma^\nu \partial_\nu \psi + \frac{g^2}{2N} (\bar{\psi} \psi)^2 \quad \sigma \sim \langle \bar{\psi} \psi \rangle \quad \text{in the large } N_f \text{ limit}$$

- ❖ Specific **ansatz** & phase diagram



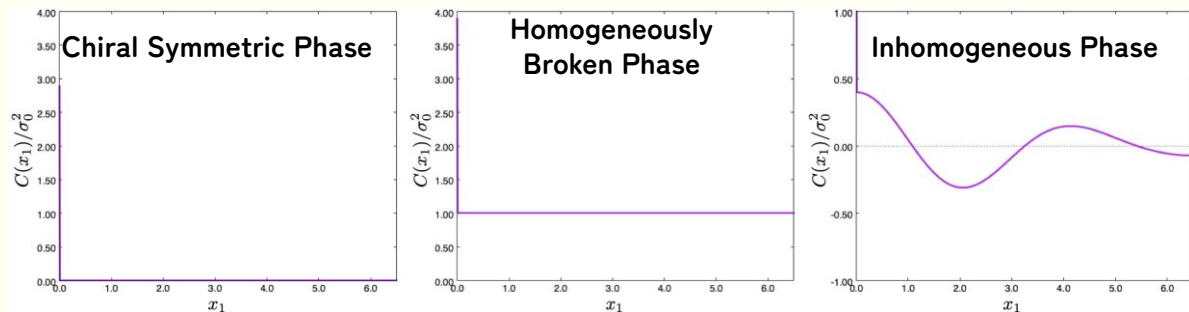
O. Schnetz, M. Thies and K. Urlichs, Annals Phys. 314, 425-447 (2004)



To calculation without ansatz, we use **lattice field theory**

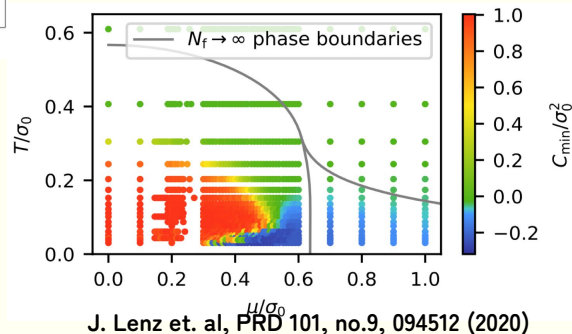
Motivation: (1+1)-dimensional GN Model @ Lattice Theory

❖ Spatial correlators in three phases



❖ Classification by **minimum of the spatial correlator**

$$C_{\min} := \min_x C(x) \begin{cases} \gg 0, & \text{the Homogeneously Broken Phase} \\ \approx 0, & \text{the Chiral Symmetric Phase} \\ \ll 0, & \text{the Inhomogeneous Phase} \end{cases}$$



Knowledge of Ansatz is used in the interpretation of the results.



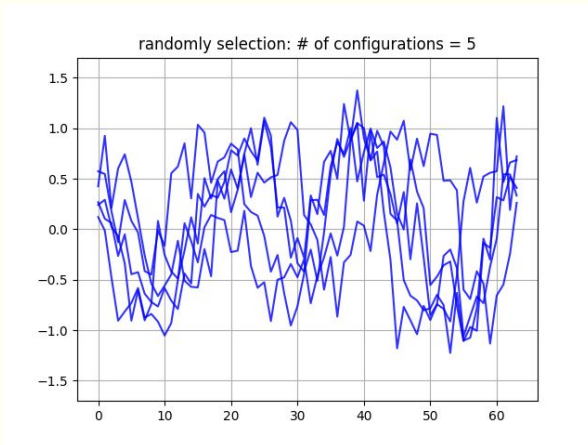
Can we **directly** extract the spatial dependence of the configurations?

Method: Shape-based Clustering Method

❖ Why is it difficult directly to extract the spatial dependence?



The configurations shifted at each Monte Carlo step



When we generate enough number of configurations, the expectation value at each point becomes zero.

→ spatial correlators

Is there a more general and direct method?

We need **shift-invariant** clustering method that focuses on the shape of configurations.



Time Series Clustering Method

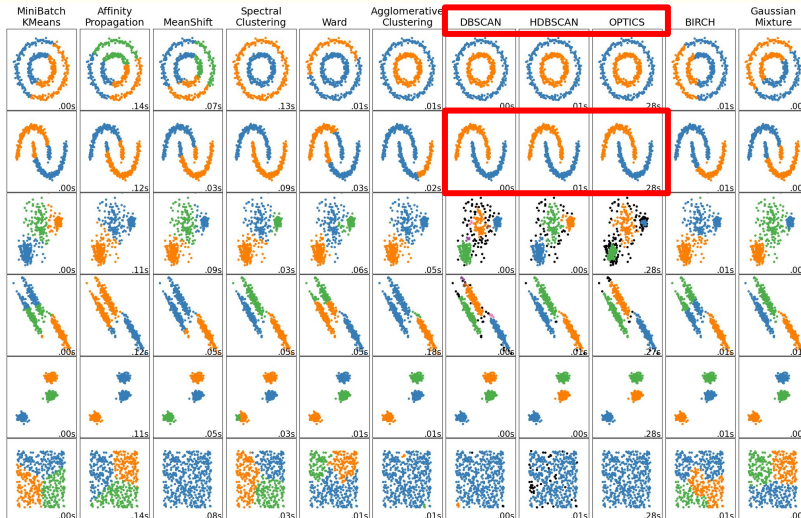
Method: Shape-based Clustering Method

❖ Clustering Method

❑ Unsupervised Learning

A method for grouping data without labeled training data

- ❑ It is important to choose a “similarity” that represents how similar two data points are.



The choice of similarity can lead to differences in the data that can be grouped.

Example:

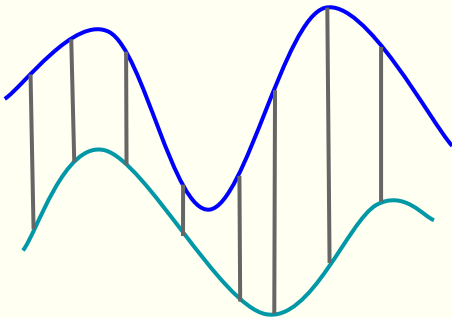
Moon-shaped data are well-suited for density-based similarity calculations such as DBSCAN.

Method: Shape-based Clustering Method

❖ Time Series Clustering Method

- ❑ One of the Clustering methods
- ❑ Clustering methods for time series (1-dimensional data):
- ❑ Major methods:
Dynamic Time Wrapping, K-Shape, k-means, etc...

❖ Simple Example: k-means method with Euclidean distance



“Similarity”:

$$d_E(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^2}$$

Note :

k-means method is not well suited for time series data because the similarity decreases when the phase is shifted.

Method: Shape-based Clustering Method

❖ K-Shape Method



This method is characterized by shift-invariance and scale-invariance

❖ Shape-based Distance (SBD) : the similarity with shift-invariance

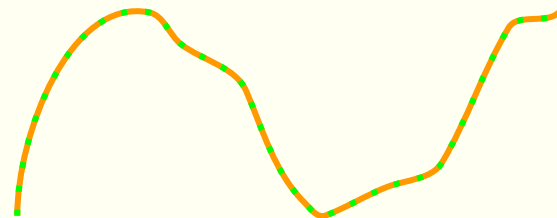
$$SBD(\sigma_1(\mathbf{x}), \sigma_2(\mathbf{x})) = 1 - \max_w \left(\frac{CCF_w(\sigma_1(\mathbf{x}), \sigma_2(\mathbf{x}))}{\sqrt{ACF(\sigma_1(\mathbf{x}))ACF(\sigma_2(\mathbf{x}))}} \right)$$

CCF : cross-correlation function
ACF : auto-correlation function

J. Paparrizos, L. Gravano, PROC. ACM SIGMOD Int. Conf. Manage. Data, pp. 1855-1870, 2015



SBD evaluate similarity
ignoring the phase shift.



Method: Shape-based Clustering Method

❖ Algorithm - Refinement step

INPUT

X is an n -by- m matrix containing n time series of length m that are initially **z-normalized**.
 k is the number of clusters to produce.



while cluster labels don't change or $iter < max$

Refinement step

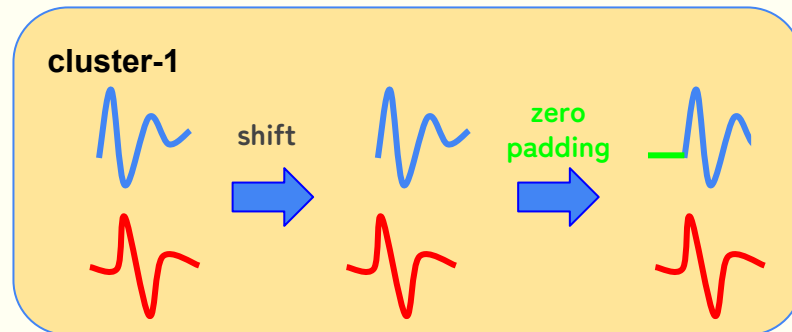
Assignment step



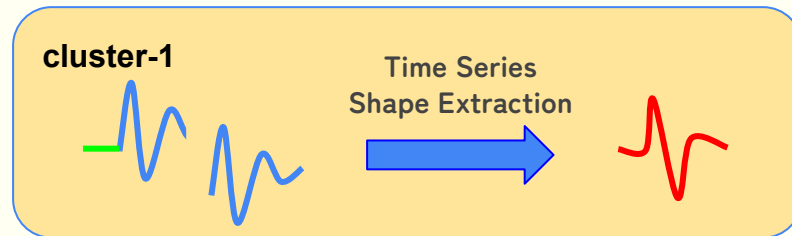
OUTPUT

IDX is an n -by-1 vector containing the assignment of n time series to k clusters (initialized randomly).
 C is a k -by- m matrix containing k **centroids** of length m (initialized as vectors with all zeros).

1. **Shift** each data to overlap with the centroid with minimized SBD



2. Calculate the optimal centroid for each data in the cluster (Time Series Shape Extraction)



Method: Shape-based Clustering Method

❖ Algorithm - Assignment step

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Refinement step

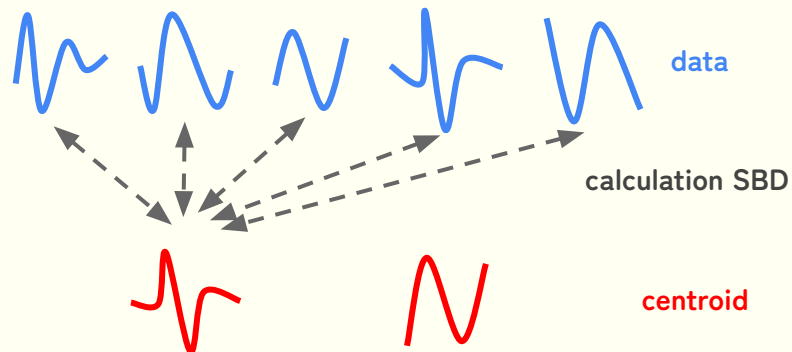
Assignment step



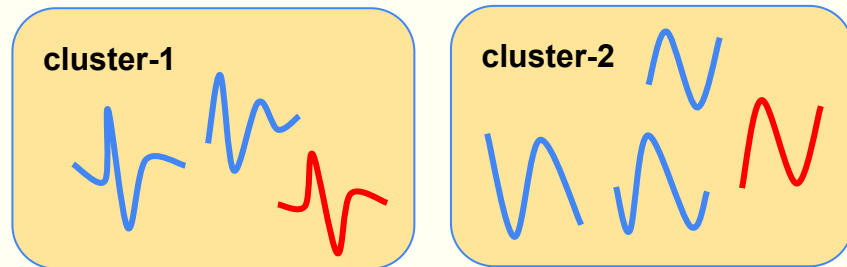
OUTPUT

IDX is an n -by-1 vector containing the assignment of n time series to k clusters (initialized randomly).
 C is a k -by- m matrix containing k **centroids** of length m (initialized as vectors with all zeros).

1. Calculate the **similarity (SBD)** between each **data** and the **centroid**



2. Assign the centroid with the minimum similarity to each data



❖ Time Series Shape Extraction

Maximization problem from SBD

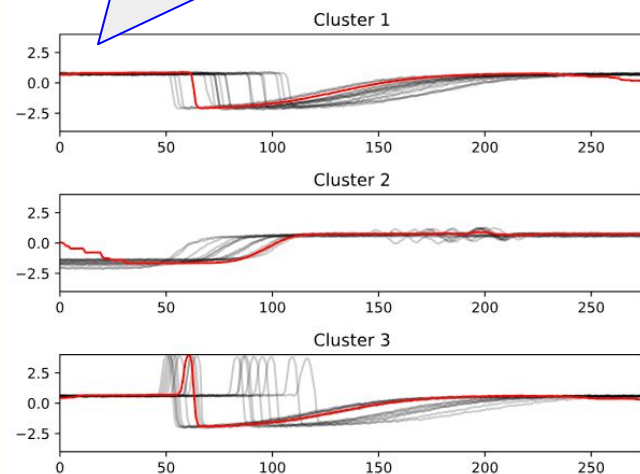
$$\mu_k^* = \operatorname{argmax}_{\mu_k} \sum_{\sigma_i \in \Sigma_k} \left(\frac{\max_w CCF_w(\sigma_i, \mu_k)}{\sqrt{ACF(\sigma)ACF(\mu_k)}} \right)^2$$

μ_k : old centroid in the cluster-k

μ_k^* : updated centroid in the cluster-k

To solve this problem,
we use Rayleigh Quotient.

Red solid lines are centroids μ_k^*



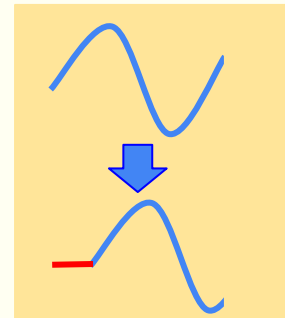
R. Tavenard et. al., JMLR, 21, no.118 (2020) <http://jmlr.org/papers/v21/20-091.html>

Method: Shape-based Clustering Method

❖ Modify K-Shape for lattice simulation

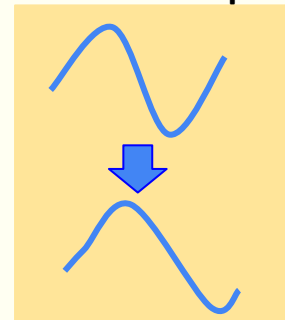
The Original K-Shape : we perform zero padding in the refinement step.

$$\mathbf{x} = \begin{cases} \overbrace{0, \dots, 0}^s, x_1, x_2, \dots, x_{m-s}, & s \geq 0 \\ x_{1-s}, \dots, x_{m-1}, x_m, \underbrace{0, \dots, 0}_{|s|} & s < 0 \end{cases}$$



The Modified K-Shape : we impose periodic boundary condition in the refinement step.

$$\mathbf{x} = \begin{cases} x_{m-s+1}, \dots, x_m, x_1, x_2, \dots, x_{m-s}, & s \geq 0 \\ x_{1-s}, \dots, x_{m-1}, x_m, x_{m+1}, \dots, x_{-s} & s < 0 \end{cases}$$



❖ Lattice Simulation Setup

- We use a standard hybrid Monte Carlo algorithm.
- Lattice discretization of fermions is a naive fermion.
- To set the scale, we use the expectation value at zero temperature and zero chemical potential.
- We use the same coupling constant as the previous study [J. Lenz et. al, PRD 101, no.9, 094512 (2020)].
- The other simulation parameters are described in the table below:

fermion	N_f	$N_s = L/a$	$N_t = 1/Ta$	g^2	$a\sigma_0$	μ/σ_0
naive	8	64	14, 24, 64	1.8132	0.42 ± 0.01	0.0, 0.5, 0.6

❖ Preprocessing

In the equilibrium, configurations do not have time dependence.

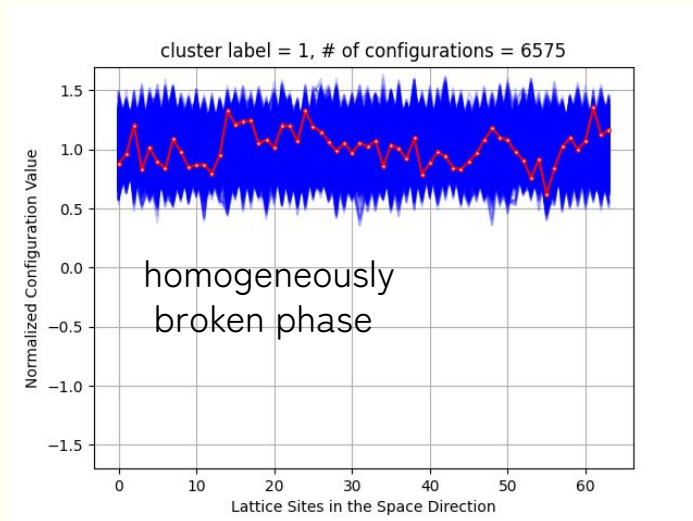
Therefore, we calculate the average of configurations along the time axis.

Results: Shape-based Clustering Method

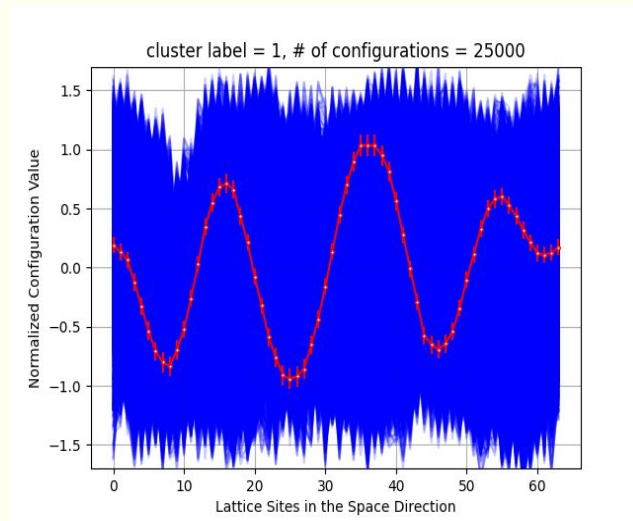
❖ Extraction the spatial dependence of the configurations

- Set the cluster number $k = 1$

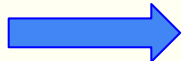
inhomogeneous phase



$$(T/\sigma_0, \mu/\sigma_0) = (0.037, 0.000)$$



$$(T/\sigma_0, \mu/\sigma_0) = (0.098, 0.630)$$



We can extract the spatial dependence without the ansatz!

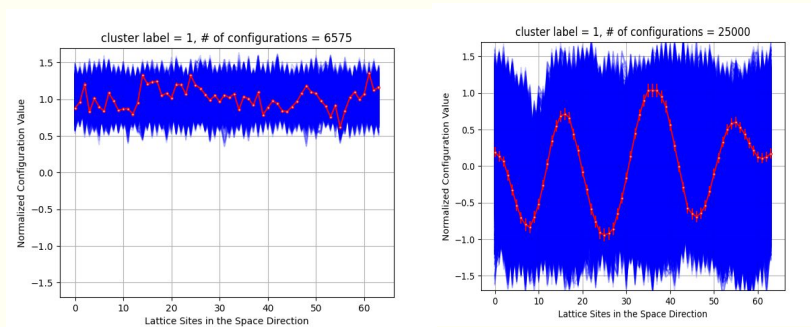
Summary:

Summary

- We applied a shape-based clustering method, a type of unsupervised learning, to the analysis of lattice configurations.
- We modified the method to make it suitable for lattice calculations, including periodic boundary condition.

$$\mathbf{x} = \begin{cases} \overbrace{0, \dots, 0}^s, x_1, x_2, \dots, x_{m-s}, & s \geq 0 \\ x_{1-s}, \dots, x_{m-1}, x_m, \underbrace{0, \dots, 0}_{|s|} & s < 0 \end{cases} \quad \longrightarrow \quad \mathbf{x} = \begin{cases} x_{m-s+1}, \dots, x_m, x_1, x_2, \dots, x_{m-s}, & s \geq 0 \\ x_{1-s}, \dots, x_{m-1}, x_m, x_{m+1}, \dots, x_{-s} & s < 0 \end{cases}$$

- We succeed in extracting the spatial dependence without the knowledge of ansatz.



Future Work

- We will apply this method to the configurations to classify the phases.
- We will use this method to another models with spatial dependent phases.