Machine Learning Study of Frustrated Classical Spin Models

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Collaborator : Hui Zhai

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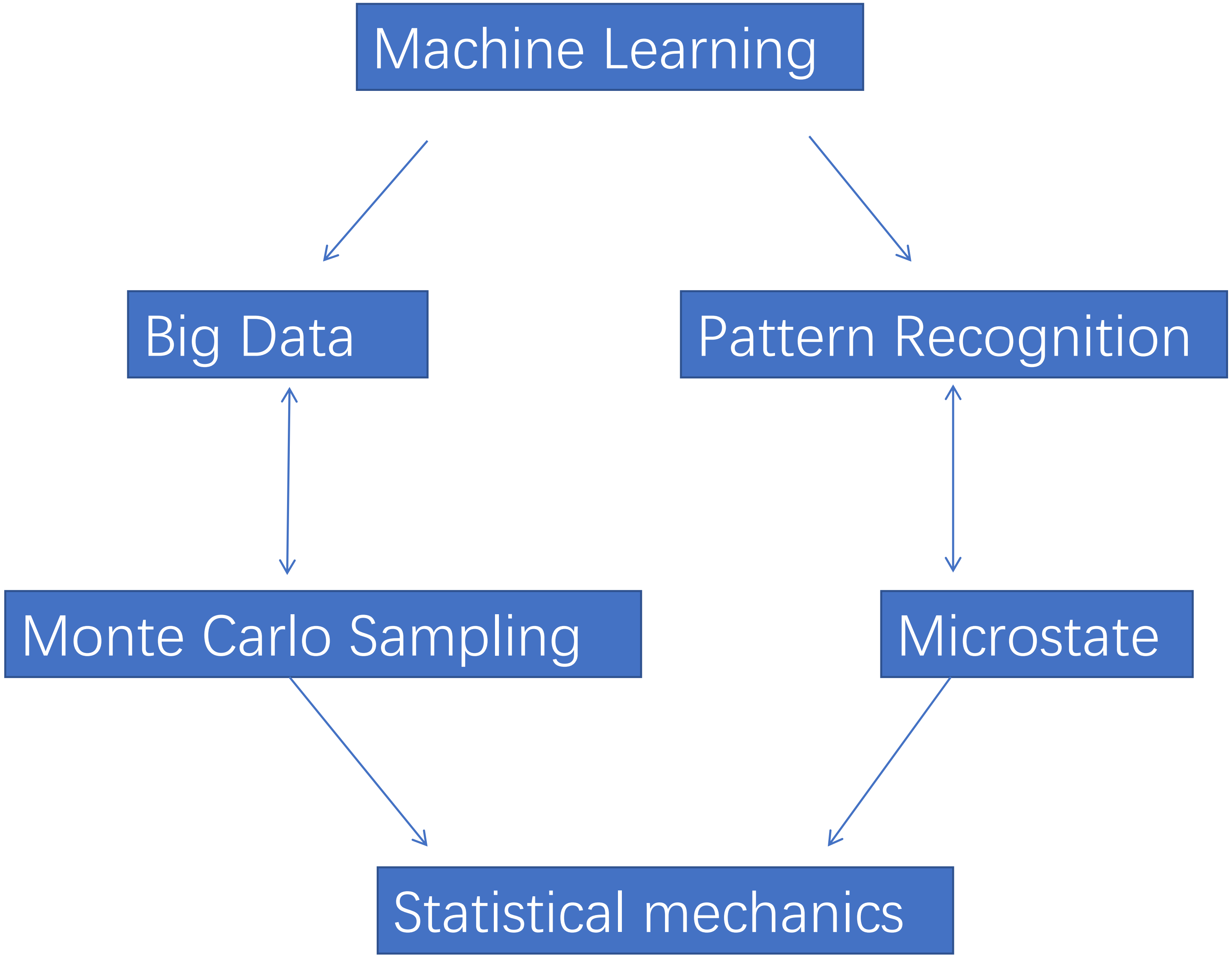
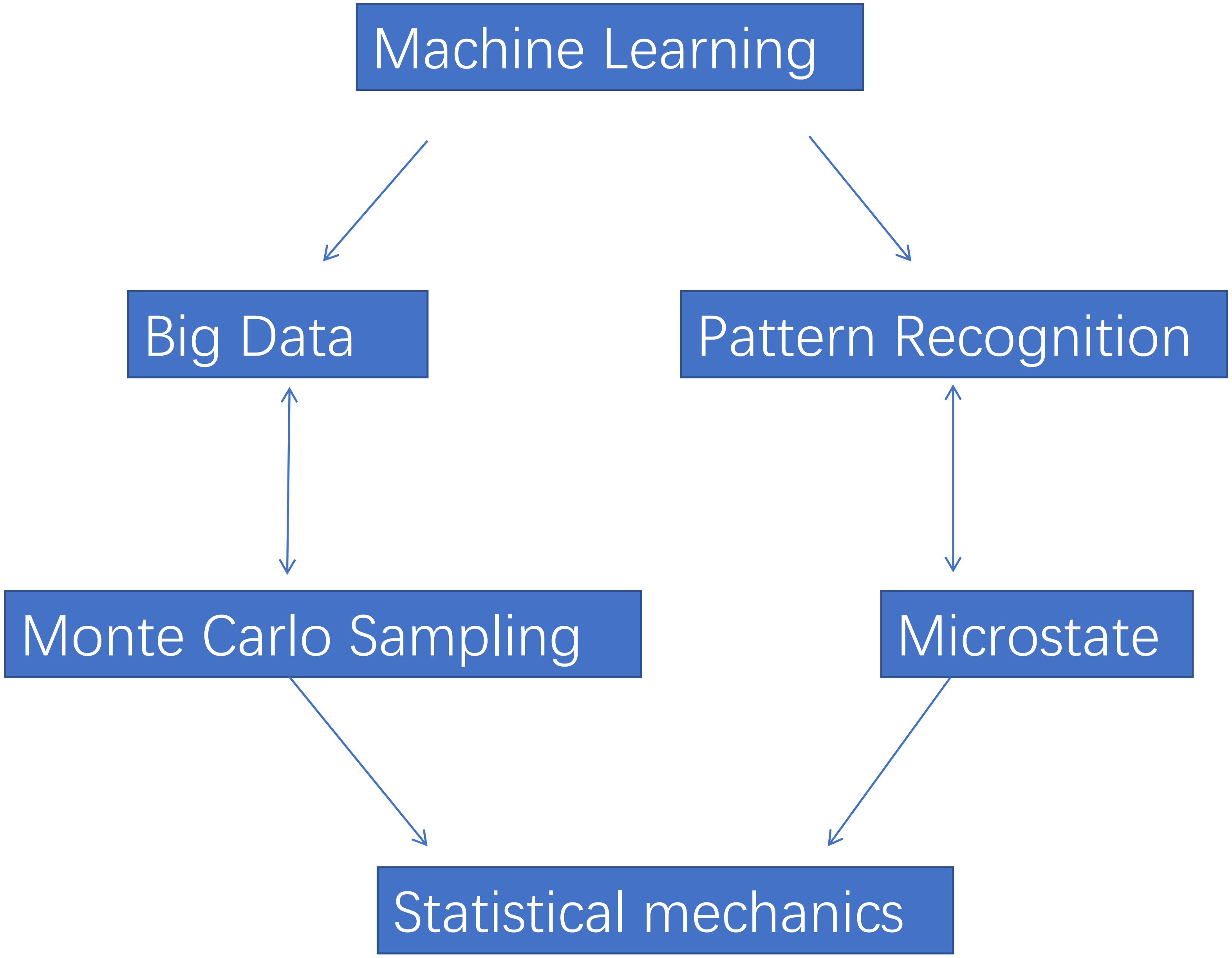
arXiv:1706.07977


Machine Learning
Big Data
Pattern Recognition
Monte Carlo Sampling
Microstate
Statistical mechanics



Supervised learning:

J. Carrasquilla, R. G.Meiko, Nat. Phy. 13, 431-434 (2017). (Ising)
P. Ponte , R. G. Melko. arXIv:1704.05848
...

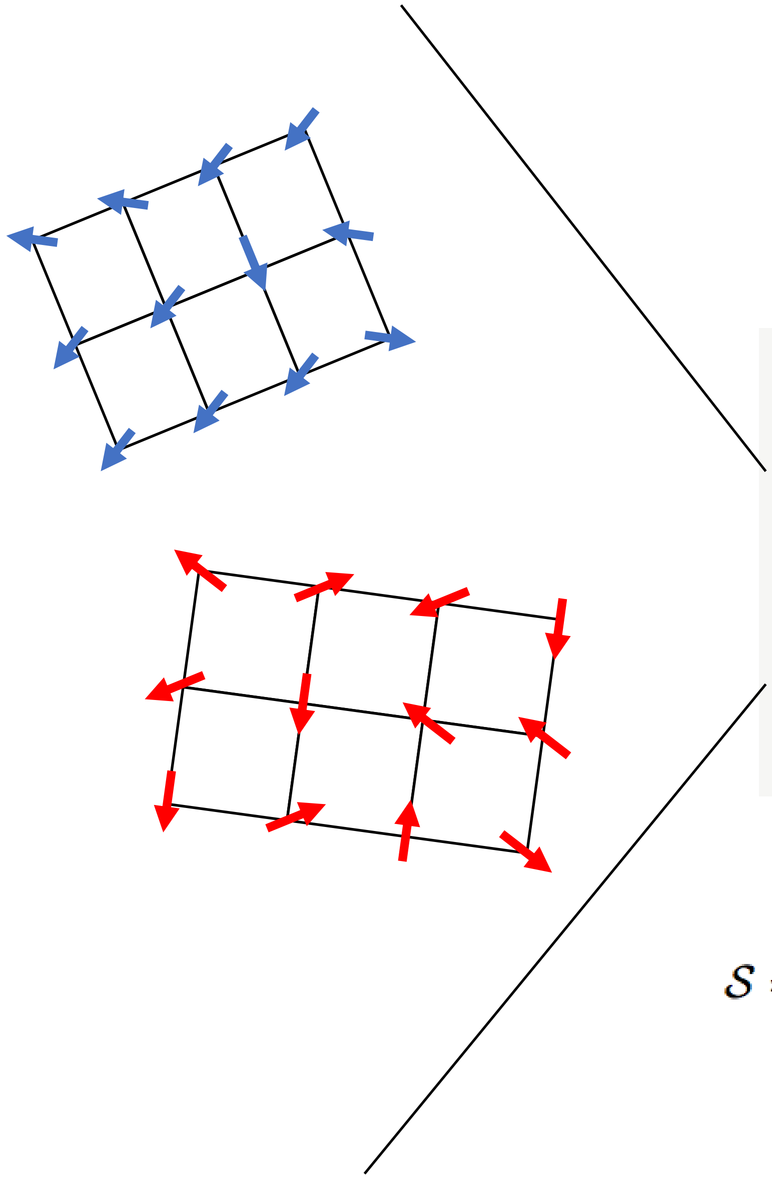
Unsupervised learning:

L. Wang, Phys. Rev. B 94.195105 (2D Ising)

S. J. Wetzel, arXiv:1703.02435 (2D Ising , 3D XY)

W.J. Hu, R. Singh, Richard Scalettar, arxiv:1704.00080. (2D Ising on triangular lattice,···, 2D XY)
...

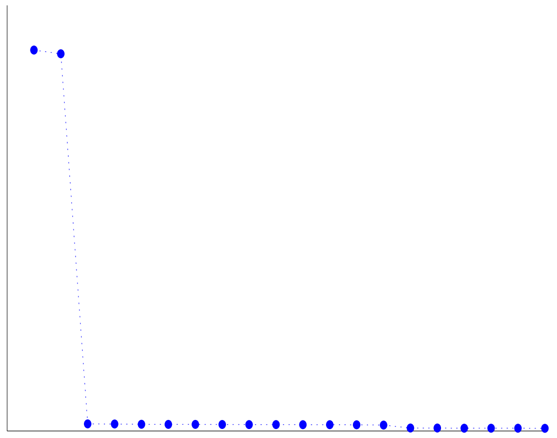
Principle component analysis



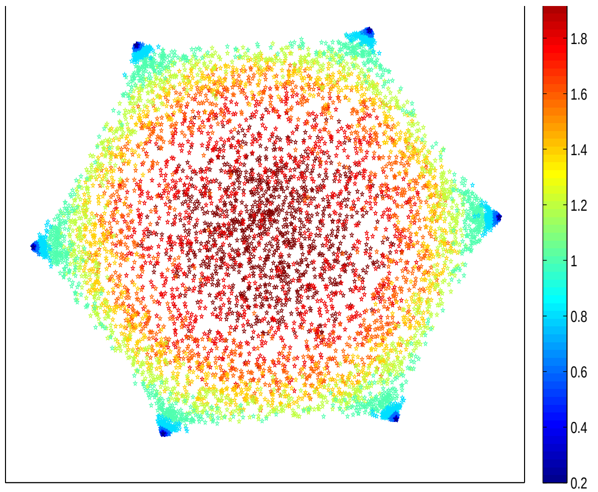
Diagonalization:

$$S = \frac{1}{N}\sum_{n}(x_n - \bar{x})(x_n - \bar{x})^T.$$

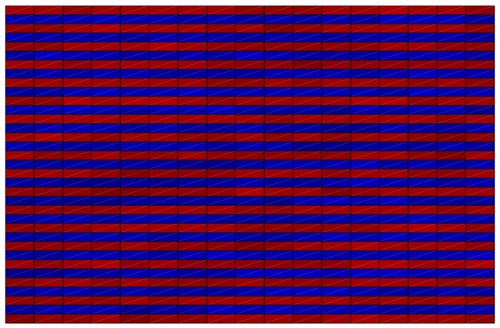
Eigenvalue λ_k



Projection $l_n^k = u_k^T x_n$

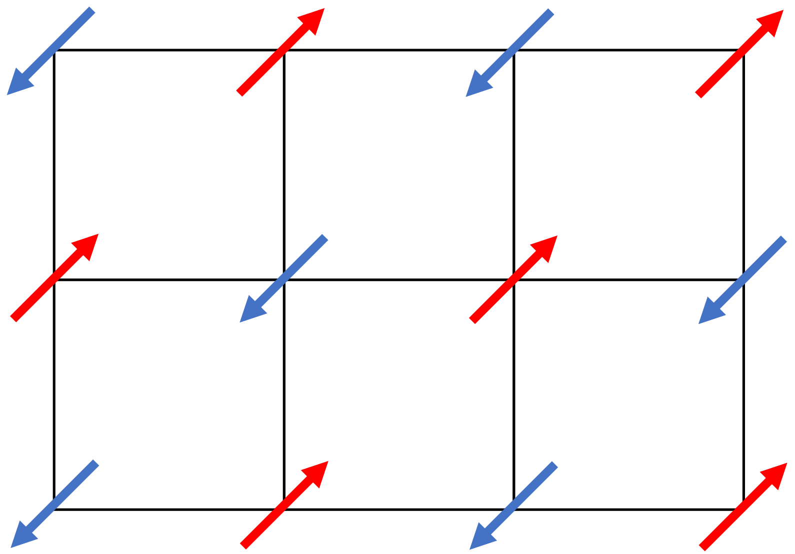


Eigenvector u_k



Example： PCA on 2D XY model on square lattice

$$\mathcal{H} = J\sum_{\langle ij\rangle}\cos(\theta_i - \theta_j)$$



S. J. Wetzel, arXiv:1703.02435
W. J. Hu et.al. arXiv:1704.0080

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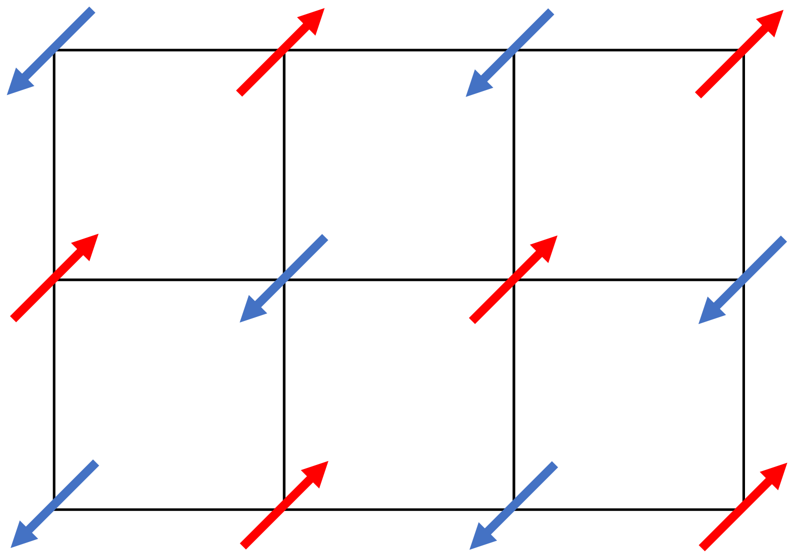

$$(\ldots, \sin\theta_i, \ldots, \cos\theta_i, \ldots)$$

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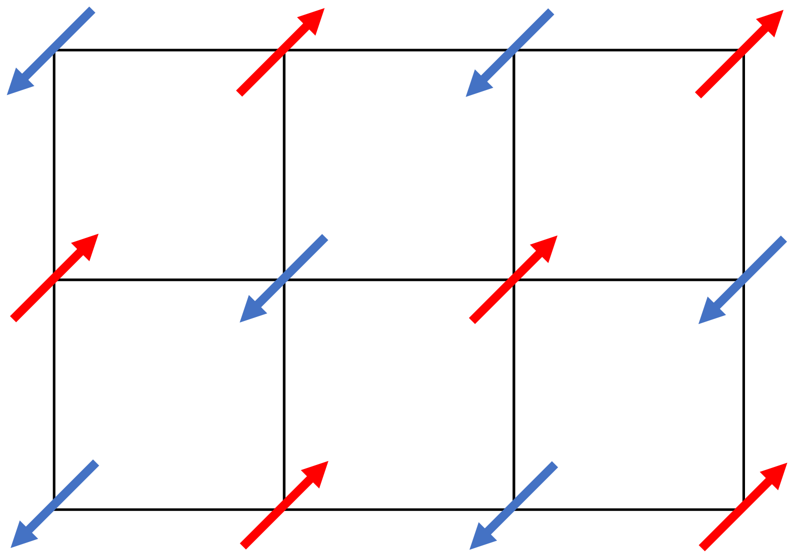

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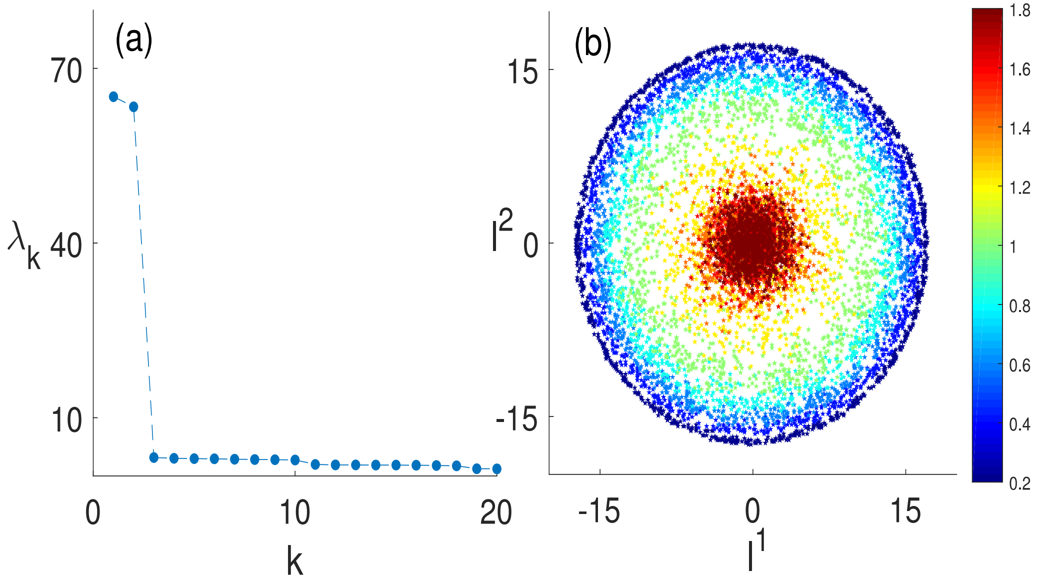
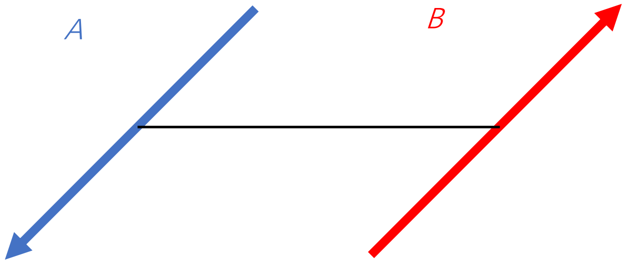


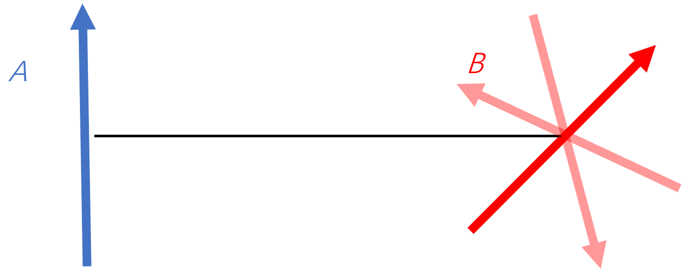
S. J. Wetzel, arXiv:1703.02435
W. J. Hu et.al. arXiv:1704.0080

A toy model

Low T: p $\theta_B = \theta_A + \pi$.

High T: 1-p θ_A θ_B uncorrelated $x_n = (\cos\theta_A, \cos\theta_B, \sin\theta_A, \sin\theta_B)$.





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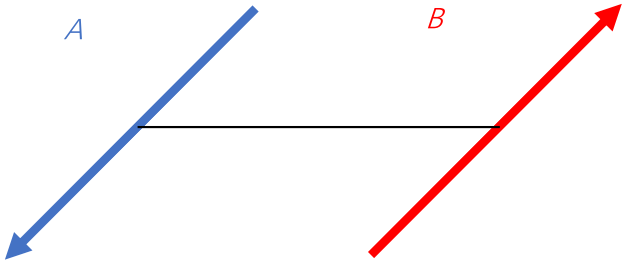

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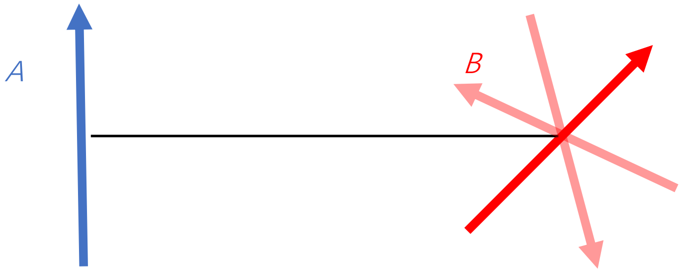

$$\mathcal{S}_l = \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda \end{pmatrix} \quad \Lambda = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

$$\mathcal{S}_h = \mathcal{I}/2,$$

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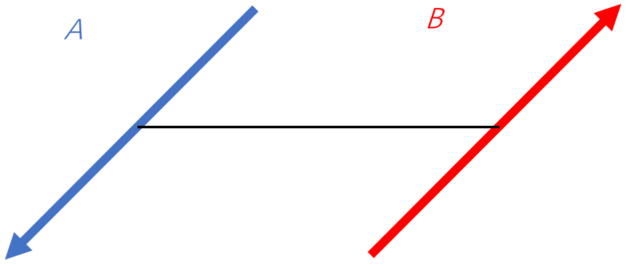

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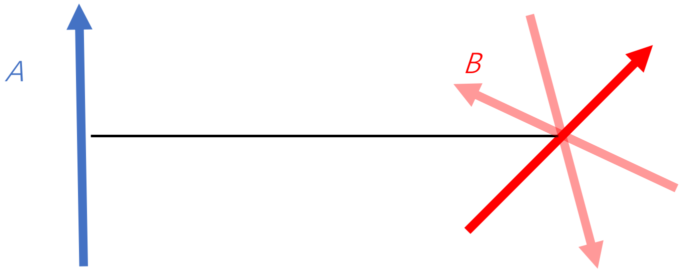

$$\mathcal{S}_h = \mathcal{I}/2,$$

$$x_n = (\cos\theta_A, \cos\theta_B, \sin\theta_A, \sin\theta_B).$$

$$\mathcal{S} = (1-p)\mathcal{S}_h + p\mathcal{S}_l,$$

$$\lambda_1 = \lambda_2 = (1+p)/2,$$

$$\lambda_3 = \lambda_4 = (1-p)/2$$

$$u_1 \propto (1, -1, 0, 0),$$

$$u_2 \propto (0, 0, 1, -1).$$

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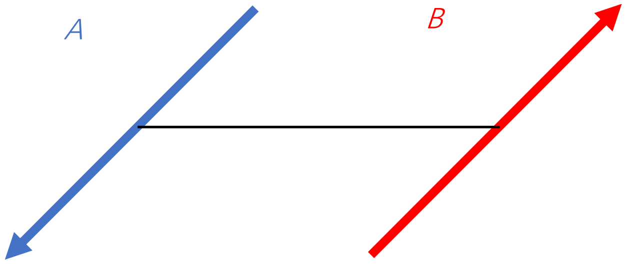

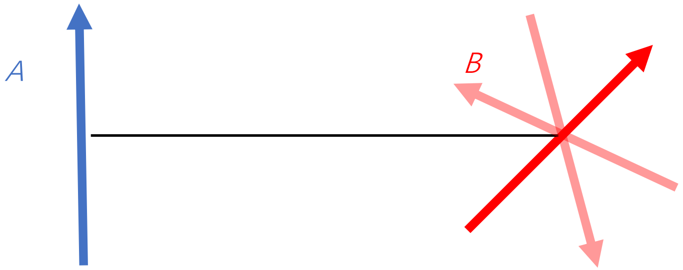

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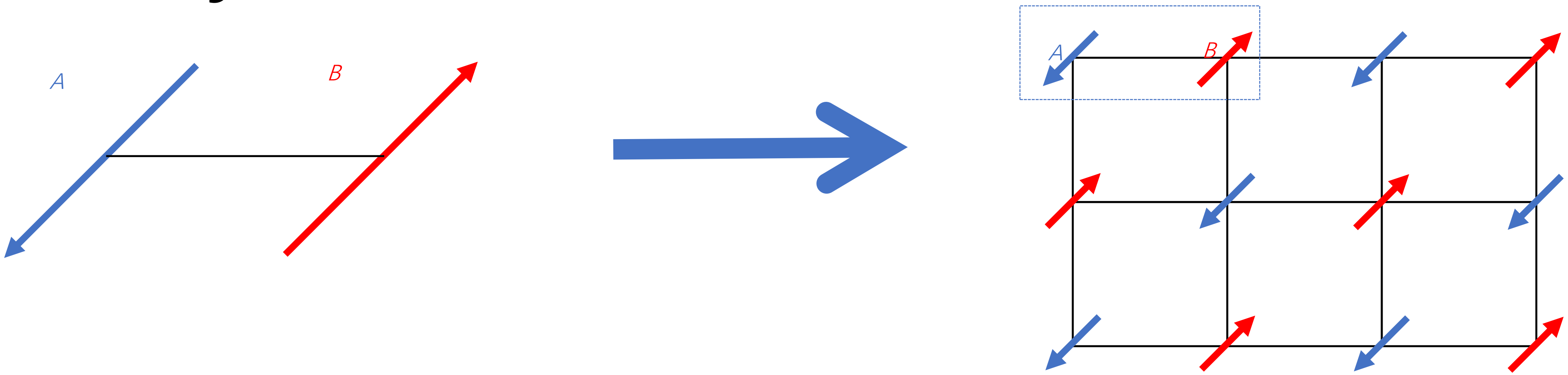
$$\mathcal{S}_h = \mathcal{I}/2,$$

$$l_n \propto (\cos\theta, \sin\theta)$$

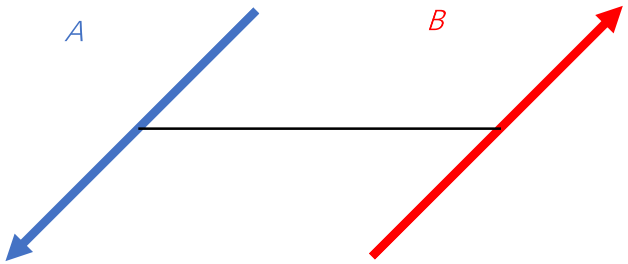
$$l_n \propto (\cos\theta_A - \cos\theta_B, \sin\theta_A - \sin\theta_B)$$

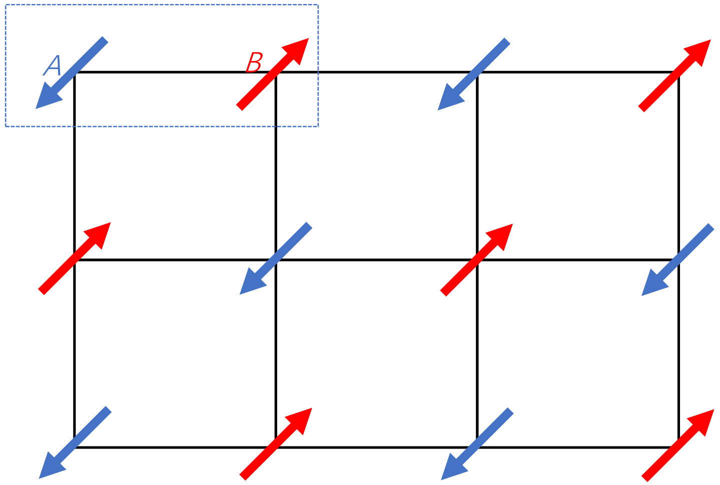
A toy model



$$x_n = (\cos\theta_1, ..., \cos\theta_i, ... \cos\theta_L, \sin\theta_1, ... \sin\theta_i, ... \sin\theta_L)$$

A toy model





$$\mathcal{S}_l = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} \otimes \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda \end{pmatrix} \qquad \mathcal{S}_h = \mathcal{I}/2,$$

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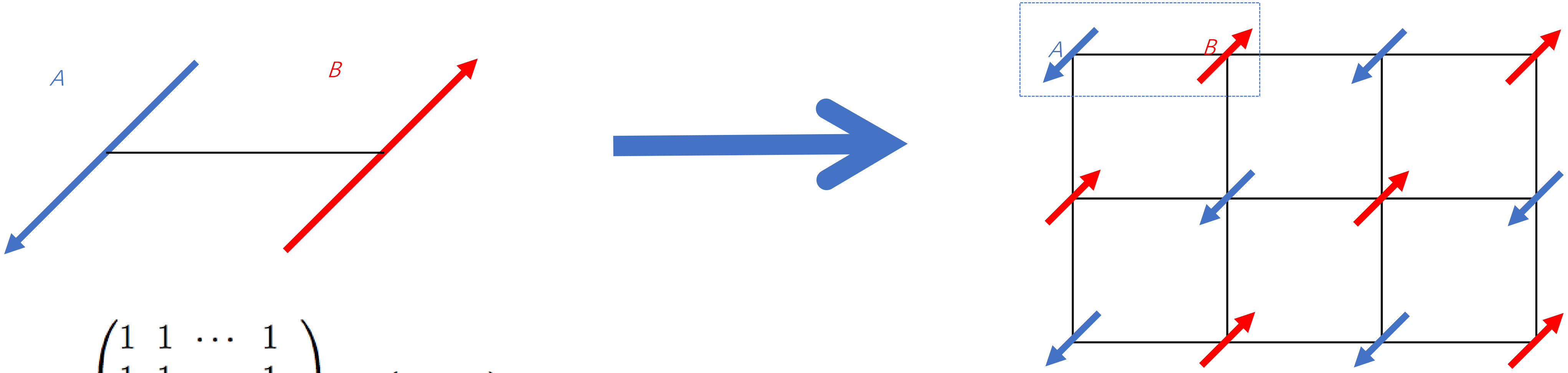
A toy model



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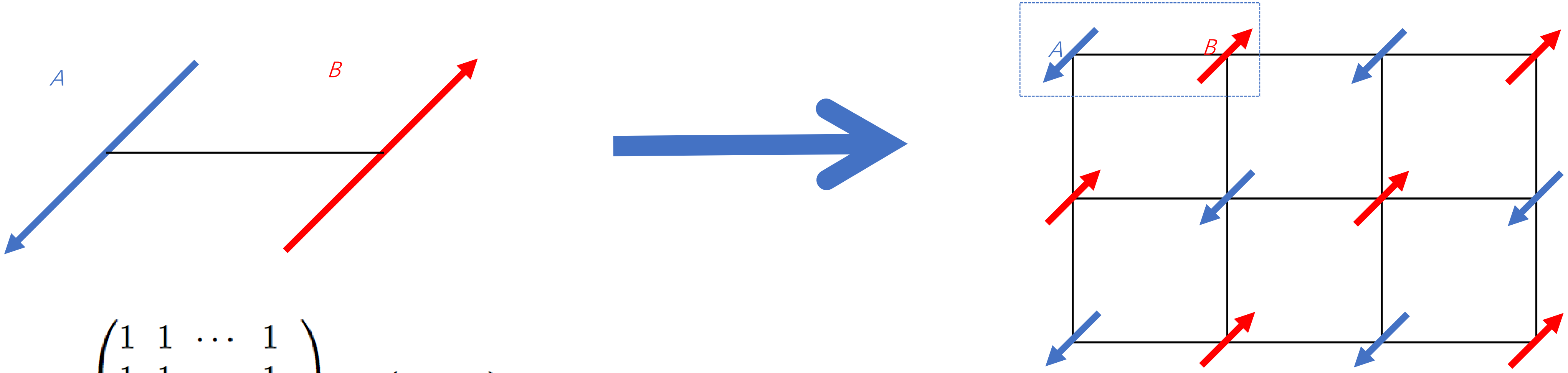
$$\lambda_1 = \lambda_2 = (1 + (L/2 - 1)p)/2 \quad \lambda_i = (1 - p)/2 \quad (i > 2)$$

$$u_1 \propto (1, -1, \ldots, 1, -1, 0, 0, \ldots, 0, 0),$$
$$u_2 \propto (0, 0, \ldots, 0, 0, 1, -1, \ldots, 1, -1).$$

Low T: $l_n \propto (\cos\theta, \sin\theta)$ *High T*: $l_n \propto (0, 0)$

A toy model



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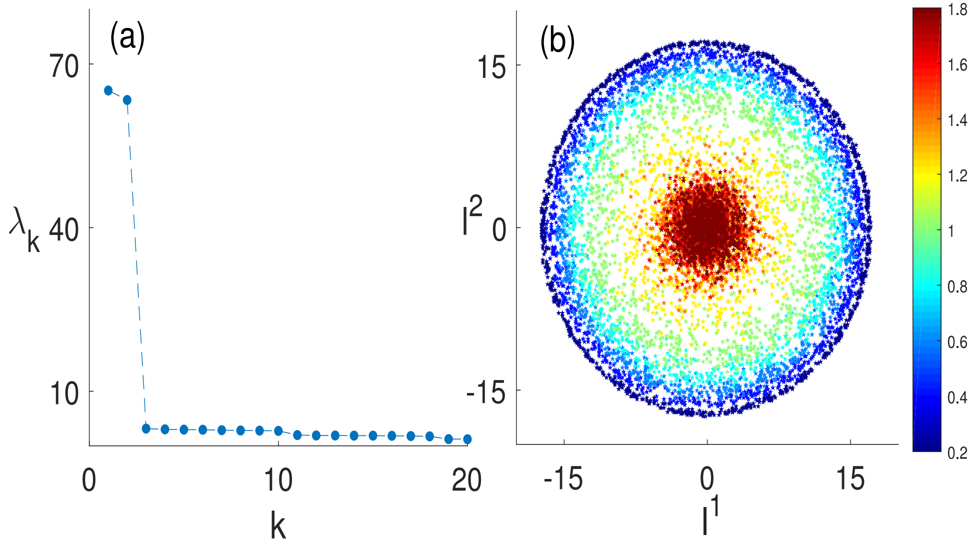
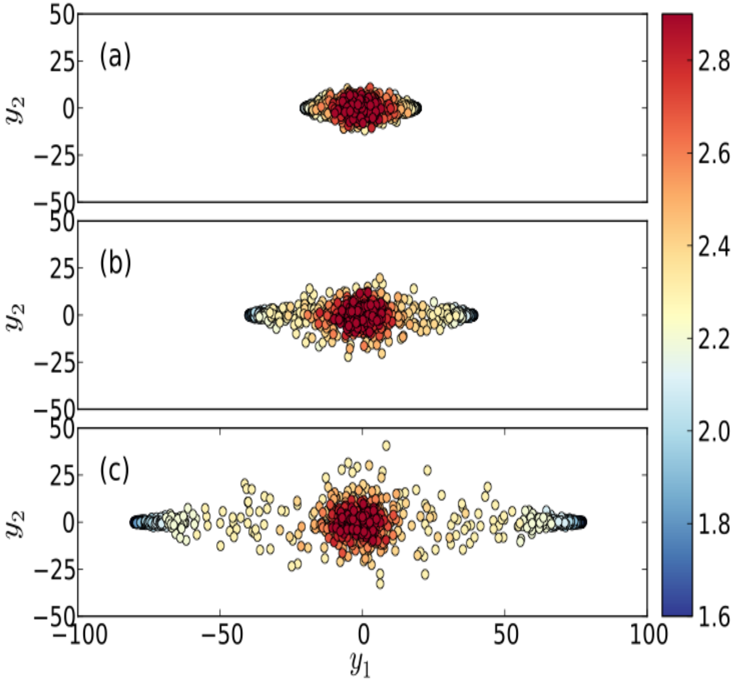
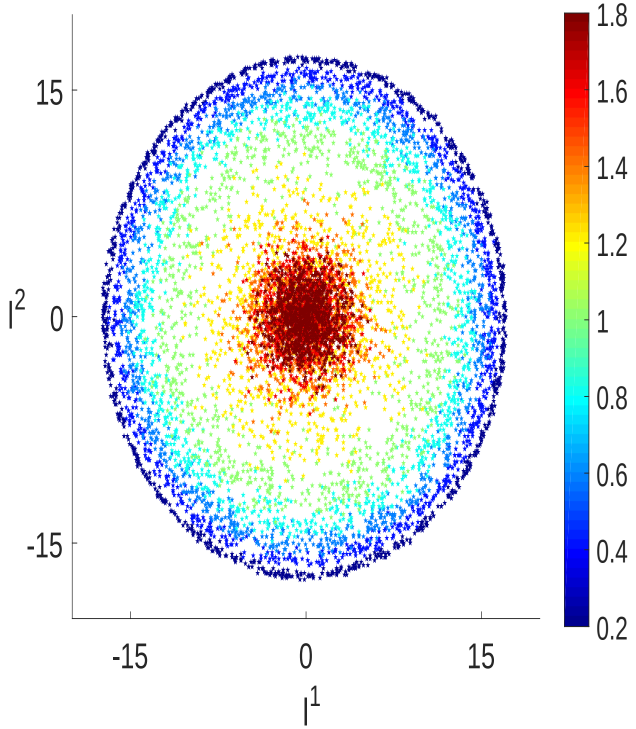


Ising model



Z_2

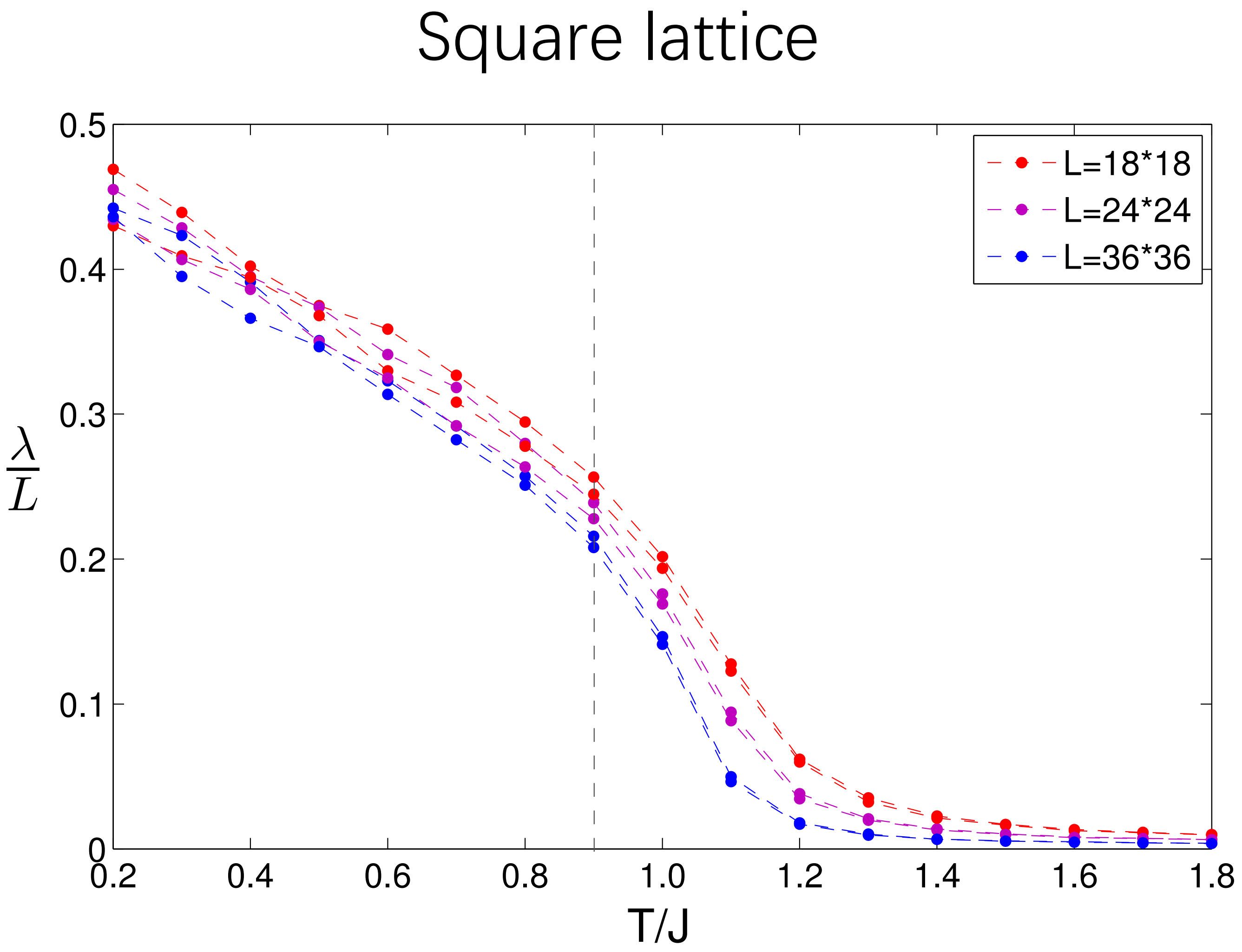
2D square lattice XY



U_1

L. Wang, Phys. Rev. B **94**.195105(2016)

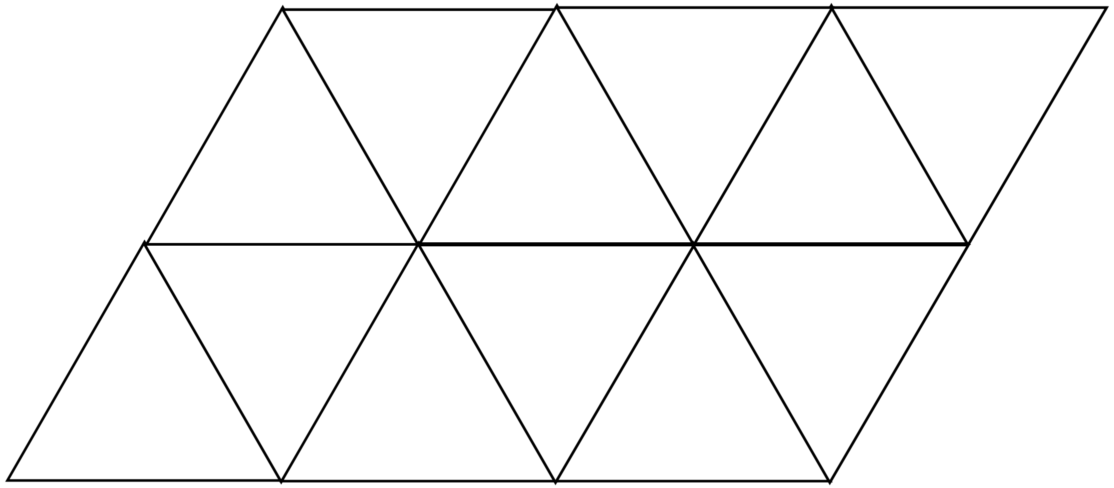
Temperature resolved PCA



What if the model has more than one order parameters or phase transitions?

Triangular lattice

Frustrated XY model : $$\mathcal{H} = J\sum_{\langle ij\rangle}\cos(\theta_i - \theta_j)$$



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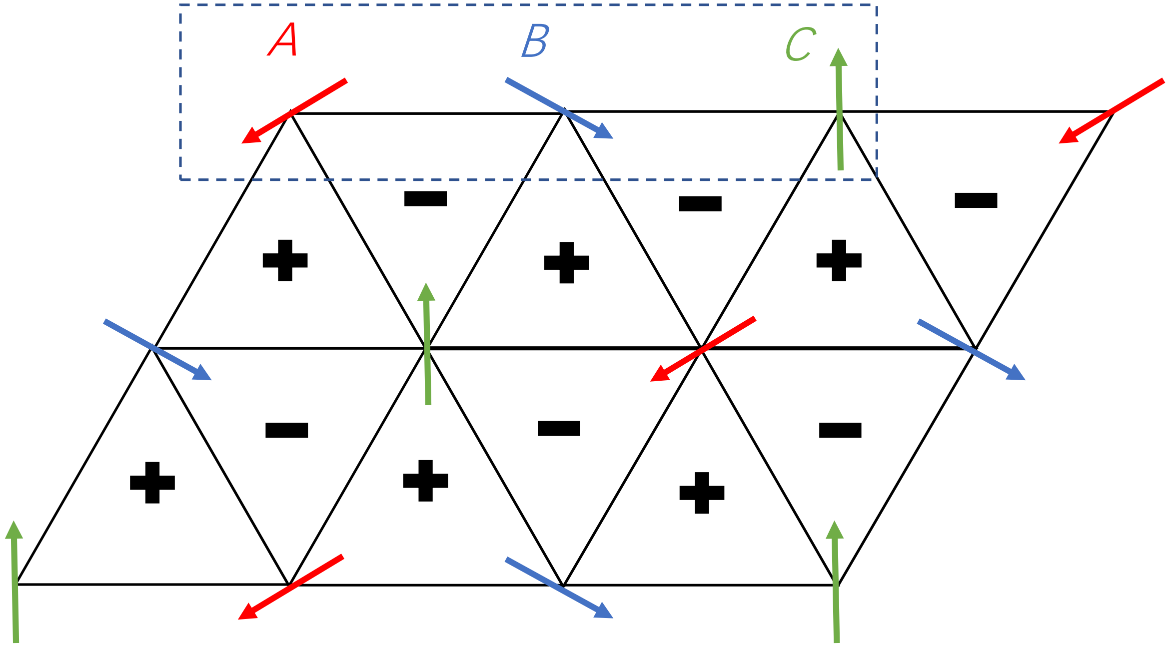

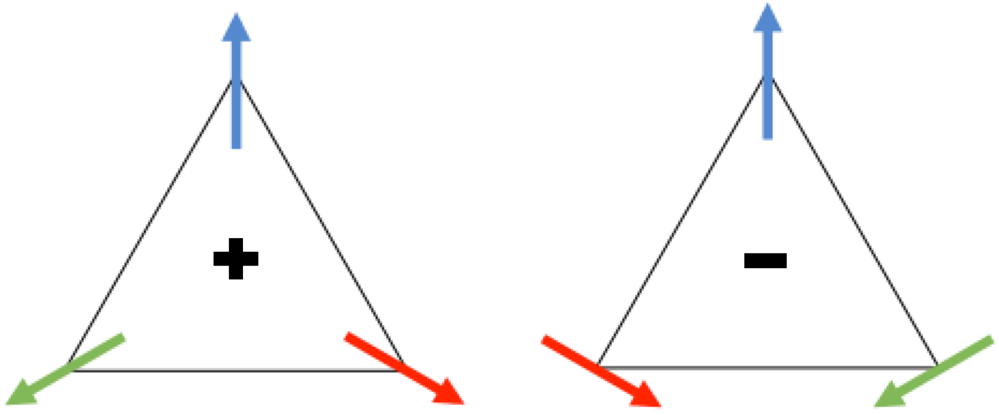

$\theta_A - \frac{4\pi}{3} = \theta_B - \frac{2\pi}{3} = \theta_C$ $\theta_A + \frac{4\pi}{3} = \theta_B + \frac{2\pi}{3} = \theta_C$

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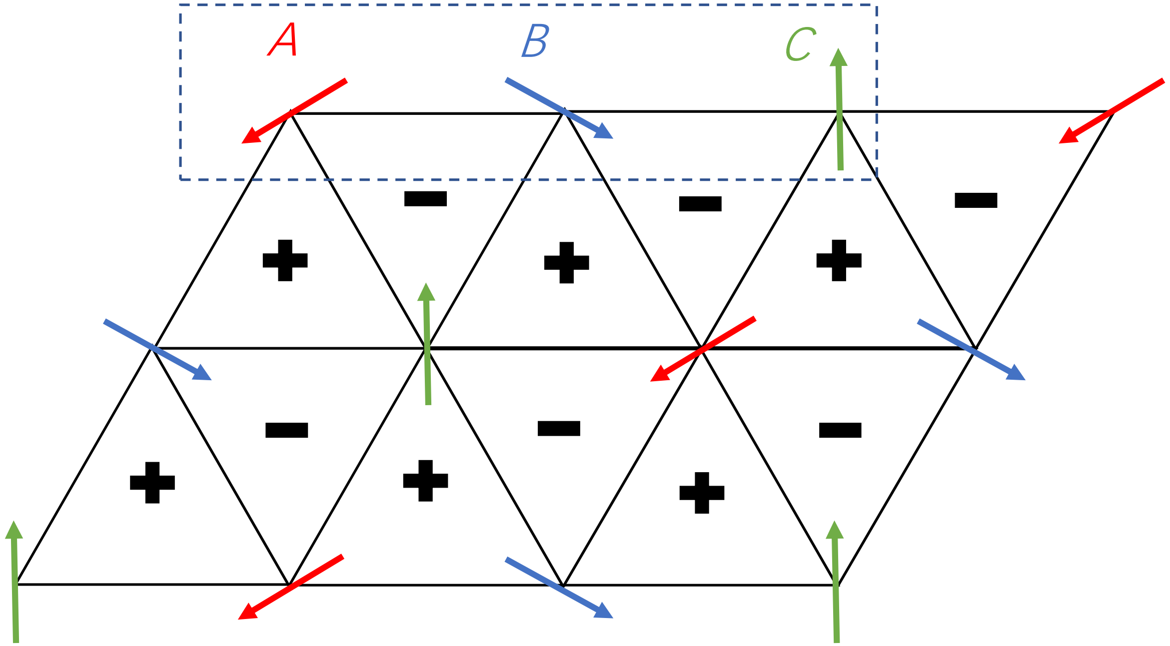

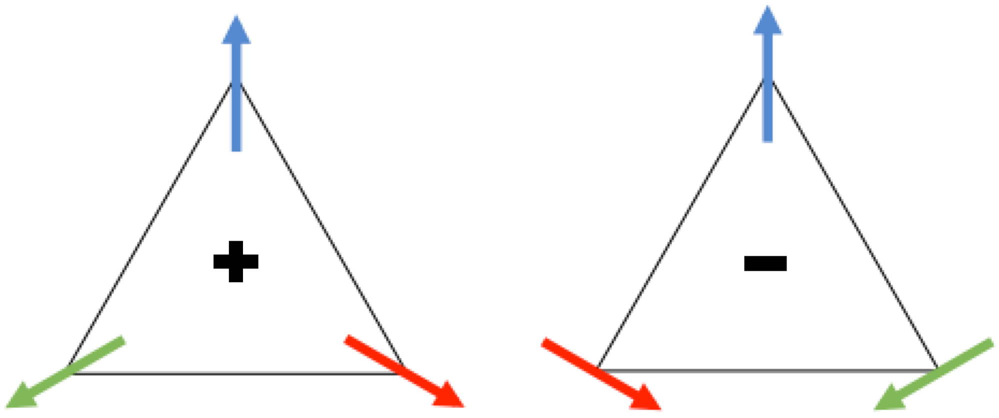

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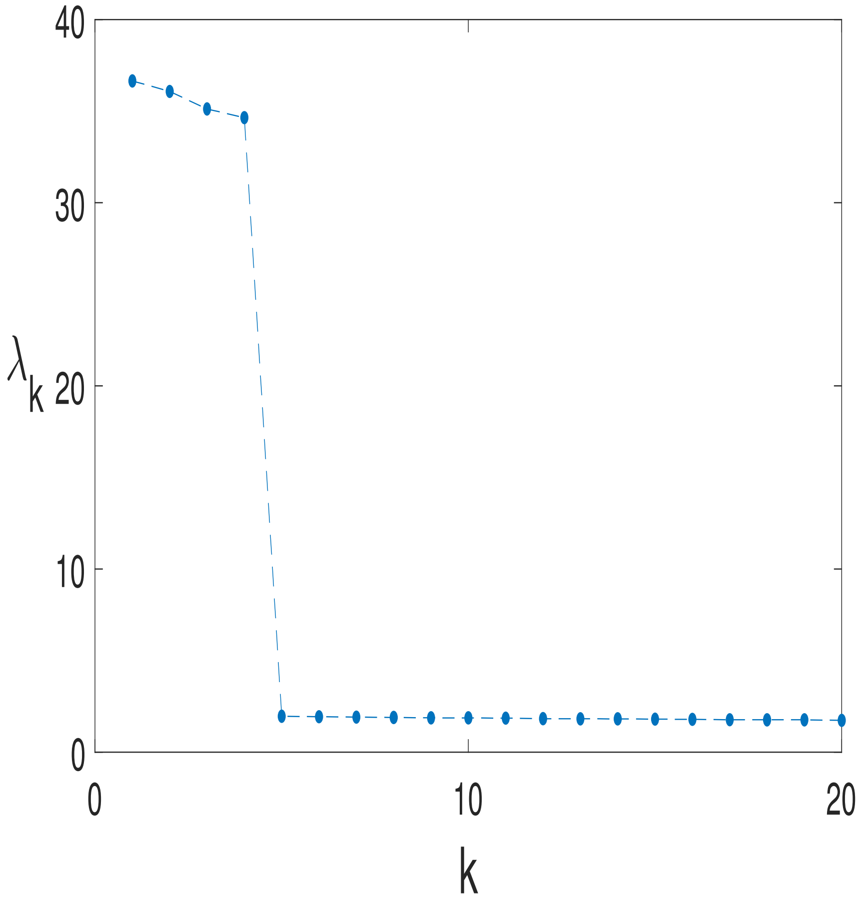
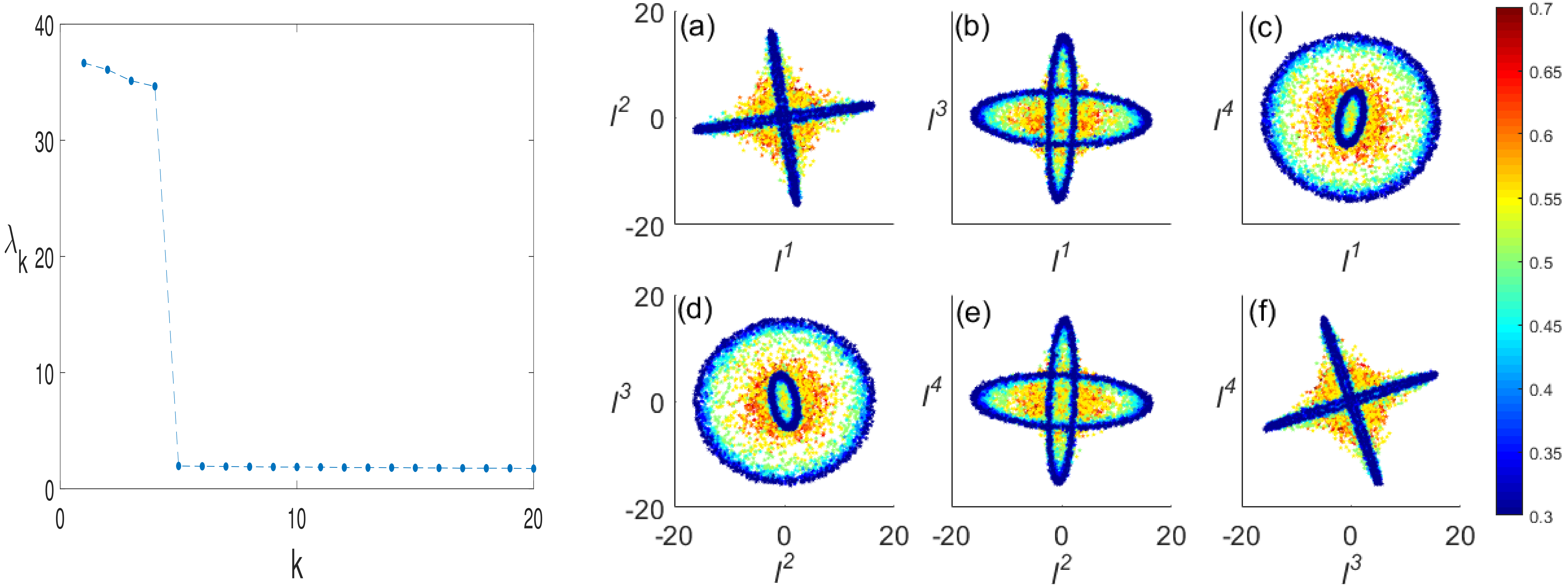
Two close phase transition:
Z2 chiral order ~ T = 0.512J
U(1) spin order ~ T = 0.504J

J. P. Lv et.al Phys. Rev. B **87**,024108 (2013)



40
30
20
10
0
λ_k
0
10
20
k

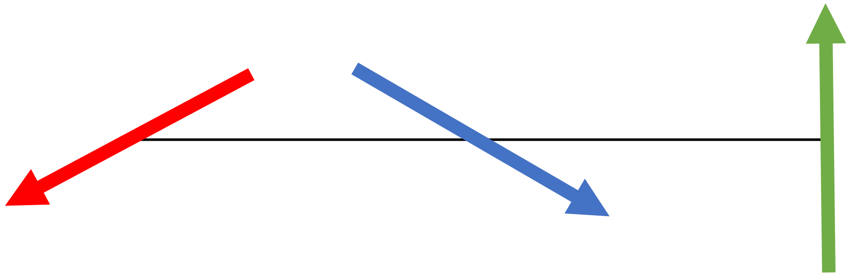


λk
k
(a)
(b)
(c)
(d)
(e)
(f)

Triangular lattice

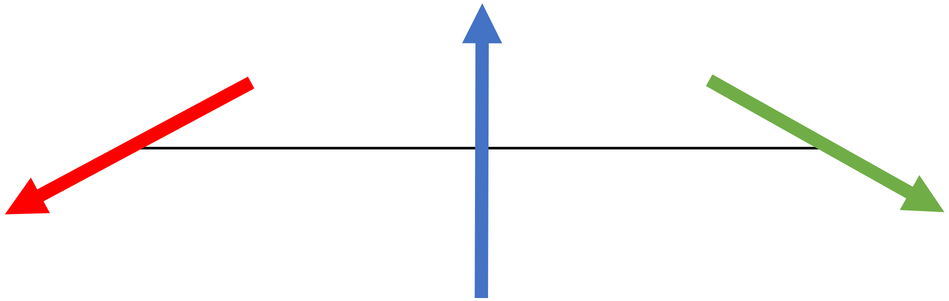
Low T: *p*/2

$$\theta_A - \frac{4\pi}{3} = \theta_B - \frac{2\pi}{3} = \theta_C$$



p/2

$$\theta_A + \frac{4\pi}{3} = \theta_B + \frac{2\pi}{3} = \theta_C$$



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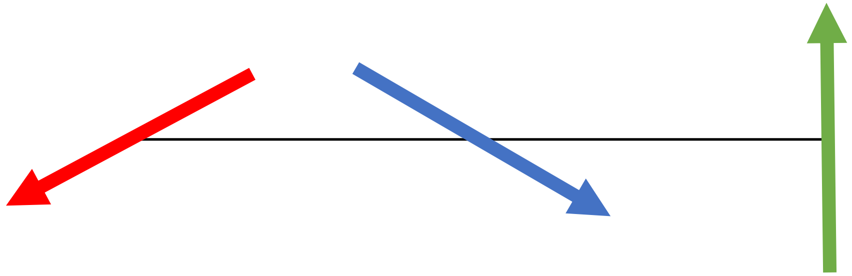

p/2

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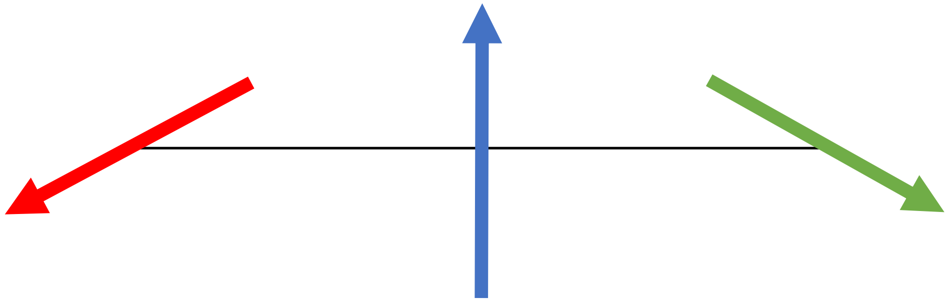

$$\mathcal{S}_l = \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda \end{pmatrix} \quad \Lambda = \frac{1}{2}\begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix}$$

Triangular lattice

Low T: *p/2*

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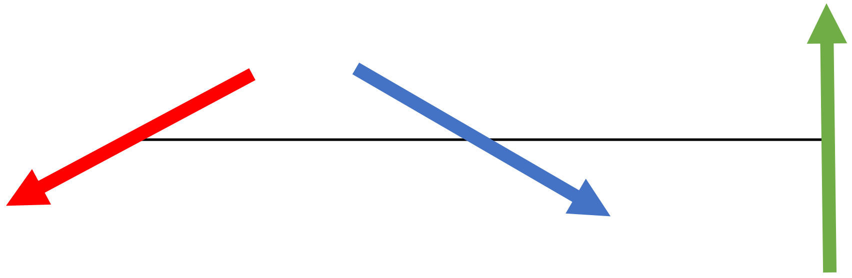
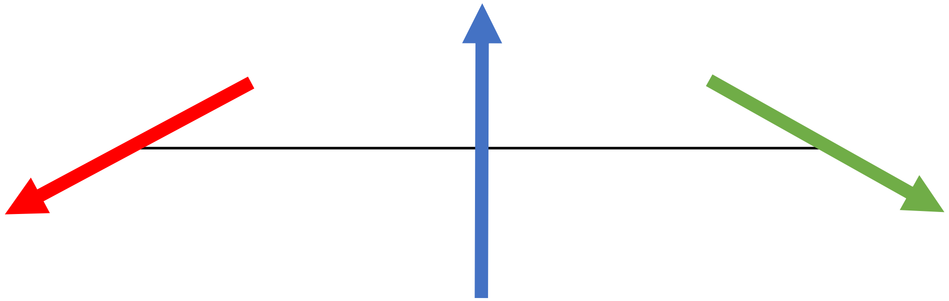


p/2

$$\theta_A + \frac{4\pi}{3} = \theta_B + \frac{2\pi}{3} = \theta_C$$



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$$u_1 = (d_2, 0);$$
$$u_2 = (0, d_2);$$
$$u_3 = (d_1, 0);$$
$$u_4 = (0, d_1).$$

$$d_1 \propto \left(1, \cos\left(\frac{2\pi}{3}\right), \cos\left(\frac{4\pi}{3}\right)\right) \propto (2, -1, -1),$$
$$d_2 \propto \left(0, \sin\left(\frac{2\pi}{3}\right), \sin\left(\frac{4\pi}{3}\right)\right) \propto (0, 1, -1).$$

Triangular lattice

Low T: *p*/2

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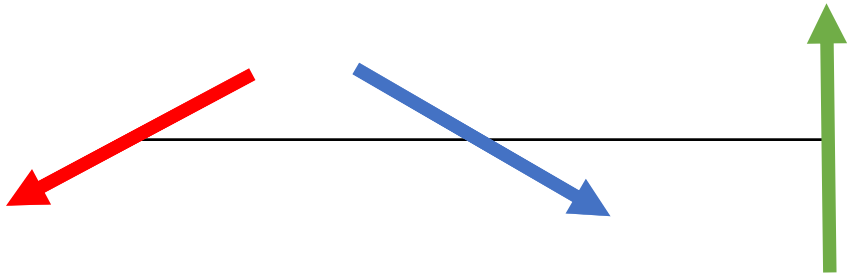

p/2

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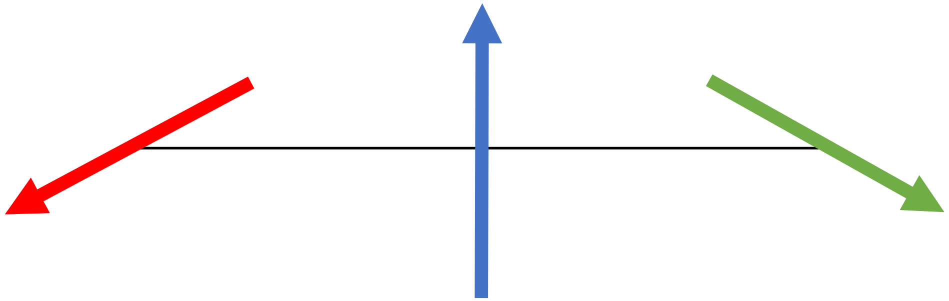

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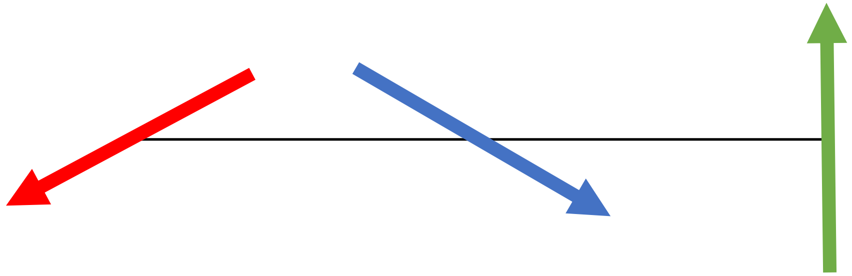
$$l_n^{\uparrow} \sim (-\sin\theta, \cos\theta, \cos\theta, -\sin\theta)$$

$$l_n^{\downarrow} \sim (\sin\theta, -\cos\theta, \cos\theta, \sin\theta)$$

Triangular lattice

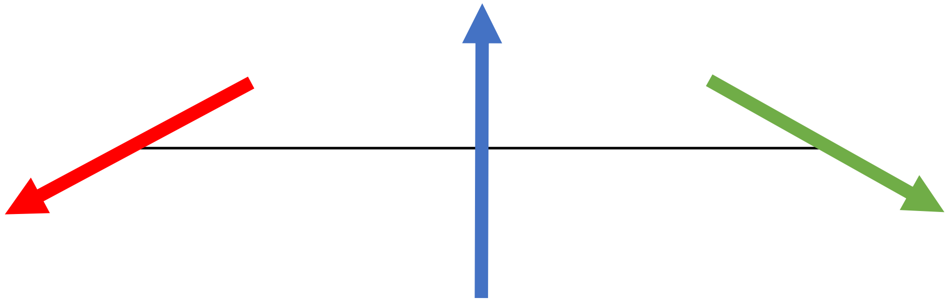
Low T: *p*/2

$$\theta_A - \frac{4\pi}{3} = \theta_B - \frac{2\pi}{3} = \theta_C$$



p/2

$$\theta_A + \frac{4\pi}{3} = \theta_B + \frac{2\pi}{3} = \theta_C$$



$$S_l = \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda \end{pmatrix} \qquad \Lambda = \frac{1}{2}\begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix}$$

$$u_1 = (d_2, 0);$$
$$u_2 = (0, d_2);$$
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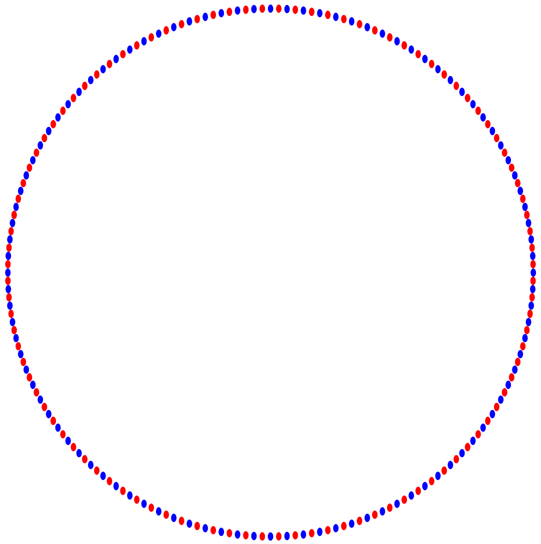

$$l_n^{\uparrow} \sim (-\sin\theta, \cos\theta, \cos\theta, -\sin\theta)$$

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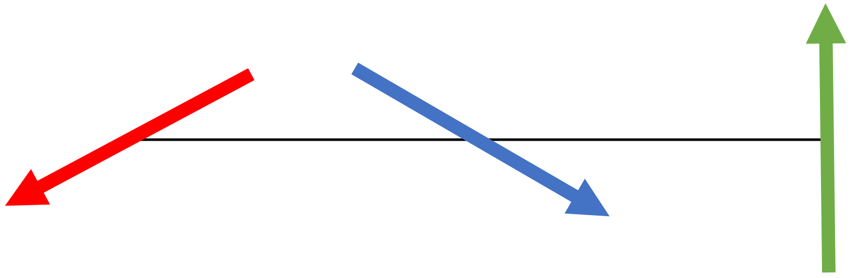
Triangular lattice

Low T: *p*/2 $\theta_A - \frac{4\pi}{3} = \theta_B - \frac{2\pi}{3} = \theta_C$



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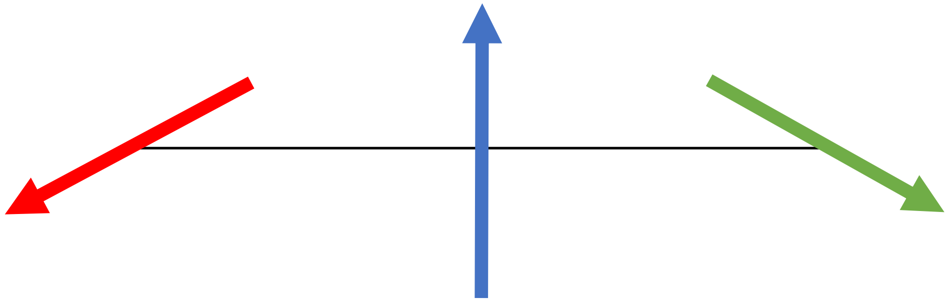

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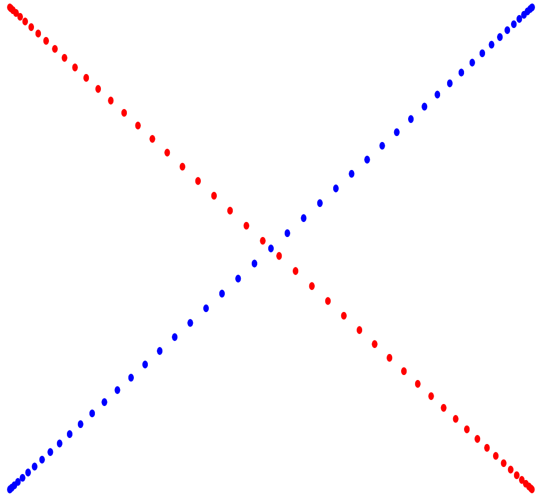

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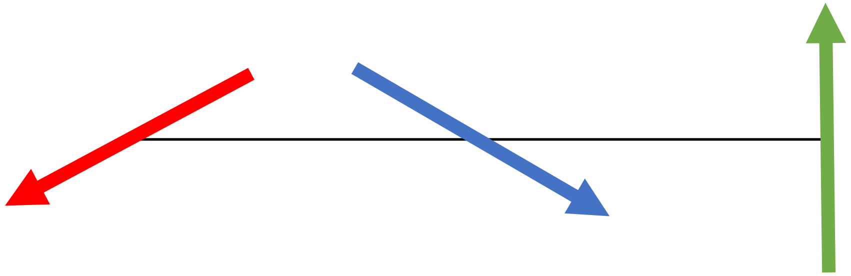
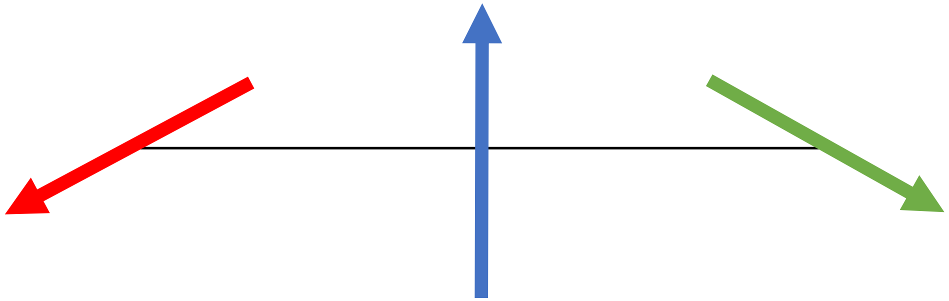


p/2

$$\theta_A + \frac{4\pi}{3} = \theta_B + \frac{2\pi}{3} = \theta_C$$



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$$\begin{aligned} u_1 &= (d_1, d_2); \\ u_2 &= (d_2, d_1); \\ u_3 &= (d_1, -d_2); \\ u_4 &= (-d_2, d_1). \end{aligned}$$

$$d_1 \propto \left(1, \cos\left(\frac{2\pi}{3}\right), \cos\left(\frac{4\pi}{3}\right)\right) \propto (2, -1, -1),$$

$$d_2 \propto \left(0, \sin\left(\frac{2\pi}{3}\right), \sin\left(\frac{4\pi}{3}\right)\right) \propto (0, 1, -1).$$

$$l_n^{\uparrow} \sim (0, \sin\theta, \cos\theta, 0)$$

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Triangular lattice

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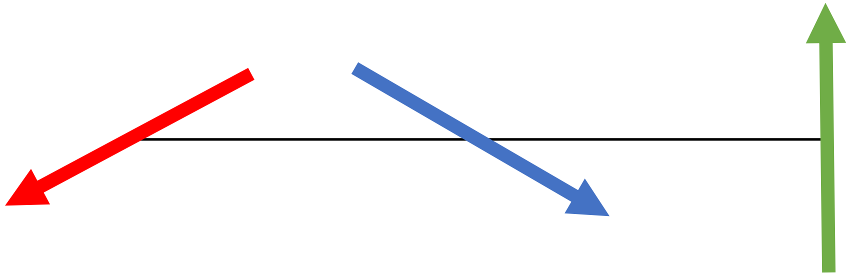

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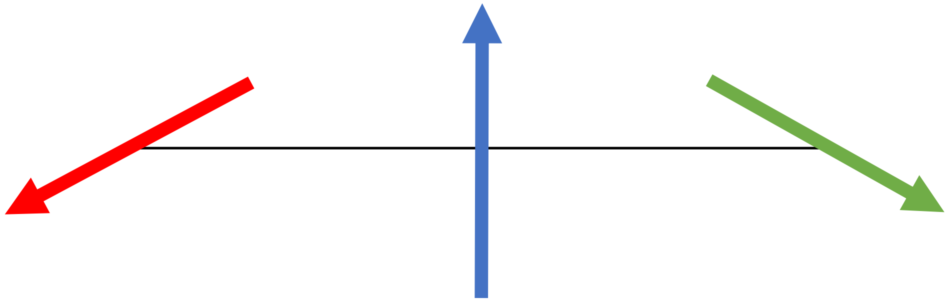

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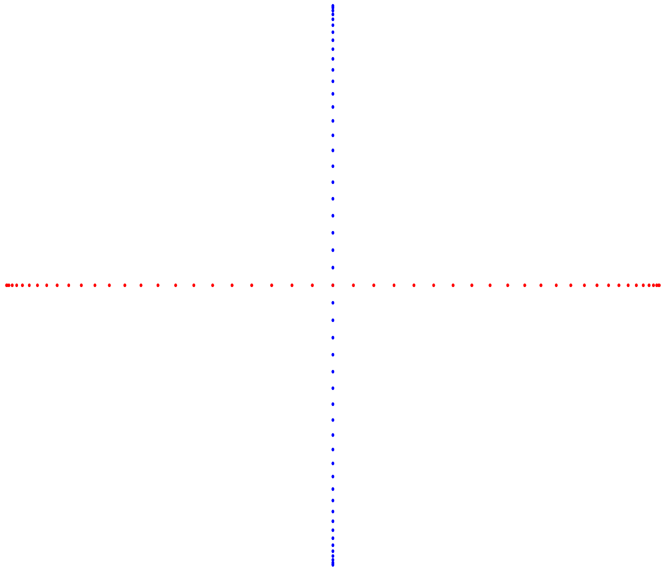

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Triangular lattice

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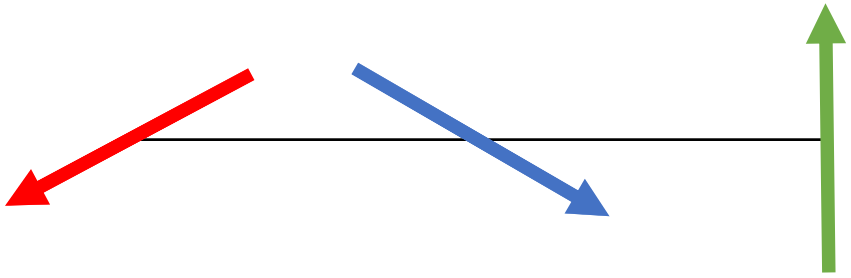

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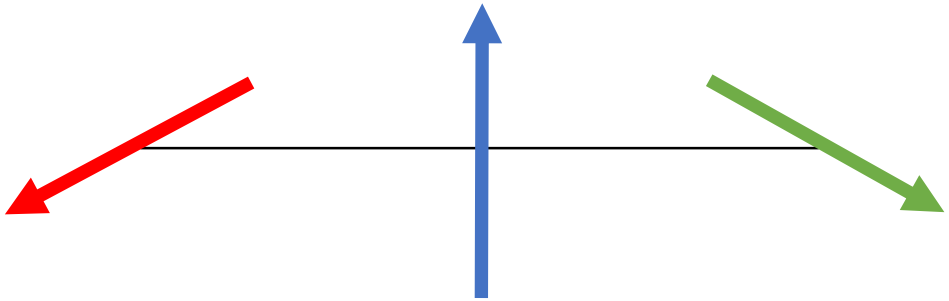

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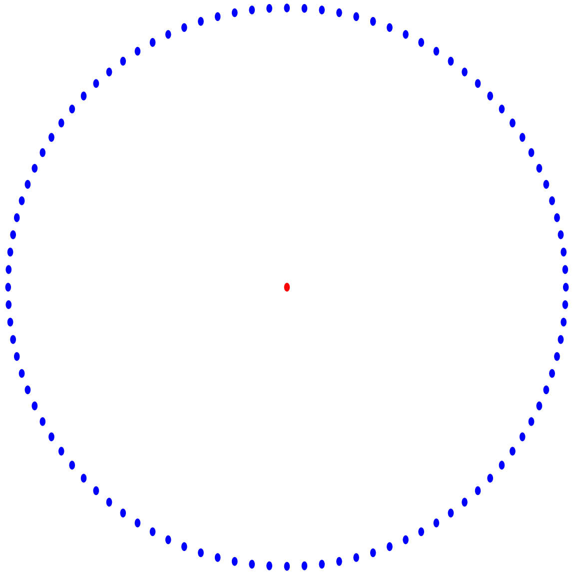

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Triangular lattice

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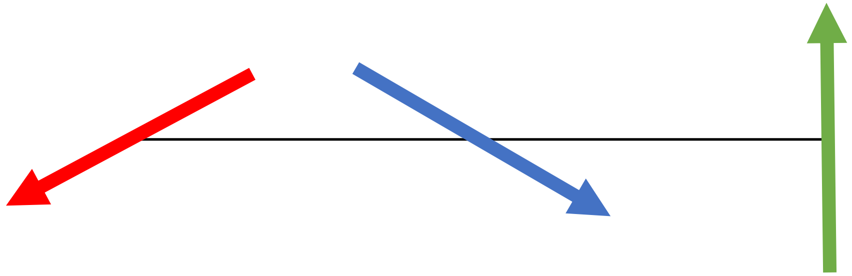

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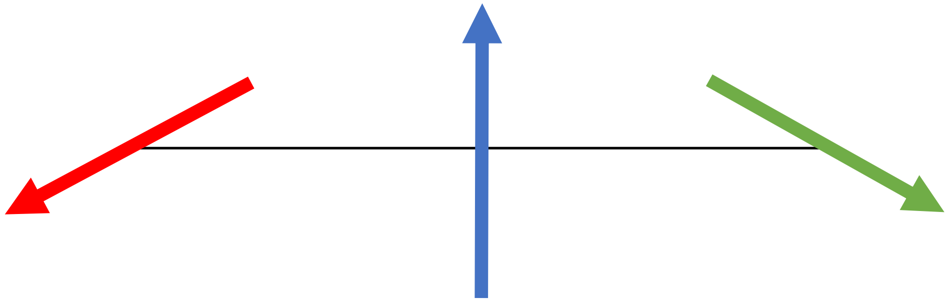

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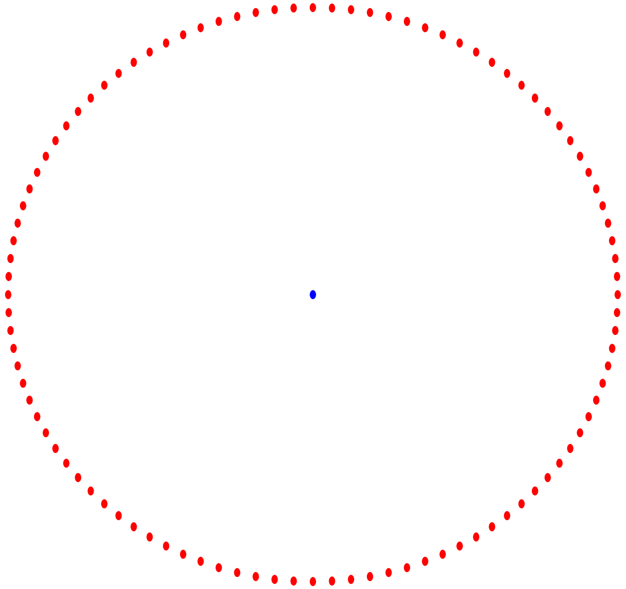

$$l_n^{\uparrow} \sim (0, \sin\theta, \cos\theta, 0)$$

$$l_n^{\downarrow} \sim (\cos\theta, 0, 0, \sin\theta)$$

$$
\begin{aligned}
u_1' &= \cos\alpha u_1 + \sin\alpha u_2;\\
u_2' &= -\sin\alpha u_1 + \cos\alpha u_2;\\
u_3' &= \cos\beta u_3 + \sin\beta u_4;\\
u_4' &= -\sin\beta u_3 + \cos\beta u_4.
\end{aligned}
$$

$$l_n^{\uparrow} \sim (\sin\alpha\sin\theta, \cos\alpha\sin\theta, \cos\beta\cos\theta, -\sin\beta\cos\theta)$$

$$l_n^{\downarrow} \sim (\cos\alpha\cos\theta, -\sin\alpha\cos\theta, \sin\beta\sin\theta, \cos\beta\sin\theta)$$

$$u'_1 = \cos\alpha u_1 + \sin\alpha u_2;$$
$$u'_2 = -\sin\alpha u_1 + \cos\alpha u_2;$$
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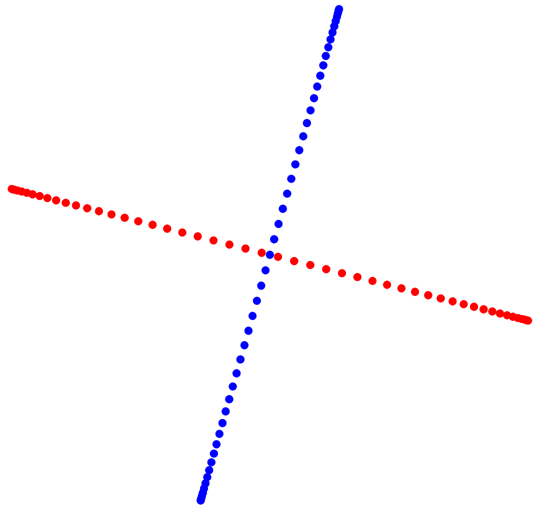

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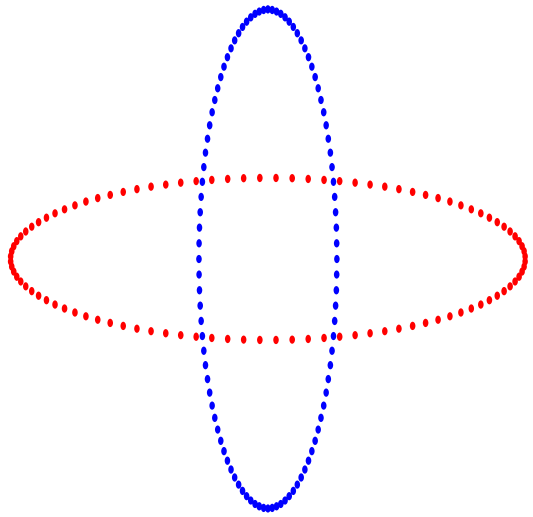

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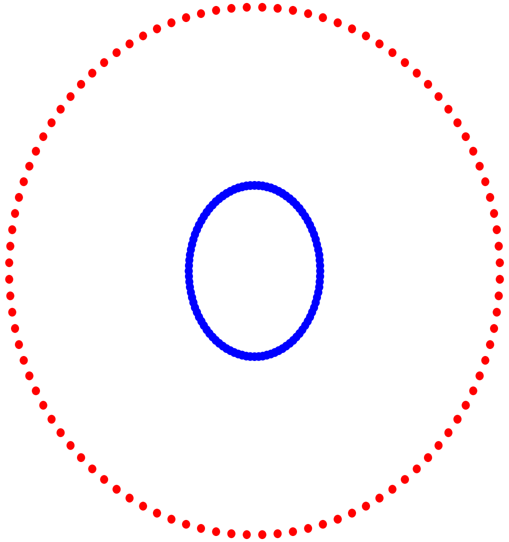

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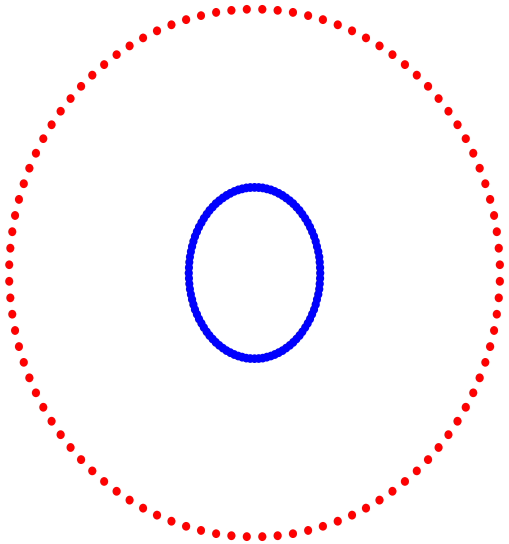

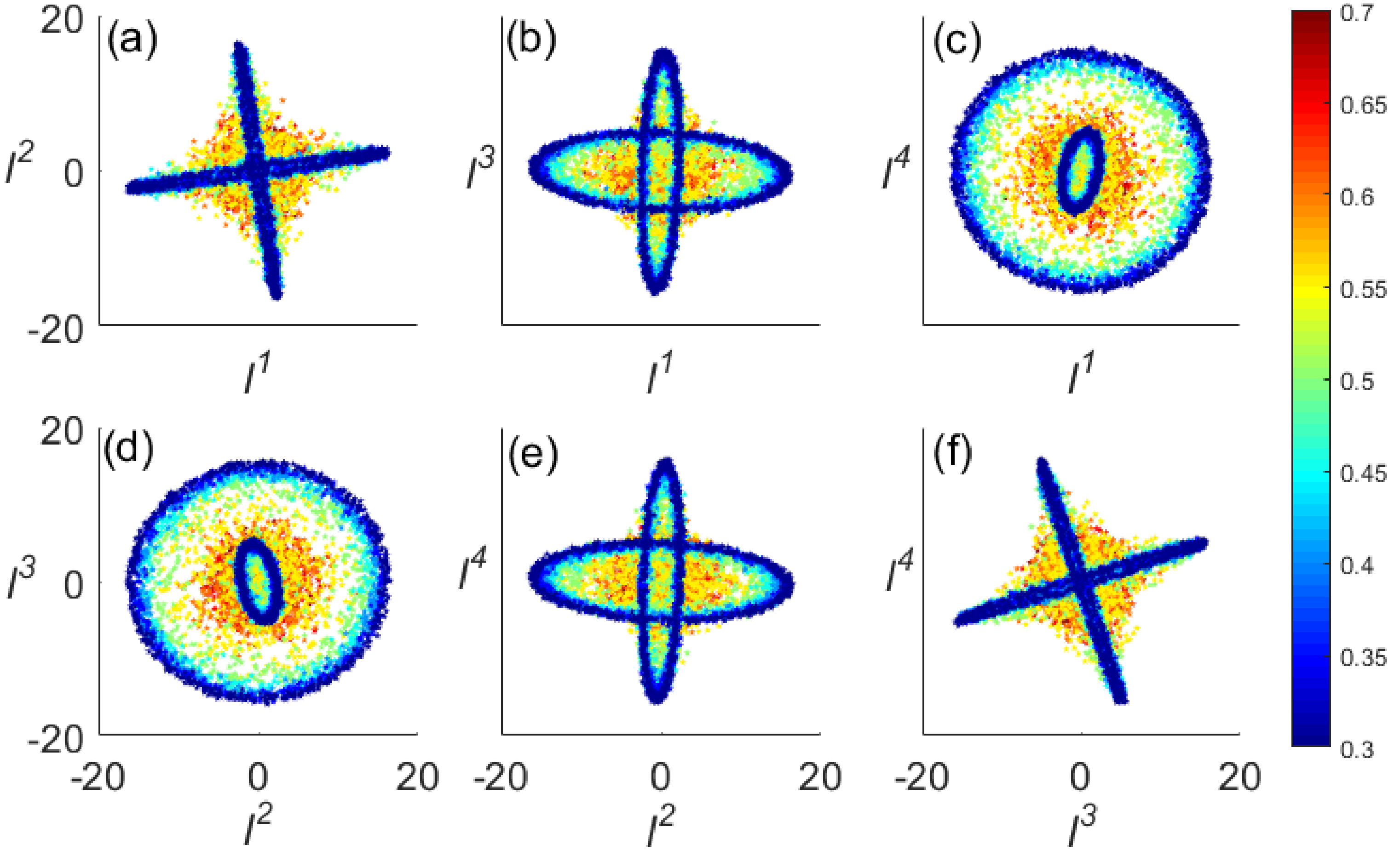

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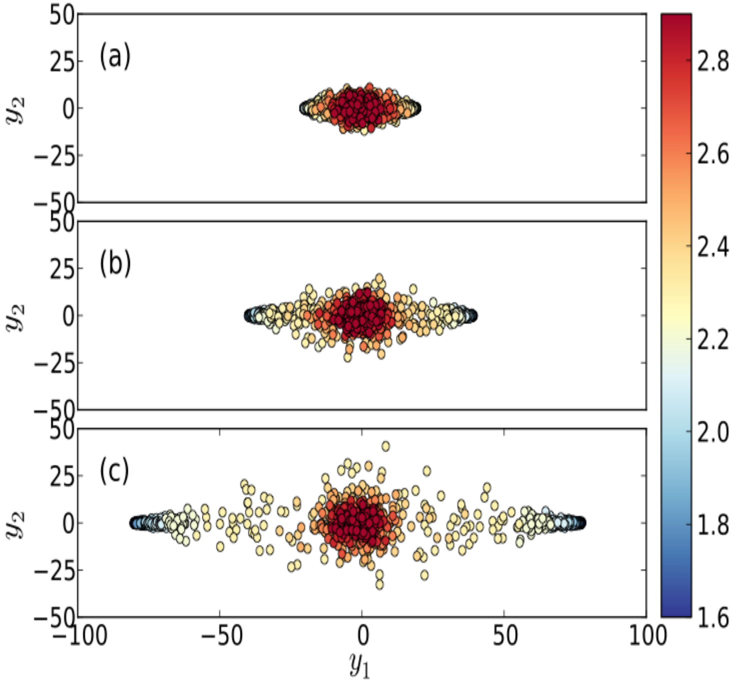
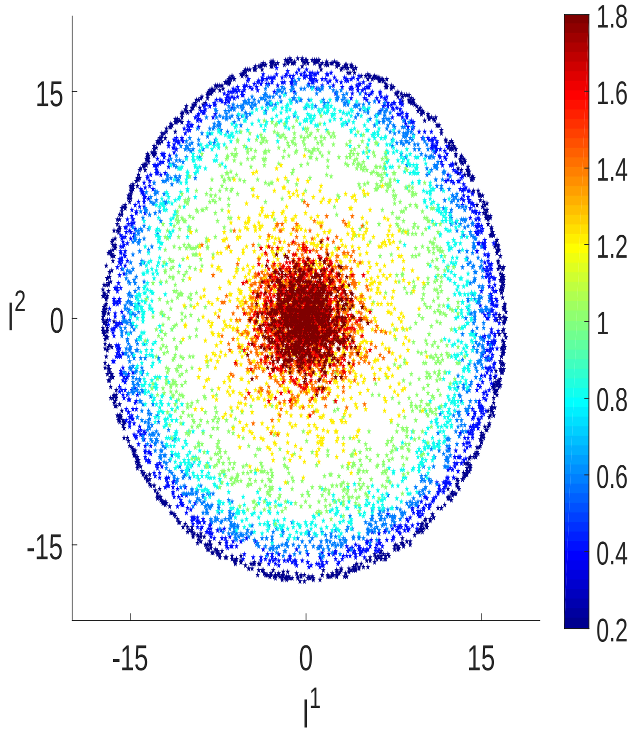
Ising model



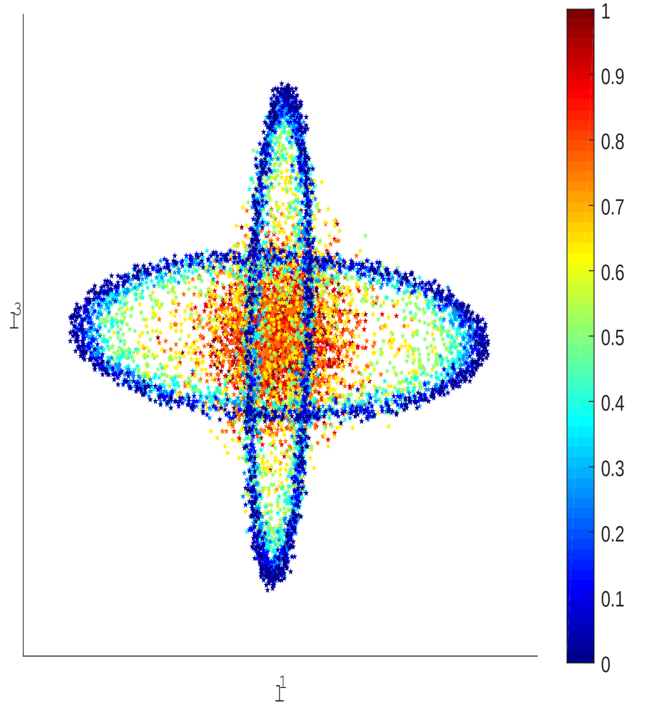
Z_2

2D square lattice XY



U_1

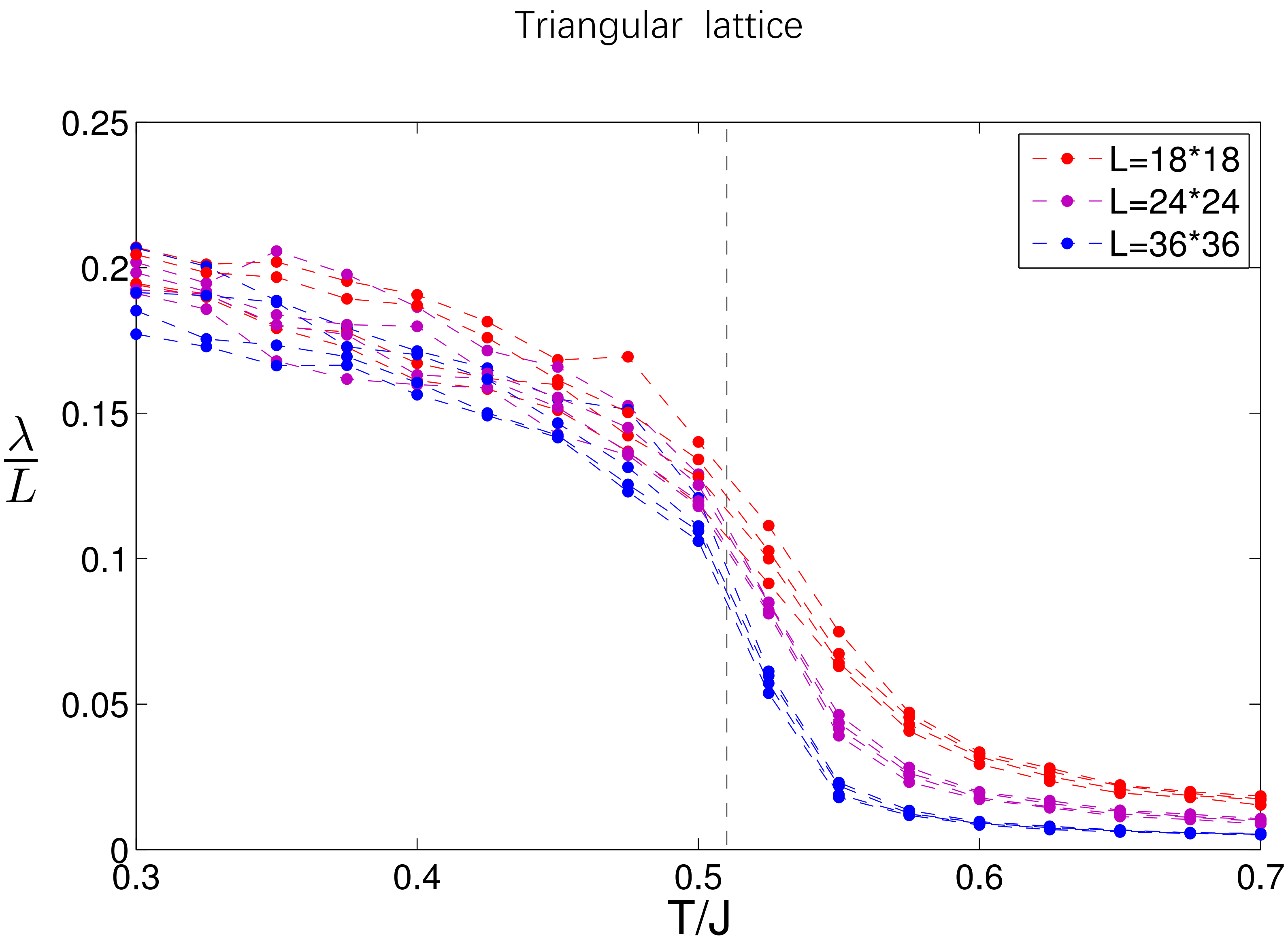
2D triangular lattice XY



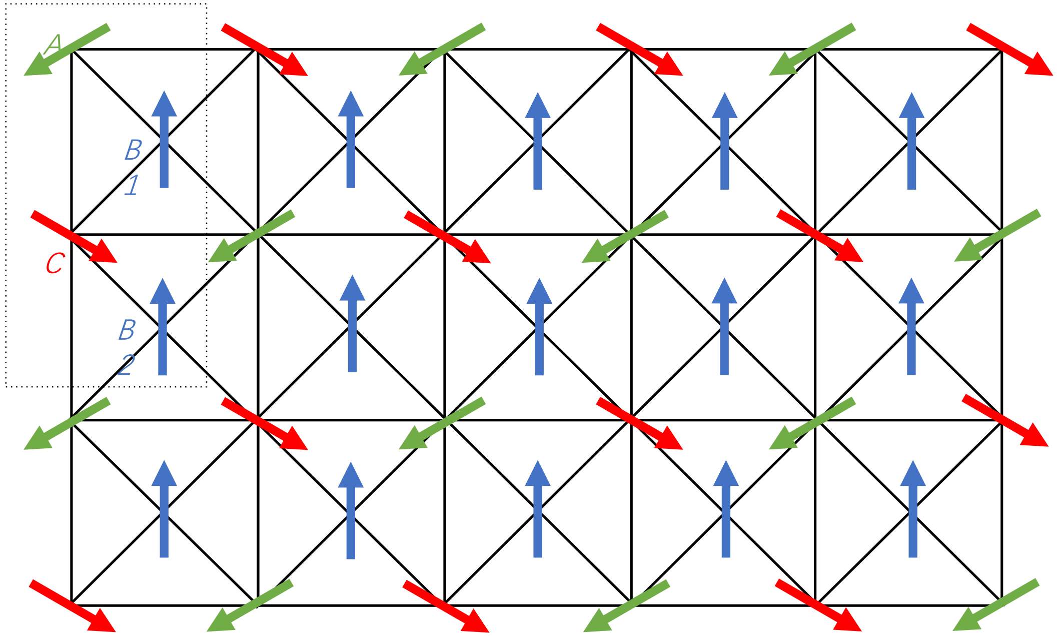
$Z_2 \times U_1$

L. Wang, Phys. Rev. B **94**.195105(2016)

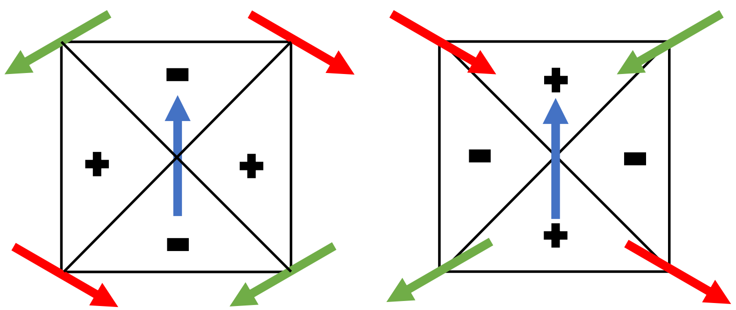
Temperature resolved PCA



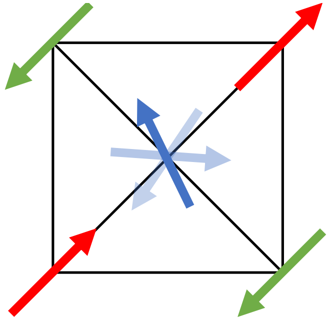
Union Jack lattice



$T < T_2$



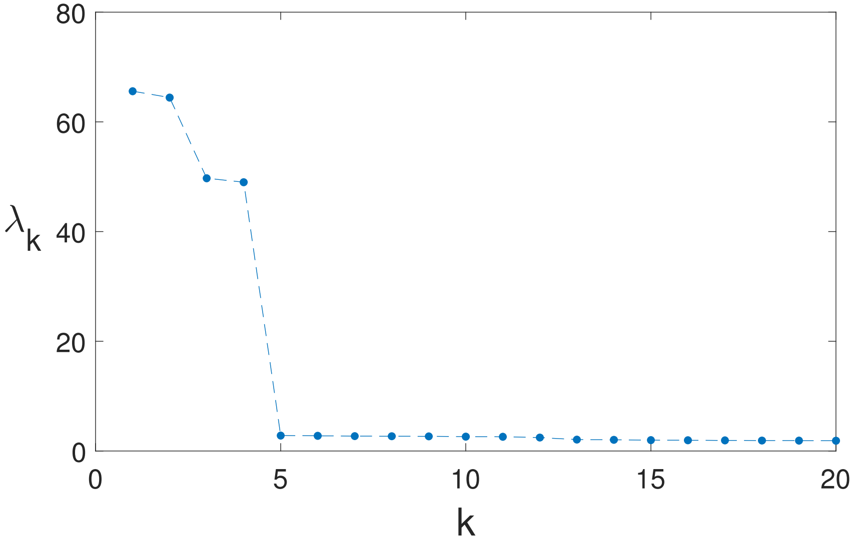
$T_2 < T < T_1$

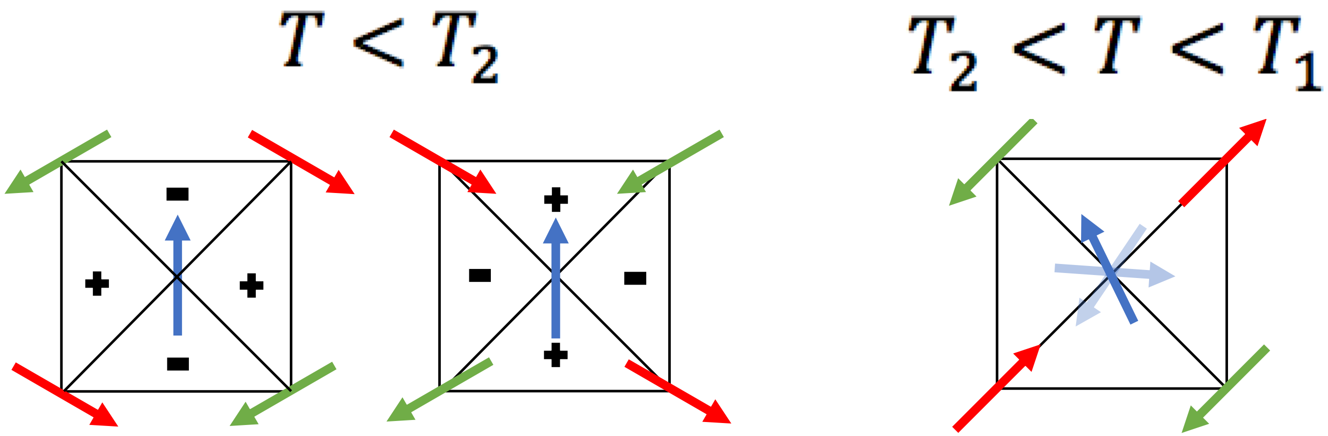


Two well separated phase transition:
T2 =0.43J Z2 chiral , U(1) on B
T1=0.64J U(1) on A,C

J. P. Lv et.al Phys. Rev. B **87**,024108 (2013)

Union Jack lattice





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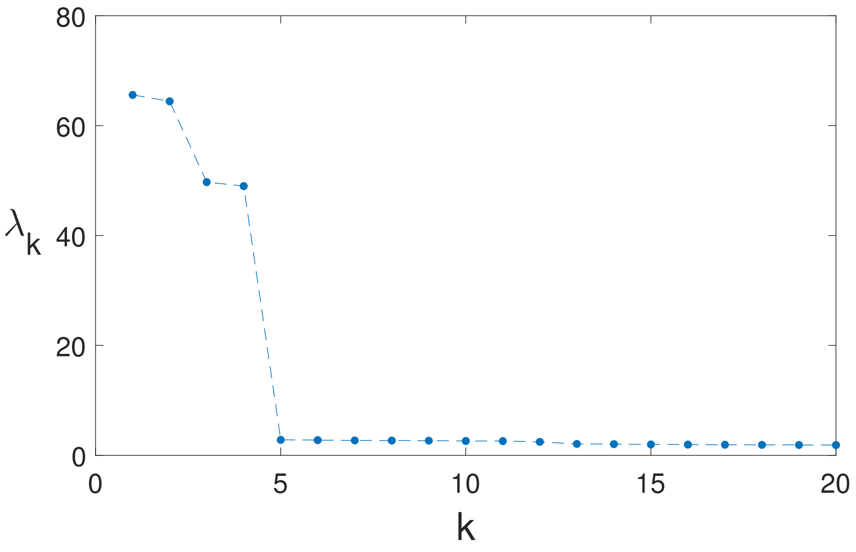

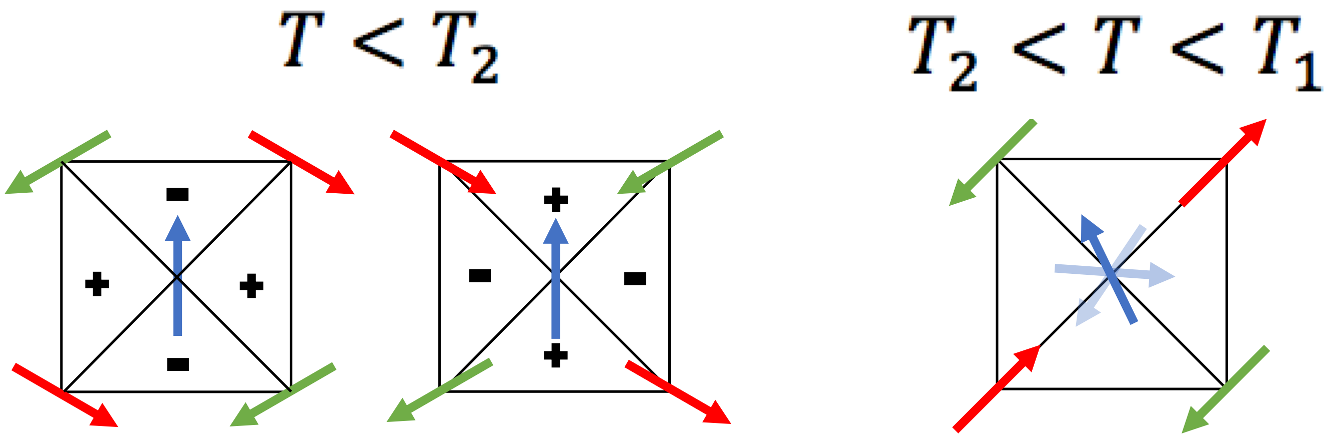

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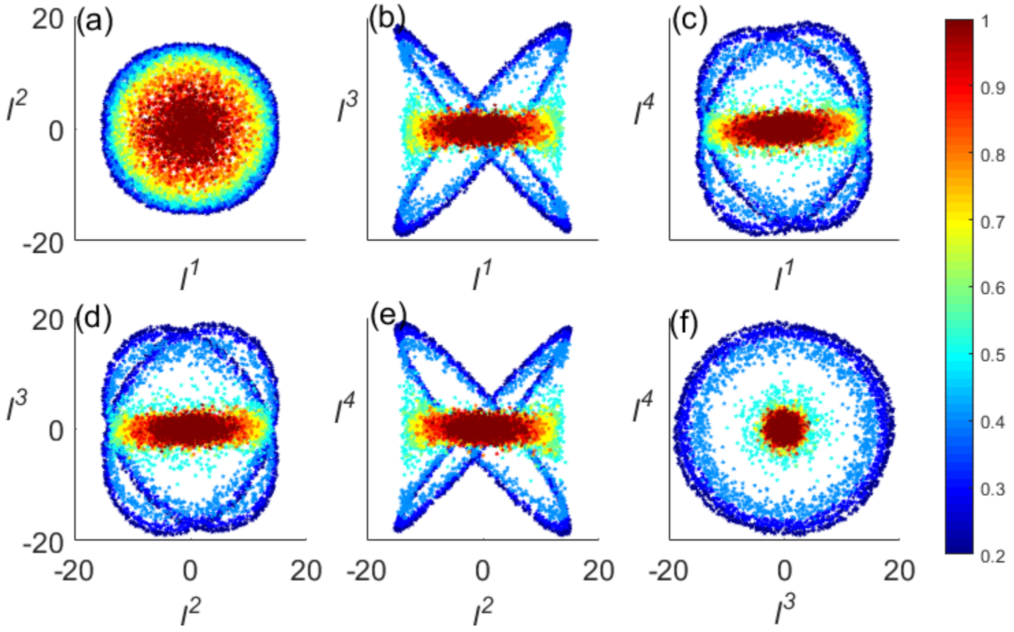

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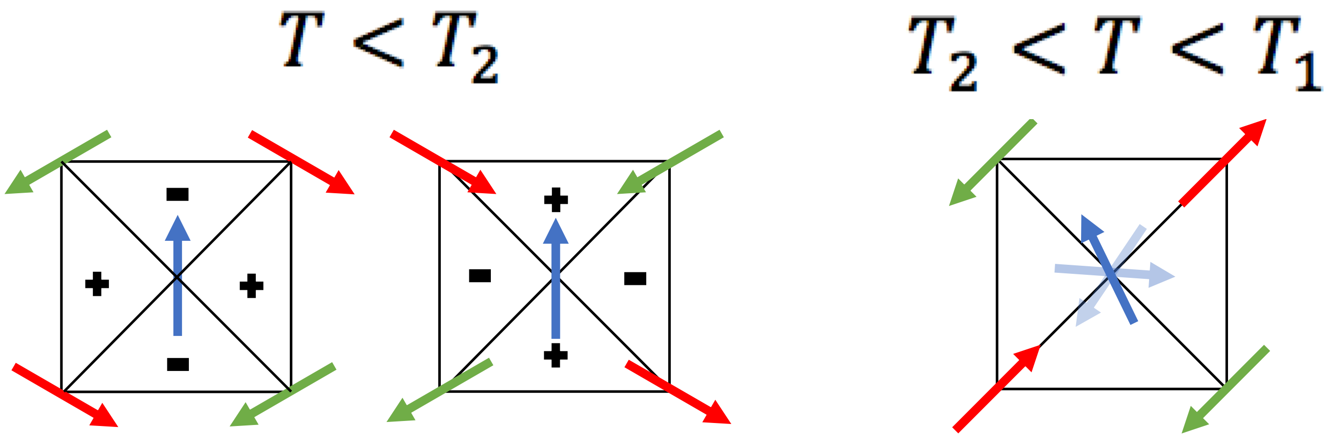

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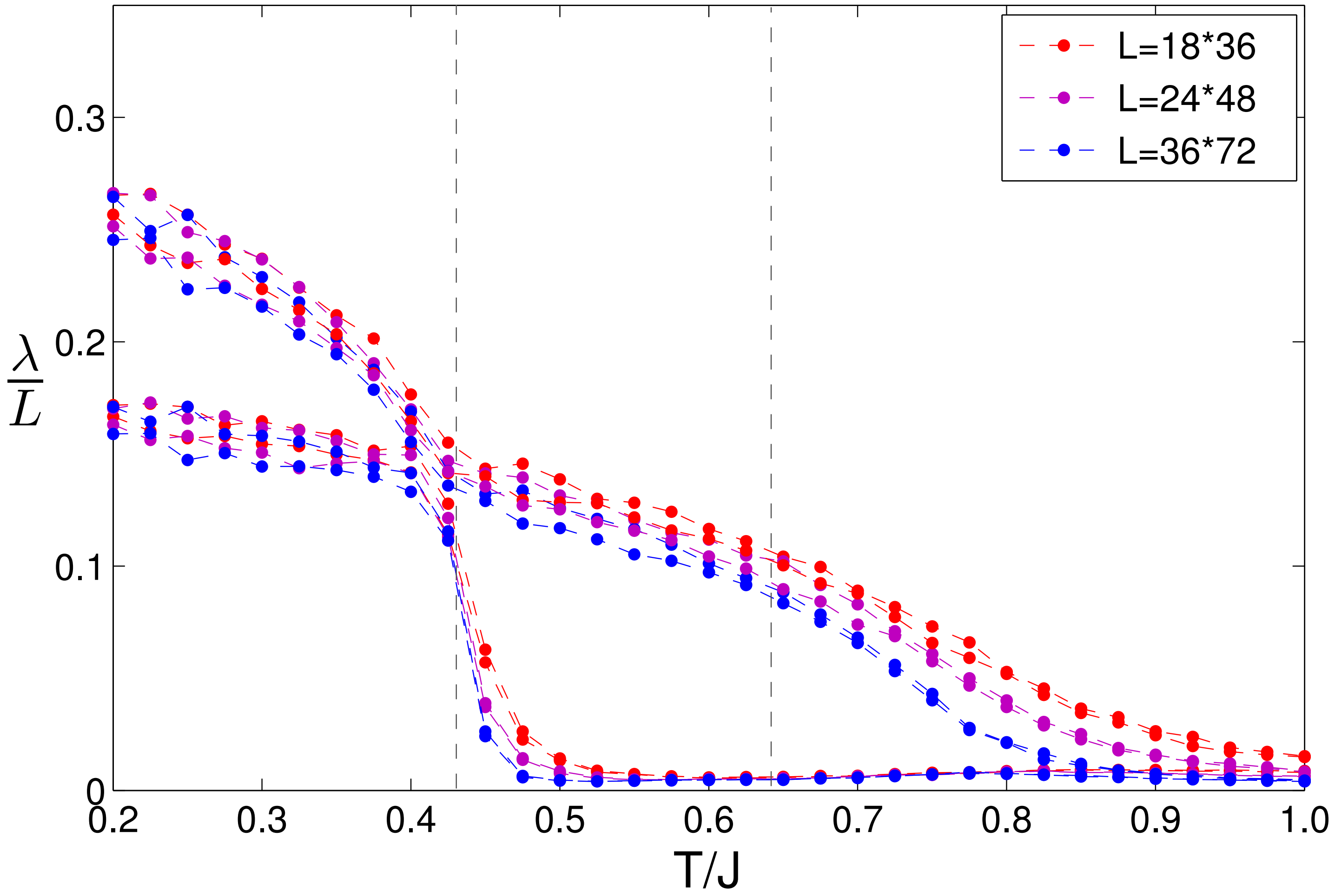

Summary

1. *PCA on XY model in square ,triangular and union-jack lattice*

2. *“Toy” model understanding*

1. *Temperature resolved analysis*

Outlook

1. *Kernel PCA*

2. *Neural network*

Thank you very much!

Introduction to kernel PCA

$$\mathcal{S} = \frac{1}{N}\sum_n (x_n - \bar{x})(x_n - \bar{x})^T.$$

$$K_{ij} = x_i^T x_j$$

$$\sum_j K_{ij} a_j = x_i^T \sum_j x_j a_j = \lambda a_i$$