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Condensation of eigen microstate in statistical ensemble and phase transition

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In a statistical ensemble with M microstates, we introduce an $M \times M$ correlation matrix with correlations among microstates as its elements. Eigen microstates of ensemble can be defined using eigenvectors of the correlation matrix. The eigenvalue normalized by M represents weight factor in the ensemble of the corresponding eigen microstate. In the limit $M \to \infty$, weight factors drop to zero in the ensemble without localization of the microstate. The finite limit of the weight factor when $M \to \infty$ indicates a condensation of the corresponding eigen microstate. This finding indicates a transition into a new phase characterized by the condensed eigen microstate. We propose a finite-size scaling relation of weight factors near critical point, which can be used to identify the phase transition and its universality class of general complex systems. The condensation of eigen microstate and the finite-size scaling relation of weight factors are confirmed using Monte Carlo data of one-dimensional and two-dimensional Ising models.

statistical ensemble, eigen microstate, condensation, phase transition, finite-size scaling

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1 Introduction

In statistical physics, the concept of ensemble in phase space serves as a starting point. An ensemble in the phase space consists of microstates of system under certain thermodynamic conditions. Thermodynamic quantities of the system can be determined by the ensemble-average with summation over all microstates of the ensemble.

Three important thermodynamic ensembles have been defined by Gibbs [1]. They are micro-canonical ensemble, canonical ensemble, and grand canonical ensemble. The micro-canonical ensemble is under the thermodynamic conditions that number of particles N, volume V, and total energy E of the system are fixed. In the canonical ensemble, the system energy is not exactly known and temperature T of the heat bath in thermal equilibrium with the system is specified. In the grand canonical ensemble, neither the energy nor particle number are fixed. However, temperature T and chemical potential μ are specified.

In computer simulations or experimental investigations of complex systems under certain conditions, snapshots of system can be taken. From these snapshots, we can obtain microstates and then a statistical ensemble of the system. In this

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paper, we study the correlations between microstates in the statistical ensemble. Considering the correlations between microstates as elements, we can obtain a correlation matrix of the microstate in the statistical ensemble. Using eigenvectors of the correlation matrix, the eigen microstates of the statistical ensemble can be defined. The eigenvalues normalized by the number of microstates represent the weight factors of the corresponding eigen microstates in the ensemble. The distribution of eigen microstates in the statistical ensemble can be described by all weight factors.

This paper is organized as follows. In sect. 2, we introduce the correlation between the microstate and a correlation matrix. Using eigenvectors, we calculate eigen microstates of the ensemble. The weight factors of eiegn microstates are determined with eigenvalues. The finite limit of weight factor at $M \to \infty$ indicates a condensation of eigen microstate. In one-dimensional and two-dimensional Ising models, the eigen microstates, weight factors, and the condensation of eigen microstate are examined using Monte Carlo (MC) simulations. In sect. 3, we propose a finite-size scaling relation of weight factors near critical point, which is confirmed by MC simulation data of Ising models. Conclusions are provided in sect. 4.

2 Eigen microstates of statistical ensemble and condensation

We consider an Ising model with the Hamiltonian

$$H = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j \,, \tag{1}$$

where $S_i = \pm 1$ is the spin on site i and J_{ij} is the interaction between spins i and j. For the Ising model with N spins, a microstate I of system can be described by a vector with N components as:

$$\boldsymbol{A}^I = \frac{1}{\sqrt{N}} \begin{bmatrix} S_1^I \\ S_2^I \\ \vdots \\ S_N^I \end{bmatrix} , \tag{2}$$

which is normalized and $|\boldsymbol{A}^I|^2 = \left[\boldsymbol{A}^I\right]^T \cdot \boldsymbol{A}^I = 1$. The total energy of system at microstate $\boldsymbol{A}^I$ can be written as $H^I = -N\left[\boldsymbol{A}^I\right]^T \cdot \hat{\boldsymbol{J}} \cdot \boldsymbol{A}^I$ with an interaction matrix $\hat{\boldsymbol{J}}$ defined by J_{ij}.

At temperature T, the microstate $\boldsymbol{A}^I$ has a probability

$$p(\boldsymbol{A}^I) = \frac{1}{Z} \mathrm{e}^{-H^I/k_\mathrm{B}T} \,, \tag{3}$$

where $Z = \sum_I \mathrm{e}^{-H^I/k_\mathrm{B}T}$ and k_B is the Boltzmann constant. In MC simulations, different microstates of system can be sampled with the probability factor. M microstates from simulation are taken to build up an ensemble. The correlation between microstates I and J is defined as:

$$C_{IJ} = \left[\boldsymbol{A}^I\right]^T \cdot \boldsymbol{A}^J \,. \tag{4}$$

If $\boldsymbol{A}^J = \boldsymbol{A}^I$, $C_{IJ} = 1$. When $\boldsymbol{A}^J = -\boldsymbol{A}^I$, $C_{IJ} = -1$. We have $-1 \le C_{IJ} \le 1$ in general.

With C_{IJ} as elements, an $M \times M$ correlation matrix $\boldsymbol{C}$ is obtained. We suppose that $\boldsymbol{C}$ has M eigenvectors $\boldsymbol{b}_1, \boldsymbol{b}_2, \cdots, \boldsymbol{b}_M$ with associated eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_M$. We arrange all eigenvalues in the order $\lambda_1 \ge \lambda_2 \cdots \ge \lambda_M$. There is a relation

$$\boldsymbol{C}\boldsymbol{b}_I = \lambda_I \boldsymbol{b}_I,\ I = 1, 2, ..., M, \tag{5}$$

where

$$\boldsymbol{b}_I = \begin{bmatrix} b_{1I} \\ b_{2I} \\ \vdots \\ b_{MI} \end{bmatrix} . \tag{6}$$

The normalized eigenvectors are orthogonal each other and follow the relation

$$\boldsymbol{b}_I^T \cdot \boldsymbol{b}_J = \sum_{l=1}^{M} b_{lI} b_{lJ} = \delta_{I,J} \,, \tag{7}$$

where $\delta_{I,J}$ is the Kronecker delta. The trace of the correlation matrix is $\mathrm{tr}\,[\boldsymbol{C}] = \sum_{I=1}^M \lambda_I = M$.

From the M eigenvectors, we can define an $M \times M$ matrix

$$\boldsymbol{U} = [\boldsymbol{b}_1 \boldsymbol{b}_2 \cdots \boldsymbol{b}_M] \tag{8}$$

with elements $U_{IJ} = b_{IJ}$. $\boldsymbol{U}$ is an orthogonal matrix and satisfies the condition $\boldsymbol{U}^T \cdot \boldsymbol{U} = \boldsymbol{U} \cdot \boldsymbol{U}^T = \boldsymbol{I}$. After the $\boldsymbol{U}$ transformation of the correlation matrix, we have $\boldsymbol{U}^T \cdot \boldsymbol{C} \cdot \boldsymbol{U} = \boldsymbol{\Lambda}$, where $\boldsymbol{\Lambda}$ is a diagonal matrix with elements $\Lambda_{IJ} = \lambda_I \delta_{I,J}$.

Using the components of an eigenvector $\boldsymbol{b}_I$, we can introduce an eigen microstate

$$\boldsymbol{E}^I = \sum_{L=1}^{M} b_{LI} \boldsymbol{A}^L,\ I = 1, 2, \cdots, M \,, \tag{9}$$

which satisfies the relation $|\boldsymbol{E}^I|^2 = \left[\boldsymbol{E}^I\right]^T \cdot \boldsymbol{E}^I = \lambda_I$. The correlation between eigen microstates I and J is

$$C_{IJ}^E = \left[\boldsymbol{E}^I\right]^T \cdot \boldsymbol{E}_J = \sum_{l,m}^{M} b_{lI} C_{lm} b_{mJ} = \lambda_I \delta_{I,J} \,. \tag{10}$$

Therefore, the correlation matrix $\boldsymbol{C}^E$ is diagonal and there is no correlation between eigen microstates.

In the ensemble consisting of original microstates, all microstates have the same weight. The weight factor of microstate I

$$w_I = C_{II}/M = 1/M \,, \tag{11}$$

which satisfies the normalization condition $\sum_{I=1}^{M} w_I = 1$.

In the ensemble consisting of eigen microstates, different microstates have different weights. We define the weight factor of eigen microstate I as:

$$w_I^E = C_{II}^E/M = \lambda_I/M , \tag{12}$$

which satisfies a normalization condition $\sum_{I=1}^{M} w_I^E = 1$.

In an ensemble without localization of microstate, all weight factors $w_I^E \to 0$ in the limit $M \to \infty$. If the largest weight factor w_1^E becomes finite in the limit $M \to \infty$, this indicates a condensation of eigen microstate $\boldsymbol{E}^1$ in the ensemble. This condensation of microstate is similar to the Bose-Einstein condensation [2]. Now system has a phase transition with the new phase characterized by the eigen microstate $\boldsymbol{E}^1$.

The eigenvalue λ_I depends on T, N, and M and $\lambda_I = \lambda_I(T, N, M)$. In the limit $M \to \infty$ at fixed $x = I/M$, an eigenvalue function $\lambda(T, N, x) \equiv \lim_{M\to\infty} \lambda_I(T, N, M)$ is obtained. The normalized condition of eigenvalue function is

$$\int_0^1 \lambda(T, N, x)\mathrm{d}x = 1 . \tag{13}$$

In the limit $M \to \infty$, the finite w_1^E implies that the eigenvalue function $\lambda(T, N, x) \to \infty$ when $x \to 0$.

Original microstates can be expressed by eigen microstates as:

$$\boldsymbol{A}^I = \sum_{J=1}^{M} b_{JI}\boldsymbol{E}^J,\ I = 1, 2, ..., M . \tag{14}$$

Since $|\boldsymbol{E}^I|^2 = \lambda_I$, a normalized eigen microstate $\bar{\boldsymbol{E}}^I = \lambda_I^{-1/2}\boldsymbol{E}^I = \sum_{L=1}^{M} b_{LI}\lambda_I^{-1/2}\boldsymbol{A}^L$ is introduced. With normalized eigen microstates, we have

$$\boldsymbol{A}^I = \sum_{J=1}^{M} b_{JI}\lambda_J^{1/2}\bar{\boldsymbol{E}}^J,\ I = 1, 2, ..., M . \tag{15}$$

In the ensemble of original microstate, the magnetization of system can be calculated as:

$$\langle m\rangle = \frac{1}{M}\sum_{I=1}^{M} m_I , \tag{16}$$

where

$$m_I = \frac{1}{\sqrt{N}}\sum_{i=1}^{N} A_i^I \tag{17}$$

is the magnetization of original microstate I.

Equivalently, we can write the magnetization of system according to eq. (14) as:

$$\langle m\rangle = \sum_{J=1}^{M} \bar{b}_J \left[w_J^E\right]^{1/2} m_J^e , \tag{18}$$

where

$$m_J^e = \frac{1}{\sqrt{N}}\sum_{i=1}^{N} \bar{E}_i^J , \tag{19}$$

$$\bar{b}_J = \frac{1}{\sqrt{M}}\sum_{I=1}^{M} b_{JI} . \tag{20}$$

Other thermodynamics quantities of system can be calculated in a similar way.

In the following, we will study the eigen microstates and their weight factors in the statistical ensembles of one-domensional and two-dimensional Ising models.

2.1 One-dimensional Ising model

The one-dimensional (1d) Ising model with the nearest-neighbour interaction has the Hamiltonian

$$H = -J\sum_{i=1}^{N} S_i S_{i+1} . \tag{21}$$

Under the periodic boundary condition $S_{N+1} = S_1$, this model can be solved exactly [3]. In the thermodynamic limit $N \to \infty$, its correlation function has an exponential form

$$\left\langle S_i S_j \right\rangle = \exp\left(-|x_i - x_j|/\xi\right) \tag{22}$$

with the correlation length

$$\xi = \tilde{a}\left(\ln\left[\coth(1/T^*)\right]\right)^{-1} , \tag{23}$$

where $\tilde{a}$ is the lattice spacing and $T^* = k_\mathrm{B}T/J$. In a finite 1d-Ising chain with periodic boundary condition, the system has susceptibility [4]

$$\chi(T^*, N) = \left(\frac{1 + \mathrm{e}^{-\tilde{a}/\xi}}{1 - \mathrm{e}^{-\tilde{a}/\xi}}\right)\left(\frac{1 - \mathrm{e}^{-L/\xi}}{1 + \mathrm{e}^{-L/\xi}}\right) , \tag{24}$$

where $L = N\tilde{a}$. The correlation length $\xi \to \infty$ when $T \to 0$. Although it has been well acknowledged that there is no phase transition in such an 1d-Ising model, we can still consider the zero temperature as a critical point since the correlation length diverges. The thermodynamic quantities of 1d-Ising model should have similar critical behaviors above T_c as that of d-dimensional Ising model with $d \geq 2$. Near $T = 0$, the susceptibility satisfies asymptotically a finite-size scaling relation

$$\chi(T^*, N) = (L/\tilde{a})^{\gamma/\nu} f_\chi(L/\xi) \tag{25}$$

with $\gamma/\nu = 1$ [3] and the finite-size scaling function

$$f_\chi(x) = \frac{2}{x}\cdot\frac{1 - \mathrm{e}^{-x}}{1 + \mathrm{e}^{-x}} . \tag{26}$$

Using the hyperscaling relation $d - 2\beta/\nu = \gamma/\nu$ for 1d-Ising model, we obtain $\beta = 0$, which is in agreement with that of ref. [3].

We simulate the microstates of 1d-Ising model using the Wolff algorithm [5]. Simulations are started with all spins aligned. To get the microstates in equilibrium, the first 10^4 microstates are not used. The subsequent microstates are chosen at an interval of 205 MC steps to keep their independence. Using the microstates obtained, we can get the correlation matrix $\boldsymbol{C}$. With the eigenvectors and eigenvalues of $\boldsymbol{C}$, we can obtain eigen microstates according to eq. (9).

The M-dependence of eigenvalue has been studied. At $M \approx 10^4$, the M-dependence of the largest three normalized eigenvalues can be neglected. We show the largest three normalized eigenvalues at $M = 2\times10^4$ in Figure 1.

We can see from Figure 1 that the weight factor becomes finite with the decrease of temperature. This indicates that there will be a phase transition. To identify the new phase of system, the corresponding eigen microstates should be studied.

At $T^* = 0.5$, the eigen microstates of the largest three eigevalues are shown in Figure 2. In these eigen microstates, spin clusters are of micro scales and distributed with alternate orientation in the real space.

The largest three eigen microstates at $T^* = 0.2$ are presented in Figure 3. The sizes of clusters are comparable to that of system. Only one cluster exists in the largest eigen microstate. The second largest eigen microstate has two clusters with opposite orientation. In the third largest eigen microstate, there are four clusters with alternate orientations.

For an overview of the weight distribution of eigen microstate, we define the cumulant

$$c(m) = \sum_{I=1}^{m} w_I^E . \tag{27}$$

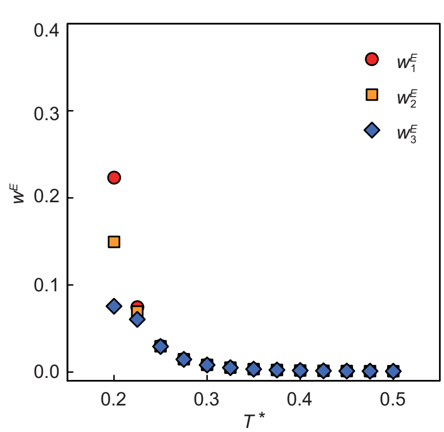

Figure 1 (Color online) The largest three normalized eigenvalues of 1d-Ising model with $N = 10^5$ spins.

In Figure 4, the weight cumulants of 1d-Ising model are plotted. At $T^* = 0.2$, the cumulant $c(m)$ reaches nearly 1 at $m \approx 200$. So the original microstates are constituted actually by about 200 eigen microstates. At $T^* = 0.5$, $c(m)$ becomes nearly 1 at $m \approx 8000$, which is still much less than $M = 2\times10^4$.

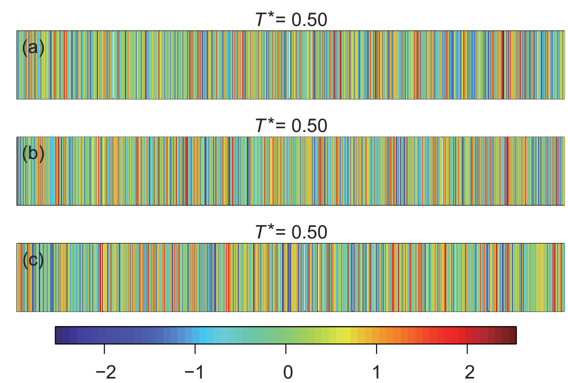

Figure 2 (Color online) The largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^1$ (a), the second largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^2$ (b), and the third largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^3$ (c) of 1d-Ising model.

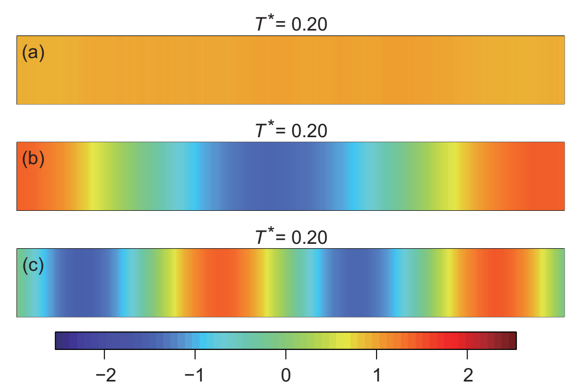

Figure 3 (Color online) The largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^1$ (a), the second largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^2$ (b), and the third largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^3$ (c) of 1d-Ising model.

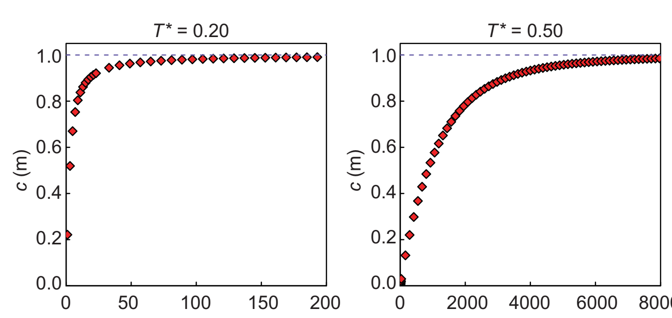

Figure 4 (Color online) Weight cumulant of eigen microstate in 1d-Ising model.

2.2 Two-dimensional Ising model

In a two-dimensional (2d) Ising model with linear length L and periodic boundary conditions, there are $N = L \times L$ spins in this system. With the nearest neighbor interaction J and square lattice, this model has a ferromagnetic phase transition at the reduced temperature $T_c^* = k_B T_c/J = 2/\ln(1+\sqrt{2}) \approx 2.269$ [6].

The microstates of the 2d-Ising model are simulated using the Wolff algorithm [5] also. In our simulations, we start with all spins aligned. The first 8000 microstates are used to reach the equilibrium. From the subsequent microstates, $M = 2 \times 10^4$ microstates at each temperature are taken at an interval of 250 MC steps. From the microstates, we can calculate the correlation matrix at first and then its eigenvalues and eigenvectors. The eigen microstates are obtained using the eigenvectors.

The largest three eigenvalues around the critical point are presented in Figure 5. The normalized eigenvalue by M is equivalent to the weight factor. At temperatures above T_c, the largest three weight factors are quite small. There is no localization of eigen microstate. The weights of eigen microstates are distributed widely. At temperatures below T_c, the largest eigenvalues become finite. This indicates a condensation of the eigen microstate . There is now a phase transition, whose nature is characterized by the condensed eigen microstate.

The largest three eigen microstates at $T^* = 6.2$ are shown in Figure 6. The sizes of the spin clusters in the eigen microstates are much smaller than system size.

In Figure 7, the eigen microstates of the largest three eigenvalues at $T_c^* \approx 2.269$ are presented. There is only one cluster in the eigen microstate of the largest eigenvalue.

We plot in Figure 8 the eigen microstates of the largest three eigenvalues at $T^* = 2.2$. In the largest eigen microstate, there is only one spin cluster. The large-M limit of its weight factor is larger than 0.6, as shown in Figure 9. There is a ferromagnetic phase transition. The second largest eigen microstate has two clusters with opposite orientation. There are four spin clusters in the third largest eigen microstate.

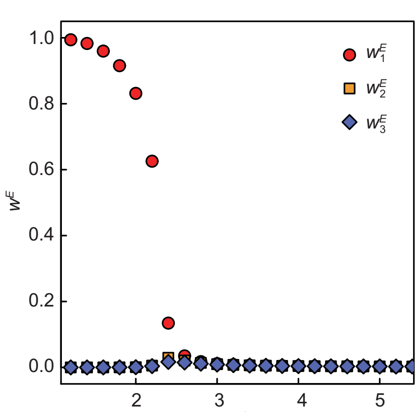

Figure 5 (Color online) The largest three weight factor of 2d-Ising model with $L = 32$.

With the further decrease of temperature, the largest eigen microstate $\boldsymbol{E}_1$ with one spin cluster becomes more dominant. The weight factor of the largest eigen microstate at $T^* = 1.4$ is larger than 0.98, which can be seen in Figure 9. Other eigen microstates have many small clusters, as shown in Figure 10.

The weight cumulants of eigen microstate at $T^* = 1.4, 2.2, 2.269, 6.2$ are shown in Figure 9. The weight cumulants reach nearly 1 at $m \approx 1000$. The 2×10^4 original microstates are composed of 1000 eigen microstates approximately.

3 Finite-size scaling of weight factor near critical point

In the region near a critical point, thermodynamic functions

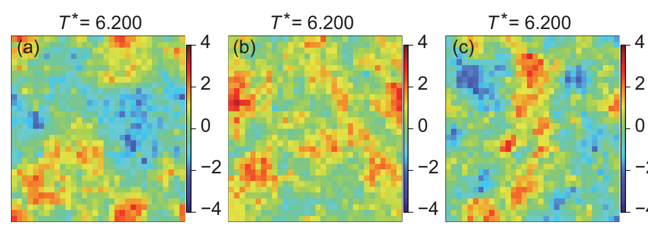

Figure 6 (Color online) The largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^1$ (a), the second largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^2$ (b), and the third largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^3$ (c) of 2d-Ising model above T_c.

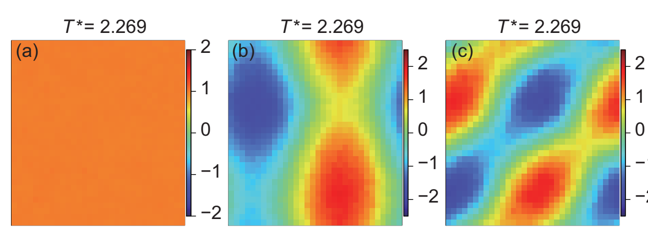

Figure 7 (Color online) The largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^1$ (a), the second largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^2$ (b), and the third largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^3$ (c) of 2d-Ising model at $T_c^* \approx 2.269$.

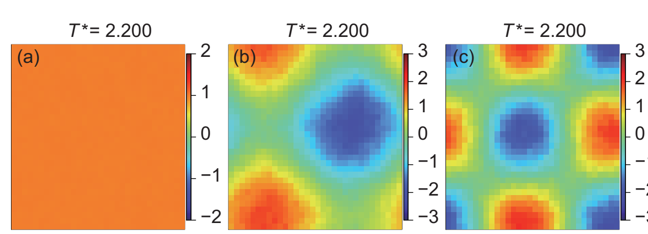

Figure 8 (Color online) The largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^1$ (a), the second largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^2$ (b), and the third largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^3$ (c) of 2d-Ising model below T_c.

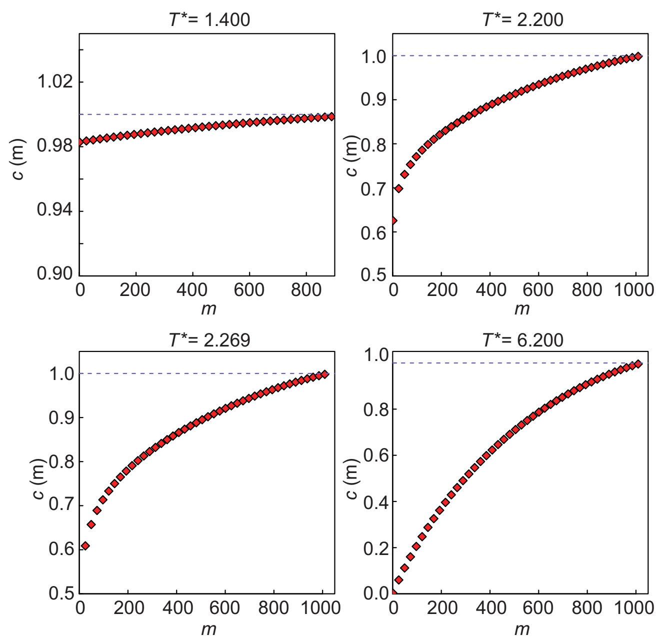

Figure 9 (Color online) Weight cumulant of eigen microstate in 2d-Ising model.

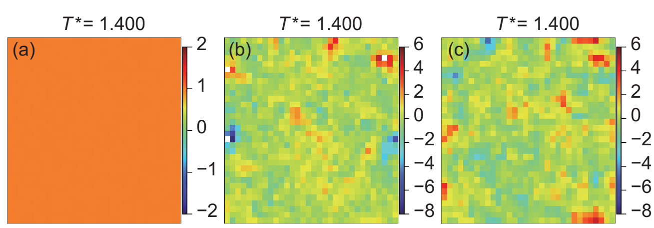

Figure 10 (Color online) The largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^1$ (a), the second largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^2$ (b), and the third largest eigen microstate $\sqrt{N}\bar{\boldsymbol{E}}^3$ (c) of 2d-Ising model below T_c.

of finite system are proposed to satisfy finite-size scaling relations [7-9]. For the order parameter, its finite-size relation is

$$\langle m\rangle(t,L) = L^{-\beta/\nu} f_m(tL^{1/\nu}), \tag{28}$$

where $t = (T - T_\mathrm{c})/T_\mathrm{c}$ is the reduced temperature, β is the critical exponent of order parameter, and ν is the critical exponent of bulk correlation length $\xi = \xi_0 t^{-\nu}$. The scaling variable $tL^{1/\nu}$ is related to the size ratio L/ξ.

The correlation length follows the finite-size scaling form $\xi(t,L) = LX(tL^{1/\nu})$ [8]. Recently, a finite-size scaling relation of correlation function was proposed [10]. Using this finite-size relation, the finite-size scaling form of correlation length can be naturally derived. For the principal fluctuation modes of complex system, there is also a finite-size scaling relation [11], which has been confirmed in 2d-Ising model.

Basing on the relation between the weight factor of eigen microstate and the order parameter, we propose a finite-size scaling form

$$w_I^E(t,L) = L^{-2\beta/\nu} F_w^I(tL^{1/\nu}) . \tag{29}$$

In 1d-Ising model, the critical exponent $\beta = 0$ and $w_I^E(T,L) = F_w^I(L/\xi)$, where ξ is given in eq. (23). We present the largest two weight factors with respect to T^* and scaling variable L/ξ in Figure 11. The finite-size scaling form of eq. (29) is confirmed in 1d-Ising model.

In 2d-Ising model, the critical exponents $\nu = 1$ and $\beta = 1/8$ [6]. On the left side of Figure 12, the largest weight factor w_1^E of $L = 32, 64, 128$ are plotted with respect to T^*. The finite-scaling form $w_1^E L^{2\beta/\nu}$ is presented with respect to $tL^{1/\nu}$ on the right side. The different curves for different L collapse together. The finite-size relation of eq. (29) is confirmed in 2d-Ising model.

In Figures 13 and 14, the second and third largest weight factors and their finite-size scaling form are presented.

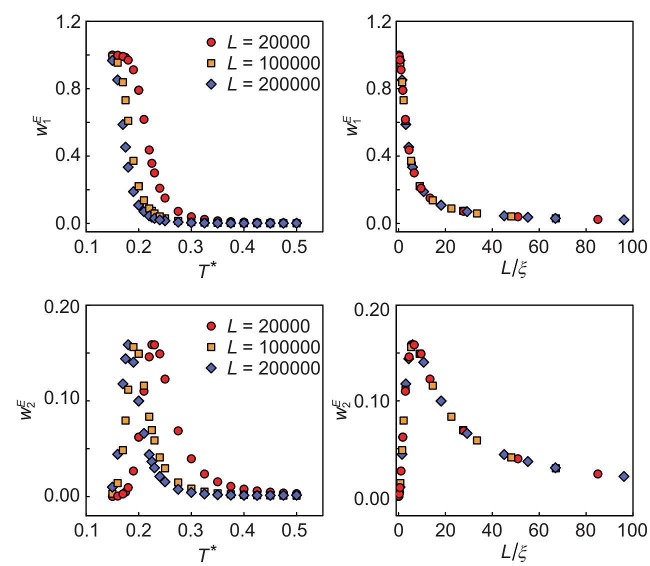

Figure 11 (Color online) The largest two weight factors of 1d-Ising model with respect to T^* and L/ξ.

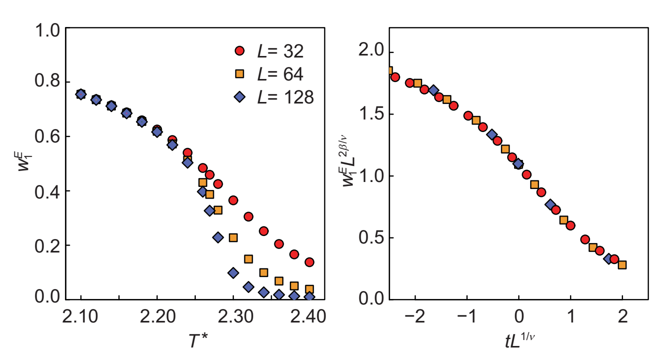

Figure 12 (Color online) The largest weight factor and its finite-size scaling form in 2d-Ising model.

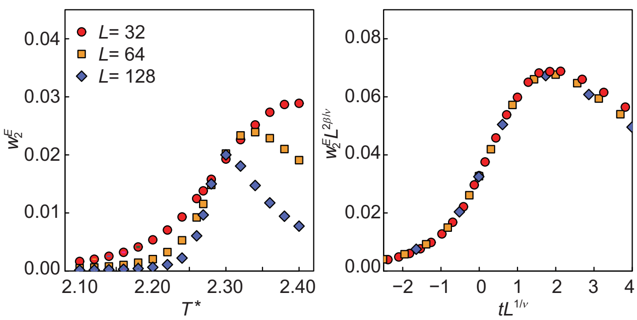

Figure 13 (Color online) The second largest weight factor and its finite-size scaling form in 2d-Ising model.

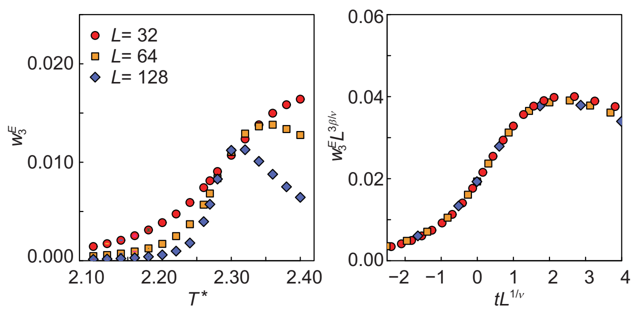

Figure 14 (Color online) The third largest weight factor and its finite-size scaling form in 2d-Ising model.

After taking logarithm of eq. (29), we obtain

$$\ln w_I^E(t, L) = -(2\beta/\nu)\ln L + \ln F_w^I(tL^{1/\nu}) , \tag{30}$$

which depends on $\ln L$ linearly at $t = 0$. This property can be used to determine the critical point and the critical exponent ratio β/ν.

In Figure 15, the log-log plot of the largest weight factor w_1^E with respect to L is presented at different reduced temperatures. The curves are curved upward at $T > T_c$ and downward at $T < T_c$. From the straight line at $T_c^* \approx 2.269$, we can obtain $2\beta/\nu = 0.246(6)$, which is in agreement with the exact value $2\beta/\nu = 1/4$ [6].

We introduce the ratio of weight factor $R \equiv w_2^E/w_1^E$, which follows the finite-size scaling form

$$R(t, L) = F_w^2/F_w^1 = \tilde{R}(tL^{1/\nu}) . \tag{31}$$

At the critical point, the ratio $R(0, L) = \tilde{R}(0)$ is independent of L. This can be used to determine the critical point also.

The ratio $R(t, L)$ of 2d-Ising model is plotted in Figure 16. With T^* as the variable, curves of different L have a fixed point at T_c. Using $tL^{1/\nu}$ as the variable, the curves collapse together.

Therefore, the finite-size scaling relation of weight factor in eq. (29) has been verified in 1d- and 2d-Ising models. We anticipate that this finite-size relation is valid for general complex systems.

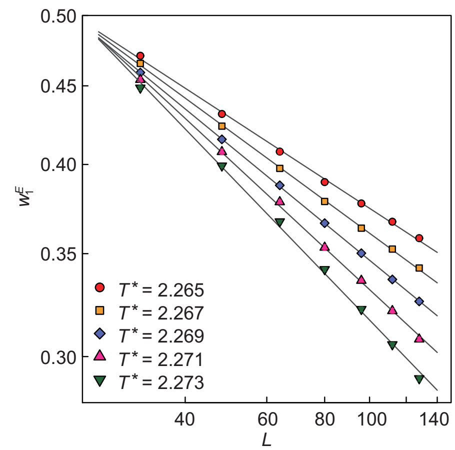

Figure 15 (Color online) Log-log plot of the largest normalized eigenvalue around T_c.

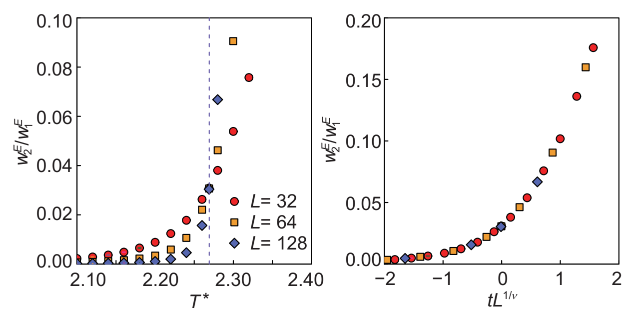

Figure 16 (Color online) Ratio of the largest eigenvalue to the second largest eigenvalue.

4 Conclusions

In the phase space of a complex system, we introduce the eigen microstates of its statistical ensemble. The microstates of the complex system under some conditions can be obtained from computer simulations or experimental studies. We introduce a correlation matrix with correlations between microstates as its elements. Using the eigenvectors of the correlation matrix, the eigen microstates of the ensemble can be defined. The normalized eigenvalues by the number of microstate M can be considered as the weight factor in the ensemble of the corresponding eigen microstates.

In an ensemble without localization of microstate, weight factors of eigen microstate go to zero when $M \to \infty$. If the largest weight factor becomes finite in the limit $M \to \infty$, there is a condensation of the eigen microstate in the ensemble. This condensation indicates a phase transition with the new phase characterized by the eigen microstate corresponding to the finite weight factor. We propose a finite-size scaling relation of the weight factors near critical point using the critical exponents of order parameter and correlation length.

The eigen microstates and their weight factors in an ensemble of 1d- and 2d-Ising models have been studied using Monte Carlo simulation. The condensation of eigen microstate in the 1d-Ising model appears when $T \to 0$. All spins of the condensed eigen microstate have the same orientation and there is a ferromagnetic phase transition. In 2d-Ising model, condensations of eigen microstate are found at the reduced temperatures $T^* < T^*_{\rm c} = 2/\ln(1+\sqrt{2})$. In the condensed eigen microstate, all spins have the same orientation and there is a ferromagnetic phase transition in 2d-Ising model. The finite-size scaling relation of weight factors is confirmed by the Monte Carlo simulation results of 1d- and 2d-Ising models. Further, we will study the eigen microstates and their weight factors of statistical ensemble for complex systems such as confined fluids [12], networks with long-range connections [13], and climate systems [14].

In the studies of phase transitions of complex systems, the definition of order parameter is sometimes a challenge. We can take collective motion as an example. Collective motion exists at almost every scale in nature, from unicellular organisms to bird flocks, fish schools, and human crowds [15]. The simple model of collective motion was introduced by Vicsek and collaborators [16]. It has been thought that the transition to collective motion in the Vicsek model (VM) is critical [16] and discontinuous [17]. More phases such as ordered "Toner-Tu" phase [18] and band phases [19-21] are suggested to exist in the VM also. The real order parameter of the transition to collective motion needs further studies and its global understanding is still lacking. We anticipate that the transition point, order parameter, and critical exponents of complex system can be determined simultaneously with the method proposed here. Our method is not restricted to systems in equilibrium.

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