

**Review Article****Historical Review on Analytic, Monte Carlo, and Renormalization Group Approaches to Critical Phenomena of Some Lattice Models\***Chin-Kun Hu<sup>†</sup>*Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan 11529*

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Analytic calculations, Monte Carlo (MC) simulations [N. Metropolis and S. Ulam, *J. Am. Stat. Asso* **44**, 335 (1949)] and renormalization group (RG) theory [K. G. Wilson, *Phys. Rev. B* **4**, 3174 and 3184 (1971)] are important methods of statistical physics to study phase transitions and critical phenomena. This paper gives a brief historical review on analytic, MC, and RG approaches to some lattice critical systems in memory of late Professors Shang-keng Ma (1940-1983) and Yu-Ming Shih (1942-2005), who played some key roles in early developments of statistical physics of critical phenomena in Taiwan. The paper first introduces some developments in the study of critical phenomena from late 19th century to early 70s in the 20th century when renormalization group theory was formulated. The paper then reviews some topics on analytic, Monte Carlo, and RG approach to some lattice models, including variational RG approach to the Ising model, slow relaxation of a spin glass model at low temperatures, iterative method for quantum spin models, percolation theory of critical phenomena of Ising-like models and hard-core particle model, histogram Monte Carlo method and histogram Monte Carlo RG method, universal finite-size scaling functions of lattice models, critical slowing down of the Ising model, finite-size corrections for critical lattice models, and self-organized critical systems. Such topics are closely related to the author's own research experience. Finally, the paper outlines some very recent developments, summarizes main results of this paper, and points out some interesting problems for further studies, e.g. why a biological system can maintain in a non-equilibrium state for a very long time.

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**I. INTRODUCTION**

The basic content of statistical physics was formulated from late 19th century to early 20th century by Ludwig Eduard Boltzmann (20 February 1844 - 5 September, 1906) [1] and Josiah Willard Gibbs (11 February 1839 - 28 April 1903) [2]. The objective of statistical physics is to understand the properties of a macroscopic system from interactions of the molecules or atoms of the macroscopic system. One important research subfield of statistical physics is the study of phase transitions and critical phenomena.

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<sup>\*</sup> A paper in memory of late Professors Shang-keng Ma (1940-1983) and Yu-Ming Shih (1942-2005)<sup>†</sup> Electronic address: huck@phys.sinica.edu.tw

Before the end of World War II, there were some experimental [3–6] and theoretical [7–17] studies of phase transitions and critical phenomena. The main theoretical methods were the mean field theory [7, 9] and analytic calculations [8, 15, 17]. The later includes the exact solutions of a one-dimensional spin model (called Ising model later) in the external magnetic field [8], and the Ising model on the square lattice in zero magnetic field [17].

After World War II, theoretical, computational, and experimental studies of phase transitions and critical phenomena became one of the active research fields in sciences. The important concepts merged from such studies include universality and scaling. In 1971, H. E. Stanley published a book to introduce and review such developments [18].

In 1971, Ken G. Wilson developed renormalization group (RG) theory [19–21] for critical phenomena, which provides a framework for understanding universality and scaling in critical systems, and can be used to calculate critical quantities of critical systems. Such developments arose a stronger trend to study phase transitions and critical phenomena.

However, before 1970 the theoretical research on phase transitions and critical phenomena in Taiwan was almost zero. The situation began to change in 1970s due to efforts of some key researchers, including Professors Shang-keng Ma (1940-1983), Yu-Ming Shih (1942-2005), Fa-Yueh Wu, Hsin-Hsiung Chen, Keh-Ying Lin, Chen-Shiung Hsue, and Felix Lee. A brief review of such developments in 1970s is given in Appendix A of the present paper.

After the development of RG theory [19–21], Shang-keng Ma (Fig. 1(a)) at University of California at San-Diego (UCSD) published a series of papers on RG theory of critical phenomena [22, 23], including Monte Carlo renormalization group method for static and dynamic critical properties of the Ising model on lattices within the framework of a kinetic Ising model [23]. Besides, Ma wrote a book [24] about RG theory of critical phenomena. After 1975, Ma also paid his attention to random systems [25].

In 1976, Kadanoff, *et al.* [26] published a variational RG method to study critical phenomena of lattice models, which can give reasonably accurate results for the critical behavior of the square lattice Ising model.

In 1977, Yu-Ming Shih invited some theoretical researchers in Taiwan (see Appendix A) to use RG theory to study critical phenomena. The group started the research by using Kadanoff's variational RG method [26] to study the Ising model.

In 1977-1978, Shang-keng Ma was a visiting professor at Department of Physics of National Tsing Hua University (NTHU) in Hsinchu, Taiwan. He coined the name “Research in Natural Science and Engineering (RINSE)” for the group organized by Y.-M. Shih. The group published two papers in 1978 about the scaling factor in RG transformation [27, 28]. In response to Ma's promotion of the usage of Chinese in scientific writing, the group published one of two papers in Chinese [28].

The RINSE group found a simple approximate method to determine the variational parameter in Kadanoff's lower bound RG transformations [29]. S.-P. Liu, D.-S. Wang and the author found that the method is exact for one-dimensional Ising model in zero external field [30]. The method may only be applied to the two-component Ising model in zero external field. Using this method [29], the author wrote a computer program and applied it to calculate the free energies of the Ising model on the body-centered cubic lattice [31].

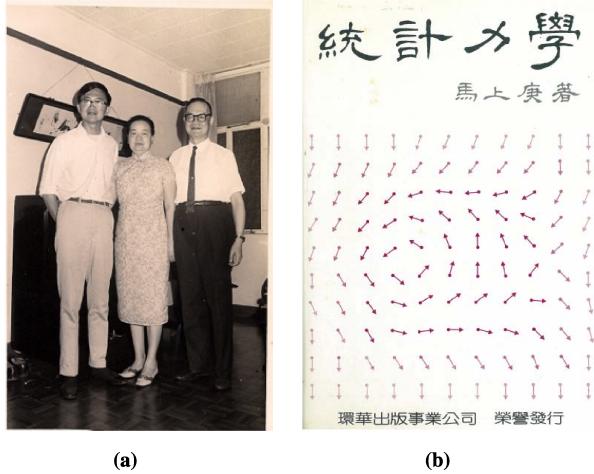


FIG. 1: (a) Photo of Sheng-Keng Ma (left) with his parents, Mr. and Mrs. Hsin-Yeh Ma. The photo was provided by Sheng-keng Ma's sister. (b) Cover of Sheng-Keng Ma's Chinese book on "Statistical Mechanics" published by Pan-Chinese Press, Taipei, in 1982 [38]. Chinese title and author of the book at the top of the cover were written by Sheng-keng Ma's mother.

From such studies, the author knew that RG transformations for interacting systems will generate a background energy.

At the end of October 1978, the author went to UCSD to work in S.-K. Ma's group as a postgraduate research physicist during November 1978–June 1979. The first problem to work in Ma's group was properties of spin glass [32–34]. Using Monte Carlo (MC) simulations and analytic calculations, Dasgupta, Ma and the author found that dynamic properties (e.g. slow relaxation) of a spin glass model at low temperatures can be understood from flipping of clusters with a distribution of barrier heights of the clusters [35]. Ma, Dasgupta and the author also developed an iterative algorithm to calculate properties of a quantum spin model with random nearest-neighbor couplings [36, 37]; the method is still widely used till now.

In 1981, Ma visited NTHU again and gave a course on statistical mechanics at Department of Physics. He also prepared a book "Statistical Mechanics" in Chinese published by a publisher in Taiwan [38] as shown in Fig. 1(b), which was translated into English [39] by M. K. Fung at Department of Physics of National Taiwan Normal University.

The purpose of this paper is not to give a comprehensive review on analytic, Monte Carlo and renormalization group approach to critical phenomena of lattice models, but to mention some key events, ideas, and references in such developments which would be useful for a general reader to understand this research field. The chosen topics are closely related to the author's own research experience.

This paper is organized as follows. In Sec. II, some developments of the theory of critical phenomena from late 19th century to the 70s in the 20th century (except renormalization group theory), especially those related to lattice phase transition models, are briefly reviewed. Some lattice phase transition models, including the Ising model, Potts model,

percolation model, and dimer model, are also introduced.

In Sec. III, theory of real space renormalization group method, including the variational renormalization group method [26], and its applications to lattice phase transition models are briefly reviewed.

In Sec. IV, the development of a theory for slow relaxation of a spin-glass model at low temperatures [35] and the application of an iterative method to study a quantum spin model [36, 37] are briefly reviewed.

In Sec. V, the connections between phase transitions of Ising-type models and lattice hard-core particle models with percolation transitions of correlated percolation models are briefly reviewed.

In Sec. VI, the histogram Monte Carlo simulation method and combination of this method with RG method to calculate critical quantity and universal finite-size scaling functions are briefly reviewed.

In Sec. VII, the study on self-organized critical systems is briefly reviewed.

In Sec. VIII, the important results of this study are summarized and discussed. Some more recent related developments are also summarized. Some interesting problems for further studies are introduced.

Appendix A gives a brief review about early studies of critical phenomena in Taiwan.

Appendix B derives the connection between the  $q$ -state Potts model and a  $q$ -state bond-correlated percolation model.

Appendix C explains how to choose aspect ratios of the square, honeycomb, and plane triangular lattices in order to get universal finite-size scaling functions for percolation and spin models on such lattices.

## II. EARLY DEVELOPMENTS IN THE THEORY OF CRITICAL PHENOMENA

In this session, some developments of the theory of critical phenomena from late 19th century to the 70s in the 20th century (except renormalization group theory), especially those related to lattice phase transition models are briefly reviewed. Some developments of RG theory will be presented in the next section.

### II-1. Critical liquid-gas systems

At the pressure  $P$  of 76 cm liquid Hg (1 atm), the liquid water has a phase transition to vapor at transition temperature  $T_t = 100^\circ\text{C}$  and the density (mass per unit volume) of liquid water  $\rho_l$  and the density of gas vapor  $\rho_g$  has a finite difference, i.e.  $\Delta\rho = \rho_l - \rho_g > 0$ . In laboratory, one can put a sample of water in a container of volume  $V$  and change the pressure  $P$  applied on the sample. As  $P$  is increased,  $T_t$  will increase and  $\Delta\rho$  will decrease and the specific heat  $C_p$ , the compressibility (change of volume due to pressure change)  $\alpha_p$ , and correlation length (linear dimension over which fluctuations can correlate with each other)  $\xi$  of the water will increase. As  $P$  is increased to reach a critical pressure  $P_c$ ,  $T_t$  will increase to reach the corresponding critical temperature  $T_c$  and  $V$  becomes critical volume

$V_c$ ,  $\Delta\rho$  becomes zero and  $C_p$ ,  $\alpha_p$ , and  $\xi$  diverge. This is called critical phenomena [18]. The critical exponents  $\beta$ ,  $\alpha$  &  $\alpha'$ ,  $\gamma$  &  $\gamma'$ , and  $\nu$  &  $\nu'$  are used to characterize critical behavior of  $\Delta\rho$ ,  $C_p$ ,  $\alpha_p$ , and  $\xi$  near the critical point, where  $\alpha$ ,  $\gamma$ , and  $\nu$  are for  $T > T_c$ , and  $\alpha'$ ,  $\gamma'$ , and  $\nu'$  are for  $T < T_c$ . At the critical temperature  $T_c$  and slightly away from the critical pressure  $P_c$  and volume  $V_c$ ,  $|V - V_c|$  varies with  $|P - P_c|$  as  $|V - V_c| \sim |P - P_c|^{1/\delta}$  with the critical exponent  $\delta$ . At the critical point, the correlation function  $\Gamma(r)$  for two particles at a large separation  $r$  has behavior  $\Gamma(r) \sim 1/r^{d-2+\eta}$  with the critical exponent  $\eta$  [18, 40].

In the later half of the 19th century, critical phenomena of many substances (e.g. CO<sub>2</sub> and H<sub>2</sub>O) were carefully studied. In 1869, Thomas Andrews (9 December 1813 - 26 November 1885) presented a detailed report on the critical phenomena of CO<sub>2</sub> [3].

In 1834, Emile Clapeyron (1799-1864) proposed the ideal gas law  $PV = RT$  for a mole ( $\approx 6.02 \times 10^{23}$  molecules or atoms) of ideal gas, where  $R$  is the ideal gas constant, and  $T$  is the absolute temperature. In 1873 Johannes Diderik van der Waals (23 November 1837 - 8 March 1923) took into account finite sizes and interactions of gas molecules to modify the ideal gas law and proposed that a mole of liquid-gas system can be described by the equation [7, 18, 41]

$$\left( P + \frac{a}{V^2} \right) (V - b) = RT, \quad (1)$$

where  $a$  and  $b$  are constants depending on the substance under study. One can use Eq. (1) to plot  $P$  as a function of  $V$  for a fixed  $T$  in the  $P$ - $V$  plane. For a constant  $T < T_c$  and a constant  $P$ , Eq. (1) could have three solutions for  $V$ ; in this case Maxwell construction (an equal area rule for the parts below and above horizontal line) can be used to obtain a curve in the  $P$ - $V$  plane, which has a horizontal portion corresponding to liquid-gas coexistence region [18]. When  $T$  is increased, the size of this region decreases. When  $T$  reaches the critical temperature  $T_c$ , the size of this region becomes 0. From this condition, one can derive that

$$V_c = 3b, \quad P_c = a/27b^2, \quad T_c = 8a/27bR, \quad (2)$$

from which one can determine  $a$ ,  $b$ , and ideal gas constant  $R$  from values of  $V_c$ ,  $P_c$ , and  $T_c$  measured by experiments. Two curves which connect boundaries of the horizontal portions for  $T \leq T_c$  form phase boundaries, which separate liquid phase, liquid-gas coexistence phase, and gas phase. For  $T \gg T_c$ , Equation (1) can be approximated by the ideal gas law  $PV = RT$ ; in this case for a constant pressure  $P$  there is only one corresponding volume  $V = RT/P$ . James Clerk Maxwell (13 June 1831-5 November 1879) considered that van der Waals' theory was an important work and reported it in Nature [42].

In 1881, van der Waals proposed “corresponding principle”. He defined reduced volume  $\phi$ , reduced pressure  $\pi$ , and reduced temperature  $\theta$  as  $\phi = V/V_c$ ,  $\pi = P/P_c$ ,  $\theta = T/T_c$ , then he rewrote Eq. (1) as

$$\left( \pi + \frac{3}{\phi^2} \right) (3\phi - 1) = 8\theta, \quad (3)$$

which has been called reduced van der Waals' equation. Equation (3) means that in terms of reduced variables, data for different substance can collapse on the same curve. Equations (3) and (1) were confirmed by experiments. In 1910, van der Waals was awarded the Nobel Prize in physics "for his work on the equation of state for gases and liquids" (see <http://www.nobelprize.org/>).

In 1924-1931, Lennard-Jones [43–45] proposed that the interaction potential between a pair of atoms or molecules at sites  $i$  and  $j$  with the distance  $r_{ij}$  is

$$v_{ij}(r_{ij}) = 4\epsilon \left( \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right), \quad (4)$$

where  $\sigma$  and  $\epsilon$  are used as units for length and energy strength, respectively. Thereafter, the potential of Eq. (4) is called Lennard-Jones potential.

In 1945, Guggenheim [46] reported that in the  $T/T_c$  versus  $\rho/\rho_c$  plane ( $\rho$  and  $\rho_c$  are density and critical density of the substance, respectively) the coexistence curves of  $N_e$ ,  $A_r$ ,  $K_r$ ,  $X_e$ ,  $N_2$ ,  $O_2$ ,  $CO$ , and  $CH_4$  are very consistent with each other. Thus van der Waals's general idea for the universality of the coexistence curves was further confirmed. However, near the critical point, Guggenheim found that  $|\rho - \rho_c| \sim |1 - (T/T_c)|^\beta$ , where the critical exponent  $\beta$  is about  $1/3$  [46], on the other hand van der Waals's equation gives  $\beta = 1/2$  [18]. The discovery of such deviation from van der Waals's theory marks modern era of critical phenomena [18].

In 1954, H. W. Habgood and W. G. Schneider carried out extensive *PVT* measurements of xenon and found the critical isotherm of xenon is considerably flatter and broader over a range of densities than that corresponding to a van der Waals equation [47], which indicates that experimental measured  $\delta$  is larger than  $\delta = 3$  calculated from van der Waals's theory [18]. In 1955, B. Widom and O. K. Rice [48] analyzed the experimental data for xenon, carbon dioxide, and hydrogen and found that the most frequently occurring value of  $\delta$  is 4.2. In 1964, B. Widom [49] presented an argument that the critical exponent  $\delta$  is related to the exponent for the order parameter  $\beta$  and the exponent for the compressibility  $\gamma$  by

$$\delta = 1 + \gamma/\beta. \quad (5)$$

In 1964, M. E. Fisher reviewed the "classical" (e.g. van der Waals) theories of the gas-liquid critical point and compared the predictions concerning the nature of the singularities of the coexistence curve, the specific heat, and the compressibility critically with experiment and with the analytical and numerical results for lattice gas models [50]. He also reviewed theories about the pair correlation function and critical scattering. He listed the deviation of the predictions of "classical" (e.g. van der Waals) theories from experimental data [50].

In 1965, B. Widom [51] identified the interface thickness of a gas-liquid system with the correlation length of that system and found that the van der Waals, Cahn-Hilliard theory [52] of interfacial tension for a fluid near its critical point becomes equivalent to the Ornstein-Zernike, Debye theory [50, 53] of molecular correlations. Widom then took into account the nonclassical behavior of the compressibility and coexistence curve, and found

that the theory is in good agreement with independently known facts in three-dimensional systems, yet slightly but unambiguously wrong in two dimensions. Widom replaced one of the hypotheses of the original theory by an alternative hypothesis and found that the resulting theory is correct in both two and three dimensions [51].

## II-2. The Ising model

Besides liquid-gas critical systems, ferromagnet to paramagnet transitions and order-disorder transitions in alloys also show critical behavior [18]. In 1895, Pierre Curie (15 May 1859 - 19 April 1906) reported that as the temperature increases, a ferromagnet can change into a paramagnet at a temperature  $T_c$  [4], which was known as Curie temperature or critical temperature. The physical quantities of a magnetic system, which correspond to  $\Delta\rho \equiv \rho_l - \rho_g$  and compressibility  $\alpha_p$  of the gas-liquid system, are the spontaneous magnetization  $M_s$  and magnetic susceptibility  $\chi$ , respectively [18]. The critical exponent of  $M_s$  is  $\beta$ , and the critical exponent of  $\chi$  are  $\gamma$  and  $\gamma'$  for  $T > T_c$  and  $T < T_c$ , respectively [18].

In early 1920s, Wilhelm Lenz (1888-1957) asked his student Ernst Ising (10 May 1900 - 11 May 1998) to study a simple model for ferromagnet to paramagnet transitions. For the model on a lattice  $G$  of  $N$  sites and  $E$  nearest neighbor bonds, the  $i$ -th site of the lattice is assigned a spin  $\sigma_i$ ,  $1 \leq i \leq N$ , which can be +1 (spin up) or -1 (spin down). When two nearest-neighbor spins are in the same (different) direction, there is an interaction energy  $-J$  ( $J$ ), where  $J$  is a coupling constant. The spin  $\sigma_i$  also couples with an external magnetic field  $h$  with an energy  $-h\sigma_i$ .

Thus the Hamiltonian (total energy) of the spin system can be written as

$$H(\sigma) = -J \sum_{(i,j)} \sigma_i \sigma_j - h \sum_i \sigma_i, \quad (6)$$

where  $\sigma$  represents the configuration of  $N$  spins, i.e.  $\sigma \equiv (\sigma_1, \dots, \sigma_N)$ , the first summation is over all  $E$  nearest-neighbor pairs of spins and the second summation is over all  $N$  sites of the lattice. According to statistical mechanics, at a given absolute temperature  $T$ , the probability for  $\sigma$  to appear  $p(\sigma)$  is proportional to the Boltzmann factor  $\exp(-\beta H(\sigma))$ , and thus is given by

$$p(\sigma) = \frac{\exp(-\beta H)}{Z_N} = \frac{\exp(K \sum_{(i,j)} \sigma_i \sigma_j + B \sum_i \sigma_i)}{Z_N}, \quad (7)$$

where  $\beta = 1/k_B T$ , with  $k_B$  being the Boltzmann constant,  $K = \beta J$ ,  $B = \beta h$ , and

$$Z_N = \sum_{(\sigma_1, \dots, \sigma_N)} \exp(-\beta H), \quad (8)$$

is the partition function of the system. The summation in the right-hand side of Eq. (8) is over  $2^N$  spin configurations.

From  $Z_N$ , one can calculate the free energy  $f_N$ , the internal energy  $U_N$ , the specific heat  $C_N$ , the magnetization  $M_N$ , and the magnetic susceptibility  $\chi_N$  per lattice site as follow [18]:

$$f_N = \frac{\ln(Z_N)}{N}, \quad U_N = -\frac{\partial f_N}{\partial \beta}, \quad C_N = \frac{\partial U_N}{\partial T}, \quad (9)$$

$$M_N = -\frac{\partial f_N}{\partial B}, \quad \chi_N = \frac{\partial M_N}{\partial B}. \quad (10)$$

Ising solved exactly the model on a one-dimensional lattice [8]. Hereafter, the model has been called Lenz-Ising model or simply the Ising model [54], and  $\sigma_i = \pm 1$  has been called the Ising spin. Ising found that his exact solution for the spin model in the limit  $N \rightarrow \infty$  does not show the phase transition for finite temperatures.

In 1941, H. A. Kramers and G. H. Wannier [15] proposed a transfer matrix method to solve exactly one-dimensional Ising model. The partition function of the Ising model on one-dimensional lattice with  $N$  sites and periodic boundary conditions can be written as

$$Z_N = \text{Trace}M^N = \lambda_1^N + \lambda_2^N, \quad (11)$$

where  $M$  is a  $2 \times 2$  matrix given by

$$M = \begin{bmatrix} \exp(K+B) & \exp(-K) \\ \exp(-K) & \exp(K-B) \end{bmatrix} \quad (12)$$

and  $\lambda_1$  and  $\lambda_2$  are eigenvalues of  $M$  given by

$$\lambda_1 = e^K \cosh B + (e^{2K}(\cosh B)^2 - e^{2K} + e^{-2K})^{\frac{1}{2}}, \quad (13)$$

$$\lambda_2 = e^K \cosh B - (e^{2K}(\cosh B)^2 - e^{2K} + e^{-2K})^{\frac{1}{2}}. \quad (14)$$

Since  $\lambda_1 > \lambda_2$ , in the thermodynamic limit  $N \rightarrow \infty$ , the free energy per spin  $f_\infty(K, h)$  is given by

$$f_\infty(K, B) = \ln(\lambda_1), \quad (15)$$

which is an analytic function of  $K$  and  $B$ , and the physical quantities of the one-dimensional Ising model do not show singular behavior at finite temperatures. Thus this system does not have a phase transition.

Please note that to get thermodynamic free energy per spin,  $f_\infty(K, B)$ , one should calculate the largest eigenvalue and to calculate exact partition function one should calculate all eigenvalues. Thus the calculation of the later is more difficult than the calculation of the former. This statement is still true when one extend the calculation to the Ising model on two-dimensional or three-dimensional lattices. Examples of two-dimensional regular square

(sq), honeycomb (hc), and plane triangular (pt) lattices are shown in the last figure of Appendix C.

For the regular sq, hc, and pt lattices, one can draw a vertical line at the middle point of each bond connecting two nearest neighbor sites. The intersection points of such vertical lines form the dual lattice of the original lattice. It is easy to show that the dual lattices of hc and pt lattices are pt and hc lattices, respectively. The dual lattice of the sq lattice is also the sq lattice and the sq lattice is called “self-dual”.

H. A. Kramers and G. H. Wannier [15] used self-duality of the Ising model on the square lattice to derive that the critical point of the Ising model on the square lattice satisfies the equation:

$$\sinh(2K_c) = 1, \quad (16)$$

whose solution gives the critical temperature  $T_c$ :

$$K_c = \frac{J}{k_B T_c} = \frac{1}{2} \ln(\sqrt{2} + 1) = 0.4406867935 \dots \quad (17)$$

In 1944, L. Onsager calculated exactly the thermodynamic free energy  $f$ , the internal energy  $U$ , and the specific heat  $C$  per lattice site of the square lattice Ising model in zero external field [17] and found that they are given by

$$\begin{aligned} f &\equiv f_\infty = \log(2 \cosh 2K) + \frac{1}{2\pi} \int_0^\pi \log\left(\frac{1}{2}\left(1 + (1 - k_1^2 \sin^2 \phi)^{\frac{1}{2}}\right)\right) d\phi, \\ U &\equiv -J \frac{df}{dK} = -J \coth 2K \left(1 + \frac{2}{\pi} k_1'' K_1\right), \\ C &\equiv k_B \frac{d^2 f}{dK^2} = k_B (K \coth 2K)^2 \frac{2}{\pi} \left(2K_1 - 2E_1 - (1 - k_1'') \left(\frac{1}{2}\pi + k_1'' K_1\right)\right), \end{aligned} \quad (18)$$

where  $k_1 = 2 \sinh K / \cosh^2 2K$ ,  $k_1'' = 2 \tanh^2 K - 1$ ;  $K_1$  and  $E_1$  are complete elliptic integrals given, respectively, by

$$K_1 = K(k_1) = \int_0^{\pi/2} (1 - k_1^2 \sin \phi)^{-\frac{1}{2}} d\phi,$$

and

$$E_1 = E(k_1) = \int_0^{\pi/2} (1 - k_1^2 \sin \phi)^{\frac{1}{2}} d\phi.$$

Onsager found that the specific heat  $C$  is divergent at the finite critical temperature [17] given by Eq. (17).

In 1949, at the first International Conference on Statistical Physics and Thermodynamics, L. Onsager presented an exact formula for the spontaneous magnetization of the Ising model on the square lattice [55], but he did not publish the procedure of his derivation.

In 1949, B. Kaufman [56] used spinor analysis to calculate exact partition function of the Ising model on the square lattice of finite sizes, and B. Kaufman and L. Onsager [57] used spinor analysis and an elliptic substitution to calculate correlation functions of the Ising model on the square lattice.

In 1952, Chen-Ning Yang [58] derived the exact spontaneous magnetization  $M_s$  of the Ising model on the square lattice with isotropic interactions.  $M_s$  is given by

$$M_s = \left[ \frac{(1+x^2)}{(1-x^2)^2} (1-6x^2+x^4)^{\frac{1}{2}} \right]^{\frac{1}{4}}, \quad (19)$$

where  $x = \exp(-2K)$ . Yang found that the critical exponent  $\beta$  of  $M_s$  is  $1/8$ .

In 1952, under the suggestion of C. N. Yang, C. H. Chang [59] derived the exact spontaneous magnetization  $M_s$  of the Ising model on a square lattice with anisotropic interactions, i.e. the coupling constants in the horizontal direction  $J_1$  and in the vertical direction  $J_2$  are different. Chang [59] found that  $M_s$  is given by

$$M_s = [1 - k^2]^{\frac{1}{8}} = \left[ 1 - \left( \frac{2x_1}{1-x_1^2} \frac{2x_2}{1-x_2^2} \right)^2 \right]^{\frac{1}{8}}, \quad (20)$$

where  $k = 1/[\sinh(2J_1/k_B T) \sinh(2J_2/k_B T)]$ ,

$$x_1 = 1 - \exp\left(-\frac{2J_1}{k_B T}\right), \quad x_2 = 1 - \exp\left(-\frac{2J_2}{k_B T}\right). \quad (21)$$

Equation (20) is consistent with that derived by L. Onsager in 1949 [55] and implies that for  $0 < J_1/J_2 < \infty$ ,  $\beta$  is always equal to  $1/8$ . C. H. Chang [59] conjectured that for other planar lattices  $\beta$  is also equal to  $1/8$ , which was confirmed by later calculations. Now it is generally believed that for the Ising model on all two-dimensional lattices, including the square (sq), the plane triangular (pt), the honeycomb (hc) lattices, etc, the specific heat exponent  $\alpha$ , the spontaneous magnetization exponent  $\beta$ , the magnetic susceptibility exponent  $\gamma$ , and the correlation length exponent  $\nu$  are 0 (logarithmic divergence),  $1/8$ ,  $7/4$ , and  $1$ , respectively [18].

In 1952, C. N. Yang and T. D. Lee proposed that the critical behavior of the gas-liquid system can be represented by a lattice-gas model [60], in which every lattice site is either occupied by an atom or vacant. They showed that the lattice gas model is equivalent to the Ising model. According to their theory, the gas-liquid systems and three dimensional (3D) Ising model should be in the same universality class and have the same set of the critical exponents, which was confirmed by later Monte Carlo simulations of the 3D Ising model and the molecular dynamics simulation (MD) of the Lennard-Jones system, to be discussed below. Yang and Lee [60] also used zeros of the partition function in the complex fugacity plane to study critical behavior of the Ising model.

In 1959, using the work of B. Kaufman and L. Onsager [57] on correlation function, M. E. Fisher [61] found that the magnetic susceptibility of the square lattice Ising model has an exact critical exponent  $\gamma = 7/4$ .

In 1963, B. Widom [62] studied a lattice gas model on the honeycomb lattice and calculated the fraction of empty sites  $f_r$  ( $r = 0, 1, 2, 3$ ) which at equilibrium are neighbored by exactly  $r$  filled sites. B. Widom found that at the critical point,  $f_0 = 3/8 + 5\sqrt{3}/24$ ,  $f_1 = 1/8 + \sqrt{3}/24$ ,  $f_2 = 1/8 - \sqrt{3}/24$ , and  $f_3 = 3/8 - 5\sqrt{3}/24$  [62].

In 1965, M. E. Fisher [63] published a paper on the zeros of the canonical partition function in the complex temperature plane of the square lattice Ising model. He showed that the partition function zeros are distributed on circles in the thermodynamic limit, and that the logarithmic singularity of the two-dimensional Ising model is related to the zero distribution.

In 1966, Robert B. Griffiths, Chi-Yuan Weng, and James S. Langer [64] used mean field theory to study relaxation from metastable to stable states of the Ising ferromagnet in which each spin interacts equally with every other spin in the system. Spins are chosen at random and flipped over with probability given by a suitable Boltzmann factor. Approximate solutions to the stochastic equations, confirmed by computer calculations on small systems, indicate a relaxation time increasing exponentially with the size of the system [64].

In 1966, T. T. Wu [65] used theory of determinants to calculate spin-spin correlations of two-dimensional Ising model. From critical point of Eq. (1.7) in [65], one can conclude that T. T. Wu considered the Ising model on the square lattice. T. T. Wu found that at the critical temperature the correlation behaves asymptotically as the inverse fourth root of the separation, i.e. the critical exponent  $\eta$  [18] is  $1/4$ .

On the basis of the exact partition function of the Ising model on a  $n \times m$  planar square lattice with periodic boundary conditions obtained by B. Kaufman [56], in 1969 Arthur E. Ferdinand and Michael E. Fisher [66] calculated finite-size corrections (FSCs) for the free energy  $f$ , the internal energy  $U$ , and the specific heat  $C$  of the Ising model for fixed  $R = m/n$  up to order  $1/n^2$ ,  $1/n$ , and  $1/n$ , respectively.

In 1971, M. Blume, V. J. Emery, and Robert B. Griffiths [67] introduced an Ising-type model for the  $\lambda$  transition and phase separation in He3-He4 mixtures and solved the model in the mean-field approximation. For reasonable values of the parameters of the model the phase diagram is qualitatively similar to that observed experimentally and the phase separation appears as a consequence of the superfluid ordering. Changing the parameters produces many different types of phase diagram, including as features  $\lambda$  lines, critical points, tricritical points, and triple points. Certain thermodynamic features which differ from the He3-He4 experiments may be artifacts of the mean-field theory [67]. This model is known as the BEG model.

### II-3. The dimer model

To study thermodynamic behavior of the absorption of diatomic molecules, e.g. O<sub>2</sub>, on the flat crystal surface, one can use the dimer model.

In 1937, R. H. Fowler and G. S. Rushbrooke published a paper on “Statistical theory of perfect solutions” in which they used an approximate method to study a system consisting of  $N_1$  dimers and  $N_2$  monomers on a lattice of  $N$  sites [10]. A dimer occupies two nearest-neighbor lattice sites and a monomer occupies one lattice site so that  $N = 2N_1 + N_2$ .

In 1961, P. W. Kasteleyn published a paper on “The statistics of dimers on a lat-

tice, I. The number of dimer arrangements on a quadratic lattice” in which he used the Pfaffian method to calculate exact partition functions for dimers fully covered (there is no monomers) finite quadratic lattices with both periodic and free boundary conditions [68].

In 1961, Michael E. Fisher solved in exact closed form for dimers on a finite  $m \times n$  plane square lattice with edges which is completely filled with  $mn/2$  dimers (close-packed limit). In terms of the activities  $x$  and  $y$  of horizontal and vertical dimers, the configurational partition function  $Z_{m,n}(x,y)$  is given in the limit of a large lattice by

$$\lim_{m,n \rightarrow \infty} \frac{Z_{m,n}(x,y)}{mn} = \frac{1}{2} \ln y + \frac{1}{\pi} \int_0^{x/y} \frac{1}{v \tan v} dv,$$

which is a continuous function of  $x$  and  $y$  [69].

In the same year, H. N. V. Temperley and Michael E. Fisher published a paper on “Dimer problem in statistical mechanics-an exact result” in which they briefly reviewed solutions of the dimer model on square lattices [70].

In 1967, Arthur E. Ferdinand [71] studied the finite-size corrections for the dimer model on  $m \times n$  rectangular lattice with free boundary conditions and periodic boundary conditions. The total free energy is calculated asymptotically for fixed  $R = n/m$  up to terms  $o(1/n^{2-c})$  for any  $c > 0$ . The bulk terms proportional to  $nm$ , the surface terms proportional to  $(n+m)$  which vanish for periodic boundary conditions, and the constant terms which reveal a parity and shape dependence are expressed explicitly using dilogarithms and elliptic theta functions [71].

#### II-4. Monte Carlo methods

In the Monte Carlo method, the computer is used to generate a sequence of random or pseudo random numbers. Such random numbers are then used to generate configurations of a many particle systems in such a way that the probability for a configuration to appear is proportional to the probability of that configuration in the equilibrium state. Physical quantities of the many body system can be calculated from the generated sequence of configurations. After the development of computers, Monte Carlo methods are developed to study various many body systems, including lattice critical systems.

In 1949, N. Metropolis and S. Ulam proposed the Monte Carlo method [72]. In 1952, R. R. Wilson used a Monte Carlo method to study shower production [73].

In 1953, Nicholas Metropolis, *et al.* used a Monte Carlo method to calculate equation of state for the two-dimensional rigid sphere system [74]. Their simulation results were compared to the free volume equation of state and to a four-term virial coefficient expansion [74].

In 1954, J. M. Hammersley and K. W. Morton gave a tutorial introduction to Monte Carlo method [75].

In 1954, Marshall N. Rosenbluth and Arianna W. Rosenbluth [76] used a Monte Carlo method to calculate the equation of state of three-dimensional hard spheres.

In 1954, F. T. Wall and L. A. Hiller [77] considered a self-avoiding walk model for the macromolecule on lattices and used a Monte Carlo method to calculate mean square end-to-end separation  $\langle r_n^2 \rangle$  of self-avoiding walks of length (step)  $n$  on simple cubic (sc)

and tetrahedral lattices. They found that for both lattices

$$\langle r_n^2 \rangle \sim n^{1.22}. \quad (22)$$

In 1955, Marshall N. Rosenbluth and Arianna W. Rosenbluth used a Monte Carlo method to calculate the average extension of molecular chains [78]. The behavior of chains of many molecules was investigated by solving a restricted random walk (i.e. self-avoiding walk) problem on the sc lattice and the square lattice. In the Monte Carlo calculation a large number of chains were generated at random, subject to the restrictions of no crossing or doubling back, to give the average extension of the chain as a function of chain length  $n$ , the number of links in the chain. A system of weights was used in order that all possible allowed chains were counted equally. Results for the true random walk problem without weights were obtained also [78]. For the sc lattice, their result is consistent with that of Eq. (22); for the square lattice, the exponent is 1.45 instead of 1.22 [78].

In 1957, W. W. Wood and F. R. Parker used a MC method to calculate equation of state of Lennard-Jones system [79]. In the same year, W. W. Wood and J. D. Jacobson used a MC method to calculate equation of state of hard spheres [80].

In 1960-1961, L. Guttman used a Monte Carlo method to study the Ising model on body-centered cubic (bcc) lattices with various sizes and concentration of +1 spins [81]. In all cases the heat capacity has a well-defined maximum. At the equatomic composition, the height of this maximum is greater in the larger crystal. Discontinuities in thermodynamic properties were not observed, and it seems reasonable that the order-disorder transition in an infinite crystal would be characterized by an infinite heat capacity as calculated by Onsager and others for two-dimensional crystals. Comparison of the results with experimental properties of Cu-Zn binary alloy suggests a remarkable applicability of the Ising model to this system. The potentialities and limitations of the Monte Carlo method for systems with phase transitions were discussed [81].

In 1968-1969, K. Binder and H. Rauch used a Monte Carlo method to calculate spin-correlation functions of the Ising model on a simple cubic lattice [82].

In 1973, E. Stoll, K. Binder, and T. Schneider used a Monte Carlo method to study dynamic critical phenomena in the two-dimensional kinetic Ising model [83].

## II-5. The percolation models

“Percolation” means spreading or penetration from one-side of the system to another. From 1900 to 1956, there are 27 publications on percolation collected in SCI extended database. Most of such publications are related to percolation of water through soil. From 1957, J. M. Hammersley published a series of papers on mathematical aspects and Monte Carlo simulations of percolation models [84, 85] and percolation becomes an important research topic in sciences after 1957.

There are several kinds of percolation models. In the bond random percolation model on a lattice  $G$  of  $N$  sites and  $E$  bonds, each bond of the lattice is occupied with a bond probability  $p$ ,  $0 < p \leq 1$ , and the sites connected by occupied bonds are defined to be in the same cluster. Since each bond can be either occupied or vacant, the total number of possible bond configurations, also called subgraphs and denoted by  $G'$ , is  $2^E$ . The probability for a

subgraph  $G'$  of  $b(G')$  occupied bonds to appear is

$$\pi(G', p) = p^{b(G')}(1 - p)^{E - b(G')}.$$
 (23)

For the site percolation model on  $G$  of  $N$  sites, each site of the lattice is occupied with a site probability  $p_s$ ,  $0 < p_s \leq 1$ , and the nearest neighbor occupied sites are defined to be in the same cluster. There are  $2^N$  different site configurations, call subgraphs and denoted by  $G'$ . The probability for a subgraph of  $v(G')$  occupied sites and  $N - v(G')$  vacant sites to appear is given by

$$\pi(G', p_s) = p_s^{v(G')}(1 - p_s)^{N - v(G')}.$$
 (24)

When  $p$  or  $p_s$  increases, the average size of the clusters also increases. The cluster which extends from the top to the bottom of the lattice is called the percolating cluster. The subgraph which contains at least one percolating cluster is called the percolating subgraph and is denoted by  $G'_p$ , otherwise the subgraph is called the non-percolating subgraph and is denoted by  $G'_f$ .

The average fraction of lattice sites in the percolating cluster is called “the percolation probability”  $P(G, p)$ . The probability that at least one percolating cluster exists is called the existence probability (also called spanning probability or crossing probability)  $E_p(G, p)$ . As the linear size of the lattice  $L$  goes to  $\infty$ ,  $P > 0$  and  $E_p(G, p) > 0$  for  $p > p_c$ , where  $p_c$  is called percolation threshold or critical point.  $E_p(G, p)$  and  $P(G, p)$  for the bond percolation on  $G$  can be written as

$$E_p(G, p) = \sum_{G'_p \subseteq G} \pi(G'_p, p),$$
 (25)

$$P(G, p) = \sum_{G'_p \subseteq G} \pi(G'_p, p) N^*(G'_p)/N,$$
 (26)

where  $\pi(G'_p, p)$  is defined by Eq. (23). The sums in Eq. (25) and Eq. (26) are over all  $G'_p$  of  $G$ ;  $N^*(G')$  is the total number of lattice sites in the percolating clusters of  $G$ . Similar equations can be written for site percolation model.

In 1961, Michael E. Fisher and John W. Essam [86] used analytic calculation to study site and bond percolation on various Bethe-like lattices and found that the percolation probability for all cases can be written in the form:  $R(p) \approx C(p - p_c)^\beta$  ( $p \geq p_c$ ), where  $C$  depends on site or bond percolation and lattice-type, but  $\beta$  always equals to 1. This is a good example for the universality of the critical exponent.

In 1961, M. E. Fisher presented some inequalities for critical points of bond and site percolation on planar lattices [87].

In 1964, M. F. Sykes and J. W. Essam [88] used an analytic method to obtain  $p_c=1/2$  for site percolation on planar triangular (pt) lattice. They also derived that  $p_c$  for bond

percolation on square (sq), pt, and honeycomb (hc) lattices are given by

$$\begin{aligned} p_c(\text{sq}) &= 1/2, \\ p_c(\text{pt}) &= 2 \sin\left(\frac{\pi}{18}\right) = 0.347296\dots, \\ p_c(\text{hc}) &= 1 - 2 \sin\left(\frac{\pi}{18}\right) = 0.6527036\dots, \end{aligned} \quad (27)$$

respectively.

In 1976, J. Hoshen and R. Kopleman proposed a multiple labelling technique [89], which is a fast algorithm for identifying which sites are in the same cluster for site or bond percolation on a lattice of  $N$  sites. The computing time of this algorithm is proportional to the number of sites  $N$  of the lattice.

## II-6. Universality and scaling laws of critical exponents

Near the critical temperature  $T_c$ , one can define  $\epsilon \equiv (T - T_c)/T_c$  to represent dimensionless deviation of the temperature  $T$  from the critical temperature  $T_c$ . As  $T$  approaches  $T_c$  from  $T < T_c$ , the spontaneous magnetization  $M_s$  decreases to 0 as  $M_s \sim (-\epsilon)^\beta$ , the magnetic susceptibility  $\chi$  goes to  $\infty$  as  $\chi \sim (-\epsilon)^{-\gamma'}$ , the specific heat  $C$  goes to  $\infty$  as  $C \sim (-\epsilon)^{-\alpha'}$ , and the correlation length  $\xi$  goes to  $\infty$  as  $\xi \sim (-\epsilon)^{-\nu'}$ . As  $T$  approaches  $T_c$  from  $T > T_c$ , the magnetic susceptibility  $\chi$  goes to  $\infty$  as  $\chi \sim (\epsilon)^{-\gamma}$ , the specific heat  $C$  goes to  $\infty$  as  $C \sim (-\epsilon)^{-\alpha}$ , and the correlation length  $\xi$  goes to  $\infty$  as  $\xi \sim (\epsilon)^{-\nu}$ . At the critical temperature  $T_c$ , the magnetization  $M$  varies with the external magnetic field  $B$  with the exponent  $\delta$  as  $M \sim B^{1/\delta}$  [18].

There were intensive studies of critical exponents in 1960's. In 1963, G. S. Rushbrooke [90] used thermodynamics arguments to deduce the inequality:

$$2\beta + \gamma' \geq 2 - \alpha'. \quad (28)$$

In 1965, Robert B. Griffiths [91] also used a thermodynamics argument to derive the inequality:

$$(1 + \delta)\beta \geq 2 - \alpha'. \quad (29)$$

In 1965, Robert B. Griffiths [92] used thermodynamic arguments to derive several inequalities relating exponents which describe the behavior of the isothermal compressibility, specific heat at constant volume, and various other quantities near the critical point. Many of the inequalities apply equally to the analogous problem of a ferromagnet near its Curie point. The thermodynamic arguments are based on the usual “stability” or “convexity” conditions on the thermodynamic potentials together with other plausible, but less general, hypotheses [92].

Research on critical physical systems till 1960s had converged to the widely accepted idea of universality: critical systems can be classified into different universality classes so that the systems in the same class have the same set of critical exponents [18]. For example, the Ising models on two-dimensional lattices are in the same universality class, but the Ising

and percolation models are in different classes; three dimensional critical systems of liquid-gas, binary alloy, binary fluid, and the Ising model are in the same universality class.

Researches on critical physical systems also found that critical exponents satisfy certain equalities, called scaling laws, e.g. the specific heat exponent  $\alpha$ , magnetization exponent  $\beta$ , magnetic susceptibility exponent  $\gamma$ , and correlation exponent  $\nu$  satisfy the equality:

$$\alpha + 2\beta + \gamma = 2, \quad \nu - d = 2 - \alpha, \quad (30)$$

where  $d$  is spatial dimensions of the system. Equation (5) is another example of scaling law.

In 1965, B. Widom [93] introduced a function  $\phi(x, y)$  with  $x$  a measure of the temperature and  $y$  of the density. Fluids obeying an equation of state of van der Waals type ("classical" fluids) are characterized by  $\phi(x, y)$  being a constant. Widom suggested that in a real fluid  $\phi(x, y)$  is a homogeneous function of  $x$  and  $y$ , with a positive degree of homogeneity. Widom found that his theory implied that inequalities of Eqs. (28) and (29) being hold as equalities [93].

In 1967, Robert B. Griffiths [94] proposed modifications to the classical analysis of equilibrium thermodynamic properties near the liquid-vapor critical point to allow for infinite singularities in the specific heat  $C_v$ , nonclassical behavior of the co-existence curve, etc. A requirement that all thermodynamic functions for the homogeneous fluid be analytic is retained and turns out to be necessary in order to justify Maxwell's prescription for modifying the Van der Waals equation of state. He presented a corresponding analysis for ferromagnets near the Curie point and discussed Widom's proposed "homogeneous" equation of state with special attention to requirements of thermodynamic stability. He constructed several examples of such homogeneous functions, including cases where the critical indices agree (very nearly, at least) with current estimates for two- and three-dimensional Ising models [94].

To give a phenomenological theory of the scaling law, it was proposed that in the critical region the singular part of the Gibbs free energy,  $G(\epsilon, h)$ , and the pair correlation function  $\Gamma(r, \epsilon)$  for two particles with a separation  $r$  are generalized homogeneous functions of their arguments, so that [18]

$$G(\lambda^{y_t} \epsilon, \lambda^{y_h} h) = \lambda^d G(\epsilon, h), \quad (31)$$

for any value of the number  $\lambda$  and  $\Gamma(r, \epsilon)$  may be written as:

$$\Gamma(r, \epsilon) = \epsilon^{2(d-y_h)/y_t} f(r\epsilon^{1/y_t}). \quad (32)$$

The critical exponents may be written in terms of the magnetic scaling power  $y_h$  and the thermal scaling power  $y_t$ , e.g.

$$\begin{aligned} \beta &= (d - y_h)/y_t, \quad \delta = y_h/(d - y_h), \\ \gamma &= \gamma' = (2y_h - d)/y_t, \quad \alpha = \alpha' = 2 - d/y_t, \quad \text{and} \quad \nu = 1/y_t. \end{aligned} \quad (33)$$

The scaling relations or laws, e.g. Eqs. (5) and (30), follow from such equations.

In 1966-1967, L. P. Kadanoff defined effective spins for cell of spins, then tried to get interactions from such effective spins. He used the transformation from the original spin-spin interaction to the effective cell spin-cell spin interactions to obtain Eqs. (31) and (32) [95, 96].

In 1967, M. E. Fisher [97, 98] gave a detail review on universality and scaling laws of critical exponents. He proposed a “microdomain” or “cluster” model of ferromagnetism with a distribution of cluster sizes, which contains parameter  $\sigma$  and  $\tau$ . The exponent  $\sigma$  is directly related to the effective surface free energy of a large microdomain. Critical exponents can be expressed in terms of  $\sigma$  and  $\tau$ , which then imply scaling relations of such exponents [97, 98]. However, later studies of the Ising model by Monte Carlo simulations and series expansion indicate that Fisher’s cluster-size distribution does not agree with Monte Carlo and series expansion results. D. Stauffer gave a review on the studies of this problem till 1979 in Sec. 6.2.3 on page 61 of [99]. This problem will be discussed further in the section about percolation theory of interacting critical systems.

## II-7. Scaling and finite-size scaling

Another important concept in the theory of critical phenomena is scaling [18]. For example, in a ferromagnetic system, e.g.  $\text{CrBr}_3$ , for temperatures  $T$  near the critical temperature  $T_c$  (also called the Curie temperature in ferromagnetic systems), if we plot  $\sigma/|\epsilon|^\beta$  as a function of  $h/|\epsilon|^{\beta+\gamma}$ , where  $\sigma$  is the magnetization,  $\epsilon = (T - T_c)/T_c$ , and  $h$  is the external magnetic field, then the experimental data for different temperatures collapse on a single curve, called the scaling function.

In 1970, M. E. Fisher proposed the theory of finite-size scaling [100]: If the dependence of a physical quantity  $Q$  of a thermodynamic system (with the number of particles approaching  $\infty$ ) on the parameter  $\epsilon$ , which vanishes at the critical point  $\epsilon = 0$ , is of the form  $Q(\epsilon) \sim |\epsilon|^a$  near the critical point, then for a finite system of linear dimension  $L$ , the corresponding quantity  $Q(L, \epsilon)$  is of the form:

$$Q(L, \epsilon) \approx L^{-ay_t} F(\epsilon L^{y_t}), \quad (34)$$

where  $y_t$  ( $=\nu^{-1}$ ) is the thermal scaling power and  $F(x)$  is the finite-size scaling function. It follows from (34) that the scaled data  $Q(L, \epsilon)L^{ay_t}$  for different values of  $L$  and  $\epsilon$  can be described as a single function  $F(x)$  of the scaling variable  $x = \epsilon L^{y_t}$ . Thus it is important to know general features of the finite-size scaling function under various conditions. At the critical point  $\epsilon = 0$ , we have

$$Q(L, \epsilon = 0) \approx L^{-ay_t} F(0). \quad (35)$$

Thus  $Q$  and  $L$  in log-log scale have a linear relationship whose slope is given by  $-ay_t = -a/\nu$ .

## II-8. The $q$ -state Potts model

In the Ising model, each spin has two components. In 1952, R. B. Potts considered the spin model in which each spin has  $q$  components [101]. Two nearest-neighbor spins

have interaction energy  $-J$  if they have the same spin components; otherwise they have zero interaction energy. The Hamiltonian of the system on a lattice  $G$  of  $N$  sites and  $E$  nearest neighbor bonds can be written as

$$H_q = -J \sum_{(i,j)} \delta(s_i, s_j), \quad (36)$$

where the summation is over  $E$  nearest-neighbor pairs of spins,  $s_i = 1, 2, \dots, q$  for  $1 \leq i \leq N$ ,  $\delta(s_i, s_j) = 1$  when  $s_i = s_j$  and  $\delta(s_i, s_j) = 0$  when  $s_i \neq s_j$ . Potts calculated exact critical points for the Hamiltonian of Eq. (36) for integer  $q$ , the model is then called the  $q$ -state Potts model (QPM).

In 1969-1972, P. W. Kasteleyn and C. M. Fortuin [102, 103] used subgraphs  $G'$  of  $G$  to express the partition function  $Z_q$  for the  $q$ -state Potts model

$$Z_q = \sum_{(s_1, \dots, s_N)} \exp(-\beta H_q) = \sum_{G'} (e^K - 1)^{b(G')} q^{n(G')}, \quad (37)$$

where  $K = J/k_B T$ , the summation is over  $2^E$  subgraph  $G'$  of  $G$ ,  $b(G')$  and  $n(G')$  are the number of occupied bonds and the number of clusters in  $G'$ , respectively. From Eq. (37), one can generalize the QPM from integer values of  $q$  to noninteger values of  $q$ . The critical point of the  $q$ -state Potts model for  $q > 0$  on the square (SQ) is given by [102, 103]

$$K_c \equiv \frac{J}{k_B T_c} = \ln(\sqrt{q} + 1). \quad (38)$$

By coupling the external field to one component of the spin, P. W. Kasteleyn and C. M. Fortuin [102, 103] showed that as  $q \rightarrow 1$  the QPM on  $G$  is equivalent to the bond random percolation model on  $G$  with the bond occupation probability given by

$$p = 1 - \exp(-K). \quad (39)$$

In 1973, Baxter [104] calculated the exact free energy of the QPM on the square lattice at the critical point  $K_c$ . There are no exact calculations of the free energy and spontaneous magnetization for the QPM for general  $q$  and  $K$  in the thermodynamic limit even for the two-dimensional systems.

In 1974, D. Kim and R. I. Joseph used the duality and star-triangle transformations together with a uniqueness assumption to get the exact transition temperature of the Potts model with  $q$  states per site for the triangular and honeycomb lattices [105]. They found that the critical temperature  $T_c$  of the triangular QPM satisfies following equation [105]:

$$\begin{aligned} \frac{1}{v_{pt}} - 1 &= 2\sqrt{q} \cos \left[ \frac{1}{3} \tan^{-1} \left( \frac{4}{q} - 1 \right)^{1/2} \right], \quad \text{for } q \leq 4; \\ &= 2\sqrt{q} \cosh \left[ \frac{1}{3} \tanh^{-1} \left( 1 - \frac{4}{q} \right)^{1/2} \right], \quad \text{for } q \geq 4, \end{aligned} \quad (40)$$

where  $v_{pt} = (\exp(K) - 1)/(\exp(K) + q - 1)$  with  $K = J/k_B T_c$ . The critical point  $K_{hc}$  for the QPM on the honeycomb lattice is given by [105]

$$K_{hc} = \ln \frac{1}{v_{pt}}. \quad (41)$$

Equations (38), (40), (41), and (39) imply that the critical point  $p_c$  of the bond percolation on the square (sq), the plane triangular (pt), and the honeycomb lattices (hc), are given by Eq. (27).

In 1978, R. J. Baxter, *et al.* obtained the free energy, the internal energy, and the latent heat of the triangular lattice Potts model at the critical point [106].

In 1978, F. Y. Wu used a subgraph expansion method to show that the partition function of the  $q$ -state Potts model can be written as Eq. (37) and the  $q$ -state Potts model is corresponding to the bond random percolation model as  $q \rightarrow 1$  [107].

In 1979, M. P. M. den Nijs used the mapping of the critical points in the  $q$ -state Potts model for  $q \leq 4$  onto the Baxter line in the eight-vertex model to get exact thermal scaling power  $y_t$  for the  $q$ -state Potts model for  $0 \leq q \leq 4$  [108].

It has been found [108, 109] the thermal scaling power  $y_t$  and the magnetic scaling power  $y_h$  of the QPM on the two-dimensional lattice for  $q \leq 4$  are given, respectively, by

$$y_t = \frac{3(1-u)}{(2-u)}, \quad (42)$$

$$y_h = \frac{(3-u)(5-u)}{4(2-u)}, \quad (43)$$

where  $u = (2/\pi) \cos^{-1}(\sqrt{q}/2)$ . For the Ising model,  $q = 2$  and thus  $u = 1/2$ ,  $y_t = 1$ , and  $y_h = 15/8$ . For the bond random percolation mode,  $q = 1$  and thus  $u = 2/3$ ,  $y_t = 3/4$ , and  $y_h = 91/48$ , which together with Eq. (33) and the assumption of universality imply that for site and bond percolation models on all two-dimensional lattices, the correlation length exponent  $\nu$ , the percolation probability exponent  $\beta$ , and the mean cluster size exponent  $\gamma$  are  $4/3$ ,  $5/36$ , and  $43/18$ , respectively.

## II-9. Other lattice models and Yang-Baxter equation

Besides the Ising model, the dimer model, percolation models, and the Potts model mentioned above, there are other interesting lattice models including the Heisenberg model, the spherical model, the  $n$ -vector model [110], the 8-vertex model [111], and chiral Potts model [112]; the 8-vertex model [111] was solved exactly by Baxter and has been called the Baxter model. Such models are not the focus of the present paper and will not be discussed further in following sections. The readers who are interested in these models can read related original papers directly.

An important equation related to analytic solution of lattice models is Yang-Baxter equation [113]. A recent review about this equation was given by Perk and Au-Yang [114].

### III. RENORMALIZATION GROUP APPROACH TO LATTICE MODELS

In early 1970s, K. G. Wilson proposed a renormalization group theory to understand the universal behaviors of critical systems [19–21]. His theory also provides a calculation scheme to obtain critical quantities. For this contribution, K. G. Wilson was awarded the Nobel Prize in Physics in 1982 [115]. After the RG theory for critical phenomena was proposed by K. G. Wilson, S.-k. Ma wrote a series of papers on RG theory [22], Monte Carlo RG (MCRG) theory [23], and a book “Modern Theory of Critical Phenomena” [24]. Ma’s MCRG theory was extended to a more general theory by R. H. Swendsen [116]. M. E. Fisher also wrote a review paper on renormalization group theory [117].

Renormalization group theory was formulated to understand a system with a large degree of freedoms, e.g. the Ising model. The basic idea of the RG theory is very similar to Sun Tzu’s thinking about how to control an army with a large number of soldiers.

In Chapter 5: Forces of the “Art of War Chapter”, Sun Tzu wrote:

“Managing a large force can be similar to managing a small force. It is a matter of organization and structure. To direct and control a large force can be similar to directing and controlling a small force. It is a matter of communications and formations.”

#### III-1. RG transformations for one-dimensional Ising model

Now let us take one-dimensional (1D) Ising model as an example to explain basic idea of the RG transformation [118, 119]. In Eq. (11), the partition function for the one-dimensional Ising model of  $N$  spin with the periodic boundary condition (a ring) is calculated from the trace of  $M^N$ . We assume that  $N = 2^L$  with a large integer  $L$ . The partition function for  $N$  spins  $Z_N(K, h)$  can be written as the partition function for  $N' = N/2$  spins as follows:

$$Z_N(K, B) = \text{Trace}M^N = \text{Trace}M'^{N/2} = \exp\left(\frac{1}{2}NK'_0\right) Z_{N/2}(K', B'), \quad (44)$$

where

$$M' = MM = \exp K'_0 \begin{bmatrix} \exp(K' + B') & \exp(-K') \\ \exp(-K') & \exp(K' - B') \end{bmatrix} \quad (45)$$

and  $K'_0$ ,  $K'$  and  $B'$  are related to  $K$  and  $B$  by following equations:

$$\begin{aligned} K' &= \frac{1}{4} \ln \cosh(2K + B) + \frac{1}{4} \ln \cosh(2K - B) - \frac{1}{2} \ln \cosh(B), \\ B' &= h + \frac{1}{2} \ln \cosh(2K + B) - \frac{1}{2} \ln \cosh(2K - B), \\ K'_0 &= K' + \ln(2) + \ln \cosh B. \end{aligned} \quad (46)$$

Equation (44) implies that in the limit  $N \rightarrow \infty$ , the free energy per spin  $f(K, B)$  satisfies the equation

$$f(K, B) = \frac{1}{2}K'_0 + \frac{1}{2}f(K', B'). \quad (47)$$

Equation(47) can be iterated up to  $l$ -times to get

$$f(K, B) = \sum_{i=1}^l \left(\frac{1}{2}\right)^i K_0^{(i)} + \left(\frac{1}{2}\right)^l f(K^{(l)}, B^{(l)}). \quad (48)$$

For  $K > 0$  and  $B > 0$ ,  $K^{(i)}$  decreases and  $B^{(i)}$  increases as  $i$  increases. For a large  $l$ ,  $K^{(i)}$  can be approximated by 0 and  $f(K^{(l)}, B^{(l)})$  can be approximated by the free energy of a free spin in the external field  $B^{(l)}$ , i.e.  $f(K^{(l)}, B^{(l)}) \approx \ln(\exp(B^{(l)}) + \exp(-B^{(l)}))$  and  $f(K, B)$  can be approximated by  $f^{(l)}(K, B)$  given by

$$f^{(l)}(K, B) = \sum_{i=1}^l \left(\frac{1}{2}\right)^i K_0^{(i)} + \left(\frac{1}{2}\right)^l \ln \left[ \exp \left( B^{(l)} \right) + \exp \left( -B^{(l)} \right) \right]. \quad (49)$$

Equations (45) to (49) can be considered as calculation of the free energy of the 1D Ising model by RG transformations. The RG transformation of Eq. (45) and its equivalent version of Eq. (46) generate a background energy  $K_0^i$ , which contribute to the free energy of the system.

In the calculation of the free energy for one-dimensional Ising model from RG transformations, Paper [118] does not include the second term of Eq. (49) and paper [119] includes the second term in Eq. (49). Table 1 of [119] shows that the later [119] converges more quickly to the exact free energy than the former when  $B \neq 0$ .

### III-2. Variational RG transformations

In 1976, Kadanoff *et al.* published a variational RG transformation (VRGT) [26] for lattice models. They considered the Hamiltonian of  $N$  original spins  $\sigma \equiv (\sigma_1, \dots, \sigma_N)$ ,  $H(\sigma)$ , can be written as

$$H(\sigma) = - \sum_{R'} v(\sigma_{R'}), \quad (50)$$

where  $v(\sigma_{R'})$  is the energy of  $z$  spins in the cell  $R'$ , then they constructed a RG transformation to generate  $v'(\mu_{R'})$  so that the Hamiltonian after RG transformation is given by

$$H^L(\mu) = - \sum_{R'} v'(\mu_{R'}), \quad (51)$$

and  $v'(\mu_{R'})$  can be obtained from  $v(\sigma_{R'})$  via the RG transformation

$$\exp(v'(\mu_{R'}) = \sum_{(\sigma_1, \dots, \sigma_z)} \exp \left[ \frac{1}{z} p_0 m_1 + p_1 \sum_i \sigma_i \mu_i \right] \exp [zv(\sigma_1, \dots, \sigma_z) - u(s_1)] \quad (52)$$

where  $p_0$  and  $p_1$  are variational parameters, and  $u(s_1)$  is given by

$$u(s_1) = \ln 2 \cosh[p_0 + p_1 s_1]$$

with  $s_1 = \sigma_1 + \dots + \sigma_z$ .

The free energy calculated from  $H^L(\mu)$ , which depends on  $p_0$  and  $p_1$ , is the lower bound of the free energy calculated from  $H(\sigma)$ . For the spin models in zero external field,  $p_0$  can be taken to be 0 and there is only one variational parameter  $p \equiv p_1$ . In the following, we consider such a simple case.

The RG transformation of Eq. (52) can be iterated up to  $l$  steps with a series of  $l$  parameters  $p^{(1)} \equiv p, p^{(2)}, \dots, p^{(l)}$ , and to generate a series of effective Hamiltonian:  $H^{(1)} \equiv H^L(\mu), H^{(2)}, \dots, H^{(l)}$ , and a series of background energy:  $K_0^{(1)}, K_0^{(2)}, \dots, K_0^{(l)}$ . For a large  $l$ , the system will approach the high temperature fixed point (HTFP) when  $T > T_c$  or the low temperature fixed point (LTFP) when  $T < T_c$ . At the HTFP or LTFP, the free energy per spin of  $H^{(l)}$ , call  $f^{(l)}$ , can be estimated from  $K_0^{(1)}, K_0^{(2)}, \dots, K_0^{(l)}$  as in Eq. (49) for the case of the HTFP.  $f^{(l)}$  is still the low bound of the free energy of the original system and depends on  $p^{(1)} \equiv p, p^{(2)}, \dots, p^{(l)}$ . One can vary  $l$  parameters  $p^{(1)} \equiv p, p^{(2)}, \dots, p^{(l)}$  to get the maximum  $f^{(l)}$ , which is a very complicated numerical procedure.

In 1977, Y. M. Shih, *et al.* proposed a simple approximate method [29] to determine the variational parameter  $p^{(i)}$ ,  $1 \leq i \leq l$ , by solving following equation

$$\frac{\sum_{(\mu_1, \dots, \mu_z)} \frac{\partial v^{(i)}}{\partial p^{(i)}} \exp[v^{(i)}(\mu_{R'})]}{\sum_{(\mu_1, \dots, \mu_z)} \exp[v^{(i)}(\mu_{R'})]} = 0. \quad (53)$$

From the original cell potential  $v(\sigma_{R'})$  of Eq. (50), one can solve Eq. (53) to determine the variational parameter  $p^{(1)}$ . Using  $p^{(1)}$  in Eq. (52), one can determine the transformed cell potential  $v^{(1)} \equiv v'(\sigma_{R'})$  of Eq. (51). Using  $v^{(1)}$  in Eq. (53), one can solve Eq. (53) to determine the variational parameter  $p^{(2)}$ . Using  $p^{(2)}$  in Eq. (52), one can determine the transformed cell potential  $v^{(2)}$ . Such calculations can be iterated to determine a series of variational parameters  $p^{(i)}$  and transformed cell potentials  $v^{(i)}$  for  $1 \leq i \leq l$ . This calculation procedure is simpler than varying  $(p^{(1)}, \dots, p^{(l)})$  simultaneously to determine the optimal variational parameters. Shih, *et al.* found that the free energies calculated from their method [29] are consistent very well with the results reported in [26].

S.-P. Liu, *et al.* [30] derived exact equations for variational parameters of VRGT [26] for three cases:

- A. One-dimensional two-component Ising model in zero external field: in such case,  $p_0 = 0$  and  $\cosh(2p) = \exp(2K)$ , which is consistent with the result of M. Droz, *et al.* [120].
- B. One-dimensional two-component Ising model in non-zero external field  $B = h/k_B T$ : in such case exact variational parameters  $p_0$  and  $p \equiv p_1$  satisfy the equations

$$\begin{aligned} \tanh(p_0) &= \frac{e^{2K} \sinh(B)}{(e^{4K} \cosh^2(B) - 1)^{1/2}}, \\ \cosh(2p) &= e^{2K} \cosh(B). \end{aligned} \quad (54)$$

- C. One-dimensional three-component spin model in zero external field.

S.-P. Liu, *et al.* [30] found that the variational parameters determined by one-cell approximation are consistent very well with exact results for Case A, but not for Case B and Case C.

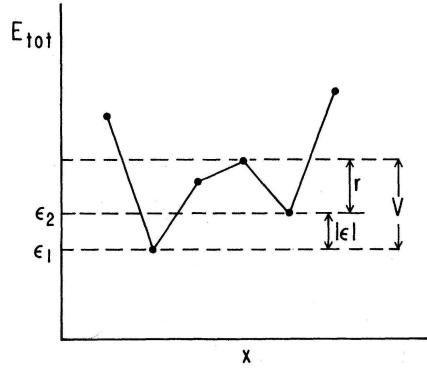


FIG. 2: Energy surface along a generalized coordinate  $x$ , that describe the flipping of a two-level cluster. Taken from Figure 2 of C. Dasgupta, S. K. Ma, and C.-K. Hu, Phys. Rev. B **20**, 3837 (1979) [35].

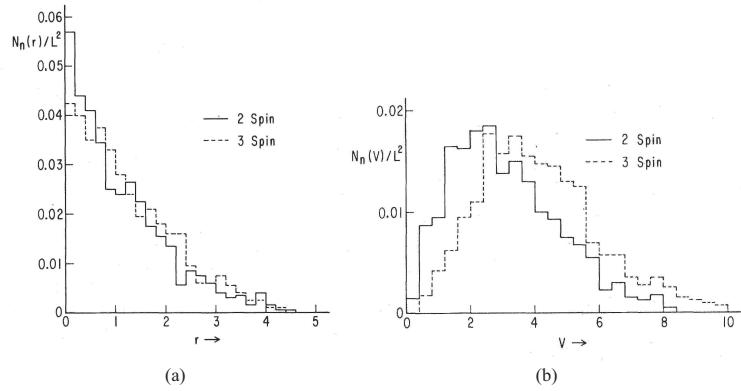


FIG. 3: (a) Distribution of barrier hight  $r$  measured from the higher of the two-spin (solid line) and three-spin (dash line) two-level clusters. (b) Distribution of barrier hight  $V = r + \epsilon$  measured from the lower of the two-spin (solid line) and three-spin (dash line) two-level clusters. (a) and (b) are taken, respectively, from Figure 3 and Figure 4 of C. Dasgupta, S. K. Ma, and C.-K. Hu, Phys. Rev. B **20**, 3837 (1979) [35].

Using the method of [29], Hu wrote a computer program and applied it to calculate the free energies of the Ising model on the body-centered cubic lattice [31]. From such studies, Hu knew that RG transformations for interacting systems will generate a background energy.

## IV. SPIN GLASS AND ONE-DIMENSIONAL QUANTUM SPIN CHAIN

### IV-1. Monte Carlo approach to a spin glass model

Near the end of October 1978, Hu went to UC-San-Diego to join Sheng-keng Ma's group. In the first day Hu entered Ma's office, Ma invited Hu to use Monte Carlo method to study a model of spin glass. Not long after Hu reached San-Diego, Ma received a preprint from Wolfgang Kinzel about remanent magnetization of a spin-glass model [34]. This paper presented many simulation results, but there is no theory to explain the results.

In 1979, Dasgupta, Ma and Hu (DMH) [35] presented a theory of the low-temperature dynamic properties of a spin-glass model with Gaussian random nearest-neighbor interactions. DMH considered the Edwards-Anderson model [33] with Ising spins  $\sigma_i$ ,  $1 \leq i \leq N = 400$ , on a  $20 \times 20$  square lattice with periodic boundary condition. The Hamiltonian for this system is given by

$$H = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j. \quad (55)$$

The summation is over all of the nearest-neighbor pairs  $\langle ij \rangle$  of spins. The nearest-neighbor coupling constants of spins,  $J_{ij}$ , follow the Gaussian distribution

$$P(J_{ij}) = \frac{1}{(2\pi)^{1/2} J} \exp(-J_{ij}^2/2J^2). \quad (56)$$

$J$  was taken to be 1.

The distribution of the low-lying energy levels of the system was studied with the aid of a numerical program. The results of this investigation suggest a simple picture of independent spins and small-size clusters of spins flipping in a frozen-random-background field as shown in Fig. 2, in which  $r$  and  $V$  are the barrier highs measured from the higher side and lower side of the cluster, respectively.

This picture is similar to the phenomenological description of amorphous materials in terms of two-level systems. Distributions of the quantities  $r$  and  $V$  which characterize a low-lying energy state in this picture were obtained numerically and are shown in Figs. 3(a) and 3(b), respectively.

A crude analytic calculation of these distributions was also included. These distributions are then used to calculate various low-temperature dynamic properties such as the time-dependent susceptibility, relaxation of the magnetization in an external magnetic field, the remanent magnetization, and the internal energy. Field cooled remanent magnetization  $M_{\text{TRM}}$  and isothermal remanent magnetization  $M_{\text{IRM}}$  [34] and internal energy  $E_{\text{TRM}}$  as functions of time  $t$  in log-log plot are shown in Fig 4(a).

The linear decreasing curves in Fig 4(a) indicate that these quantities have a power-law decay and can be written as

$$M_{\text{TRM(IRM)}}(t) \sim M_0 t^{\alpha_{\text{TRM(IRM)}}}, \quad (57)$$

$$M_{\text{TRM}}(t) \sim E_0 t^{\alpha_E}. \quad (58)$$

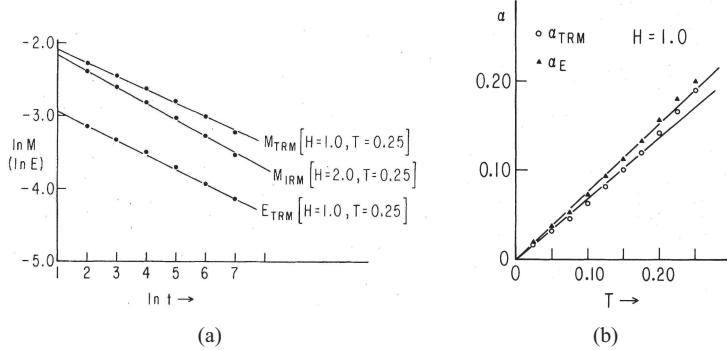


FIG. 4: (a) Remanent magnetization ( $M_{\text{TRM}}$  and  $M_{\text{IRM}}$ ) and internal energy ( $E_{\text{TRM}}$ ) as a function of time  $t$  in log-log plot showing a power-law decay. (b) Temperature dependence of the exponents  $\alpha_{\text{TRM}}$  and  $\alpha_E$ . (a) and (b) taken, respectively, from Figure 12 and Figure 13 of C. Dasgupta, S. K. Ma, and C.-K. Hu, Phys. Rev. B **20**, 3837 (1979) [35].

The temperature dependence of  $\alpha_{\text{TRM}}$  and  $\alpha_E$  was shown in Fig. 4(b).

The simple description of the spin glass model in [35] provides qualitative explanations of a large number of simulation results obtained in [34]. This is an interesting example to show that a simple model can be useful for understanding complicated phenomena.

#### IV-2. Iterative Approach to a one-dimensional quantum spin chain

In the spring of 1979, Sheng-Keng Ma, C. Dasgupta and Hu (MDH) began to work on a model of one-dimensional quantum spin chain [36]. They considered the random one-dimensional Heisenberg anti-ferromagnetic chain with the Hamiltonian

$$H = \sum_{i=1} K_r \vec{S}_r \cdot \vec{S}_{r+1}, \quad (59)$$

where  $\vec{S}_r$  are spin  $\frac{1}{2}$  operators. The coupling constants  $K_r$  are different for different  $r$ . Their values are distributed randomly following a distribution  $P(K, J)$ ,  $0 < K < J$ .

MDH proposed an approximate iteration method to study the system of Eq. (59). The method is based on successive elimination transformations, each of which eliminates a pair of neighboring spins, say  $\vec{S}_1$  and  $\vec{S}_2$ , with the maximum of coupling  $J$ .  $\vec{S}_1$  also couples with  $\vec{S}'_1$  with coupling  $K_1$  and  $\vec{S}_2$  also couples with  $\vec{S}'_2$  with coupling  $K_2$ . The part of Hamiltonian involving  $\vec{S}_1$  and  $\vec{S}_2$  is

$$H_{12} = K_1 \vec{S}'_1 \cdot \vec{S}_1 + J \vec{S}_1 \cdot \vec{S}_2 + K_2 \vec{S}_2 \cdot \vec{S}'_2. \quad (60)$$

Keeping  $\vec{S}'_1$  and  $\vec{S}'_2$  as fixed vectors and taking trace over  $\vec{S}_1$  and  $\vec{S}_2$ , one can get following effective Hamiltonian

$$\begin{aligned} H'_{12} &= -T \ln \text{Tr} \exp(-H_{12}/T) \\ &= F'_{12} + K' \vec{S}'_1 \cdot \vec{S}'_2. \end{aligned} \quad (61)$$

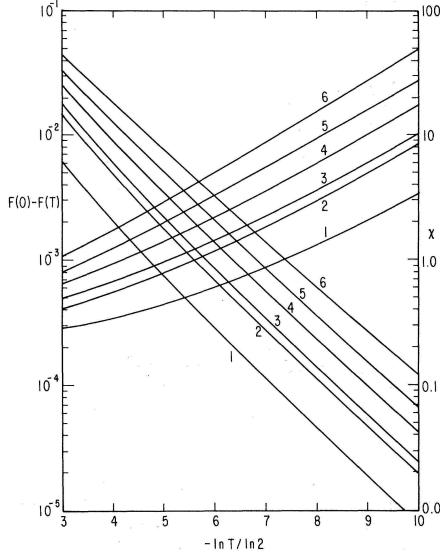


FIG. 5: Free energies  $F(0) - F(T)$  and zero-field susceptibilities  $\chi$  for the assorted distributions. The labels 1 through 6 denotes the distributions of  $P(K)$ ,  $0 < K < 1$ , as follows: 1.  $2\theta(K - 1/2)$ ; 2. 1; 3.  $1.58e^{-K}$ ,  $1.34e^{-K^2}$ ,  $(2/3)K^{-1/3}$ ; 4.  $(1/2)K^{-1/2}$ ; 5.  $(1/3)K^{-2/3}$ ; 6.  $(1/5)K^{-4/5}$ . Taken from Figure 1 of S.-K. Ma, C. Dasgupta and C.-K. Hu, Phys. Rev. Lett. **43**, 1434 (1979) [36].

Here

$$\begin{aligned} F'_{12} &= -\frac{3}{4}J - T \ln(1 + 3e^{-J/T}) - \frac{3}{16J}(K_1^2 + K_2^2)V\left(\frac{J}{T}\right), \\ K' &= K_1 K_2 W(J/T)/2J, \end{aligned} \quad (62)$$

where

$$\begin{aligned} V(y) &= \frac{1 - e^{-y}(1 - y)}{1 + 3e^{-y}}, \\ W(y) &= \frac{1 - e^{-y}(1 + y)}{1 + 3e^{-y}}. \end{aligned} \quad (63)$$

These results are correct up to the second order in  $K_1$  and  $K_2$ .

Now  $H_{12}$  is removed from  $H$  and  $K'\vec{S}'_1 \cdot \vec{S}'_2$  is added back to get the new Hamiltonian  $H'$  with  $(L - 2)$  spins. The free energy  $F(H')$  calculated from  $H'$  is related to the old free energy  $F(H)$  by

$$F(H) = F(H') + F'_{12}. \quad (64)$$

Equations (62) and (64) are similar to Eqs. (46) and (47) for the 1D Ising model. In both cases, the old system is transformed into a new (renormalized) system with a small number of degree of freedoms. Thus Eqs. (62) and (64) can be considered as RG transformations for the quantum spin system. Such transformations can be iterated step by step, and the

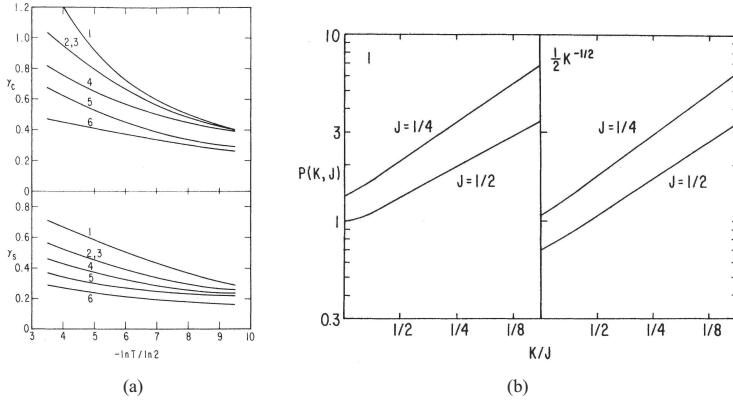


FIG. 6: (a) The specific heat exponent  $\gamma_c$ , and the susceptibility exponent  $\gamma_s$  as a function of  $-\ln T / \ln 2$ .  $\gamma_c$  and  $\gamma_s$ , are obtained by respectively differentiating the free energy and the susceptibility. The labels are the same as in Fig. 5. (b) Transformed distributions  $P(K, J)$  for  $P(K, 1) = 1$ , and  $\frac{1}{2}K^{-1/2}$ . (a) and (b) taken, respectively, from Figure 2 and Figure 3 of S.-K. Ma, C. Dasgupta and C.-K. Hu, Phys. Rev. Lett. **43**, 1434 (1979) [36].

corresponding  $P(K, J)$  is also modified with  $J$  becomes smaller and smaller. Equation (64) implies that the modification of  $P$  is determined by solving the equation

$$-\frac{\partial}{\partial J}P(K, J) = P(J, J) \int_0^J dK_1 dK_2 P(K_1, J) P(K_2, J) \delta(K - K_1 K_2 W(J/T)/2J). \quad (65)$$

Iterative transformations were used to calculate the low-temperature free energy  $F(T)$ , specific heat  $C$ , and zero-field susceptibilities  $\chi$  as function of the temperature  $T$  for several distributions  $P(K, J)$  listed in the figure caption of Fig. 5. The results for  $F(0) - F(T)$  and  $\chi$  were shown in Fig. 5. It was found that  $C$  and  $\chi$  have the approximate power-law dependence on  $T$ :

$$\begin{aligned} C &\sim T^{\gamma_c}, \\ \chi &\sim T^{\gamma_s-1}. \end{aligned} \quad (66)$$

The exponents  $\gamma_c$  and  $\gamma_s$  are slowly decreasing function of  $\ln(1/T)$  as shown in Fig. 6(a). Numerical solution of Eq. (65) was used to calculate the transformation distribution  $P(K, J)$  for  $J = 1/2$  and  $1/4$  from initial  $P(K, J = 1) = 1$  and  $\frac{1}{2}K^{-1/2}$ . The calculated results are plotted in Fig. 6(b), which shows that very different initial  $P(K, 1)$  can give very similar  $P(K, 1/2)$  and  $P(K, 1/4)$ .

A more detailed description of the method of [36] was presented later by C. Dasgupta and S. K. Ma in [37], for which Hu had helped to do some calculations (see Acknowledgments in [37]).

The idea of [36, 37] was used by R. N. Bhatt and P. A. Lee to study scaling of highly disordered spin-1/2 antiferromagnetic systems [121], and extended by D. S. Fisher to study properties of spin-1/2 antiferromagnetic chains with various types of random exchange coupling and critical behavior of random transverse-field Ising spin chains [122].

## V. PERCOLATION THEORY OF INTERACTING CRITICAL SYSTEMS

In the random percolation model, one has a geometrical picture to understand that the singular behavior near the critical point is related to the first appearance of the percolating cluster at the critical point. The critical exponents of the system can be understood and calculated from geometrical quantities such as percolation probability, mean cluster sizes, etc., of the model system.

The academic question is whether one can define clusters for the Ising model (and other interacting lattice models) so that the singular behavior of the Ising model near the critical temperature  $T_c$  is related to the first appearance of the percolating cluster at the critical point  $T_c$  and critical exponents of the Ising model can be understood and calculated from percolation probability, mean cluster sizes, etc., of the clusters for the Ising model. If the answer is positive, then we have a unified theory for the critical behavior of the random percolation model and the Ising model.

In 1967, M. E. Fisher proposed a “microdomain” or “cluster” model for the ferromagnetic Ising model. For temperature  $T$  below  $T_c$ , most Ising spins are in the direction of the magnetic field  $h$  and Ising spins in the opposite direction form clusters [97, 98]. Fisher proposed a phenomenological equation for cluster-size distribution, which contains parameter  $\sigma$  and  $\tau$ . The exponent  $\sigma$  is directly related to the effective surface free energy of a large microdomain. Critical exponents can be expressed in terms of  $\sigma$  and  $\tau$ , which then imply scaling relations of such exponents [97, 98]. However, later studies of the Ising model indicate that Fisher’s cluster-size distribution does not agree with Monte Carlo [123] and series expansion results [124]. From an analysis of low temperature series, M. F. Sykes and D. S. Gaunt [124] concluded that for a two-dimensional Ising model in zero magnetic field the mean size probably diverges at the Ising critical temperature,  $T_c$ , as  $(T_c - T)^\theta$ , with  $\theta = 1.91 \pm 0.01 > \gamma' = 1.75$  the corresponding Ising susceptibility exponent. For a three-dimensional lattice they tentatively concluded that the mean size diverges at some temperature  $T^* < T_c$ . D. Stauffer gave a review on the studies of this problem till 1979 in Sec. 6.2.3 on page 61 of [99]. In 1980, A. Coniglio and W. Klein [125] used a renormalisation group approach to introduce a bond probability  $p = 1 - \exp(-K)$  between spins in Fisher’s clusters so that the mean cluster-size of the newly defined clusters has the same exponent as the Ising magnetic susceptibility. However, this approach is not elegant.

There was another related development of the percolation theory for interacting systems. In 1979-1980, H. E. Stanley and J. Teixeira [126] proposed a percolation theory for water molecules on the lattice to explain the unusual behavior of supercooled water. They assumed that the probability  $p_w$  for two neighboring water molecules to be in the same cluster increases as the temperature  $T$  decreases. However, they did not derive the dependence of  $p_w$  on  $T$  from the coupling between neighboring water molecules.

Hu knew both problems and solved them together elegantly starting from the study of lattice models with sublattice vacancies to be discussed below.

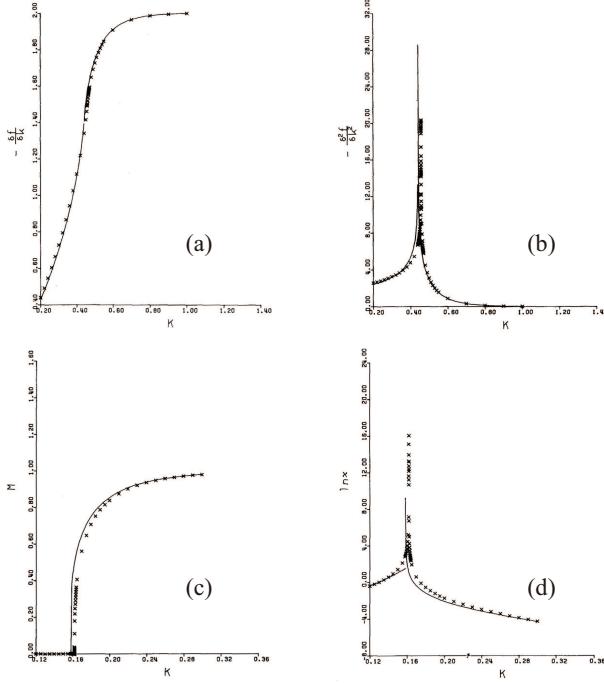


FIG. 7: Direct calculations for the derivatives of the free energy for the Ising model. The data with “x” are our calculated results. (a) the first derivative of the free energy w.r.t.  $K$ ,  $-\frac{\delta f}{\delta K}$ ; (b) the second derivative of the free energy w.r.t.  $K$ ,  $-\frac{\delta^2 f}{\delta K^2}$ ; (c) the spontaneous magnetization,  $M$ ; (d) the magnetic susceptibility,  $\ln \chi$ . The solid lines in Figs. 7(a) and 7(b) were calculated from Onsager’s exact solution for the square lattice Ising model [17]; the solid line in Fig. 7(c) represents C. N. Yang’s exact solution for the spontaneous magnetization of the square lattice Ising model [58]; the solid lines in Fig. 7(d) were obtained from series expansion [128, 129]. Taken from Fig. 1 of C.-K. Hu and P. Kleban, J. Comp. Phys. **43**, 289 (1981) [127].

### V-1. Ising model with the sublattice vacancies

During July 1979-August 1981, Hu worked at University of Maine at Orono. Hu extended the computer program for variational renormalization group transformations so that one can use the program to calculate directly the internal energy, the specific heat, the spontaneous magnetization, and the magnetic susceptibility of the Ising model on various two and three dimensional lattices [127]. The method was applied to calculate the internal energy, the specific heat, the spontaneous magnetization, and the magnetic susceptibility of the Ising model on the square lattice and calculated results are shown as “x” in Fig. 7. The solid lines in Figs. 7(a) and 7(b) were calculated from Onsager’s exact solution for the square lattice Ising model [17]; the solid line in Fig. 7(c) represents C. N. Yang’s exact solution for the spontaneous magnetization of the square lattice Ising model [58]; the solid lines in Fig. 7(d) were obtained from low temperature series expansions [128] and high temperature series expansions [129].

In the summer of 1980, Hu met Dr. Y. D. Yao at Institute of Physics of Academia

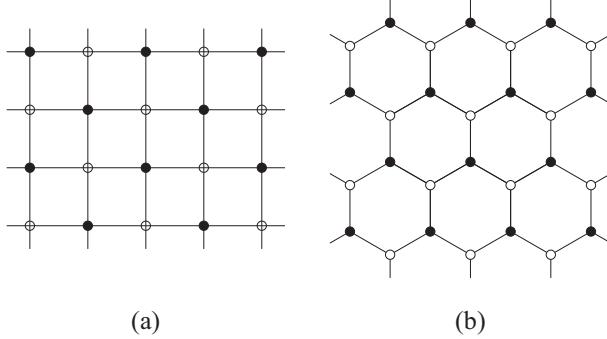


FIG. 8: A lattice of lattice constant  $a$  is divided into two sublattices (a) A square lattice of lattice constant  $a$  is divided into two square sublattices of lattice constant  $\sqrt{2}a$ , (b) a honeycomb lattice is divided into two triangular sublattices. Taken from Fig. 6 of [131].

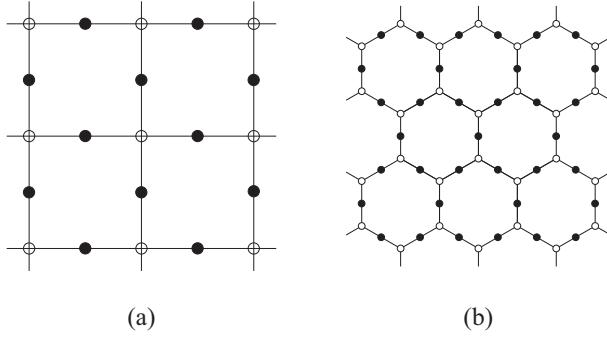


FIG. 9: A lattice is divided into two sublattices: (a) A decorated square lattice is divided into two square sublattices; (b) a decorated honeycomb lattice is divided into two honeycomb sublattices. Taken from Fig. 7 of [131].

Sinica and knew that he found the ferromagnetic Curie temperature of Ni-Ti decreases linearly with small Ti concentration [130]. The method of [127] was used to calculate phase diagrams for the dependence of the critical temperature  $T_c$  of the Ising model on the square (sq) and body-center cubic (bcc) lattice on the concentration  $< n >$  of vacancies on a sublattice. The structure of the sq lattice with sublattice vacancies is shown in Fig. 8(a) taken from [131]. For small  $< n >$ ,  $T_c$  decreases linearly with  $< n >$  [132].

## V-2. Finite-size scaling for first-order phase transitions

In March 1981, Hu attended American Physical Society March Meeting and presented a paper on “A new criterion for phenomenological renormalization-group transformation” [133]. In this paper, Hu and Peter Kleban used a phenomenological renormalization-group theory to argue that the specific heat of a physical system at the phase transition point of the first-order phase transition is proportional to the number of particles in the system.

On 7 and 8 May 1981, Hu and Peter Kleban went to Rutgers University to attend

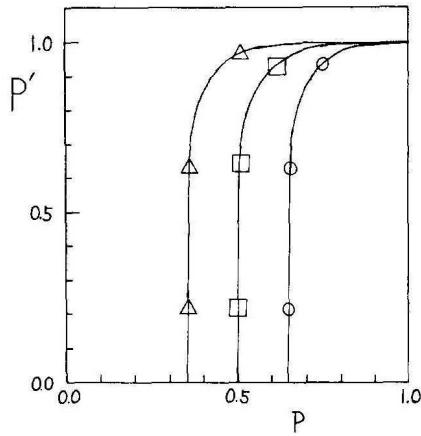


FIG. 10: Percolation probability  $P'$  as a function of renormalized bond probability  $p$ . The curves from left to right are for plane triangular (pt), square (sq), and honeycomb (hc) lattices, respectively. The critical points of pt, sq, and hc lattices, are  $0.3522 \dots$ ,  $0.5$ , and  $0.6477 \dots$ , respectively. Taken from Fig. 2 of C.-K. Hu, Physica A **119**, 609 (1983) [137].

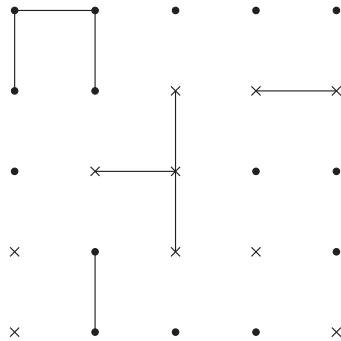


FIG. 11: Subgraph  $G'$  of a  $5 \times 5$  square lattice and a spin configuration on the  $G'$ . The solid lines represent occupied bonds in  $G'$ . The crosses represent the Ising spin in one direction and the solid disks represent Ising spin in the opposite direction. Taken from Fig. 1 of C.-K. Hu, Phys. Rev. B **29**, 5103 (1984) [138].

the 45th Statistical Mechanics Meeting. During a coffee break, Peter Kleban wrote on the blackboard our theory about finite-size scaling for first-order phase transition [133]. After the coffee break, he used the information on the blackboard to present a talk on “Criterion for First-order Phase Transitions” by P. Kleban and Chin-Kun Hu [134]. M. E. Fisher and A. N. Berker attended this talk and later published a paper on “Scaling for first-order phase transitions in thermodynamic and finite systems” [135].

### V-3. Percolation and phase transition of Ising-like models

At the 45th Statistical Mechanics Meeting, Hu presented a talk on “Phase diagram of an Ising model with random sublattice vacancies” by Chin-Kun Hu and P. Kleban (see also [132, 134]). A. N. Berker gave a comment that the phase diagram of a similar model on the honeycomb lattice may be exactly calculated. A few days later, Hu calculated the phase diagram of the Ising model on the honeycomb lattice with sublattice vacancies (Fig. 8(b)) and found that for  $T \rightarrow 0$  the critical concentration of vacant sites on the sublattice, which is a plane triangular lattice, for the disappearance of the long range order is  $1/2$ , which is the same as the critical concentration of site random percolation on the plane triangular lattice. Hu conjectured that perhaps one might obtain critical concentration of the bond random percolation model in a similar way. Hu put a lattice site in the middle of each bond of a lattice  $G$  and considered such new lattice sites constitute the sublattice  $D$ , whose sites may be either occupied or nonoccupied as shown in Fig. 9(a) and 9(b) for the sq and hc lattices, respectively. Hu calculated the critical concentration  $p_c$  of occupied sites on the sublattice  $D$  for the appearance of long range order as  $T \rightarrow 0$  and found that  $p_c$  for  $G$  being the square, the plane triangular, and the honeycomb lattices are  $1/2$ ,  $0.3522 \dots$ , and  $0.6477 \dots$ , respectively, but the corresponding  $p_c$  for the bond random percolation model on the square, the plane triangular, and the honeycomb lattices are  $0.5$ ,  $0.34729$ , and  $0.65271$ , respectively, as shown in Eq. (27).

Therefore, the sublattice dilute Ising model on bond-decorated lattices at  $T \rightarrow 0$  may not represent the bond random percolation model. Using the subgraph expansion method considered by Wu [107], in the summer of 1981 Hu found that the sublattice dilute Ising model at  $T \rightarrow 0$  represents a bond-correlated percolation model such that the probability weight for a subgraph  $G'$  depends not only on the number of occupied bonds in  $G'$ , but also on the number of clusters in  $G'$ .

In September 1981, Hu moved to University of Toronto. Hu extended the connection between the sublattice dilute Ising model and a bond-correlated percolation model to the connection between a sublattice-dilute  $q$ -state Potts model and a  $q$ -state bond-correlated percolation model (QBCPM) and wrote his first paper on percolation theory [136]. In the summer of 1982, Hu found that the 2 state BCPM of Ref. [136] is also corresponding to the simple Ising model at finite temperatures [137]. Figure 10 shows percolation probability  $P'$  as a function of renormalized bond probability  $p$  for the bond-correlated percolation model on the sq, hc and pt lattices.

Soon after finding this result, Hu found that the connection between the Ising model and 2 state BCPM may be obtained directly from the subgraph expansion of the Ising model in an external field [138, 139]. Figure 11 shows how to define clusters for the Ising model in such a connection between the Ising model and a bond-correlated percolation model [138].

In the first section of [138], Hu gave a brief review about percolation theory of critical phenomena in interacting lattice models and pointed out some conceptual problems in A. Coniglio and W. Klein’s approach [125]. From the comparison of [138, 139] and [125], one can easily reach the conclusion that Hu’s approach is more elegant, and can be easily extended to other interacting lattice model. Hu also realized that such a connection may

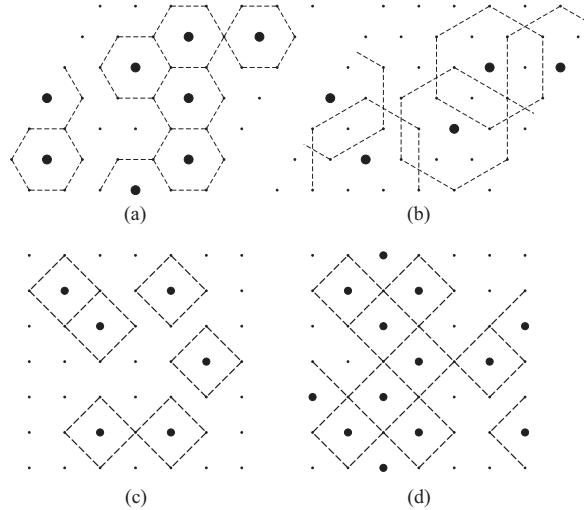


FIG. 12: Hard-core particles (represented by “•” on lattices with exclusion volume interactions (represented by dotted lines). (a) Eight hard-core particles on a  $7 \times 7$  plane triangular (PT) lattice with the nearest neighbor exclusion interactions. The problem is equivalent to the hard hexagons (dotted lines) on the PT lattice. When two hard hexagons have a common side, they are considered to be in the same cluster. (b) Five hard core particles on a  $7 \times 7$  PT lattice with the first and the second neighbor exclusion interactions. The exclusion region of a particle is represented by dotted line When two particles are in the same sublattice and they have the shortest possible separation, they are considered to be in the same cluster. (c) Six hard core particles on the square (SQ) lattice with the nearest neighbor exclusion interactions. The problem is equivalent to the hard squares (dotted lines) on the SQ lattice. Two hard squares have a common side are considered to be in the same cluster. This figure has 5 non-percolating clusters. (d) Thirteen hard squares on a  $7 \times 7$  SQ lattice. This figure has one percolating cluster and two non-percolating clusters. Taken from Figure 1 and 2 of C.-K. Hu and K.-S. Mak, Phys. Rev. B **39**, 2948 (1989) [154].

be extended easily to many Ising-type spin models, including a lattice model of supercooled water [140], various  $q$ -state Potts model and dilute Potts model (see last section in [138] and [139]).

In particular, Hu has shown that phase transitions of the  $q$ -state Potts model (QPM) are percolation transitions of a  $q$ -state bond-correlated percolation model (QBCPM) [138, 139], in which a subgraphs  $G'$  of  $b(G')$  occupied bonds and  $n(G')$  clusters will appear with the probability weight:

$$\pi(G', p, q) = p^{b(G')} (1 - p)^{E - b(G')} q^{n(G')}, \quad (67)$$

where  $p = 1 - \exp(-K) = 1 - \exp(-\beta J)$  with  $J$  being the nearest neighbor ferromagnetic coupling constant and  $\beta = (k_B T)^{-1}$ . The spontaneous magnetization  $M$  and the magnetic susceptibility  $\chi$  of the QPM are related to the percolation probability  $P$  and the mean cluster size  $S$  of the QBCPM, respectively [138, 139]. A detail derivation of the connection between the QPM and the QBCPM is given in Appendix B.

In September 1983, Hu came back to Taiwan and began to work at the Institute of

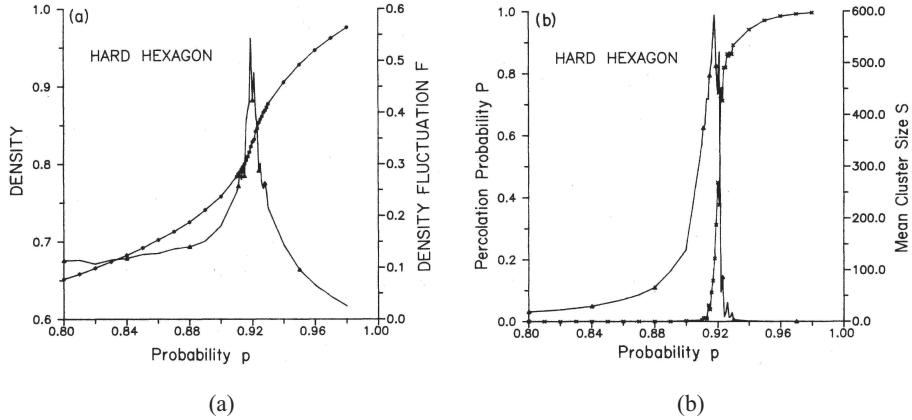


FIG. 13: Monte Carlo simulations of hard-core particles on a  $128 \times 128$  plane triangular lattice with the nearest neighbor exclusion interactions. (a) The density and the density fluctuations ( $F$ ) as a function of  $p$  with the maximum of  $F$  appears at  $p_c(F) = 0.919$ ; (b) the percolation probability  $P$  and the mean cluster size  $S$  as a function of  $p$  with the maximum of  $S$  appears at  $p_c(S) = 0.918$ , where  $p = \exp(\Delta)/(1 + \exp(\Delta))$  with  $\Delta$  being the dimensionless chemical potential. Note that  $p_c(F)$  and  $p_c(S)$  are consistent with Baxter's exact solution  $p_c = \exp(\Delta_c)/[1 + \exp(\Delta_c)] \approx 0.917$  with  $\Delta_c = \ln[11 + 5\sqrt{5}]/2$ . Taken from Figure 3 of C.-K. Hu and K.-S. Mak, Phys. Rev. B **39**, 2948 (1989) [154].

Physics of Academia Sinica. He reviewed [141] the subgraph expansion method in [138, 139] and applied such method to show that phase transitions of a lattice sol-gel model [142], an Ising model with multispin interactions [142], a dilute-Potts model [143], etc are percolation transitions. The dilute-Potts model [143] is an extension of the BEG model proposed by M. Blume, V. J. Emery, and Robert B. Griffiths [67]. In the former, each lattice site is either vacant or occupied by a spin of  $q$  components; in the latter, each lattice site is either vacant or occupied by a spin of 2 components.

Using the connection between the  $q$ -state Potts model (QPM) and the  $q$ -state bond-correlated percolation model (QBCPM), Hu defined the percolating geometrical factor  $g_p$  and the nonpercolating geometrical factor  $g_f$  [144–146]. The thermal properties of the QPM may be calculated from  $g_p$  and  $g_f$  [144–146].

Using the connection between the QPM and the QBCPM, Larsson proposed a percolation renormalization group method for the QPM [147]. However, Larsson's RG equations are not self consistent. In Ref. [148], Hu pointed out that the problem may be removed by introducing a background energy in RG equations. Hu had this idea from his research experience on the variational renormalization group transformations [31, 127]. However, Hu did not actually use this idea to carry out RG transformations for the QPM. The calculations were carried out later by Chi-Ning Chen.

From early 1987 to 1990, Hu was the thesis advisor of Chi-Ning Chen. Hu and Chen used the percolation renormalization group method [148] to calculate the free energy, the critical point, the critical exponent, and the order parameter of the Potts model [149]. In

such studies, the geometrical factors of the Potts model was calculated exactly using a fast algorithm [150]. Using the connection between the QPM and QBCPM, Hu and Chen also found a geometrical meaning of the thermal scaling power  $y_t$  [151].

#### V-4. Percolation and phase transitions of lattice hard-core particle models

Besides the Ising-type spin models, it is of interest to know whether phase transitions of other systems may also be related to percolation transitions. In this subsection, the phase transition of hard-core particles on lattices with exclusion volume interactions will be considered. Figure 12 show typical configures of hard core particles on the plane triangular (PT) and the square (SQ) lattices. In the simplest case, besides exclusion volume interactions, there is no other interactions. The hard-core particles on the PT lattice with the nearest-neighbor exclusion is corresponding to the hard hexagon model as shown in Fig. 12(a), and hard-core particles on the SQ lattice with the nearest-neighbor exclusion is corresponding to the hard square model as shown in Figs. 12(c) and 12(d).

For hard-core particles on lattices, one can use a normalized (dimensionless) chemical potential  $\Delta$  to control the density of the system. From  $\Delta$ , one can define

$$p = \exp(\Delta)/[1 + \exp(\Delta)], \quad (68)$$

which is between 0 and 1. As  $\Delta$  increases from  $-\Delta$  to  $\Delta$ ,  $p$  increases from 0 to 1. At the critical point  $\Delta_c$  and the corresponding  $p_c = \exp(\Delta_c)/[1 + \exp(\Delta_c)]$ , the fluctuations of the number of particles per site  $F$  becomes divergent.

In 1965, D. S. Gaunt and M. E. Fisher [152] used the series expansion to study the hard square model and found that the system has a second-order phase transition with a critical exponent of the order parameter  $\beta \approx 1/8$ , i.e. in the universality class of the two-dimensional Ising model.

In 1980, R. J. Baxter [153] solved exactly hard-hexagon model and found that the exact critical point is  $\Delta_c = \ln[11 + 5\sqrt{5}]/2$ .

During September 1986-June 1987 and August 1987-August 1989, K.-S. Mak worked with Hu as an master degree student and a research assistant, respectively. Hu and Mak used Monte Carlo simulations to study phase transitions of hard-core particles on lattices without [154] and with [155] other pair interactions. They found that phase transitions of hard-core particles on the SQ, the PT, and the simple cubic lattices are percolation transitions [154, 155]. Figure 13 shows that singular point of the fluctuations of the number of particles (a) is consistent with singular point of the percolation transition. Thus the phase transition of hard-core particles on the lattice is also a percolation transition.

Using such a connection, C.-N. Chen and Hu used the percolation renormalization group method to calculate the thermal scaling power of the hard-core particles on the square lattice, i.e. the hard square model [156]. The result indicates that the hard square model is in the universality class of the Ising model, which is consistent with the result reported by D. S. Gaunt and M. E. Fisher [152].

In 1994, J. L. Lebowitz visited Institute of Mathematics of Academia Sinica. Hu told him the results in Refs. [154–156]. Giacomin, Lebowitz, and Maes showed rigorously that the phase transition of the hard square model is indeed a percolation transition [157].

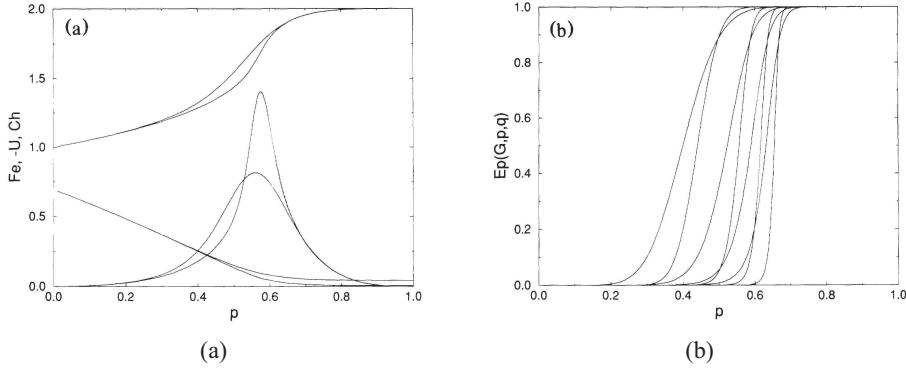


FIG. 14: Calculated results for the  $q$ -state Potts model (QPM) on the sq lattices with  $L = 4, 6$  and  $12$ ,  $N_R = 10^5$  for  $L = 4$  and  $N_R = 2 \times 10^5$  for  $L = 6$  and  $12$ , and  $w = 459$  for every case. (a) The free energy  $F_E$ , the internal energy  $-U$ , and the specific heat  $C_h$  for the Ising model as a function of  $p$ . We set  $k_B = J = 1$ . As a function of  $p$ ,  $F_E$  is decreasing,  $-U$  is increasing, and  $C_h$  has a maximum. The upper curves of  $F_E$  and  $U$  are for  $L = 4$ ; the lower curves are for  $L = 12$ . Near  $p = 0.58$  the curves for  $C_h$  from down to up positions are for  $L$  being 4 and 12, respectively. Our results and the exact results of Ferdinand and Fisher [66] are shown by solid and dotted lines, respectively. The invisibility of the dotted line means that our results and exact results are consistent. (b) The existence probability  $E_p$  as a function of  $p$ . The curves which intersect at a point near  $E_p = 0.8$  come from the same  $q$  value. The intersections from left to right are for  $q$  being 1, 2, 3, and 4, respectively. Below an intersection, the curve at the left is for  $L = 6$  and the curve at the right is for  $L = 12$ . Taken from Fig. 1 of C.-K. Hu, Phys. Rev. Lett. **69**, 2739 (1992) [164].

### V-5. Monte Carlo simulation of percolation transition of the Potts model

Using the connection between the QPM and the QBCPM [138, 139], Swendsen and Wang [158] proposed a cluster Monte Carlo simulation method. The systems simulated by the cluster algorithm may reach equilibrium much more quickly than the traditional MC simulation method [158]. Using the cluster Monte Carlo simulation method, Mak and Hu prepared a computer program to study the QPM on the square and the simple cubic lattices [159]. Table I of Ref. [159] shows that percolation transition points of the QBCPM, estimated from the maximum of the mean cluster sizes, are consistent very well with exact critical points of the square lattice Potts model and approximate critical points of the simple cubic lattice estimated by series expansion method, other Monte Carlo simulation method, and Monte Carlo RG method [159].

L.-J. Chen and Hu improved the computer program for such study so that it becomes more efficient [160]. The program was used by S.-S. Hsiao and Hu to calculate the critical points the QPM on hypercubic lattices [161].

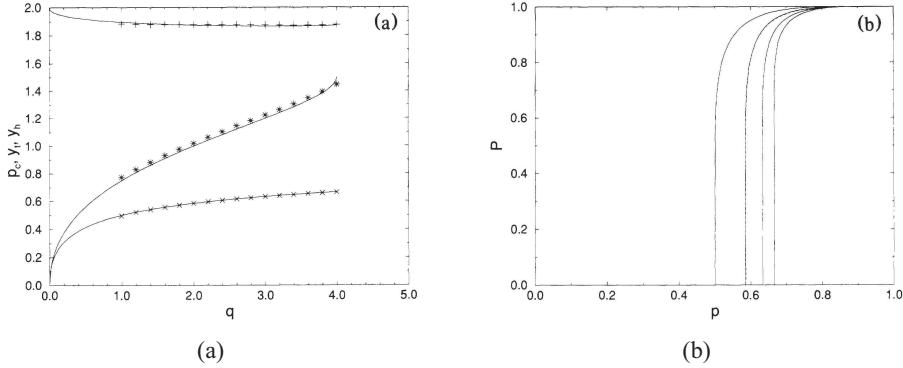


FIG. 15: HMCRG approach to the QPM on the sq lattice with  $L_1 = 16$ ,  $N_R = 6 \times 10^5$ ,  $w = 369$ , and  $L_2 = 8$ ,  $N_R = 12 \times 10^5$ ,  $w = 369$ . (a) The critical point  $p_c(\times)$ , the thermal scaling power  $y_t(*)$ , and the field scaling power  $y_h(+)$  as a function of  $q$ . The solid curves from down to up positions represent exact solutions for  $p_c$ ,  $y_t$ , and  $y_h$ , respectively. (b) The percolation probability  $P$  as a function of  $p$ . The solid curves from left to right are for  $q$  being 1, 2, 3, and 4, respectively, they represent our results. The dotted line represent Yang's exact solution [58]. For  $q = 1$  alone, we use  $N_R = 10^5$  for  $L_1 = 20$ ,  $N_R = 5 \times 10^5$  for  $L_2 = 10$ , and  $w = 459$  for both cases. Taken from Fig. 2 of C.-K. Hu, Phys. Rev. Lett. **69**, 2739 (1992) [164].

## VI. HISTOGRAM MONTE CARLO METHOD AND UNIVERSAL FINITE-SIZE SCALING FUNCTIONS

The fast algorithm proposed by Chen and Hu [150] may only produce the geometrical factors for lattices of order  $5 \times 5$  with personal computers in 1987-1991. Thus the critical point  $p_c$ , thermal scaling power  $y_t$ , and field scaling power  $y_h$  calculated from percolation renormalization group method [149] still do not agree very well with exact equations for  $K_c$ ,  $y_t$ , and  $y_h$  given in Eqs. (38), (42), and (43), respectively.

In October 1991-June 1993, Hu visited Department of Physics of Harvard University in Boston region [162]. In order to obtain geometrical factors for larger lattices, in early 1992 Hu proposed a histogram Monte Carlo simulation method (HMCSM) for percolation and phase transition models [163–165]. Instead of calculating the percolation probability  $P$ , the mean cluster size  $S$ , etc, at various discrete bond or site occupation probabilities  $p$  for percolation problems, Hu used the Monte Carlo simulation method to calculate the histograms of various important quantities from which the geometrical factors, the percolation probability  $P$ , the mean clusters  $S$ , and the existence probability  $E_p$  for finite systems at any bond or site occupation probability  $p$  may be calculated [163]. Using the percolation renormalization group method [148, 149] and the data of histograms, one may obtain very accurate critical points, critical exponents, and the thermodynamic order parameters for percolation and Potts models on the square lattice [163, 164].

The calculated free energy  $F_e$ , the internal energy  $-U$ , and the specific heat  $C_h$  for the Ising model as a function of  $p$  are shown in Fig. 14(a). The calculated data are consistent very well with exact values calculated from equations in Ref. [66]. The calculated existence

probabilities  $E_p$  as a function of  $p$  for different linear dimensions of lattices and  $q$  values are shown in Fig. 14(b). The intersection points give the critical points.

The calculated critical point  $p_c = 1 - \exp(K_c)$ , thermal scaling power  $p_t$ , and field scaling power  $p_h$  as functions of  $q$  are shown in Fig. 15(a), which are consistent very well with exact equations for  $K_c$ ,  $y_t$ , and  $y_h$  given in Eqs. (38), (42), and (43), respectively. The calculated order parameter of the QBCPM and QPM for  $q=1, 2, 3$ , and 4 are shown in Fig. 15(b). The result for the Ising model ( $q = 2$ ) is consistent very well with C. N. Yang's exact solution [58].

The HMCSM was used to calculate the critical point of the Kagome Potts model [166] and the free energy and its derivatives of various planar Potts model [167]. Hu found that in the large cell-to-cell renormalization group transformations to obtain the thermodynamic free energy and order parameter of a phase transition system one needs only iterate the transformations until the correlation length of the system is smaller than the linear dimensions of the cells [168]. Hu applied this idea to the histogram Monte Carlo simulation method and obtained very accurate thermodynamic order parameter for the site random percolation model on the square and the simple cubic lattices [168].

In Refs. [163] and [165], Hu pointed out that one could use the cluster algorithm [158] to simulate subgraphs for the QBCPM and use the histogram method to analyze the simulated data. Such method is simpler than Ferrenberg and Swendsen's multiple histogram Monte Carlo method [169]. J.-A. Chen, who worked with Hu on his doctoral thesis from September 1989-January 1994, and Hu realized this idea for the Potts model [170]. The free energy, the internal energy, and the specific heat of the Ising model calculated by Chen and Hu agree very well with exact results [170]. Such method is useful for studying larger interacting systems, e.g. the Kagome Potts model [166], in order to get more accurate results.

The HMCSM was used to calculate scaling functions of the  $q$ -state bond-correlated percolation model on planar lattices [171, 172] and of the bond random percolation model on three-dimensional lattices [173]. In such calculations, the periodic boundary condition was imposed. Hu also used the histogram Monte Carlo simulation method [163] to calculate the existence probability  $E_p$  and the percolation probability  $P$  of the site random percolation model on the square lattice with free and periodic boundary conditions and with various linear dimensions. For a given percolation model with a given boundary condition, the calculated  $E_p$  and  $P$  have very good scaling behavior. Hu found different scaling functions for the periodic and the free boundary conditions. However, when Hu applied the histogram Monte Carlo renormalization group method [163, 164, 168] to  $E_p$  and  $P$  of the periodic and free boundary conditions, Hu obtained the consistent critical point  $p_c$ , critical exponents, and the thermodynamic order parameter [174]. The thermodynamic order parameters reported in [168, 174] are very accurate. Such results may be used to compare with experimental order parameters of dilute magnets at low temperatures [175].

In the next subsection, the histogram Monte Carlo simulation method for percolation models will be briefly described.

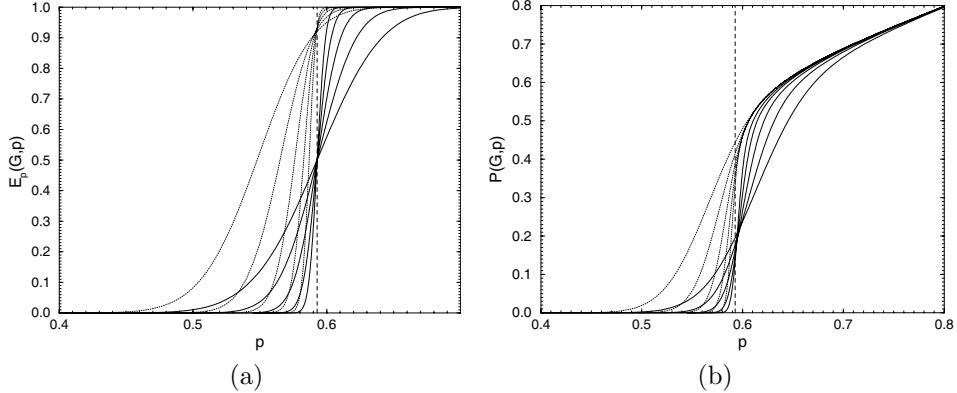


FIG. 16: The calculated results for the site random percolation model on the square lattices with linear dimensions  $L$ : 32, 64, 128, 256, and 512, where the  $(w, N_R)$  values are  $(420, 9 \times 10^5)$ ,  $(389, 9 \times 10^5)$ ,  $(369, 9 \times 10^5)$ ,  $(369, 1.8 \times 10^5)$ , and  $(420, 7.2 \times 10^4)$ , respectively, for the free boundary condition. For the periodic boundary condition,  $7.2 \times 10^4$  is replaced by  $9.6 \times 10^4$ . (a)  $E_p$  as a function of  $p$ . The vertical line intersects  $p$  axis at  $p_c = 0.5927460$ . At  $p_c$ , the lower 5 curves are for the free boundary condition and the upper 5 curves are for the periodic boundary condition. (b)  $P$  as a function of  $p$ . The vertical line intersects  $p$  axis at  $p_c = 0.5927460$ . At  $p_c$ , the lower 5 curves are for the free boundary condition and the upper 5 curves are for the periodic boundary condition. Taken from Fig. 1 of C.-K. Hu, J. Phys. A **27**, L813 (1994) [174].

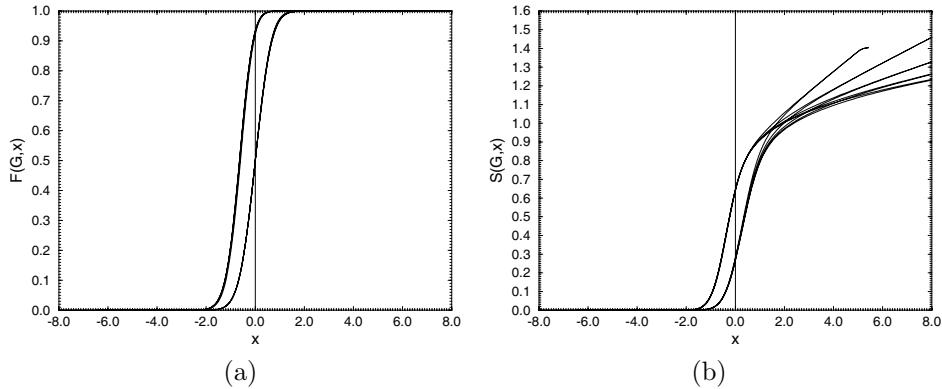


FIG. 17: (a) The calculated  $E_p$  for the square lattice as a function of  $x$ , where  $x = (p - p_c)L^{y_t}$ . The function is the scaling function  $F(G,x)$ . (b) The calculated  $P/L^{-\beta y_t}$  for the square lattice as a function of  $x$ , where  $x = (p - p_c)L^{-\beta y_t}$ . The function is the scaling function  $S(G,x)$ . Taken from Fig. 2 of C.-K. Hu, J. Phys. A **27**, L813 (1994) [174].

## VI-1. HISTOGRAM MONTE CARLO METHOD AND MCRG

Percolation is of much interest in recent decades [175–179]. In the following, the HMCSM is applied to calculate  $E_p$ ,  $P$ ,  $p_c$ ,  $y_t$ ,  $y_h$ , and the thermodynamic order parameter  $P_\infty(G,p)$  of the site random percolation model on the square and simple cubic lattices to show the basic ideas in this approach.

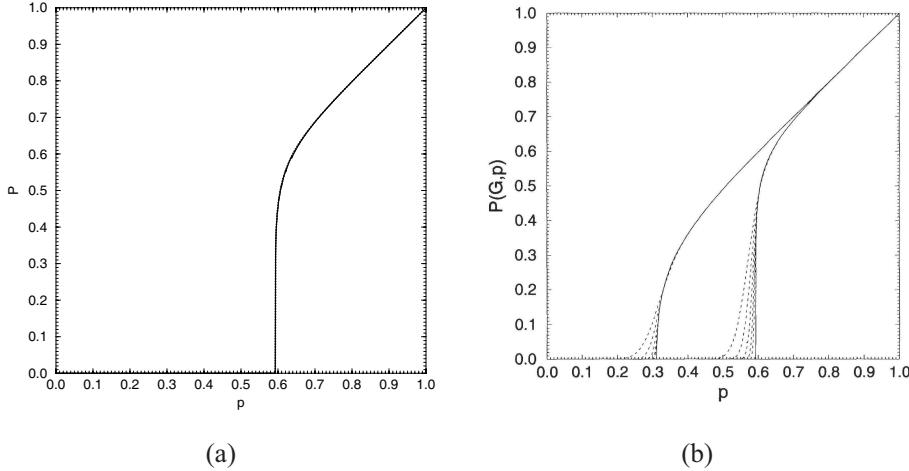


FIG. 18: The calculated thermodynamic order parameters  $P_\infty(G, p)$  of the site random percolation model on the square and the simple cubic lattices. The solid and dotted lines starting from 0.592(8) are for the square lattice with the free and periodic boundary conditions, respectively. Another solid line in (b) is for the simple cubic lattice. (a) Taken from Fig. 3 of C.-K. Hu, J. Phys. A **27**, L813 (1994) [174]. (b) Taken from Fig. 2 of C.-K. Hu, Phys. Rev. B **51**, 3922 (1995) [168].

In the site random percolation model (SRPM) on a  $d$ -dimensional lattice  $G$  of  $N$  sites and  $E$  nearest neighbor bonds, each site of  $G$  is occupied with a probability  $p$ , where  $0 \leq p \leq 1$ . The probability weight for the appearance of a subgraph  $G'$  of  $v(G')$  occupied sites is given by:

$$\pi(G', p) = p^{v(G')}(1 - p)^{N - v(G')}. \quad (69)$$

The nearest-neighbor occupied sites are said to be in the same cluster. The cluster which extends from one side of  $G$  to the opposite side of  $G$  is called a percolating cluster. The subgraph which contains at least one percolating cluster is called a percolating subgraph and will be denoted by  $G'_p$ . The subgraph which does not contain any percolating cluster is called a nonpercolating subgraph and will be denoted by  $G'_f$ . The existence probability  $E_p(G, p)$  and the percolation probability  $P(G, p)$  for the SRPM on  $G$  are given by:

$$E_p(G, p) = \sum_{G'_p \subseteq G} \pi(G'_p, p), \quad (70)$$

$$P(G, p) = \sum_{G'_p \subseteq G} \pi(G'_p, p) N^*(G'_p)/N, \quad (71)$$

where  $\pi(G'_p, p)$  is defined by Eq. (69). The sums in Eq. (70) and Eq. (71) are over all  $G'_p$  of  $G$ ;  $N^*(G')$  is the total number of lattice sites in the percolating clusters of  $G$ .  $E_p(G, p)$  will be useful in the percolation renormalization group calculation of the critical point  $p_c$

and the thermal scaling power  $y_t$ . Now one may proceed to use the histogram Monte Carlo simulation method [163, 164] to calculate  $E_p$  and  $P$ .

The  $N$  lattice sites of  $G$  are labelled by  $i = 1, 2, 3, \dots, N$  in the following. To each site of  $G$ , say the  $i$ -th site, one can assign a random number  $r_i$ . Such random numbers constitute a random vector of length  $N$ :  $V = (r_1, r_2, r_3, \dots, r_N)$ . One then considers a sequence of site probabilities of increasing magnitudes:  $0 < p_1 < p_2 < p_3 \dots < p_w < 1$ . For a given  $p_j$ ,  $1 \leq j \leq w$ , if  $r_i \leq p_j$ , then the corresponding  $i$ -th site of  $G$  is occupied. In this way, one generates a site subgraph  $G'$  for each  $p_j$ . The multiple labeling technique of Hoshen and Kopelman [89] is used to identify sites which are belong to the same clusters and then calculate the total number of sites in the percolating clusters, i.e.  $N^*(G')$ . Of course, for nonpercolating subgraphs,  $N^*(G')$  is 0.

One can generate  $N_R$  random vectors. For each random vector, one can generate  $w$  different  $G'$  corresponding to  $w$  different values of  $p$ . The data obtained from  $wN_R$  different  $G'$  are then used to construct three arrays of length  $N$  with elements  $N_p(v)$ ,  $N_f(v)$ , and  $N_{pp}(v)$ ,  $0 \leq v \leq N$ , which are, respectively, the total numbers of generated percolating subgraphs with  $v$  occupied sites, the total number of generated nonpercolating subgraphs with  $v$  occupied sites, and the sum of  $N^*(G')$  over subgraphs with  $v$  occupied sites. In the large number of simulations, one can expect that the total number of percolating subgraphs with  $v$  occupied sites,  $N_{tp}(v)$ , and the total number of nonpercolating subgraphs with  $v$  occupied sites,  $N_{tf}(v)$  should be proportional to  $N_p(v)$  and  $N_f(v)$  with the same proportional constant  $C(v)$ , which may be determined from the following equation:

$$C(v)[N_p(v) + N_f(v)] = N_{tp}(v) + N_{tf}(v) = C_v^N. \quad (72)$$

The existence probability  $E_p$  and the percolation probability  $P$  at any value of the site occupation probability  $p$  may be calculated from following equations:

$$E_p(G, p) = \sum_{v=0}^N p^v (1-p)^{N-v} N_{tp} = \sum_{v=0}^N p^v (1-p)^{N-v} C_v^N \frac{N_p(v)}{N_p(v) + N_f(v)}, \quad (73)$$

$$P(G, p) = \sum_{v=0}^N p^v (1-p)^{N-v} C_v^N \frac{N_{pp}(v)/N}{N_p(v) + N_f(v)}. \quad (74)$$

Please note that  $E_p$  and  $P$  of Eqs. (73) and (74) are continuous function of  $p$ . This is quite different from the results obtained by traditional Monte Carlo simulation methods [180].

According to the theory of finite-size scaling [100, 175, 181, 182], if the dependence of a physical quantity  $Q$  of a thermodynamic system on the reduced probability  $t = p - p_c$  may be written as  $Q(t) \sim t^a$  near the critical point  $p_c$ , then for a finite system of linear dimension  $L$  at reduced probability  $t$ , the corresponding quantity  $Q(L, t)$  may be written as

$$Q(L, t) \sim L^{-ay_t} F(tL^{y_t}), \quad (75)$$

where  $y_t$  (being  $\nu^{-1}$ ) is the thermal scaling power and  $F(x)$  is called a scaling function.

If  $Q(L, t) \equiv \langle N^* \rangle / N$  represents the percolation probability with the critical exponent  $\beta$ , where  $\langle N^* \rangle$  is the average number of sites in percolating clusters and  $L = L^d$  is the total number of lattice sites with  $d$  being the space dimensions, then at the critical point  $t = 0$  we have

$$\langle N^* \rangle \sim L^D \sim L^{d-\beta/\nu} F(0), \quad (76)$$

with  $D$  being the fractal dimension of the percolating cluster at the critical point. Equation (76) implies that  $D = d - \beta/\nu = y_h$  [171, 176], i.e.  $y_h$  can be calculated from the fractal dimensions of the critical percolation clusters.

Suppose one already carries out histogram Monte Carlo simulations on lattices  $G_1$  and  $G_2$  of linear dimensions  $L_1$  and  $L_2$ , respectively, where  $L_1 > L_2$ . The percolation renormalization group (PRG) transformation from lattice  $G_1$  to lattice  $G_2$  is given by the equation [163, 164]:

$$E_p(G_2, p') = E_p(G_1, p), \quad (77)$$

which gives the renormalized site probability  $p'$  as a function of  $p$ . The fixed point of Eq. (77) gives the critical point  $p_c$ , i.e.

$$E_p(G_2, p_c) = E_p(G_1, p_c). \quad (78)$$

The thermal scaling power  $y_t$  and the field scaling power  $y_h = D$  [171, 176] may be obtained from the equations:

$$\frac{1}{\nu} = y_t = \frac{\ln \left( \frac{\partial p'}{\partial p} \right)_{p_c}}{\ln \frac{L_1}{L_2}}, \quad y_h = D = \frac{\ln \frac{P(G'_1, p_c) L_1^d}{P(G'_2, p_c) L_2^d}}{\ln \frac{L_1}{L_2}}. \quad (79)$$

One may associate with each site of the lattice an adimensional “magnetic moment”  $m_0$  and consider the renormalization of  $m_0$  under the PRG transformation to give the renormalized “magnetic moment”  $m'_0$  [183]

$$m'_0 P(G_2, p') L_2^d = m_0 P(G_1, p) L_1^d, \quad (80)$$

which means that the total “magnetization” is preserved after the PRG transformation. After a series of PRG transformations, one has a series of renormalized site probability  $p$ ,  $p^{(1)} (= p')$ ,  $p^{(2)}$ , ...,  $p^{(n)}$  and the renormalized magnetic moments  $m_0$ ,  $m_0^{(1)} (= m'_0)$ ,  $m_0^{(2)}$ , ...,  $m_0^{(n)}$ . The thermodynamic percolation probability of the original systems,  $P_\infty(p)$ , may be related to the thermodynamic percolation probability of the  $n$ -th transformed system,  $P_\infty(p^{(n)})$ , by the equation:

$$P_\infty(p) = \frac{m_0^{(n)}}{\lambda^{nd} m_0} P_\infty(p^{(n)}), \quad (81)$$

for  $p > p_c$  with  $\lambda = L_1/L_2$ . In the traditional small cell renormalization group transformation (RGT) [183], one iterates the RGT's until  $p^{(n)}$  approaches the “lower temperature” fixed point  $p_c = 1$  then  $P_\infty(p^{(n)})$  of Eq. (81) is given by 1. However, in the large cell-to-cell RGT's considered here, one needs only iterate the RGT's until the correlation length of the  $n$ -th transformed system is smaller than the linear dimensions of the transformed cell. In such case, the transformed cell may well represent the thermodynamic systems and we may use  $P(G_2, p^{(n)})$  to represent  $P_\infty(p^{(n)})$  of Eq. (81) and obtain [168]

$$P_\infty(p) = \frac{m_0^{(n)}}{\lambda^{nd} m_0} P(G, p^{(n)}). \quad (82)$$

Hu had used Eqs. (73) and (74) to calculate the existence probability  $E_p(G, p)$  and the percolation probability  $P(G, p)$  of the site random percolation model on the square lattices with linear dimensions  $L = 32, 64, 128, 256$ , and 512 with both the free and periodic boundary conditions. Typical calculated results of  $E_p$  and  $P$  are shown in Fig. 16(a) and Fig. 16(b), respectively. For the SRPM on the square lattice, it is generally believed that the exact  $y_t$  and  $y_h$  are  $3/4=0.75$  and  $91/48=1.89583 \dots$ , respectively [175], and Ziff [179] has done extensive Monte Carlo simulation on  $1024 \times 1024$  lattice to obtain  $p_c = 0.5927460 \pm 0.0000005$ . Using the exact value of  $y_t$  [175] and the numerical value of  $p_c$  [179], Hu plotted the data for  $E_p(G, p)$  represented in Fig. 16(a) as a function of  $x = (p - p_c)L^{y_t}$  in Fig. 17(a). Since the critical exponent of  $E_p$  is zero [175], we need not divide  $E_p$  by the factor  $L^{-ay_t}$ . Using same values of  $y_t$  and  $p_c$ , we have also plotted  $P(G, p)/L^{-\beta y_t}$  for  $P(G, p)$  presented in Fig. 16(b) as a function of  $x = (p - p_c)L^{y_t}$  in Fig. 17(b).

Figures 17(a) and 17(b) show that  $E_p$  and  $P$  have nice finite-size scaling behavior. However, the scaling functions for the periodic and the free boundary conditions are quite different. As  $L$  approaches very large values,  $E_p(G, p_c)$  approaches 1/2 for the free boundary condition and approaches 0.93 for the periodic boundary condition. We studied the case: a cluster is percolating if it percolates in one directions, i.e. from top to bottom [174]. Hu found that such definition gives different scaling functions than the case of two-direction percolation. For the periodic boundary condition and the free boundary conditions,  $E_p(G, p_c)$  equals 0.93 and 0.50, respectively, which are larger than the corresponding values for *two direction* percolation.

Hu used Eqs. (78) and (79) to calculate the critical point  $p_c$ , the thermal scaling power  $y_t$ , and the field scaling power  $y_h$  for the SRPM on the square lattice. For the free boundary condition, Hu used  $w = 420$  and  $N_R = 72000$  for  $L_1 = 512$ , and  $w = 369$  and  $N_R = 180000$  for  $L_2 = 256$  to obtain  $p_c(\text{sq}) = 0.592(8)$ ,  $y_t = 0.7(5)$ , and  $y_h = 1.89(1)$ . For the periodic boundary condition, Hu used  $w = 420$  and  $N_R = 96000$  for  $L_1 = 512$ , and  $w = 369$  and  $N_R = 180000$  for  $L_2 = 256$  to obtain  $p_c(\text{sq}) = 0.592(8)$ ,  $y_t = 0.7(5)$ , and  $y_h = 1.89(6)$ . Two results are consistent. The numerical results are very close to exact results [175] or the numerical results of Ziff [179]. More recent results are summarized on the “Percolation Threshold” wikipedia page.

For the simple cubic (sc) lattice, Hu used  $N_R = 54000$  for  $L_1 = 80$ ,  $N_R = 56000$  for  $L_2 = 64$ , and  $w = 429$  for both cases to obtain  $p_c(\text{sc}) = 0.311(4)$ ,  $y_t = 1.1(0)$ , and

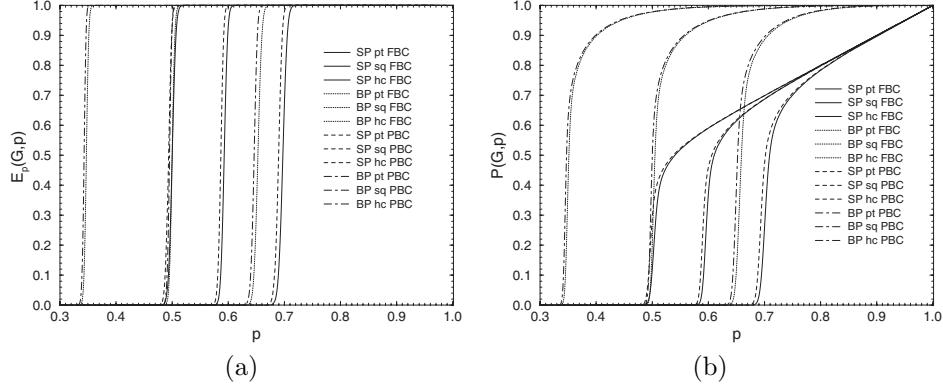


FIG. 19: Results for site percolation (SP) and bond percolation (BP) on the plane triangular (pt), the square (sq), and the honeycomb (hc) lattices. The solid (dotted) lines from left to right are for site (bond) percolation on pt, sq, and hc lattices with free boundary conditions (FBC). The dashed (dot-dashed) lines from left to right are for site (bond) percolation on pt, sq, and hc lattices with periodic boundary conditions (PBC). (a)  $E_p$  as a function of  $p$ . (b)  $P$  as a function of  $p$ . Taken from Fig. 1 of C.-K. Hu, C.-Y. Lin, and J.-A. Chen, Phys. Rev. Lett. **75**, 193 (1995) [184].

$y_h = 2.4(9)$ . It is of interest to compare such results with other results. Ziff and Stell [178] had done Monte Carlo simulation on a virtual lattice of  $1024^3$  sites to obtain  $p_c = 0.311605 \pm 0.000010$ ,  $y_t = 1.14 \pm 0.01$ , and  $y_h = D = 2.52 \pm 0.02$ . Hu's numerical results are consistent with the numerical results of Ziff and Stell [178].

Hu used Eq. (82) to calculate the thermodynamic order parameter  $P_\infty$  for the SRPM on the square lattice with the free and periodic boundary conditions, which are shown by solid and dotted lines in Fig. 18(a), respectively. Two results are consistent. Hu also calculated the thermodynamic order parameter for the SRPM on the simple cubic lattice. The result is also shown in Fig. 18(b). Such results may be used to compare with experimental order parameters of dilute magnets at low temperatures [168, 175].

## VI-2. Universal finite-size scaling functions for percolation models

In 1984, Privman and Fisher [182] proposed the idea of universal finite-size scaling functions (UFSSFs) and nonuniversal metric factors for static critical phenomena [182] for  $T$  near  $T_c$  and the external magnetic field  $h$  near 0. Specifically, they proposed that, near  $\epsilon = 0$  and  $h = 0$ , the singular part of the free energy for a ferromagnetic system can be written as

$$f_s(\epsilon, h, L) \approx L^{-d} Y(C_1 \epsilon L^{1/\nu}, C_2 h L^{(\beta+\gamma)/\nu}), \quad (83)$$

where  $d$  is the spatial dimensionality of the lattice,  $Y$  is a universal finite-size scaling function, and  $C_1$  and  $C_2$  are adjustable nonuniversal metric factors [182] which depend on the specific lattice structure. From Eq. (83) and the scaling relations  $\nu d = 2 - \alpha$  and  $\alpha + 2\beta + \gamma = 2$  of Eq. (30) [18], one obtains the scaling expression for the finite-size

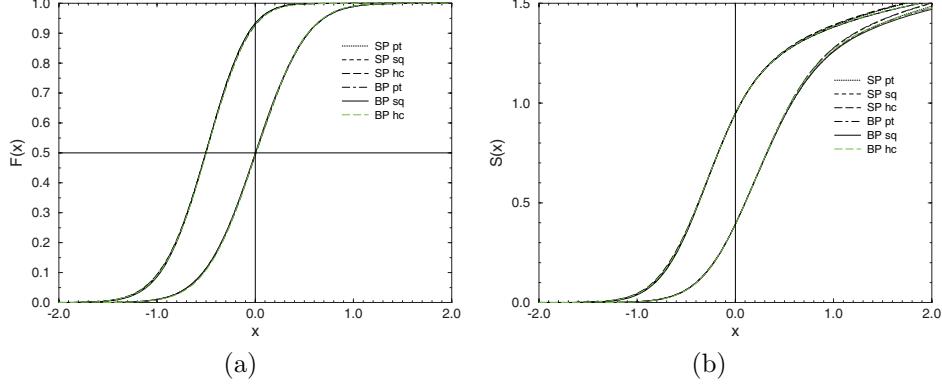


FIG. 20: (a) The calculated  $E_p$  for the site and bond percolation on pt, sq, and hc lattices as a function of  $x$ , where  $x = D_1(p - p_c)L^{y_t}$ . The scaling function is  $F(x)$ . The lower (upper) curves are for free (periodic) boundary conditions. (b) The calculated  $D_3P/L^{-\beta y_t}$  for the site and bond percolations on pt, sq, and hc lattices as a function of  $x$ , where  $x = D_2(p - p_c)L^{y_t}$ . The scaling function is  $S(x)$ . The lower (upper) curves are for free (periodic) boundary conditions. Taken from Fig. 2 of C.-K. Hu, C.-Y. Lin, and J.-A. Chen, Phys. Rev. Lett. **75**, 193 (1995) [184].

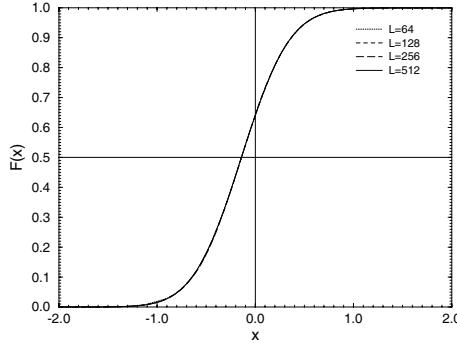


FIG. 21: The calculated  $E_p$  as a function of  $x = (p - p_c)L^{1/\nu}$  for the bond percolation on the square lattice with the periodic boundary conditions in the horizontal direction and free boundary conditions in the vertical direction, where  $L=64, 128, 256$ , and  $512$ . Taken from Fig. 1 of C.-K. Hu, Phys. Rev. Lett **76**, 3875 (1996) [187].

magnetization [182]

$$m = -\frac{\partial}{\partial h} f_s(\epsilon, h, L) \approx C_2 L^{-\beta/\nu} Y^{(1)}(C_1 \epsilon L^{1/\nu}, C_2 h L^{(\beta+\gamma)/\nu}), \quad (84)$$

which is the order parameter of the system. From 1984 to 1994, the progress in research on UFSSF was very slow. The title of Privman and Fisher's paper [182] is "Universal critical amplitudes in finite-size scaling" and most papers related to [182] only address the problem about the universality of critical amplitudes rather than universality of finite-size scaling functions.

In the following two-dimensional percolation models will be used to show that critical

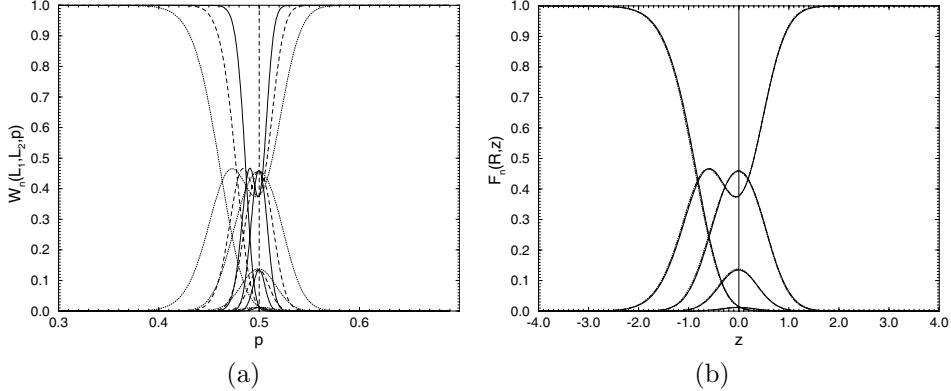


FIG. 22: (a)  $W_n(L_1, L_2, p)$  for bond percolation on  $128 \times 32$ ,  $256 \times 64$ , and  $512 \times 128$  sq lattices, which are represented by dotted, dashed, and solid lines, respectively. (b) The data of (a) are plotted as a function of  $z = (p - p_c)L^{1/\nu}$ . The scaling function for  $W_n(L_1, L_2, p)$  is denoted by  $F_n(R, z)$ , where  $R = L_1/L_2$ . The monotonic decreasing function is for  $F_0(R, z)$ . The S shape curve is for  $F_1(R, z)$ . The bell shape curves from top to bottom are for  $F_n(R, z)$  with  $n$  being 2, 3, and 4, respectively. Taken from Fig. 1 of C.-K. Hu and C.-Y. Lin, Phys. Rev. Lett. **77**, 8 (1996) [190].

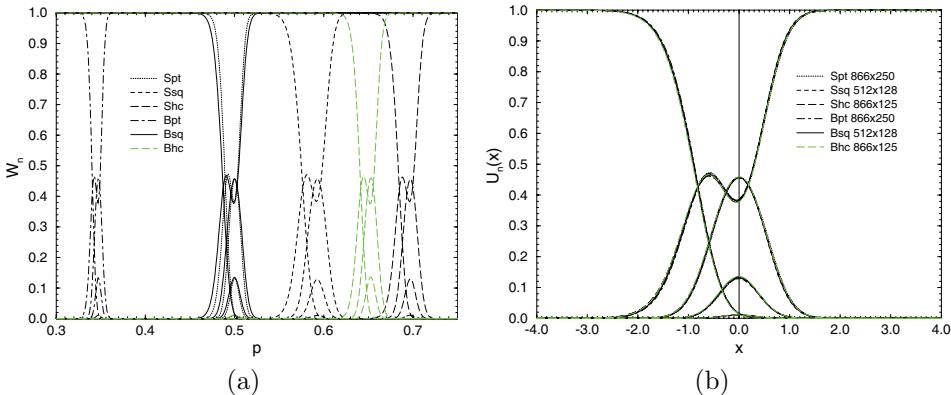


FIG. 23: (a)  $W_n$  for bond and site percolation on  $866 \times 250$  pt,  $512 \times 128$  sq, and  $866 \times 125$  hc lattices. (b) The data of (a) are plotted as a function of  $x = D_1(p - p_c)L^{1/\nu}$ . The universal scaling function for  $W_n$  is denoted by  $U_n(x)$ . Taken from Fig. 2 of C.-K. Hu and C.-Y. Lin, Phys. Rev. Lett. **77**, 8 (1996) [190].

systems can have very good finite-size scaling behaviors and universal finite-size scaling functions.

In 1995, Hu, Lin and Chen (HLC) applied the HMCSM [163, 164] to calculate the existence probability  $E_p$  and the percolation probability  $P$  of the bond and site percolation on finite  $L_1 \times L_2$  square (sq), honeycomb (hc), and planar triangular (pt) lattices with free boundary conditions (FBC) and periodic boundary conditions (PBC), where  $L_1$  and  $L_2$  are linear dimensions of the lattice in the horizontal and vertical directions, respectively. As in [163, 164], the PBC in both horizontal and vertical directions are considered.

The simulated data of  $E_p$  and  $P$  are shown in Figs. 19(a) and 19(b), respectively. HLC found that, by choosing aspect ratio  $L_1/L_2$  for sq, pt, and hc lattices to be about 1,  $\sqrt{3}$ , and  $\sqrt{3}/2$ , respectively, and nonuniversal metric factors for each model,  $E_p$  and  $P$  for six percolation models on planar lattices have universal finite-size scaling functions (UFSSF's) as shown in Figs. 20(a) and 20(b), respectively [184]. The reason for choosing aspect ratio  $L_1/L_2$  for sq, pt, and hc lattices to be about 1,  $\sqrt{3}$ , and  $\sqrt{3}/2$ , respectively, in order to get the UFSSF is explained in Appendix C. In [185], Hu, Lin and Chen found that the non-universal metric factors do not change when aspect ratios of sq, hc, and pt lattices are multiplied by the same factor.

After the publication of [184], J.-P. Hovi and A. Aharony [186] noted that at the critical point,  $E_p$  for PBC in [184] is about 0.93, but they found the value is about 0.63. Hu found that HA [186] and HLC [184] used different definitions of PBC; the former considered PBC only in the horizontal direction, while the later considered PBC in both horizontal and vertical directions.

Hu used the HMCSM to calculate  $E_p$  as a function of  $x = (p - p_c)L^{1/\nu}$  for the bond percolation on the square lattice with the periodic boundary conditions in the horizontal direction and free boundary conditions in the vertical direction, where  $L = 64, 128, 256$ , and 512, and got the results shown in Fig. 21 taken from [187]. The value of  $E_p$  at the critical point in Fig. 21 is consistent with that in [186].

Motivated by the work by I. M. Ruzin, N. R. Cooper, and B. I. Halperin [188], Hu defined the probability for the appearance of  $n$  percolating clusters from the top to the bottom of the lattice  $W_n$  for bond percolation on  $L_1 \times L_2 \equiv RL \times L \equiv L_2$  sq lattice:

$$W_n(L_1, L_2, p) = \sum_{G'_n} p^{b(G'_n)} (1-p)^{E-b(G'_n)}, \quad (85)$$

where the summation is over subgraphs  $G'_n$  with  $n$  percolating clusters from the top to the bottom of the lattice. Hu found that for a fixed aspect ratio  $R$ , data of  $W_n$  for different  $L$  have good finite-size scaling [189]. In 1996, Hu and Chai-Yu Lin found that bond and site percolation on sq, hc, and pt lattices with aspect ratios satisfying  $R(\text{sq}) : R(\text{hc}) : R(\text{pt}) = 1 : \sqrt{3} : \sqrt{3}/2$  have universal UFSSFs [190]. Figure 22 shows that  $W_n$  have very nice finite-size scaling behavior. Figure 23 shows that bond and site percolation models on sq, hc, and pt lattices have very nice UFSSFs [190].

Before the publication of [190], it was widely believed that there is only one percolation cluster in two dimensional lattices, see [191] for a brief review. Thus [190] has inspired subsequent studies on multiple percolation clusters [191].

In 1997, Hu and B. I. Halperin published scaling function for the number of alternating percolation clusters on self-dual finite square lattices [192], which can represent better the experimental sample considered in [188].

In 1997, Hu and Wang used a random deposition Monte Carlo method to find that the continuum percolation of soft disks and hard disks have the same UFSSF as percolation on planar lattices [193]. In 2001, Hsu, Lin and Hu used Monte Carlo simulations to find that the bond percolation on random lattices has the same UFSSFs as the percolation model on regular lattices [194]. In summary, bond and site percolation on sq, hc, pt regular

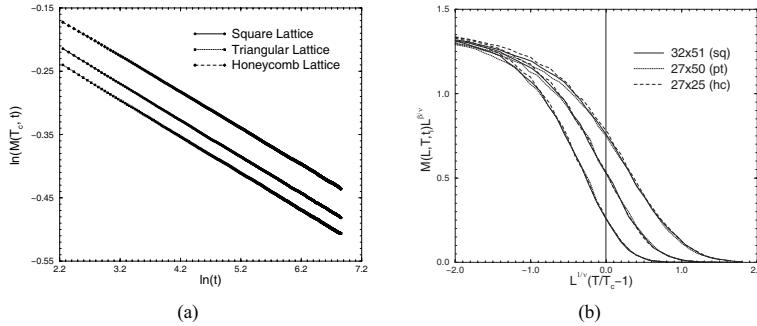


FIG. 24: (a) Decay of the critical magnetization  $M(T_c, t)$  of the Ising model on the square (sq), triangular (pt), and honeycomb (hc) lattices at the critical temperature  $T_c$  for each lattice. This figure shows  $\ln M(T_c, t)$  vs.  $\ln(t)$  for the Ising model on sq, pt and hc lattices with linear dimension  $L = 1000$  and time  $t = 10 \sim 1000$  MCS. The slope of the curve is  $b \equiv \beta/\nu z$  with  $\beta = 1/8$ ,  $\nu = 1$ , and  $z$  was estimated to be  $2.166 \pm 0.007$ ,  $2.164 \pm 0.007$ ,  $2.170 \pm 0.010$  for sq, pt, and hc lattices, respectively. (b)  $D_i M(L, T, t_i)L^{\beta/\nu}$  vs.  $E_i L^{1/\nu}(T/T_c - 1)$  with  $D_i = E_i = 1$  for  $1 \leq i \leq 3$  for the Ising model on sq, pt, and hc lattices near the critical temperature of each lattice and for the scaled times  $C_i t_i L^{-z} = 1.658g$  with  $g$  being 0.5, 1, and 2.  $C_1 = 1$ ,  $C_2 = 1.222 \pm 0.009$ , and  $C_3 = 0.693 \pm 0.018$ , for sq, pt, and hc lattices, respectively. At  $T = T_c$ , the curves from top to bottom are for  $g$  being 0.5, 1.0, and 2.0, respectively. (a) and (b) taken, respectively, from Fig. 1 and Fig. 3 of F.-G. Wang and C.-K. Hu, Phys. Rev. E **56**, 2310 (1997) [198].

lattices, bond percolation on random lattices, and continuum percolation of soft disks and hard disks have identical UFSSFs.

In 1998, Lin and Hu used HMCSM to study site and bond percolation on three dimensional lattices and found consistent critical exponents and UFSSFs [195].

Hu gave the computer program of the histogram Monte Carlo simulation method [163] to Hiroshi Watanabe who and collaborators used that program to find superscaling behavior of bond percolation on  $RL \times L$  two-dimensional rectangular domains with a width  $L$  and aspect ratio  $R$ : the existence probability of the percolating cluster  $E_p(L, t, R)$  as a function of  $L$ ,  $R$ , and deviation from the effective critical point  $t$  can be expressed as  $F(tL^{y_t}R^a)$ , where  $y_t = 1/\nu$  is the thermal scaling power,  $a$  is a new exponent, and  $F$  is a scaling function [196].

### VI-3. Dynamic universal Finite-Size Scaling Function for the Ising model

Critical systems relax very slow [18]. It is of interest to study such critical slowing down in the Ising model. The dynamic critical exponent  $z$  related to critical slowing down can be evaluated by studying the relaxation of the magnetization  $M$  on a lattice with a linear dimension  $L$  and  $N$  lattice sites, which has following form at the critical temperature  $T_c$  [197],

$$M(T_c, t) \equiv M(L \rightarrow \infty, T_c, t) \sim t^{-\beta/\nu z} \equiv t^{-b}, \quad (86)$$

where  $\beta$  and  $\nu$  are universal static exponents for  $M$  and correlation length, respectively, and are  $1/8$  and  $1$  for the two-dimensional Ising model, and  $t$  is the number of Monte Carlo

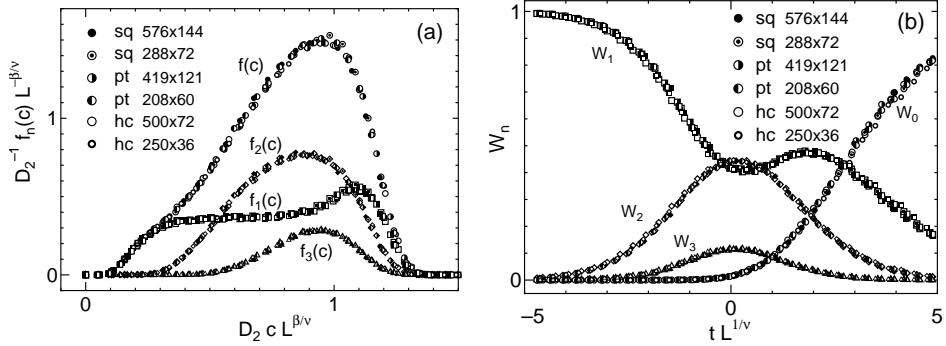


FIG. 25: Universal finite-size scaling functions for the Ising clusters on the sq, pt, and hc lattices. (a)  $D_2^{-1} f_n(c)L^{-\beta/\nu}$  and  $D_2^{-1} f(c)L^{-\beta/\nu}$  at the critical point as a function of  $D_2 c L^{\beta/\nu}$ , where  $f_n(c)$  is the distribution function for the fraction ( $c$ ) of lattice sites in percolating clusters in subgraphs with  $n$  percolating clusters; (b) the probability for the appearance of  $n$  percolating cluster  $W_n$  as a function of  $t L^{1/\nu}$ . Taken from Fig. 1 of Y. Tomita, Y. Okabe and C.-K. Hu, Phys. Rev. E **60**, 2716 (1999) [200].

steps with the unit of one sweep of all lattice sites.

Wang and Hu [198] used a heat bath dynamics to evaluate the dynamic critical exponent  $z$  and the dynamic finite-size scaling function of an Ising model on square (sq), planar triangular (pt or TP), and honeycomb (hc) lattices. They found convincing evidences that  $z$  is universal as shown in Fig. 24(a) and, by choosing an aspect ratio and a nonuniversal metric factor for the scaled time of each lattice, they obtained a universal dynamic finite-size scaling function for the Ising model on the planar lattices as shown in Fig. 24(b). Figure 24(b) shows that critical slowing down appears near the critical region, not just at the critical point.

#### VI-4. Monte carlo calculations of static universal finite-size scaling function for the Ising model

In 1999, Y. Okabe, K. Kaneda, M. Kikuchi, and C.-K. Hu [199] calculated finite-size scaling functions (FSSF's) of Binder parameter  $g$  and magnetization distribution function  $p(m)$  for the Ising model on  $L_1 \times L_2$  square lattices with periodic boundary conditions in the horizontal  $L_1$  direction and tilted boundary conditions in the vertical  $L_2$  direction such that the  $i$ -th site in the first row is connected with the mod( $i + cL_1, L_1$ )-th site in the  $L_2$  row of the lattice, where  $1 \geq i \geq L_1$ . For fixed sets of  $(a, c)$  with  $a = L_1/L_2$ , the FSSF's of  $g$  and  $p(m)$  are universal and in such cases  $a/(c^2 + a^2)$  is an invariant [199].

Based on the connection between the Ising model and a correlated bond-correlated percolation model [137, 138], Y. Tomita, Y. Okabe and C.-K. Hu (TOH) calculated the distribution function for the fraction ( $c$ ) of lattice sites in percolating clusters in subgraphs with  $n$  percolating clusters,  $f_n(c)$ , and the distribution function for magnetization ( $m$ ) in subgraphs with  $n$  percolating clusters,  $p_n(m)$ . TOH found that  $f_n(c)$  and  $p_n(m)$  have very good finite-size scaling behavior and that they have universal finite-size scaling functions for

the model on square (sq), plane triangular (pt), and honeycomb (hc) lattices when aspect ratios of these lattices have the proportions  $1 : \sqrt{3}/2 : \sqrt{3}$  [200]. TOH also found that the probabilities for the appearance of  $n$  percolating cluster  $W_n$  have UFSSFs [200]. Universal finite-size scaling functions of  $f_n(c)$  and  $W_n$  for the Ising clusters on the sq, pt, and hc lattices are shown in Fig. 25(a) and 25(b), respectively.

### VI-5. Partition function zeros of the $q$ -state Potts model

Since the method of [164] can be used to calculate the partition function of the  $q$ -state Potts model, F. Y. Wu proposed to Hu to use the method of [164] to calculate partition function zeros of the  $q$ -state Potts model as in [60, 63] for the Ising model. Hu considered that partition function zeros should be sensitively dependent on the value of the partition function and thus it is better to use exact partition functions of the  $q$ -state Potts model to calculate their zeros. Hu invited Chi-Ning Chen to use exact exact partition functions obtained by the fast algorithm of [150] to study such a problem. Chen, Hu and Wu found that such zeros distribute on the unit circle of the complex  $x = (e^K - 1)/\sqrt{q}$  plane for the self-dual square lattices when the real component of the zero is positive [201].

### VI-6. Finite-size corrections for critical lattice models

For a physical quantity  $f_N$  of a lattice model on a lattice of  $N$  site, one can calculate  $f_N$  for a finite  $N$  and its limit  $f_\infty$  as  $N \rightarrow \infty$ . The difference  $f_N - f_\infty$  is called the finite-size correction (FSC).

Low order FSCs of the Ising model and the dimer model on the square lattice had been calculated by Ferdinand and Fisher [66] and Ferdinand [71] and had been mentioned in sub-section II-2 and II-3, respectively.

In 1997, R. M. Ziff, S. R. Finch, and V. S. Adamchik (ZFA) published a paper on “Universality of finite-size corrections to the number of critical percolation clusters” [202]. ZFA found that FSCs for the number of clusters per site of various percolation models on lattices of  $S$  sites with periodic boundary conditions decreases linearly with  $1/S$  with an universal positive slope  $b$ . ZFA argued that  $b$  is the average number of clusters wrapping around the toroidal system. It should be noted that Hu and Lin had shown the number of percolating clusters for site and bond percolation of sq, hc, and pt lattices is universal when sq, hc, and pt lattices have aspect ratios:  $1 : \sqrt{3} : \sqrt{3}/2$  (see also Appendix C) [190].

In 1998, P. Kleban and R. M. Ziff published a paper on “Exact results at the two-dimensional percolation point” [203], which gives analytic equation for  $b$  as a function of the aspect ratio of the lattice.

After knowing ZFA’s result [202], Hu asked J. A. Chen to calculate FSCs for the number of clusters of the  $q$ -state bond-correlated percolation model (QBCPM) corresponding to the  $q$ -state Potts model [137–139, 145] for  $q$  being 1, 2, 3 and 4. The curve for the FSC  $n - n_c$  as a function of  $1/L^2$  ( $L^2$  is the total number of lattice sites) for  $q = 1$  has a positive slope which is consistent with the result in [202]. However, the curves for  $q = 2, 3$  and 4 have negative slopes. Hu invited N. S. Izmailian [204] and P. Kleban to collaborate to solve this “negative slope” problem and published a paper on “Geometry, thermodynamics, and

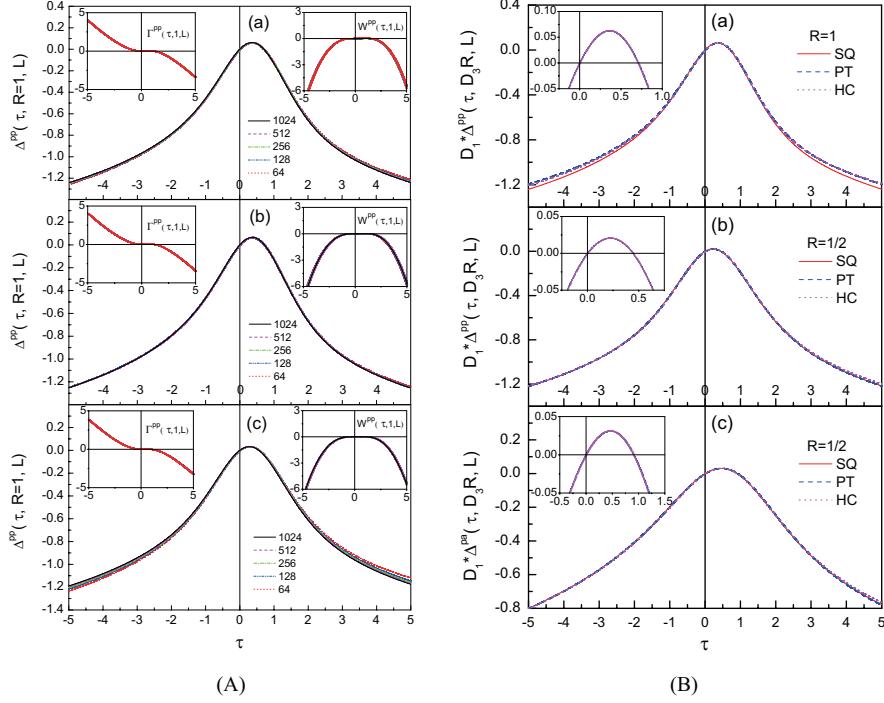


FIG. 26: (A) The scaling functions  $\Delta^{pp}(\tau, R = 1, L)$ ,  $\Gamma^{pp}(\tau, R = 1, L)$ , and  $W^{pp}(\tau, R = 1, L)$  as a function of  $\tau$  with  $D_2 = 1$  for (a) SQ, (b) PT, (c) HC lattices under periodic-periodic (pp) BC's.  $\Gamma^{pp}$  and  $W^{pp}$  are shown as left and right insets, respectively.  $R = L_1/L_2$  is the aspect ratio of the lattice. (B) The universal scaling function  $D_1 \Delta^B(\tau, D_3 R, L)$  as a function of  $\tau$  for SQ, PT, and HC lattices.  $D_1$ ,  $D_2$ , and  $D_3$  are non-universal metric factors defined in [208]. (a)  $R = 1$ , pp BC's,  $L_1 = 1024$ ,  $D_1^{\text{PT}} = 0.957\dots$ , and  $D_1^{\text{HC}} = 0.9896\dots$ , (b)  $R = 1/2$ , pp BC's,  $L_1 = 768$ ,  $D_1^{\text{PT}} = 0.9898\dots$ , and  $D_1^{\text{HC}} = 1.018\dots$ , and (c)  $R = 1/2$ , pa BC's,  $L_1 = 768$ ,  $D_1^{\text{PT}} = 0.9997\dots$ , and  $D_1^{\text{HC}} = 1.0167\dots$ . The insets show the curves near  $\tau = 0$  in more detail. (A) and (B) taken, respectively, from Fig. 1 and Fig. 2 of M.-C. Wu, C.-K. Hu, and N. Sh. Izmailian, Phys. Rev. E. **67**, 065103(R) (2003) [208].

finite-size corrections in the critical Potts model” [205]. For  $q > 1$ , there is a correction term in  $n - n_c$  which is related to the internal energy of the QPM. In order to calculate this correction term, the results in [66] should be extended to higher order terms. After this work, N. S. Izmailian turned his attention from spin models on Bethe lattices [204] to FSCs and worked with Hu, *et al.* on FSCs for the Ising model [206–209], dimer model [207, 210–212], quantum spin chains [206], and critical dense polymer [214] on regular lattices.

In [206], N. S. Izmailian and C.-K. Hu found that the Ising model on square, plane triangular, honeycomb lattices, and a quantum spin model have universal amplitude ratios for corrections to the free energy and the correlation length.

In [207], E. V. Ivashkevich, N. Sh. Izmailian, and C.-K. Hu formulated a general calculation procedure to obtain exact finite-size corrections from the exact partition function of the Ising and the dimer model on finite lattices.

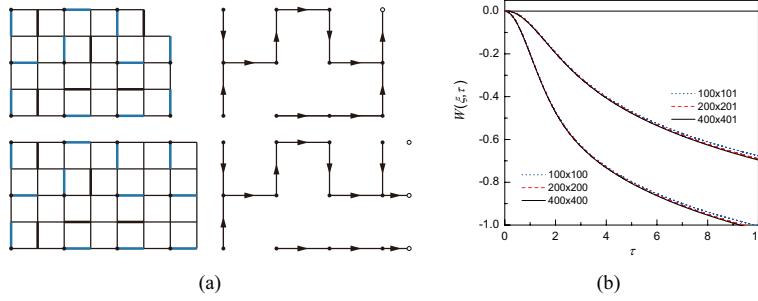


FIG. 27: (a) (Color online) Mapping of a dimer covering to a spanning tree on the odd sublattice, for an  $M \times N = 5 \times 7$  lattice (top) and a  $5 \times 8$  lattice (bottom). In both cases, the solid dots represent the sites of the odd sublattice  $G$ , and the open dots are the roots of the trees. (b) Scaling function  $W$  as a function of  $\tau$  for the different lattice sizes, where  $\tau = tS^{1/2}$  with  $S$  being the total number of lattice sites. (a) and (b) taken, respectively, from Fig. 1 of N. Sh. Izmailian, V. B. Priezzhev, P. Ruelle, and C.-K. Hu, Phys. Rev. Lett. **95**, 260602 (2005) [211] and Fig. 8 of N. Sh. Izmailian, *et al.*, Phys. Rev. E **73**, 016128 (2006) [212].

In [208], M. C. Wu, C.-K. Hu and N. S. Izmailian used exact partition functions of the Ising model on finite square (SQ), plane triangular (PT), and honeycomb (HC) lattices [213] with the aspect ratios considered in Appendix C, and the method of [207] to calculate universal finite-size scaling functions (UFSSFs) of the free energy, the internal energy, and the specific heat of the Ising model on SQ, PT, and HC lattices. The obtained UFSSFs are based on analytic equations rather than Monte Carlo data. The obtained results are shown in Fig. 26. Figure 26(A) shows that finite-size correction parts of the free energy  $W$  (right inset), of the internal energy  $\Gamma$  (left inset), and of the specific heat  $\Delta$  (central part) have very good finite-size scaling behaviors for linear dimensions  $L$  from 64 to 1024. Figure 26(B) shows that finite-size correction parts of the specific heat  $\Delta$  for SQ, PT, and HC lattices have universal finite-size scaling functions.

In [211], N. Sh. Izmailian, V. B. Priezzhev, P. Ruelle, and C.-K. Hu solved a well known puzzle about finite-size corrections of the dimer model on  $\infty \times N$  lattices. They found that finite-size corrections for such dimer system can be described by central charge  $c = -2$  universality class for both even and odd  $N$ , and for both free and periodic boundary conditions. In such study, the mapping of a dimer covering to a spanning tree on the odd sublattice shown in Fig. 27(a) was used.

In [212], N. Sh. Izmailian, K. B. Oganesyan, M. C. Wu, and C.-K. Hu calculated finite-size scaling function of the dimer model on  $M \times M$  and  $M \times (M + 1)$  triangular lattices, where  $M = 100, 200$ , and  $400$ . They found that even number  $\times$  even number lattices and even number  $\times$  odd number lattices have very different finite-size scaling functions as shown in Fig. 27(b).

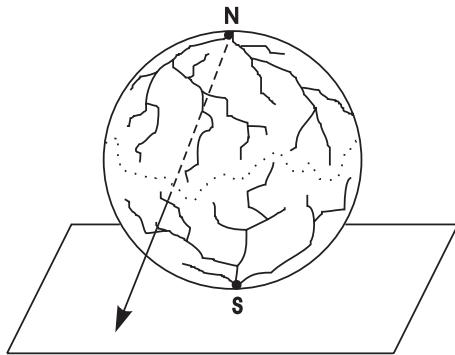


FIG. 28: The stereographic projection from the plane onto the sphere. From Fig. 1 of C.-K. Hu, *et al.*, Phys. Rev. Lett. **85**, 4048 (2000) [221].

## VII. SELF-ORGANIZED CRITICAL SYSTEMS AND AVALANCHE PROCESS

In the critical systems mentioned above, one should tune a parameter (e.g. temperature  $T$  in liquid-gas systems and the Ising model or bond probability  $p$  for the bond percolation model) so that the systems can reach its critical state. However, there are still many systems which show scaling behavior without turning any parameter [215, 216]. Such systems exhibit self-organized criticality (SOC) and are called self-organized critical systems. There are many examples of self-organized critical systems [215, 216].

### VII-1. ZIPF'S law

In 1949, George Zipf published an interesting result about statistical data in human writing [217]. He found that in a given text corpus there is an approximate mathematical relation between the frequency of the occurrence of each word and its rank in the list of all the words in the text ordered by decreasing frequency [217]. Such frequency distribution is called the Zipf distribution

### VII-2. BAK-TANG-WIESENFELD (BTW) sandpile

In 1987, Bak, Tang, and Wiesenfeld (BTW) first proposed the idea of SOC and also proposed a lattice sandpile model to show this phenomena [215, 216]. Since then, many researchers have been working on lattice models of SOC [218–222].

BTW's sandpile model on a general lattice  $\mathfrak{R}$  of  $N$  sites is defined as follows [215, 221, 222]. Each site of  $\mathfrak{R}$  is assigned a height integer; the  $i$ -th site is assigned  $z_i$  for  $1 \leq i \leq N$ . In a stable configuration the height  $z_i$  at any site  $i \in \mathfrak{R}$  takes values  $0, 1, \dots$ , or  $z_i^c - 1$ , where the critical height  $z_i^c$  is the coordination number (the number of the nearest neighbors) of the  $i$ -th site. A particle is added at a randomly chosen site and the addition of the particle increases the height at that site by one. If this height equals or exceeds the critical value  $z_i^c$ , then particles at that site are unstable and topple, and on toppling its height decreases by  $z_i^c$  and the heights at all of its  $z_i^c$  neighbors increase by 1. These neighboring sites may

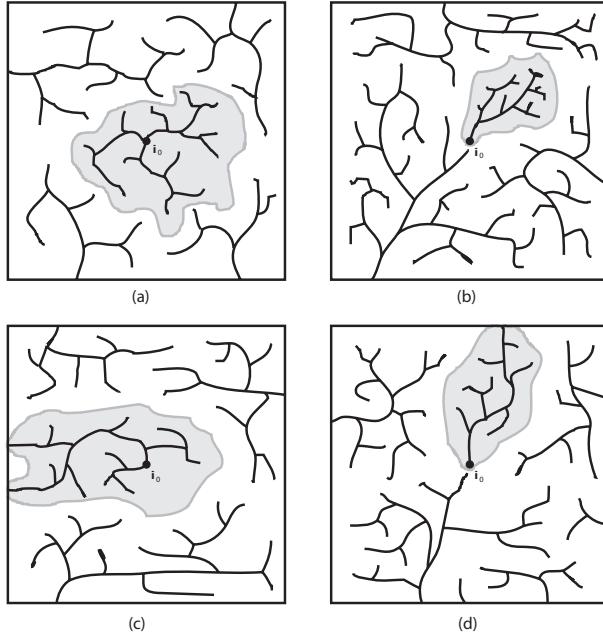


FIG. 29: Two-component spanning trees corresponding to: (a) all, (b) last, (c) dissipating and (d) dissipating last waves. From Fig. 2 of C.-K. Hu, *et al.*, Phys. Rev. Lett. **85**, 4048 (2000) [221].

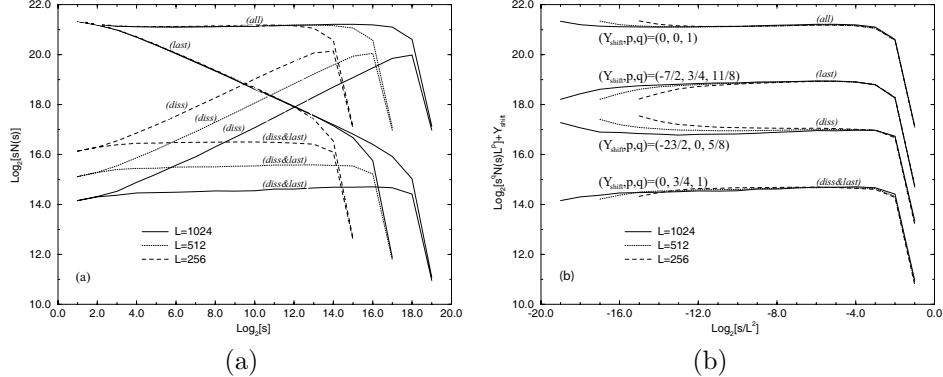


FIG. 30: (a) (a) The distribution of all (*all*), last (*last*), dissipating (*diss*) and dissipating last waves (*diss&last*) for  $L = 1024$  (solid line),  $512$  (dotted line), and  $256$  (dashed line). (b) The collapse of the data from (a) with parameters  $(Y_{shift}, p, q)$ . From Fig. 3 of C.-K. Hu, *et al.*, Phys. Rev. Lett. **85**, 4048 (2000) [221].

become unstable in their turn and the toppling process continues causing an avalanche. The open boundary conditions are used so that when particles at a boundary site topple, some particles can leave the system. The dynamical process continues until  $z_i < z_i^c$  for  $1 \leq i \leq N$ . In this way, a set of toppling sites with area  $s$ , occurs and forms an avalanche.

Every avalanche may be represented as a sequence of more elementary events, waves

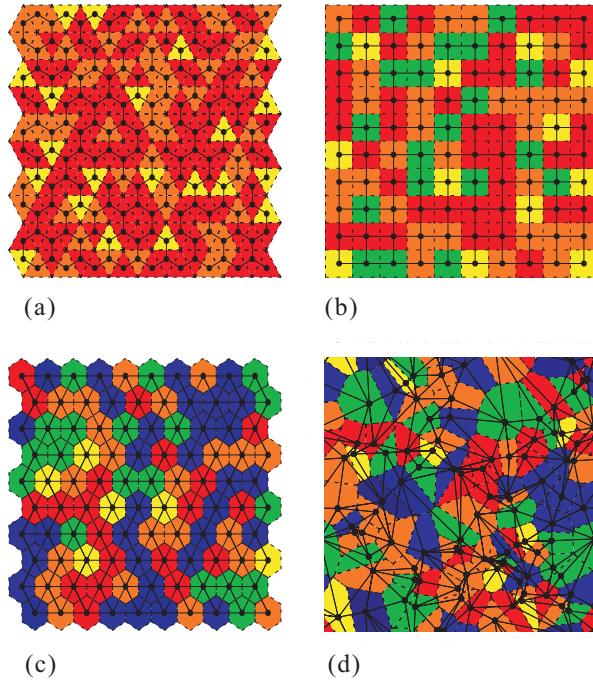


FIG. 31: (Color online) Typical stable sandpile configuration on (a) honeycomb (hc), (b) square (sq), (c) triangle (ta), and random (d) lattices. For every lattice, sites are represented by solid black dots and links between neighboring sites are represented by solid lines. The dual of a given lattice is represented by dotted lines. Each site of a lattice has a corresponding cell of the dual lattice, which encloses the site. Thus the color of a cell is used to represent the height of the enclosed site. Red, orange, and yellow are used to represent the height  $z_i$  being  $z_i^c - 1$ ,  $z_i^c - 2$ , and 0, respectively. In (b), (c), and (d), green represents  $z_i^c - 3$ . In (c) and (d), purple represents  $z_i^c - 4$ . In (c), blue represents 1. In (d), different depth of blue represents different values from 1 to  $z_i^c - 5$ . When a particle is added at a red site, the site begins to topple and initiate an avalanche. Taken from Fig. 1 of C.-K. Hu and C.-Y. Lin, Physica A **318**, 92 (2003) [222].

of topplings, which can be organized as follows: if the site  $i$  to which a grain was added becomes unstable, topple it once and then topple all other sites of the lattice that become unstable, keeping the initial site  $i$  from a second toppling. The set of sites toppled thus far is called *the first wave of topplings*. After the first wave is completed, site  $i$  is allowed to topple the second time, not permitting it to topple again until *the second wave of topplings* is finished. The process continues until site  $i$  becomes stable and the avalanche stops, then we have *the last wave of toppling*. Since the BTW sandpile model is Abelian [218], the final stable configuration does not depend on how the waves of toppling are organized.

Waves of toppling on the square domain can be mapped into waves on the surface of a sphere by a stereographic projection as shown in Fig. 28.

Waves of toppling, being more elementary events than avalanches, also have much simpler properties. All the waves are individually compact, so we will characterize the waves of toppling only by their area,  $s$ , and calculate total numbers and probability distributions

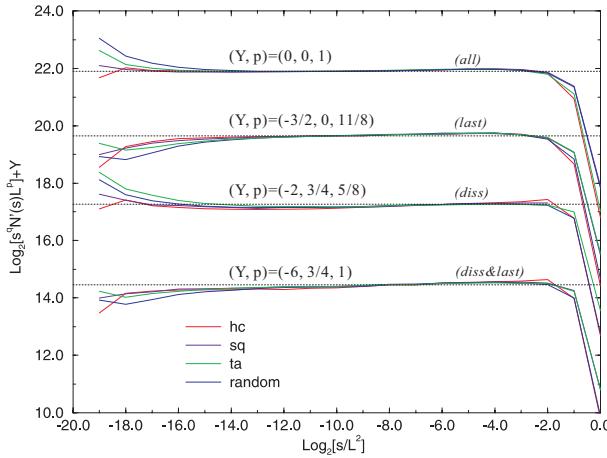


FIG. 32: (Color online)  $\text{Log}_2[s^q N'(s)L^p] + Y$  as a function of  $\text{Log}_2[s/L^2]$  for hc, sq, ta, and random lattices with linear dimension  $L = 1024$ , where  $q$  is the exact critical exponent and is 1,  $11/8$ ,  $5/8$ , and 1 for all, last, dissipating, and dissipating last waves, respectively. The shift parameter  $Y$  is introduced so that we can show curves for four kinds of waves in the same figure. We used ten independent set of data in the region  $2^{-12} \leq s/L^2 \leq 2^{-3}$  to calculate critical exponents for four kinds of waves on four different lattices. All, last, dissipating, and dissipating last waves have exponents  $1.00 \pm 0.01$ ,  $1.37 \pm 0.01$ ,  $0.61 \pm 0.02$ , and  $1.02 \pm 0.02$  for the hc lattice; exponents  $1.01 \pm 0.01$ ,  $1.36 \pm 0.02$ ,  $0.61 \pm 0.02$ , and  $1.02 \pm 0.02$  for the sq lattice; exponents  $1.01 \pm 0.01$ ,  $1.36 \pm 0.02$ ,  $0.62 \pm 0.01$ , and  $1.01 \pm 0.02$  for the ta lattice; exponents  $1.01 \pm 0.01$ ,  $1.36 \pm 0.02$ ,  $0.62 \pm 0.02$ , and  $1.02 \pm 0.02$  for the random lattice. The exponents for four lattices are consistent with each other and also consistent with predicted exact values. This figure was plotted with data from Fig. 4 of C.-K. Hu and C.-Y. Lin, Physica A **318**, 92 (2003) [222].

of areas  $s$  for four categories of waves (Fig. 29) (1) All waves. (2) Last waves. Each avalanche has exactly one last wave. When a particle is added to the  $i$ -th site with height  $z_i^c - 1$ , an avalanche is induced. Thus the total number of last waves is approximately equal to the product of the number of added particles and average fraction of lattice sites with height  $z_i^c - 1$  (red sites in Fig. 31 below). (3) Dissipating waves which have particles leave the system from the boundary. (4) Dissipating last waves which are both dissipating and last [221].

For a given probability distribution of waves,  $\mathcal{N}(s)$ , the normalized condition  $\int_{a^2}^{L^2} \mathcal{N}(s)ds = 1$  is imposed, where  $a$  is the lattice constant. In fact, Ivashkevich, Ktitarev, and Priezzhev [220] proposed that for  $a^2 \ll s \ll L^2$ , the probability distribution of areas  $s$  for all waves of toppling is given by

$$\mathcal{N}_{\text{all}}(s) ds \sim \frac{ds}{s}. \quad (87)$$

Dhar and Manna [219] proposed that the asymptotic probability distribution of the last

wave is given by

$$\mathcal{N}_{last}(s) \, ds \sim \left(\frac{a^2}{s}\right)^{3/8} \frac{ds}{s}, \quad (88)$$

for  $a^2 \ll s \ll L^2$ . Hu *et al.* [221] observed that Eq. (87) is invariant under the inversion transformation (Fig. 28) and argued that the asymptotic probability distribution of dissipating waves is :

$$\mathcal{N}_{diss}(s) \, ds \sim \left(\frac{s}{L^2}\right)^{3/8} \frac{ds}{s}. \quad (89)$$

Hu *et al.* [221] assumed that the events for last waves and dissipating waves are independent and obtained

$$\mathcal{N}_{diss\&last}(s) \, ds \sim \left(\frac{a}{L}\right)^{3/4} \frac{ds}{s}. \quad (90)$$

The critical exponents for Eqs. (87), (88), (89), and (90) are exactly 1, 11/8, 5/8, and 1, respectively.

In summary, in 2000 C.-K. Hu, E. V. Ivashkevich, C. Y. Lin, and V. B. Priezzhev used an inversion symmetry as shown in Fig. 28 to show that in the Abelian sandpile model [215, 216] the probability distribution of dissipating waves of toppling that touch the boundary of the system as defined in Fig. 29 shows a power-law relationship with critical exponent 5/8 and the probability distribution of those dissipating waves that are also last in an avalanche has an exponent of 1 [221] as shown in Fig. 30. Their extensive numerical simulations not only support these predictions, but also show that inversion symmetry is useful for the analysis of the two-wave probability distributions [221].

Hu and Lin [222] studied BTW models on two-dimensional systems, including hc, sq, triangle (ta), and random lattices as shown in Fig. 31.

The random lattice is constructed by randomly selecting points in the given domain and then connecting neighboring points by bonds; the method was described in Hsu *et al.* [194]. The coordinate numbers of hc, sq, and ta lattices are 3, 4, and 6, respectively; the coordinate numbers of the random lattice change from site to site with the most probable number being 6.

Hu and Lin [222] simulated the BTW sandpile model on hc, sq, ta, and random lattices with linear dimensions  $L = 32 - 1024$ , and  $N = L^2$ . For each  $L$  and lattice, they first generated a random stable configuration, and add  $10^6$  particles at randomly chosen sites to drive the system into critical recurrent configurations [218]. They then began to take data by adding  $n = 4 \times 10^7$  particles at randomly chosen sites. The total numbers of all waves  $A_{all}$ , last waves  $A_{last}$ , dissipating waves  $A_{diss}$ , and dissipating last waves  $A_{diss\&last}$  for these lattices as a function of  $L$  in log-log scale are plotted in Fig. 2 of [222]. The data can be well represented by straight lines and slopes of the lines for four kinds of lattices are consistent with each other within numerical uncertainties. The average slopes for all, last, dissipating, and dissipating last waves are  $0.19 \pm 0.01$ ,  $0.01 \pm 0.01$ ,  $-0.18 \pm 0.02$ , and  $-0.71 \pm 0.01$ , respectively.

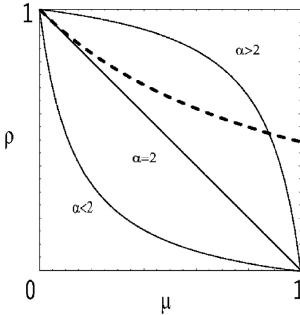


FIG. 33: The phase diagrams of the density  $\rho = P/N$  as a function of the parameter  $\mu$  for different toppling rules. The broken line separates the intermittent flow phase from the continuous flow phase for the case  $\mu_n = \mu(1 - \mu_{n-1})$ . Solid lines represent phase boundaries for models parameterized by  $\alpha$  for  $\alpha=1/4, 2$ , and  $16$  for the case  $\mu_n/(1 - \mu_n) = [2\mu/(1 - \mu)][(n - 2 + \alpha)/n\alpha]$ . From Fig. 1 of V. B. Priezzhev, E. V. Ivashkevich, A. M. Povolotsky, and C.-K. Hu, Phys. Rev. Lett. **87**, 084301 (2001) [225].

To check whether waves of the BTW sandpile model on regular and random lattices have the same set of critical exponents predicted by Eqs. (87)–(90), they used the data for  $1024 \times 1024$  hc, sq, ta, and random lattices to plot  $\text{Log}_2[s^q N'(s)L^p] + Y$  as a function of  $\text{Log}_2[s/L^2]$  in Fig. 4 of [222], reproduced as Fig. 32 of the present paper. They used ten independent set of data in the region  $2^{-12} \leq s/L^2 \leq 2^{-3}$  to calculate critical exponents for four kinds of waves on four different lattices. All, last, dissipating, and dissipating last waves have exponents  $1.00 \pm 0.01$ ,  $1.37 \pm 0.01$ ,  $0.61 \pm 0.02$ , and  $1.02 \pm 0.02$  for the hc lattice; exponents  $1.01 \pm 0.01$ ,  $1.36 \pm 0.02$ ,  $0.61 \pm 0.02$ , and  $1.02 \pm 0.02$  for the sq lattice; exponents  $1.01 \pm 0.01$ ,  $1.36 \pm 0.02$ ,  $0.62 \pm 0.01$ , and  $1.01 \pm 0.02$  for the ta lattice; exponents  $1.01 \pm 0.01$ ,  $1.36 \pm 0.02$ ,  $0.62 \pm 0.02$ , and  $1.02 \pm 0.02$  for the random lattice. The exponents for four lattices are consistent with each other and also consistent with predicted exact values of Eqs. (87)–(90) when  $2^{-12} \leq s/L^2 \leq 2^{-3}$ .

In summary, Hu and Lin simulated the BTW sandpile model on hc, sq, ta, and random lattices and found that total numbers of waves and area distributions of waves on these lattices have nice finite-size scaling behavior and the same set of critical exponents. Thus the critical behavior of toppling waves is insensitive to the details of the lattices, which is similar to the critical behavior in ordinary critical systems.

### VII-3. Avalanche process

It is of interest to know whether one can observe SOC in laboratory systems. For this purpose, in 1996, V. Frette, *et al.*, in Oslo [223] used rice pile experiments to observe SOC behavior. To describe such SOC behavior, K. Christensen, *et al.* proposed an Oslo model [224] and used the numerical method to find that the Oslo model can give the SOC behavior similar to that observed in experiments. In 2001, V. B. Priezzhev, E. V. Ivashkevich, A. M. Povolotsky, and C.-K. Hu proposed an asymmetric avalanche process (ASAP) on a ring (one dimensional lattice with the periodic boundary conditions) [225]. The ASAP reads as

follows: In a stable state,  $P \leq N$  particles are located on a ring of  $N$  sites. During the infinitesimal time interval  $dt$ , each particle has a probability  $dt$  of jumping one step to the right. If any site  $x$  contains a number of particles  $n(x) > 1$ , it becomes unstable, and must relax immediately by spilling to its right either  $n$  particles with probability  $\mu_n$  or  $n - 1$  particles with probability  $1 - \mu_n$ . The relaxation stops when all sites become stable again with  $n(x) \leq 1$  [225]. The exact phase diagram of the ASAP was obtained as shown in Fig. 33.

In 2003, A. M. Povolotsky, V. B. Priezzhev, and C.-K. Hu used a discrete-time formulation of the ASAP [225] of  $P$  particles on a finite ring of  $N$  sites to obtain an exact expression for the average avalanche size as a function of toppling probabilities and particle density  $\rho = P/N$  [226]. By mapping the model onto driven interface problems, they found that the ASAP incorporates the annealed Kardar-Parisi-Zhang [227] and quenched tilted interface dynamics for  $\rho < \rho_c$  and  $\rho > \rho_c$ , respectively, with  $\rho_c$  being the critical density for given toppling probabilities and  $N \rightarrow \infty$  [226].

## VIII. SUMMARY, DISCUSSION, AND RECENT DEVELOPMENTS

### VIII-1. Summary and recent developments

In summary, this paper gives a historical review on analytic, Monte Carlo, and renormalization group approaches to critical phenomena of lattice models, including the developments of Monte Carlo and renormalization group approach to critical phenomena, such as the histogram Monte Carlo renormalization group (MCRG) method, which may be used to obtain very accurate critical points, critical exponents, and the thermodynamic order parameters. The MCRG method may be applied to many phase transition and percolation models, including those mentioned at the end of [164]. Since the computing facilities advance very rapidly, we expect that the importance of this method will also increase.

Universality is an important concept in the study of critical phenomena. In Sec. V, it is pointed out that one can use a universal mechanism to understand critical behavior in random percolation models, correlated percolation models corresponding to Ising-type lattice models, and hard-core particles on lattices.

In Section VI, it is pointed out that bond and site percolation on sq, hc, and pt lattices, continuum percolation of soft disks and hard disks, and bond percolation on random lattice have universal finite-size scaling functions. In 1998, Lin and Hu used HMCSM to study site and bond percolation on three dimensional lattices and found consistent critical exponents and UFSSFs [195].

It is found that the value of  $E_p$  at  $p_c$  depends on the boundary condition and also on the rule used to identify the percolating cluster. The histogram Monte Carlo simulation method [163, 164] is useful for identifying the *universality classes* of  $E_p(G, p_c)$ , which is a problem of much interest [228], and for obtaining the scaling functions for  $E_p$  and  $P$ .

Another example of the universality of critical exponents is related to lattice Ising model. In 1952, C. N. Yang and T. D. Lee proposed that the Ising model can be used to describe liquid-gas systems [60]. In 1995-1996, Blöte and collaborators [229, 230] used Monte

Carlo simulations to find that the critical exponent  $\beta$  of the spontaneous magnetization and  $\nu$  of the correlation length [18] of a three-dimensional (3D) Ising model are 0.3269(6) [230] and 0.6301(8) [229], respectively. In 2009, Sengers and Shanks [231] reviewed the experimental data for liquid-gas critical systems and reported that the order parameter and the correlation length have critical exponents  $\beta = 0.3245$  and  $\nu = 0.629 \pm 0.003$ , respectively. In 2012, Watanabe, Ito and Hu [232] used molecular dynamics simulations to find that  $\beta$  and  $\nu$  of a 3D Lennard-Jones (L-J) model system [43, 44] are 0.3285(7) and 0.63(4), respectively. The values of  $\beta$  and  $\nu$  obtained for simple model systems reported in Refs. [229, 230, 232] are highly consistent with experimental data reported in [46, 231].

Very recently, Au-Yang and Fisher calculated critical behavior of alternating layered Ising models based on analytic equations [233] and ordinary percolation model was extended to explosive percolation models [234], which can have a very sharp transition.

Instead of using Monte Carlo as in [77, 78], very recently Chen, Hsieh, and Hu calculated the exact partition of the interacting self-avoiding walks up to chain length  $N = 27$  on the simple cubic lattice. They used partition function zeros to decompose the specific heat and identify a collapse transition at a higher temperature and a freezing transition at a low temperature [235].

### VIII-2. Discussion and future work

Figure 4(b) indicates that at very low temperature,  $\alpha_{\text{TRM}}$  and  $\alpha_E$  can be smaller than 0.025 [34, 35], which is much smaller than the critical decay exponent  $b = \beta y_t/z \approx 0.058$  of magnetization  $M \sim t^{-b}$  of the square-lattice Ising model with  $\beta = 1/8$ ,  $y_t = 1$ , and dynamic critical exponent  $z = 2.166$  [198], i.e. the spin glass system can relax slower than the critical slowing down of the Ising system at low temperatures [236]. Glassy behavior has also been found in interacting polymer chains with strong bending and torsion angle dependent interactions [237, 238], and in native collagen fibril [239]. Since many important biological macromolecules, such as DNA, RNA, proteins, etc, are polymer, the results of [237–239] about the glassy behavior of polymers or proteins are useful for understanding the mechanism for a biological system to maintain in a non-equilibrium state, including ancient seeds [240, 241], which can maintain in a viable non-equilibrium state for a very long time. To draw such a connection, one should try to understand better the relation between simulation time and real time in biological systems.

Besides liquid-gas critical phenomena, lattices models are also useful for understanding structures, folding, and aggregation of proteins [242]. This topic deserves another review.

Lattice spin models can not only be applied to understand phase transitions and critical phenomena in physical systems, they can also be applied to molecular theory of biological evolution and the origin of life [243–245]. This has becoming an active research field in recent decades, see e.g. [246–248] and references in these papers. Such developments also deserve another review paper.

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## APPENDIX A: EARLY STUDIES OF CRITICAL PHENOMENA IN TAIWAN

In 1960's, the Institute of Physics of the National Tsing Hua University (IOP/NTHU) in Hsinchu, Taiwan established the first Doctor of Science (Ph.D.) program in Taiwan. A Ph.D. student should first passed an oral examination of the institute, then another oral examination organized by the Ministry of Education of Taiwan government. The Ph.D. degree was then granted by the Minister of Education. National Tsing Hua University began to have a bachelor degree program in physics in 1965.

Yee-Yen Lee was born on 26 August 1937. In 1955, he entered Department of Electrical Engineering of National Taiwan University in Taipei, then transferred to Electrical Engineering of Northwestern University in 1956 and got a bachelor degree in 1959. He then entered Department of Physics of Michigan University in USA, and received a Ph.D. degree from that department in 1964 with Ph.D. thesis on particle theory. Samuel C. C. Ting was his classmate. In 1964, Yee-Yen Lee joined Institute of Physics of National Tsing Hua University. In 1966-1967, he was Director of Institute of Physics of National Tsing Hua University and Physics Research Promotion Center [249].

Yu-Ming Shih was the first student in the Ph.D. program at IOP/NTHU with Yee-Yen Lee as his thesis advisor. Mr. Shih worked on field theory and particle physics [250] and was Chairman of Department of Physics of Tamkang College of Arts and Sciences (which became Tamkang University later) from August 1970 to July 1971. On 1 February 1971, Mr. Shih passed the oral examination arranged by the Ministry of Education and received the first Doctor of Science (Ph.D.) diploma from the Ministry of Education of the Republic of China in Taiwan. After receiving a Ph.D. degree, Y. M. Shih went to visit the Department of Physics of Northwestern University to work with Chia-Wei Woo on the theory of liquid helium [251] and liquid crystals [252] and changed his research field from particle physics to statistical physics. After returning to Taiwan, Y.-M. Shih continued to work at the Department of Physics of Tamkang College of Arts and Sciences, and was Chairman of that department from August 1978 to July 1980.

Fa-Yueh Wu obtained a B.S. degree from Chinese Naval College of Technology in

Taiwan in 1954, an M.S. degree from National Tsing Hua University in Hsinchu, Taiwan in 1959, and a Ph.D. degree from Washington University in St. Louis in 1963. In 1963-1967, he was an Assistant Professor at Virginia Polytechnic Institute. In 1967, he joined Department of Physics of Northeastern University [253]. He often visited Institute of Physics of National Tsing Hua University in Hsinchu and worked with K. Y. Lin and C. S. Hsue on the vertex model [254]. He also helped to supervise K. S. Chang, the second person to receive a Ph.D. degree from IOP/NTHU, to work on ice-rule ferroelectric models [255].

Keh-Ying Lin obtained a bachelor degree from Department of Electrical Engineering of National Taiwan University in Taipei in 1959, and a Ph.D. degree from Carnegie Institute of Technology in 1966 [256] with a Ph.D. thesis on particle theory [257]. He continued to work on particle theory at Cornell University (1966/7-1968/8), Rockefeller University (1968/9-1969/8), and CERN (1969/9-1970/8). In September 1970, he joined the Department of Physics of National Tsing Hua University and began to publish papers on statistical physics of lattice models in 1974 [254, 258]. Afterward, he spent most of his research effort on statistical physics of lattice models [256].

Hsin-Hsiung Chen obtained a bachelor degree from the Department of Electrical Engineering of National Chen Kung University in Tainan, Taiwan in 1966, a Ph.D. degree from the Department of Electrical Engineering of The Johns Hopkins University in 1970 [259] with R. I. Joseph as his thesis advisor. He worked with Joseph on models of phase transitions and critical phenomena [260]. After one year research at the Department of Physics, New York University, he joined the Department of Physics of National Tsing Hua University in August 1971. After joining NTHU, he supervised Mr. D. C. Jou to finish his Ph.D. research on anisotropic Heisenberg ferromagnets and antiferromagnets [261]. Mr. Kuo-Gen Chen obtained a Master's Degree in June 1972 at IOP/NTHU and became a Lecture at the Department of Physics of Suchou University in Taipei. He was also a Ph.D. student of H. H. Chen and C. S. Hsue to work on the classical Heisenberg model [262].

The author of the present paper (Chin-Kun Hu) was born in Tu Cheng of Taipei County (now New Taipei City) in 1948. Hu did not have good health in his childhood and thus entered Ding Pu Elementary School in Tu Cheng in 1955 at age 7 and graduated from that school in 1961. Hu studied at Panchiao Junior High School in 1961-1964 and Jianguo Senior High School in 1964-1967. During September 1967-June 1971, Hu studied at the Department of Physics of National Tsing Hua University in Hsinchu, Taiwan. In the summer of 1970, Hu took a summer job to help the library of the Physics Research Promotion Center to prepare a Fortran computer program to sort books collected in that library. Thus Hu had good experience to prepare a complicated computer program to solve complicated problems, which turned out to be useful in future career in computational physics.

During September 1971- June 1973, Hu studied at the Institute of Physics of National Hsing Hua University as a Master's Degree student. Professor Yee-Yen Lee was his thesis advisor. In 1972, Physics Today had a report that Stevan Weinberg's theory of lepton was proved by himself to be renormalizable [263]. Hu's Master degree thesis was about a renormalization problem of this model [264].

During September 1973- June 1976, Hu studied at the Institute of Physics of National Hsing Hua University as a Ph.D. degree student. Professor Y. Y. Lee was still Hu's thesis advisor. On 2 December 1974, Samuel C. C. Ting's group and Burton Richter's group independently published two papers about the discovery of a new  $J/\psi$  elementary particle [265]. Part of Hu's Ph.D. dissertation was about a phenomenological models for  $J/\psi$  particle and other particles [266]. Mr. Wen-Den Chen was also a Ph.D. student of Prof. Y. Y. Lee, received a Ph.D. degree in 1975, and became an associate professor at the Department of Physics of National Taiwan Normal University. After receiving his doctoral degree in June 1976, Hu went to military service and worked at the Institute of Applied Physics of Chung Cheng Institute of Technology (CCIT) as an Associate Professor during January 1977-May 1978. In January 1977, Professor S.-P. Liu invited Hu to supervise Mr. D.-S. Wang, a Master's degree student at CCIT.

In February 1977, CCIT hosted the annual meeting of the Physical Society of the Republic of China. After the meeting, Y. M. Shih and Hu took the same bus from CCIT to Taipei. Hu told Y. M. Shih that he was not satisfied with renormalization method in quantum field theory, in which one should subtract an infinite quantity from another infinity quantity to get a finite quantity for comparing with experimental data. Y. M. Shih told Hu that in statistical physics there is a new approach, called renormalization group (RG) theory developed by K. G. Wilson [19–21], which can be used to study systems with infinite degree of freedoms. He suggested Hu to study renormalization group theory and gave Hu a paper by Leo P. Kadanoff, *et al.* [26].

In the Spring of 1977, Y. M. Shih invited D. C. Jou, C. K. Pan, W. S. Lee, W. D. Chen, H. M. Huang, K. G. Chen, H. C. Tseng, and C.-K. Hu to form a research group to work on renormalization group theory of critical phenomena. While Hu studied at Department and Instutute of Physics of National Tsing Hua University in 1967-1976, he took only one semester course on basic thermodynamics and statistical mechanics and one semester course on statistical mechanics. Hu started to work on phase transitions and critical phenomena from reading Ref. [26] by Kadanoff, *et al.*, and the classic book “Introduction to Phase Transitions and Critical Phenomena” by H. E. Stanley [18].

Shang-keng Ma was born in Chungking, China on 24 September 1940. His father Hsin Yeh Ma was a high official of National Party. In 1949, Shang-keng Ma moved with his family to Taipei, Taiwan. He finished high school education in Taipei and entered Department of Civil Engineering of National Taiwan University in 1958. In 1959, he transferred from National Taiwan University to Department of Physics of the University of California, Berkeley (UC-Berkerley) when his father was appointed as the Ambassador to Panama by Republic of China in Taiwan. He received his B.S. (1962) and Ph.D. (1966) degrees from UC-Berkerley. His Ph.D. thesis “Correlations of Photons from a Thermal Source” was under the supervision of Kenneth Watson. Figure 1(a) shows a photo of Shang-keng Ma with his parents at his home in Taipei no long after he received his Ph.D. degree.

After received a Ph.D. degree, Ma moved to Department of Physics of UC-San Diego as a postdoctoral fellow, and as a faculty member in less than one year. He became a tenured member of the UCSD physics department in 1971. During 1966-1968, Chia-Wei Woo was a postdoctoral research fellow at Department of Physics of UC-San Diego. Ma

and Woo finished two research papers on theory of a charged bose gas [267], which were the first two journal papers published by Ma.

In 1977-1978, Shang-keng Ma was a visiting professor at Department of Physics of National Tsing Hua University in Hsinchu, Taiwan.

In May 1978, Hu finished the military service and worked at Precision Instrument Development Center inside National Tsing Hua University and joined a group to read S.-K. Ma's book [24] during June-October 1978. At the end of October 1978, Hu went to UCSD to work in S.-K. Ma's group as a postgraduate research physicist during November 1978-June 1979 to work on the theory of a spin glass model at low temperatures [35] and a quantum spin model with random nearest-neighbor couplings [36].

## APPENDIX B: CONNECTION BETWEEN THE $q$ -STATE POTTS MODEL AND THE $q$ -STATE BOND CORRELATED PERCOLATION MODEL

As an illustrative example, now we show that the phase transition of the  $q$ -state Potts model (QPM) is equivalent to the percolation transition of a  $q$ -state bond-correlated percolation model (QBCPM), the physical quantities of the former are corresponding to the geometrical quantities of the later. The derivation below is a simple extension of the derivation presented in [138, 139] and has also been given in [141, 145, 159].

The  $q$ -state Potts model on a lattice  $G$  of  $N$  sites and  $E$  nearest-neighbor bonds has been defined in Section II-7 in which each spin has component  $1, 2, \dots, q$ . In [102, 103, 107], the authors coupled one of the spin component to the external magnetic field and showed that as  $q \rightarrow 1$  the magnetization of the QPM is corresponding to the percolation probability of the bond random percolation model in which the probability for a subgraph  $G'$  to appear is given by Eq. (23). To show the equivalence between the QPM and the QBCPM for any  $q$ , as in [136, 139, 141, 145] we consider a  $q$ -state Potts spin  $s_i$  has components:  $-j, -j+1, \dots, j-1$ , and  $j$ , where  $1 \leq i \leq N$ ,  $2j+1 = q$ , and  $q$  is an integer. The Hamiltonian of the QPM may be written as

$$-H/k_B T = K \sum_{\langle i,j \rangle} \delta(s_i, s_j) + B \sum_i s_i. \quad (\text{B.1})$$

Here the first summation is a sum over all nearest neighbors,  $\delta(s_i, s_j) = 1$  or 0 when  $s_i = s_j$  or  $s_i \neq s_j$ , respectively,  $K = J/k_B T$  is the normalized NN coupling constant, and  $B = h/k_B T$  is the normalized external magnetic field. The partition function for Hamiltonian of Eq. (B.1) may be written as

$$\begin{aligned} Z_N &= \sum_{s_i=-j}^j \prod_{\langle i,j \rangle} \exp[K\delta(s_i, s_j)] \prod_i \exp(Bs_i) \\ &= \sum_{s_i=-j}^j \prod_{\langle i,j \rangle} [1 + (\exp(K) - 1)\delta(s_i, s_j)] \prod_i \exp(Bs_i). \end{aligned} \quad (\text{B.2})$$

Now we expand the first product in Eq. (B.2) and use the subgraphs  $G' \subseteq G$  to represent the terms in the expansion. For each NN pair of sites  $\langle i, j \rangle$ , there occurs in Eq. (B.2) the two terms: 1 and  $[\exp(K) - 1]\delta(s_i, s_j)$ ; subgraphs  $G'$  with no  $\langle i, j \rangle$  bond correspond to the former, and those with an  $\langle i, j \rangle$  bond to the latter. There are  $b(G')$  bonds in the subgraphs  $G'$ ,  $0 \leq b(G') \leq E$ . The clusters are defined in the same way as they are in usual bond percolation problem. After sum over spin states, we have

$$\begin{aligned} Z_N &= \sum_{G' \subseteq G} (e^K - 1)^{b(G')} \prod_c \{\exp(Bn_{cj}) + \exp[Bn_c(j-1)] + \dots + \exp(-Bn_{cj})\} \\ &= e^{KE} \sum_{G' \subseteq G} p^{b(G')} (1-p)^{E-b(G')} \prod_c [\exp(Bn_{cj}) + \dots + \exp(-Bn_{cj})], \end{aligned} \quad (\text{B.3})$$

where the sum is over all subgraphs  $G'$  of  $G$ , the product extends over all clusters  $c$  in a given  $G'$ ,  $n_c = n_c(G')$  is the number of sites in the cluster  $c$ , and  $p$  is given in Eq. (38).

Let  $N^*(G')$  and  $n_f(G')$  denote, respectively, the total number of sites in the percolating clusters of  $G'$  and the total number of nonpercolating clusters in  $G'$ . Using  $Z_N$  of Eq. (B.3), we may derive following expressions for the spontaneous magnetization  $M$ , the zero-field magnetic susceptibility  $\chi$ , the internal energy  $U$ , and the specific heat  $C_h$  of the  $q$ -state Potts model in  $N \rightarrow \infty$ :

$$\begin{aligned} M &= \lim_{B \rightarrow 0^+} \lim_{N \rightarrow \infty} \frac{\partial}{\partial B} \ln Z_N/N \\ &= \lim_{N \rightarrow \infty} W^{-1} \sum_{G' \subseteq G} \pi(G', p, q) [N^*(G')/N] j \equiv j P, \end{aligned} \quad (\text{B.4})$$

$$\begin{aligned} \chi &= \lim_{B \rightarrow 0^+} \lim_{N \rightarrow \infty} \frac{\partial^2}{\partial B^2} \ln Z_N/N \\ &= AS + \lim_{N \rightarrow \infty} j^2 W^{-2} \sum_{G' \subseteq G} \sum_{G'' \subseteq G} \pi(G', p, q) \\ &\quad \times \pi(G'', p, q) [N^*(G') - N^*(G'')]^2 / (2N), \end{aligned} \quad (\text{B.5})$$

$$\begin{aligned} U &= - \lim_{B \rightarrow 0^+} \lim_{N \rightarrow \infty} \frac{\partial}{\partial \beta} \ln Z_N/N \\ &= -\frac{J}{p} \langle b(G') \rangle_0 \equiv -\frac{zJ}{2p} \bar{p} \end{aligned} \quad (\text{B.6})$$

$$C_h = \frac{\partial}{\partial T} U = \frac{k_B K^2}{p^2} [-(1-p) \frac{z}{2} \bar{p} + F]. \quad (\text{B.7})$$

Here  $A = [j^2 + (j-1)^2 + \dots + (-j+1)^2 + (-j)^2]/q = (q^2 - 1)/12$ ,  $z$  is the coordinate number of  $G$ ,  $\pi(G', p, q)$  is defined by Eq. (67),  $W = \sum_{G' \subseteq G} \pi(G', p, q)$ ,  $P = \lim_{N \rightarrow \infty} W^{-1} \sum_{G' \subseteq G} \pi(G', p, q) [N^*(G')/N]$ ,

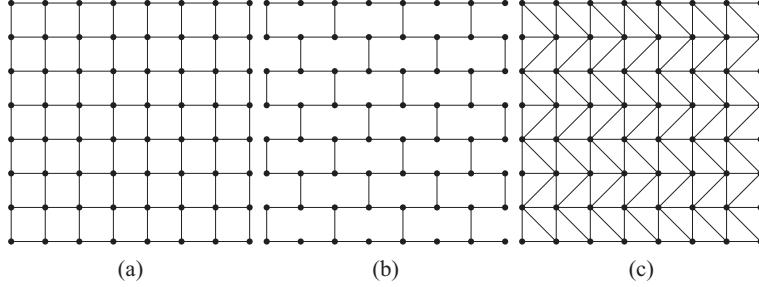


FIG. 34: (a) A  $8 \times 8$  square lattice, (b) a  $8 \times 8$  honeycomb (hc) lattice obtained from the sq lattice by deleting half of the vertical bonds, (c) a  $8 \times 8$  plane triangular (pt) lattice obtained from the square lattice by adding the diagonal bonds. Taken from Figure 5 of C.-K. Hu, Proc. NSC ROC (1999) [268].

$$\begin{aligned} S &= \lim_{N \rightarrow \infty} W^{-1} \sum_{G' \subseteq G} \pi(G', p, q) \left[ \frac{\sum_c^f n_c^2(G')/N}{\sum_c^f n_c(G')/N} \right], \quad \bar{p} = \\ &\lim_{N \rightarrow \infty} W^{-1} \sum_{G' \subseteq G} \pi(G', p, q) [b(G')/E], \quad F = \lim_{N \rightarrow \infty} W^{-1} \sum_{G' \subseteq G} \pi(G', p, q) [b(G') - \\ &[b(G')]_{av}]^2/N, \quad [b(G')]_{av} = W^{-1} \sum_{G' \subseteq G} \pi(G', p, q) b(G'), \text{ and } \sum_c^f \text{ for } S \text{ sums over all} \\ &\text{non-percolating clusters in } G'. \end{aligned}$$

It is obvious that the divergent behavior of  $C_h$  is dominated by  $F$ .  $P$ ,  $S$ ,  $\bar{p}$ , and  $F$  are, respectively, the percolation probability, the mean cluster size, the average number of occupied bonds, and the fluctuations of occupied bonds of the following q-state bond-correlated percolation model (QBCPM):

- a. All sites of  $G'$  are occupied and each bond of  $G$  is attached with the bond probability  $p$ . This process generates subgraphs  $G' \subseteq G$ .
- b. The overall probability weight of a  $G' \subseteq G$ , is enhanced by a factor  $q$  for each finite cluster in  $G'$ .

## APPENDIX C: HOW TO CHOOSE RATIOS OF ASPECT RATIOS TO GET UNIVERSAL FINITE-SIZE SCALING FUNCTIONS

In this Appendix, how to choose ratios of aspect ratios to get universal finite-size scaling functions for lattice models will be discussed.

Equation (34) for  $E_p$  implies that  $E_p$  for all models in the same universality class must be equal at the critical point in order to have universal finite-size scaling functions (UFSSF's). In 1992, Ziff found that  $E_p=0.5$  for site and bond percolation on large square lattices with free boundary conditions [179], and Langlands, Pichet, Pouliot, and Saint-Aubin (LPPS) proposed that when aspect ratios for the square (sq), honeycomb (hc), and plane triangular (pt) lattices have the relative proportions  $1:\sqrt{3}:\sqrt{3}/2$ , then site and bond percolation on such lattices have the same value of  $E_p$  at the critical point [269]. In 1992, Cardy used a conformal theory to write down a formula for the critical  $E_p$  as a function of aspect ratio for percolation on lattices with free boundary conditions [270]. Cardy's formula

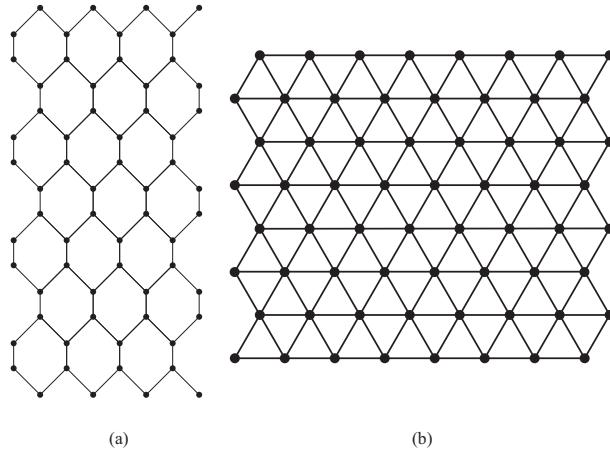


FIG. 35: (a) A  $8 \times 8$  square lattice, (b) a  $8 \times 8$  honeycomb (hc) lattice obtained from the sq lattice by deleting half of the vertical bonds, (c) a  $8 \times 8$  plane triangular (pt) lattice obtained from the square lattice by adding the diagonal bonds. Taken from Figure 6 of C.-K. Hu, Proc. NSC ROC (1999) [268].

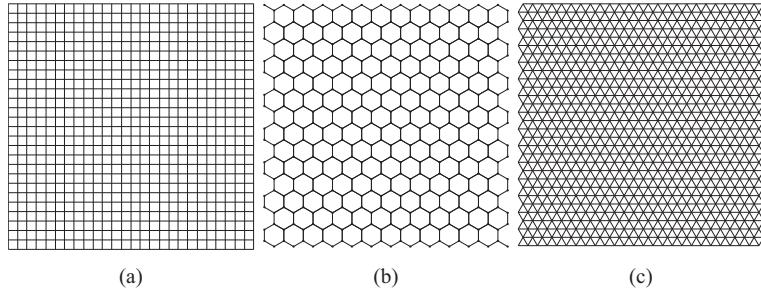


FIG. 36: (a) A  $26 \times 26$  sq lattice, (b) a  $26 \times 15$  hc lattice, (c) a  $26 \times 30$  pt lattice. Taken from Figure 7 of C.-K. Hu, Proc. NSC ROC (1999) [268].

is consistent with LPPS's numerical results. Cardy and LPPS did not discuss the values of  $E_p$  for  $p \neq p_c$ .

LPPS's result about the relative proportions  $1:\sqrt{3}:\sqrt{3}/2$  for sq, hc, and pt lattices can be understood as follows. Figure 34(a) shows a typical  $L \times L$  sq lattice. An  $L \times L$  hc and an  $L \times L$  pt lattices can be obtained from the sq lattice of Fig. 34(a) by removing or adding bonds, respectively, as shown in Fig. 34(b) and Fig. 34(c), which are equivalent to Fig. 35(a) and Fig. 35(b), respectively. If lattice sites in the horizontal direction of Fig. 35(a) and Fig. 35(b) are enlarged by a factor  $\sqrt{3}$  and  $\sqrt{3}/2$ , respectively, the domains of hc and pt lattices are similar to  $L \times L$  square lattices. To illustrate this point, we show  $26 \times 26$  sq,  $26 \times 15$  hc, and  $26 \times 30$  pt lattices in Figs. 36(a), 36(b), and 36(c), whose aspect ratios approximately match the ratio  $1:\sqrt{3}:\sqrt{3}/2$  considered by LSSP. It is obvious that three figures in Fig. 36 have similar domains.

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