PHYSICAL REVIEW E **78**, 021138 (2008)

Effect of thermal bond excitations on the critical properties of covalent Ising networks

S. Davatolhagh, L. Separdar, and M. Barati
Department of Physics, College of Sciences, Shiraz University, Shiraz 71454, Iran

(Received 30 January 2008; revised manuscript received 12 June 2008; published 28 August 2008)

We introduce a bond-diluted Ising model with *temperature-dependent* concentration of bonds, which is intended to simulate the excitations of bond degrees of freedom as in covalently bonded network liquids arising from the thermal electronic transitions between bonding and antibonding electronic states. The critical behavior of this simplified model system, called the thermalized-bond Ising model, is investigated in terms of the Monte Carlo simulation results of finite-size *regular* Ising systems, as input for the method of chemical potentials that is generally used to obtain the thermodynamic properties of annealed impurity models. A finite-size scaling analysis of the susceptibility and the fourth-order cumulant results in a reliable estimation of the renormalized critical exponents. The exponents are found to be consistent with the phenomenological renormalization relations, due to Fisher, despite the temperature-dependent bond dilution.

DOI: 10.1103/PhysRevE.78.021138 PACS number(s): 64.60.De, 68.35.Rh, 05.20.−y

I. INTRODUCTION

Models with annealed bond disorder were once considered by Thorpe and Beeman [1], among others [2], and investigated in detail using the method of chemical potentials and the grand-canonical ensemble [3]. However, such models of disorder were not pursued any further because of their lack of a spin-glass phase that was in so much demand in those days. The absence of a spin-glass transition is attributed to the correlations introduced among the bonds by annealing, such that like bonds have a tendency to form clusters particularly close to the transition point [1]. Such correlations are entirely absent in spin glasses, which are characterized by uncorrelated quenched-in disorder, thus resulting in frustration [4]. In the annealed case the system as a whole, including the disorder, is allowed to come into complete thermal equilibrium at every temperature. Thus, the system has the liberty of choosing optimal spatial arrangements of the disorder variables in order to further minimize its free energy. In the annealed impurity models studied so far [1,2], however, the concentration of the disorder is kept constant with the temperature.

As a way to revive some interest in models with annealed bond disorder, in this paper we extend the method of chemical potentials to study a bond-diluted Ising model that is different from others by virtue of its temperature-dependent annealed bond dilution. By introducing the thermalized-bond Ising model (TBIM), we would like to investigate the effect the thermally induced bond excitations have on the critical behavior of a covalent liquid at its critical point, which is generally believed to be in the universality class of the three-dimensional lattice-gas model or equivalently the ferromagnetic Ising model. In the case of TBIM, every covalent bond linking a nearest-neighbor pair of atoms is allowed thermally induced electronic transitions between bonding and antibonding electronic states. Hence, it can be regarded as containing annealed bond defects with a temperature-dependent concentration. Every bond at every instant is characterized by a coupling constant $J=0, J_0$ such that $J=0$ corresponds to a broken bond (antibonding electronic state), while $J=J_0$ means an attractive coupling between the two atoms (bonding electronic state) as illustrated schematically in Fig. 1. Like the annealed case, and given enough time, our model system has the liberty of lowering its free energy by choosing optimal arrangements for the bond variables, and reaching complete thermal equilibrium with the lattice or the structural variables. This of course introduces correlations among neighboring bonds, which is in sharp contrast with random quenched impurity models. We believe that the thermalized bond model introduced here, and the many conceivable variants thereof, can be of broader interest in the research field of phase transitions in systems with predominantly covalent bonding, such as the lattice polymers [5] and the lattice protein [6], as they can provide for a natural bond breaking mechanism in lattice models of covalent structures. A rather similar model, called as the bond-lattice excitations model, has been introduced and studied before in the context of the supercooled glass-forming liquids [7].

TBIM is exactly soluble in one and two dimensions [8], as the solution can be mapped on to a regular Ising model with a rescaled temperature on the same lattice [1]. In the following, we focus on TBIM in three dimensions for which no exact solution is anticipated. Thus, we rely on the statistics obtained from Monte Carlo (MC) simulations of finite lattices of the reference pure system in order to calculate the rescaled temperatures of the corresponding finite thermalized-bond lattices. A careful finite-size scaling analysis of the susceptibility and the fourth-order cumulant then provides reliable estimates for the critical exponents and the overall critical behavior exhibited by TBIM in three dimensions.

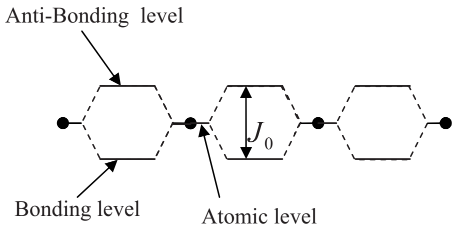

FIG. 1. A schematic illustration of the electronic energy states of the covalent bonds linking a chain of atoms. The energy gap between the bonding and the antibonding level is denoted by J_0.

The rest of this paper is organized as follows. In Sec. II, we present the microscopic Hamiltonian that characterizes the thermalized-bond Ising model. In Sec. III, the method of chemical potentials that is generally used to investigate the thermodynamic properties of annealed impurity models is briefly reviewed, paying particular attention to those aspects that are directly relevant to the present work. This method is then applied in Sec. IV to calculate the thermodynamic properties of interest for finite-size TBIM systems, using the Monte Carlo simulation results of finite-size regular Ising systems as input. In Sec. V, a finite-size scaling analysis is carried out to calculate the critical exponents of TBIM in the thermodynamic limit. Our main results are discussed in Sec. VI, and the paper is concluded in Sec. VII with a summary.

II. THERMALIZED-BOND ISING MODEL

We introduce an Ising model with a temperature-dependent bond dilution, arising from the thermally induced electronic transitions of the covalent bonds between bonding and antibonding electronic states, referred to as thermalized-bond Ising model or TBIM. The bond dilution is annealed in the sense that any relaxation time associated with the bond defects is much shorter than the experimental or the observation time scale. Thus, the system is allowed to further lower its free energy by choosing optimal spatial arrangements of the defects. We denote the thermally averaged bond concentration by p. $(1-p)$ is therefore the concentration of broken bonds due to thermal excitations. To keep the analysis simple, we shall treat the covalent bonds as independent two-level systems with energy gap J_0 (as sketched in Fig. 1), obeying classical Maxwell-Boltzmann statistics, and in thermal equilibrium with the lattice. Thus, the ratio of the bonds to the broken bonds in equilibrium is given by the ratio of the corresponding Boltzmann factors: $p/(1-p)=\exp(\beta J_0)$. On solving for bond concentration p, we have

$$p = 1/(1+e^{-\beta J_0}), \tag{1}$$

where $\beta=1/k_B T$ is the reciprocal temperature of the TBIM, and k_B is the Boltzmann constant. We certainly do not rule out other forms of the bond concentration p. In fact, in a more realistic application, one may wish to consider bonds that obey Fermi-Dirac statistics, and treat the electronic occupation numbers accordingly. However, as we shall explain later in this paper, our main results stay the same no matter which one statistics is used for the treatment of the bonds. Thus, to keep the treatment simple, we shall adopt the classical Maxwell-Boltzmann statistics for the treatment of the bonds. It is clear from Eq. (1) that the bond concentration p decreases from unity at $T=0$ to one-half at infinitely large temperatures, while the concentration of broken bonds $(1-p)$ increases from zero at the absolute zero of temperature to one-half at infinite temperature. It must be pointed out that the bond concentration p remains well above the bond percolation threshold for the cubic lattice, $p_c=0.2488$ [9], at all temperatures: as the bonds percolate at all temperatures, the bond percolation problem does not appear to be directly relevant to the thermodynamic transition studied later in this paper.

The bond distribution function for our thermalized-bond model system is of the form

$$P_J(\beta) = p\,\delta_{J,J_0} + (1-p)\,\delta_{J,0}, \tag{2}$$

where p is given by Eq. (1) and δ denotes the Kronecker delta. $J=J_0$ is the coupling associated with a bond, and $J=0$ is that due to a broken bond. Each atom of a nearest-neighbor pair contributes an electron to the covalent bond, and the thermalization of the bond allows for thermally induced electronic transitions between the two electronic states at finite temperature. Indeed this provides for a natural bond-breaking mechanism that may be suitably incorporated in the lattice models of covalently bonded structures. The microscopic Hamiltonian of the system under consideration can be formally defined by

$$H = -\sum_{\langle ij\rangle} J_{ij}\sigma_i\sigma_j, \tag{3}$$

where $\sigma_i=\pm 1$ is the structural variable associated with the site i of the underlying simple cubic lattice, and $J_{ij}=0$, J_0 represents the *annealed* bond variable associated with the nearest-neighbor sites $\langle ij\rangle$ that is described by the bond distribution function given as Eq. (2). The Ising variable σ_i must be interpreted as a structural variable (as opposed to interaction/gauge variable), the thermal average of which defines the order parameter for the model system under consideration. It is well known that the lattice-gas model in three dimensions (or, equivalently, the ferromagnetic Ising model) largely captures the universal behavior of fluids at their critical point, despite the lattice or the simple mathematical structure. By introducing the thermalized-bond Ising model, we wish to incorporate a bond-breaking mechanism suitable for covalent bonds, and investigate the effect on the critical behavior of a covalent liquid at its critical point. Indeed, the renormalizing effect of the "hidden variables" (or annealed impurity subject to a constraint) on the critical exponents of magnets and fluids has been recognized for many years [10]. (See also Table I in Ref. [10] for a comparison of the experimental exponents with the theoretical exponents, highlighting some of the discrepancies.) In doing so, we also extend the method of chemical potentials to investigate systems with temperature-dependent annealed bond impurity. A variant of this model was introduced and studied by Monte Carlo simulation, albeit for a fixed bond concentration, in Ref. [11]. A rather similar model involving excitations of a bond lattice has also been studied before in the context of the supercooled glass-forming liquids [7].

III. THEORETICAL BACKGROUND

The following is a review of those aspects of the method of chemical potentials that are directly relevant to the present work. Throughout this section, we shall use the notation and the mathematical structure introduced by Thorpe and Beeman [1]. The model Hamiltonian (3) may be written as a sum over nearest-neighbor pairs of atoms

$$H = \sum_{\langle ij \rangle} H_{ij}, \tag{4}$$

where

$$H_{12} = - \sum_{i=1,2} J_i f_i \sigma_1 \sigma_2 - \sum_{i=1,2} f_i \xi_i. \tag{5}$$

Thus, each bond has a coupling associated with it, J_i, which characterizes the electronic state of the covalent bond: $J_1 \equiv J_0$ denotes the bonding state, while $J_2 \equiv 0$ is the antibonding state. In Eq. (5), the bond indicator function f_i is unity if the coupling is J_i and zero otherwise. The thermal average, $\langle f_i \rangle$, is physically the same as the bond distribution function $P_J(\beta)$ given as Eq. (2). The chemical potential ξ_i coupled to the bond indicator f_i is introduced into the Hamiltonian only to produce the desired bond distribution. (It drops out of consideration at the end.) As in the case of the annealed impurity models, one averages the partition function over the disorder, rather than averaging the free energy. Thus, the grand partition function involves a trace over both the structural variables, σ_i, and the bond variables f_i,

$$\Xi = \sum_{\{f_i\}} \sum_{\{\sigma_j\}} e^{-\beta H}. \tag{6}$$

A partial trace over the $\{f_i\}$ allows for an expression of the result in terms of the partition function of a regular Ising model on the same lattice, but with a different temperature. The result is

$$\Xi = A^{Nz/2} Z(K), \tag{7}$$

where $Z(K)$ is the partition function of a *regular* Ising model with reciprocal temperature K, z is the coordination number of the lattice, and N is the total number of atoms. $Nz/2$ is therefore the total number of bonds. K is interpreted as the reciprocal temperature of the regular Ising model or the reference system in terms of which the thermodynamic properties of the TBIM at a rescaled reciprocal temperature β can be derived. More explicitly, K and A are, respectively, given by

$$e^{2K} = \left(\sum_i e^{\beta \xi_i + \beta J_i} \right) \Big/ \left(\sum_j e^{\beta \xi_j - \beta J_j} \right),$$

$$A^2 = \left(\sum_i e^{\beta \xi_i + \beta J_i} \right) \left(\sum_j e^{\beta \xi_j - \beta J_j} \right). \tag{8}$$

Now, the concentration $\langle f_i \rangle$ is given by

$$\beta \langle f_i \rangle = \frac{2}{Nz} \frac{\partial \ln \Xi}{\partial \xi_i} = \frac{\partial \ln A}{\partial \xi_i} + \epsilon(K) \frac{\partial K}{\partial \xi_i}, \tag{9}$$

where $\epsilon(K) = \langle \sigma_1 \sigma_2 \rangle$ is the nearest-neighbor pair correlation function of the regular Ising model, and is simply given by the negative energy of the reference system normalized to the number of bonds $Nz/2$. From Eqs. (8) and (9), and on eliminating the unwanted chemical potentials, one gets an implicit equation giving the rescaled temperature of the annealed system in terms of the temperature of the reference system [1],

$$\sum_{i=1,2} \frac{\langle f_i \rangle}{[1 + \epsilon(K)] + [1 - \epsilon(K)] e^{2K - 2\beta J_i}} = \frac{1}{2}. \tag{10}$$

It must be emphasized that relations (7)–(10) remain valid even if $\langle f_i \rangle$ is temperature-dependent [12]. On replacing $\langle f_i \rangle$ by its explicit form $P_J(\beta)$, the above can be written as

$$\sum_{J=0,J_0} \frac{P_J(\beta)}{[1 + \epsilon(K)] + [1 - \epsilon(K)] e^{2K - 2\beta J}} = \frac{1}{2}. \tag{11}$$

Equation (11) is an implicit relation in terms of which β can be obtained as a function of K. An important point one needs to recognize, however, is that the critical point singularities of the thermodynamic functions that do not involve a temperature derivative of the free energy, such as the order parameter and its higher-order cumulants, are only renormalized due to the rescaling of the temperature given by Eq. (11). This can be seen in view of the fact that the definition of the order parameter, given as Eq. (12) below, does not involve the bond indicator function f_i. Equation (11) is central to the analysis presented in the following section, where we present our results for the order parameter and the susceptibility of finite-size TBIM systems.

IV. STATISTICS OF FINITE-SIZE TBIM SYSTEMS

As outlined in the Introduction, we shall only be concerned with the critical behavior of the TBIM in three dimensions, where Monte Carlo simulation results of finite-size regular Ising systems are used as input to find the thermodynamic properties of the corresponding finite-size TBIM systems. A finite-size scaling analysis of the statistics thus obtained reveals the critical behavior expected of TBIM in the thermodynamic limit.

Although in one and two dimensions the regular Ising model has been solved analytically [13,14], an exact solution in three dimensions is still lacking. In order to obtain the properties of the reference Ising system, we have simulated simple cubic lattices of size $N = L^3$ with periodic boundary conditions for five different linear system sizes $L = 16$, 20, 30, 40, and 50 using a dedicated Metropolis Monte Carlo code [15], with sequential spin-flip attempts through the lattice, over its critical region. At every temperature, the system was allowed 4000 equilibration passes (complete lattice updates), and data points were accumulated by averaging over 400 000 accumulation passes. The accumulation passes were divided into 10 bins, and the binned averages were used to estimate the statistical errors, which in most cases are no more than a few percent of the corresponding mean values. In order to check the accuracy of our data, we calculated the critical exponents of the reference Ising system and compared our results with the extensive literature available on the subject [16]. Very good agreement was obtained.

In order to determine the rescaled temperatures of the finite-size TBIM systems, we computed the energy per bond, $-\epsilon_L(K)$, of the finite-size regular Ising systems. $\epsilon_L(K)$, when substituted in Eq. (11), gives the rescaled temperature of the corresponding finite-size TBIM system. Figure 2 shows the rescaled temperature T_L plotted against the temperature of

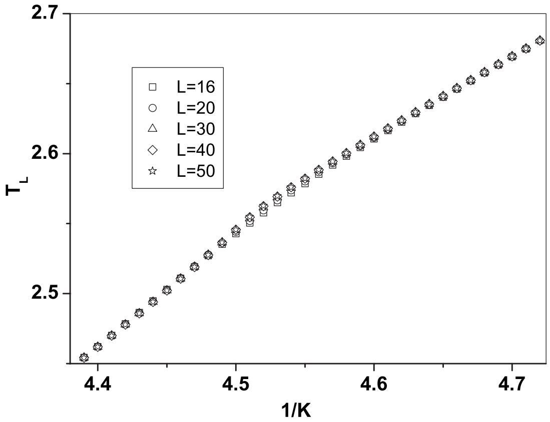

FIG. 2. The temperature of finite-size TBIM versus that of the reference system for different system sizes in the critical region. Both temperatures are measured in units of J_0/k_B.

the reference system $1/K$ for various system sizes. Both temperatures are measured in units of J_0/k_B. The finite-size effect on T_L, though small, must be taken into account in a careful finite-size scaling analysis of the data, which we present in the next section. The order parameter of the TBIM, defined by

$$\langle m_L\rangle = \left\langle \left| \sum_{i=1}^{N} \sigma_i \right| \right\rangle \Bigg/ N, \tag{12}$$

is plotted in Fig. 3 against the rescaled temperature for various system sizes. The corresponding susceptibility

$$\chi_L = \frac{N}{k_B T_L}(\langle m_L^2\rangle - \langle m_L\rangle^2) \tag{13}$$

is shown in Fig. 4. In addition to the above, we have determined the fourth-order cumulant, given by Eq. (14) below, for finite-size TBIM systems, which provides a convenient route to finite-size scaling analysis as presented in the next section.

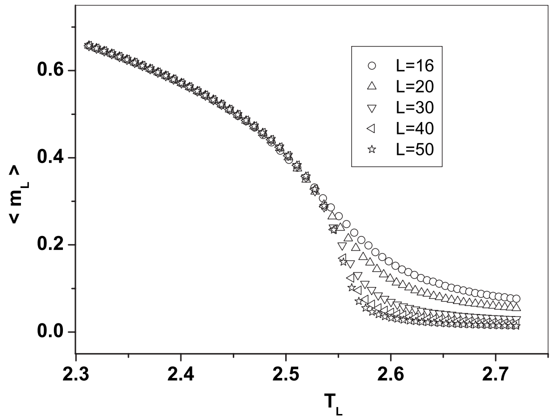

FIG. 3. The order parameter for finite-size TBIM systems is plotted against the corresponding rescaled temperatures in the critical region.

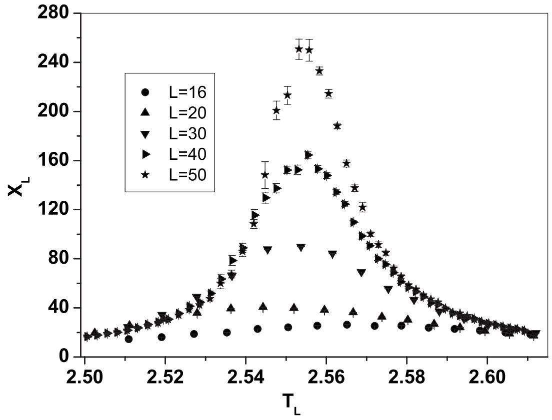

FIG. 4. The susceptibility of finite-size TBIM systems vs the corresponding rescaled temperatures in the vicinity of the critical point.

V. FINITE-SIZE SCALING ANALYSIS

The singularities of the free energy can only evolve in the thermodynamic limit of the infinite system size, $L\to\infty$, and the finite size of the systems employed causes a systematic rounding of the critical singularities, as seen explicitly in Figs. 3 and 4. Such finite-size effects, however, can be turned into a powerful tool through finite-size scaling analysis for determining the critical exponents [17].

A convenient way of studying critical phenomena is through the fourth-order cumulant due to Binder [18],

$$U_L = 1 - \frac{\langle m_L^4\rangle}{3\langle m_L^2\rangle^2}, \tag{14}$$

which asymptotically approaches zero for $T>T_c$, and two-thirds for $T<T_c$. This dimensionless quantity has the finite-size scaling form

$$U_L(T_L) = \widetilde{U}[L^{1/\nu}(T_L - T_c)] \tag{15}$$

that is independent of L at the critical point $T_L=T_c$, where T_L is the rescaled temperature of a finite-size TBIM lattice obtained from Eq. (11). In order to locate the critical temperature of the TBIM, we have relied on the cumulant crossing method [18]. In Fig. 5, $U_L(T_L)$ is plotted against T_L for different system sizes. The inset shows a zoom on the crossing for the larger system sizes, the width of which is used to estimate bounds for T_c. The plot gives evidence of a continuous phase transition of the conventional type at $T_c=2.557(1)$. T_c is indeed much lower than the critical temperature of the regular Ising model $1/K_c=4.5115(5)$ [19]. The lowering of the transition point is expected in the light of the annealed bond disorder present. Furthermore, the correlation length exponent ν, defined by $\xi\sim|T-T_c|^{-\nu}$, is estimated from the scaling plot of $U_L(x)$ against $x=L^{1/\nu}(T_L-T_c)$. This is shown in Fig. 6, for $\nu=0.70$, and $T_c=2.557$. By varying ν, and evaluating the quality of the data collapse, our best estimate of the correlation length exponent is $\nu=0.70(1)$. To obtain bounds for an exponent, we rely on a lower and an upper bound that give a good data collapse, beyond which the collapse of the data is visibly worsened.

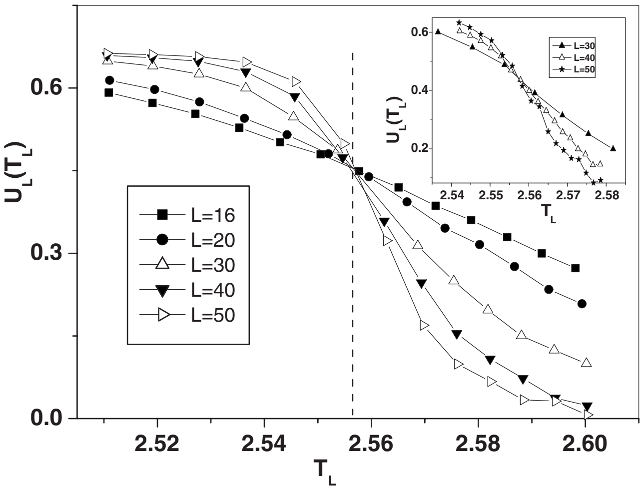

FIG. 5. Plot of the fourth-order cumulant vs rescaled temperature for various system sizes. The point of intersection corresponds to the critical temperature, T_c=2.557(1), of TBIM in the limit of the infinite lattice size. The inset is a zoom on the crossing for the larger system sizes.

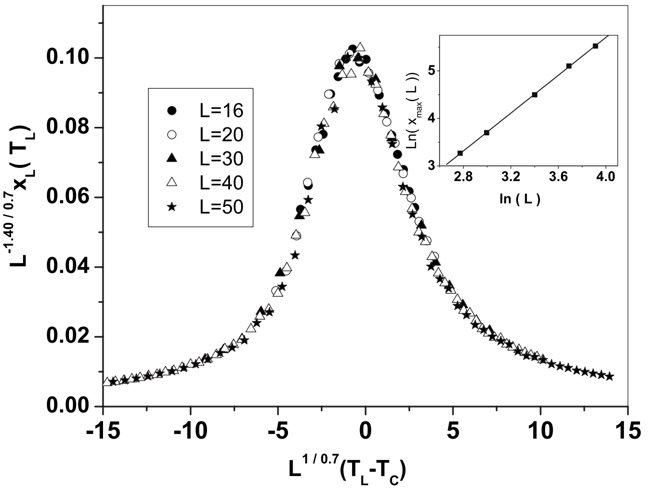

FIG. 7. A scaling plot of the susceptibility with γ=1.40, ν=0.70, and T_c=2.557, according to the finite-size scaling form given in Eq. (16). All available data have collapsed onto the corresponding universal scaling function, $\tilde{\chi}$. The inset shows a log-log plot of $\chi_{\max}(L)$ against L.

We have also carried out a finite-size scaling analysis of the susceptibility χ_L, which has the finite-size scaling form

$$\chi_L(T_L) = L^{\gamma/\nu}\tilde{\chi}[L^{1/\nu}(T_L - T_c)], \qquad (16)$$

where γ is the susceptibility exponent defined by $\chi \sim |T - T_c|^{-\gamma}$. The ratio γ/ν is closely related to the anomalous dimension exponent, η, which describes the power-law decay of correlations at the transition point T_c, through the Fisher scaling law $\gamma/\nu = 2-\eta$ [20]. $\tilde{\chi}$ is a universal scaling function such that an appropriate choice of the exponent γ, in this case γ=1.40(1), results in a data collapse in a scaling plot as can be seen in Fig. 7. It must also be pointed out that Eqs. (15) and (16) represent only the leading term in finite-size scaling, as for the system sizes considered, the correction to scaling is expected to be rather small. This expectation is validated by the inset of Fig. 7, showing a log-log plot of $\chi_{\max}(L)$ (i.e., maximum value of χ_L) against L, which must be a straight line with a slope equal to γ/ν, if Eq. (16) is a valid representation of the finite-size scaling for the system sizes considered. This is indeed the case, and the slope of the straight line fit γ/ν=1.990(15) is in good agreement with the exponent ratio γ/ν=2.000(14) obtained from the scaling plots shown in Figs. 6 and 7.

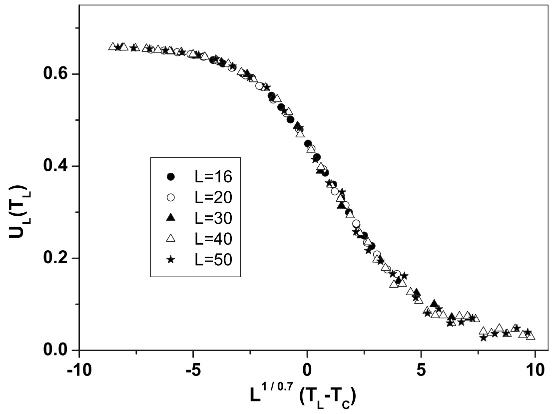

FIG. 6. A scaling plot of the fourth-order cumulant with ν=0.70 and T_c=2.557 according to the finite-size scaling form in Eq. (15). These values give the best data collapse that we have been able to observe.

Having estimated two of the critical exponents, the rest can be obtained from a variety of scaling laws relating the exponents. The scaling laws are particularly useful in the instance of accurate estimation of the specific-heat exponent α, defined by $C \sim |T-T_c|^{-\alpha}$, where a finite-size scaling analysis is always rendered inaccurate by a large nonsingular background contribution. The hyperscaling law $\alpha = 2 - d\nu$ [21], where d is the space dimensions, gives $\alpha = -0.10(3)$ for d=3. The negative sign is indicative of the fact that the specific-heat divergence in the regular Ising model has been reduced to a finite cusp singularity. Furthermore, the order-parameter exponent β, defined by $\langle m \rangle \sim (T_c - T)^{\beta}$, can be obtained from the scaling law [21], $2\beta + \alpha + \gamma = 2$, thus giving β=0.35(2) for our thermalized-bond model system.

VI. DISCUSSION

It is interesting to note the consistency of the critical exponents of the TBIM with certain phenomenological relations due to Fisher [10], which give the renormalization of the critical exponents, by the so-called hidden variables, in terms of the known exponents of the regular model system. The term "hidden variable" applies to the annealed impurity that may exist in addition to the statistical variables already incorporated in the regular model Hamiltonian. Thus, it is believed that the exponents describing the critical behavior of the thermodynamic functions that do not involve a temperature derivative of the free energy, such as the order parameter and the corresponding susceptibility, are renormalized according to $\beta = \beta_r/(1-\alpha_r)$, and $\gamma = \gamma_r/(1-\alpha_r)$,

TABLE I. The critical exponents of TBIM are compared with those obtained from the renormalization relations. The critical exponents of the regular Ising model are also included for completeness. The last row contains some experimental data on simple and binary fluids adopted from Table I in Ref. [10].

Critical exponent	ν	γ	α	β
Three-dimensional TBIM	0.70(1)	1.40(1)	−0.10(3)	0.35(2)
Renormalization relations [10]	0.7086(35)	1.3907(75)	−0.1258(38)	0.3675(17)
Three-dimensional Ising model [16]	0.6294(10)	1.2353(25)	0.1118(30)	0.3265(4)
Simple and binary fluids		1.35-1.40	≤ 0	0.33–0.36

respectively, where a subscript r on the exponent means the regular/reference system. On the other hand, the exponent α describing the specific-heat singularity is believed to be given by $\alpha = -\alpha_r/(1-\alpha_r)$ [10]. (Note the negative sign.) In Table I, we have listed for comparison the critical exponents we have found for the TBIM along with those obtained from the above renormalization relations. They agree very well within statistical errors. The exponents of the regular Ising model [16], which have been used in connection with the above renormalization relations, are also included for completeness. Fisher, however, considered the effect of the hidden variables in the form of the annealed impurity subject to a constraint such as a fixed number of impurity atoms (concentration). Furthermore, a variety of solvable models were discussed to check the renormalization relations explicitly, all of which involved a temperature-independent impurity concentration [10]. Hence, our results may be regarded as independent verification of the above renormalization relations for systems involving temperature-dependent annealed bond impurity. Physically, this consistency should be interpreted in light of the fact that the minute details of the microscopic interactions of a physical system, in this case the temperature dependence of the bond dilution, may not alter the large-scale behavior at a critical point, thus preserving the renormalized exponents and their universality.

This work only dealt with the effect the thermal bond excitations have on a continuous phase transition. It is, however, more common for a covalent liquid to undergo an abrupt or first-order phase transition to a solid or a gaseous phase. Thus, one may again invoke a lattice model such as the q-state Potts model (with $q > 4$ in two dimensions and $q > 2$ in three dimensions) to investigate the effect the thermal bond excitations have on a first-order transition point. Whether it has any weakening effect on the latent heat, and whether the effect is significant enough to change the order of a weak first-order phase transition, are the kind of questions one may wish to consider. More generally, we believe that in the lattice models of covalently bonded structures such as the supercooled liquids [7], polymers [5], lattice protein [6], etc., the thermalization of bonds can provide for a natural bond-breaking mechanism when suitably employed. It should also be pointed out that in order to keep the treatment simple, we have treated covalent bonds as independent, two-level systems obeying classical Maxwell-Boltzmann statistics. However, this does not rule out other forms. In particular, a Fermi-Dirac distribution for the bond electrons, is another plausible candidate. However, our main results are not likely to change no matter which statistics is used here, because the present work clearly shows that the bond thermalization preserves the expected renormalization of the exponents—universality prevails.

VII. SUMMARY

In summary, the method of chemical potentials is extended to systems with temperature-dependent annealed bond impurity by using it to calculate the critical behavior of the thermalized-bond Ising model in three dimensions. The critical exponents are found by a finite-size scaling analysis. It is a matter of interest to note that the TBIM exponents are consistent with the renormalization relations due to Fisher despite the temperature-dependent bond dilution, thus preserving the universality of the renormalized exponents.

---

[1] M. F. Thorpe and D. Beeman, Phys. Rev. B **14**, 188 (1976).
[2] D. C. Rapaport, J. Phys. C **5**, 1830 (1972).
[3] L. Syozi, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 1, p. 269.
[4] K. Binder and A. P. Young, Rev. Mod. Phys. **58**, 801 (1986).
[5] A. Bakk and J. S. Høye, Physica A **323**, 504 (2003).
[6] K. F. Lau and K. A. Dill, Macromolecules **22**, 3986 (1989); A. Irbäck and E. Sandelin, J. Chem. Phys. **108**, 2245 (1998).
[7] C. T. Moynihan and C. A. Angell, J. Non-Cryst. Solids **274**, 131 (2000); C. A. Angell and C. T. Moynihan, Metall. Mater. Trans. B **31B**, 587 (2000).
[8] A preliminary account of this work appears in S. Davatolhagh, L. Separdar, and M. Barati, Proceedings of the 13th Condensed Matter Meeting (Institute for Advanced Stuides in Basic Sciences Press, Zanjan-Iran, 2007).
[9] See, e.g., D. Stauffer and A. Aharony, *Introduction to Percolation Theory* (Taylor & Francis, London, 1994).
[10] M. E. Fisher, Phys. Rev. **176**, 257 (1968).
[11] S. Davatolhagh and B. R. Patton, Phys. Rev. B **64**, 224206 (2001).
[12] M. F. Thorpe (private communication).
[13] E. Ising, Z. Phys. **31**, 253 (1925).
[14] L. Onsager, Phys. Rev. **65**, 117 (1944).

[15] See, e.g., D. P. Landau and K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics*, 2nd ed. (Cambridge University Press, Cambridge, 2005).

[16] H. G. Ballesteros, L. A. Fernandez, V. Martin-Mayor, G. Parisi, and J. J. Ruiz-Lorenzo, J. Phys. A **32**, 1 (1999).

[17] See, e.g., *Finite-Size Scaling and Numerical Simulations of Statistical Systems*, edited by V. Privman (World Scientific, Singapore, 1990).

[18] K. Binder, Phys. Rev. Lett. **47**, 693 (1981); Z. Phys. B: Condens. Matter **43**, 119 (1981).

[19] A. M. Ferrenberg and D. P. Landau, Phys. Rev. B **44**, 5081 (1991).

[20] M. E. Fisher, J. Math. Phys. **5**, 944 (1964).

[21] See, e.g., L. P. Kadanoff *et al.*, Rev. Mod. Phys. **39**, 395 (1967).