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# Critical behavior of the two-dimensional thermalized bond Ising model

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ABSTRACT

A suitably modified Wolff single-cluster Monte Carlo simulation has been performed to investigate the critical behavior of a two-dimensional Ising model with *temperature-dependent* annealed bond dilution, also known as the thermalized bond Ising model, which is intended to simulate the thermal excitations of electronic bond degrees of freedom as in covalently bonded network liquids. A finite-size scaling analysis of the susceptibility and the fourth-order cumulant, results in a reliable estimation of the critical exponents in the thermodynamic limit. The exponents are found to be consistent with those predicted by the Fisher renormalization relations, despite the well known violations of the renormalization relations when approximate methods such as real space renormalization group are employed to investigate two-dimensional Ising model with annealed bond dilution, and the temperature variation of the bond concentration in thermalized bond model system.

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## 1. Introduction

The lattice models with annealed disorder are among the interesting cases in the study of critical phenomena. A variety of annealed disorder models have been considered by Thorpe and Beeman [1], among others [2–5], in which the concentration of disorder is kept constant with the temperature. The disorder is said to be annealed in the sense that any relaxation time associated with the defects is much shorter than the observation or the experimental time-scale such that the system is able to further minimize its free energy by choosing optimal spacial arrangements of the disorder variables. Thus, the whole system, including the disorder, is allowed to come into complete thermal equilibrium at any given temperature. The case of annealed bond disorder can be simply modeled by an extra variable in the middle of the bond, also known as bond decoration [2]. An important aspect of bond decoration is that, because the bond variable interacts only with its two neighboring sites, its local environment is like a 1d chain, as a result of which the bond variable can be traced out and the annealed system can be mapped onto an equivalent regular (pure) one with a rescaled temperature [1–3]. The annealed bond variable, however, may lead to a so-called renormalization of the critical exponents [4,6]. According to the Fisher renormalization relations, if the specific heat exponent of the regular system $\alpha_r$ is positive, the annealed critical exponents are 'renormalized', still satisfying the usual scaling laws. If $\alpha_r$ is negative, however, the annealed exponents are the same as the regular ones. The applications of approximate techniques such as real space renormalization group to bond-diluted Ising square lattice, however, are found to violate the Fisher renormalization relations [7].

Here, we would like to model and investigate the effect of thermally induced electronic bond excitations on the critical behavior of a covalent liquid at its critical point, which is generally believed to be in the universality class of the lattice gas model or equivalently the ferromagnetic Ising model. In the case of the Thermalized Bond Ising Model (TBIM) each covalent bond linking a nearest neighbor pair of atoms is allowed thermally induced electronic transitions between bonding and anti-bonding electronic states [8]. Hence, it can be regarded as containing annealed bond defects with a temperature-dependent concentration. Every bond at every instant is characterized by a binary coupling constant $J_{ij} = 0, J_0$, such that

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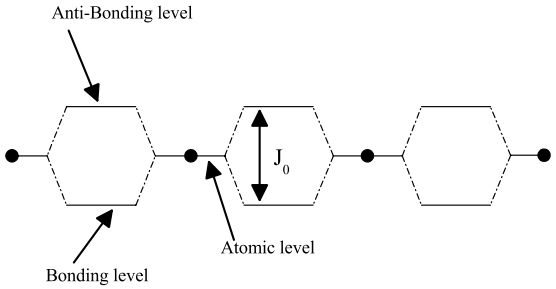


**Fig. 1.** Schematic illustration of the electronic energy states of the covalent bonds linking a chain of atoms. The energy gap between the bonding and the antibonding level is denoted by $J_0$.

zero corresponds to a broken bond (anti-bonding electronic state), while $J_0$ 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 freedom to lower its free energy by choosing optimal arrangements of the bond variables, and to reach complete thermal equilibrium with the lattice or the structural variables. We believe that the thermalized bond Ising model [8], 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 lattice polymers and lattice protein, as they can provide for a natural bond breaking mechanism in lattice models of covalent structures. A rather similar model, known as the bond-lattice excitation model, has been introduced and studied in the context of supercooled glass-forming liquids [9].

In the following, we focus on TBIM in two dimensions, and rely on the statistics obtained from Monte Carlo (MC) simulations of finite lattices in order to investigate the critical behavior of the system. The 3d TBIM was investigated in Ref. [8] using the method of chemical potential and the grand canonical ensemble [1]. In this paper, however, the critical behavior of 2d TBIM is investigated using the canonical ensemble Monte Carlo simulations of the model system by a suitably modified Wolff single-cluster algorithm. 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 the TBIM in two dimensions.

The rest of this paper is organized as follows. In Section 2, the thermalized bond Ising model is reviewed in more detail. A suitably modified Wolff single-cluster algorithm is applied in Section 3 to compute the thermodynamic properties of interest for finite-size 2d TBIM lattices. In Section 4 a finite-size scaling analysis is carried out to obtain the critical exponents of 2$d$ TBIM in the thermodynamic limit. Our main results are discussed in Section 5, and the paper is concluded with a summary.

## 2. Model system

Denoting the thermally averaged bond concentration by $p$, $(1-p)$ therefore represents the concentration of broken bonds due to thermal excitations. To keep the analysis simple, the covalent bonds are treated as independent two-level systems with energy gap $J_0$, as sketched in Fig. 1, obeying classical statistics, and in thermal equilibrium with the lattice at temperature $T$. Thus, the ratio of the bonds to the broken bonds in equilibrium, is given by the ratio of the corresponding Boltzmann factors $p/(1-p) = \exp(\beta J_0)$, or

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

where $\beta = 1/k_B T$ is the reciprocal temperature and $k_B$ is the Boltzmann constant [8]. 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 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 form of statistics is used for the treatment of the bonds. As can be seen in Fig. 2, the bond concentration $p$ decreases from unity at absolute zero to one-half at infinitely large temperatures, while the concentration of broken bonds $(1-p)$ increases from zero at the absolute zero to one-half at infinite temperature. It must be noted that the bond concentration $p$ remains above the bond percolation threshold for the square lattice, $p_c = 1/2$ [10], at all temperatures: as bonds percolate, 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 the thermalized-bond model system is of the form

$$P_{J_{ij}}(\beta) = p\ \delta_{J_{ij},J_0} + (1-p)\ \delta_{J_{ij},0} \tag{2}$$

where $p$ is given by Eq. (1), and $\delta$ denotes the Kronecker delta [8]. $J_{ij} = J_0$ is the coupling associated with a bond, and $J_{ij} = 0$ 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

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