Wetting transition in the McCoy-Wu model

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The wetting transition is studied in the McCoy-Wu model in which the random bonds are perfectly correlated in the direction parallel to the walls. It is shown that the wetting transition is the first order. The disorder of the random bond does not round the transition contrary to many known systems. For a fixed surface field, the wetting transition temperature is sample dependent, even if the size of the system goes to infinity.

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I. INTRODUCTION

The disorder is ubiquitous in nature. The influence of quenched disorder on the phase transition has been of great interest in the theoretical and experimental physics [1]. The disorder can cause various effects. In the three-dimensional Ising model, the quenched disorder leads to a new critical point with exponents different from the pure ones [2,3]. In the McCoy-Wu model, the disorder causes the Griffiths-McCoy singularity, where some thermodynamic quantities are singular in a range of temperature, rather than just at the critical point [4,5]. The disorder may suppress the first order phase transition. It is shown rigorously that in 2D quenched randomness results in the suppression of first-order phase transitions in the random-field Ising model, random bond Potts model and spin glasses [6]. The disorder can also drive the critical point to be lack of self-averaging, for example, the ratio between the variation and the average of magnetization remains finite as the system size goes to infinity in the site-diluted d = 3 Ising model [7].

In this paper I show two novel effects of the disorder in the wetting transition in the McCoy-Wu model. Firstly the phase transition is the first order even with the disorder. Secondly for a fixed surface field the wetting transition temperature is sample dependent and does not converge to a limit as the size of the system goes to infinity. To our knowledge, in the all previous studied disordered systems the phase transition temperature converges to a limit as the system size goes to infinity, i.e. in the thermodynamic limit.

The wetting transition in the random bond systems has been studied extensively and intensively [8,9]. However the random bonds are not correlated. In the McCoy-Wu Ising model the random bonds are perfectly correlated in a direction [10].

For the Ising model without disorder, if two opposite external field are applied on the boundary, there exist a wetting transition. In the Abraham’s exact solution, it is shown that at the wetting transition the average distance of the interface (separating the predominantly + and −phases) from the boundary diverges smoothly to infinity [12]. Forgacs, Svrtak and Privman obtained another exact solution that the wetting transition is the first order if one adds a line defect in the middle of the system [13]. In a sense, the McCoy-Wu model can be regarded as an Ising model being added many line defects. The wetting transition in the McCoy-Wu model is an extension of the model Forgacs et. al proposed. However the wetting transition in this model show some unusual properties mentioned above.

We solve the model on large size lattices with Bond Propagation Algorithm (BPA) [20–22]. This algorithm is very accurate and can be carried out on very large lattices. In our numerical calculation, the largest size of the lattice is 200^2 × 200. We can calculate the specific heat and the magnetization of each site with relative accuracy less than 10^{-6}. The results show that the wetting transition is the first order. The interface is pinned at the boundary at the nonwet phase and jumps to a position far form the boundary. The jumping takes place at the pseudo-phase-transition temperature, at which the specific heat is maximal. We solved the model on the lattices with different sizes. We find that the distribution width of the pseudo-phase-transition temperature does not decrease as the size of lattice increases. We show that the distribution width of the phase transition temperature remains finite even if the size of lattice goes to infinity, i.e. in the thermodynamic limit.

The paper is arranged as follows. In Sec. II, we define the model and discuss the algorithm of BPA. In Sec. III, the distribution of the pseudo-phase-transition temperature on the finite size lattices is shown. In Sec. IV, the mechanism of the wetting transition is discussed. We find that the thermodynamics at the wet phase is dominated by the group with most adjacent line defects and at the nonwet phase by the bonds near the boundary. Therefore the transition temperature is sample dependent. In Sec. V, we propose two semi-random models to improve our conclusions further. Sec. VI is a discussion.

II. THE MODEL

The McCoy-Wu model with surface fields is sketched in Fig. 1(a), in which all the vertical bonds are the same, while the horizontal bonds are identical to each other.
within each column but differ from column to column. Consider a set of spins \( \sigma(n, m) = \pm 1 \) located at points \((n, m)\) of the planar square lattice such that \(1 \leq n \leq N, 1 \leq m \leq M\). The energy of a configuration \(\{\sigma\}\) of spins is given by

\[
E = -J \sum_{m=1}^{M-1} \sum_{n=1}^{N} \sigma(n, m)\sigma(n, m + 1)
- J \sum_{n=1}^{M} \sum_{m=1}^{N-1} a_n \sigma(n, m)\sigma(n + 1, m)
- \sum_{m=1}^{M} [H_1 \sigma(1,m) + H_N \sigma(N,m)]
\]

(1)

where \(H_1\) and \(H_N\) are the surface field. The left and right boundary are often referred to competing walls. The random bond \(a_n\) is the horizontal bond in the \(n\)th column. In this paper we use the binary bond disorder probability distribution:

\[
p(a_n) = \frac{1}{2} \delta(a_n - 1) + \delta(a_n - 0.9).
\]

(2)

The horizontal bonds are either strong \(J\) or weak \(0.9J\) with half probability. We use this special case to show the general conclusions. The normalized canonical probability is \(P(\sigma) = Z^{-1} \exp(-\beta E)\) where \(Z\) is the canonical partition function. We set \(J/k_B = 1\), where \(k_B\) is the Boltzmann constant. We solve this model on finite size lattices with bond propagation algorithm, which is very efficient and accurate and can be carried out on very large size lattices \([20, 22]\). In the model, the top and bottom boundary are open because of our algorithm.

We consider two types of boundary conditions as done in Abraham’s model \([12]\):

\[
+-: \quad H_N = 1, \quad H_1 = -a_0 \quad \quad +:+: \quad H_N = 1, \quad H_1 = a_0
\]

(3)

where \(a_0 > 0\). Throughout this paper, we set \(a_0 = 0.4\) in the numerical calculation. Under the boundary condition \(+ -\), there is an interface. Then the interfacial free energy (density) is defined

\[
f = -\frac{k_B T}{M} \ln \frac{Z_{+-}}{Z_{++}}
\]

(4)

Fixing surface field \(a_0\), there is a wetting transition for the boundary condition \(+ -\) as the temperature changes. Correspondingly, we define the interfacial internal energy density by \(u = \frac{\partial (\beta f)}{\partial \beta}\) and the interfacial specific heat by \(c = \frac{\partial u}{\partial T}\).

With the bond propagation algorithm with a surface filed \([22]\), we calculate the interfacial free energy, specific heat, and magnetization \(\langle \sigma_{n,m} \rangle\), which is the thermodynamic average of the spin at the site \((n, m)\) on finite size lattices. In the numerical calculation, we set \(M = N^2\) and study the lattices with size \(M \times N\) and \(N = 80, 120, 160, 200\) respectively. For all these quantities the accuracy can reach \(10^{-6}\) at least.

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**FIG. 1.** (a) The sketch of the McCoy-Wu model with surface fields. The surface fields act on the spins at the first and last column. The horizontal segments in different colors represent random horizontal bonds. (b) The interfacial specific heat for four samples with \(N = 120\). (c) The magnetization profile \(\langle \sigma(n, M/2) \rangle\) for the four samples in (b). (d) The interface positions VS temperature for the samples in (b).

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**III. THE DISTRIBUTION OF THE PSEUDO-PHASE-TRANSITION TEMPERATURE AND THE MAXIMUM OF THE SPECIFIC HEAT**

Figure 1(b) shows the interfacial specific heat for four typical samples with \(L = 120\). We call a given configuration of disorder \(\{a_n\}\) a sample. All the samples, especially sample 2 and 3, show very narrow and high peaks. The pseudo-transition temperatures \(T_w\), at which a maximum in the specific heat of the sample occurs, are different for sample to sample. Moreover, the difference between the pseudo-transition temperatures for any two samples is much larger than their half widths of the specific heat peaks.

The jumping of the interface can be seen directly in the Fig. 1(d), which shows the interface’s positions VS temperature for the four samples. The rounding of the jumping is due to the finite size effect. The temperatures at the jump of the interface’s position coincide with those at the maximal interfacial specific heat in Fig. 1(b). The interface position is obtained from the magnetization profile, which are shown in Fig. 1(c). At \(T = 2.083\), the systems are at the wet phase for the four samples, where the interfaces are far from the left wall. At \(T = 1.852\), the systems are at the nonwet phase, where the interfaces are pinned at the left wall.

To show the statistical properties of transition, we calculated 200 configurations of disorder for each size \(N = 80, 120, 160, 200\). For each sample, we obtained the pseudo-transition temperatures \(T_w\), maximal specific heat \(c_m\) and the half width of the specific heat peak \(\tau\) \([24]\). Fig. 2 shows the spreading of \(T_w, c_m, \tau\) directly.
There are two obvious trends as the lattice size increases. The first is that in average the specific heat peaks increase with the size as shown in Fig. 2(a). The second is that that in average the half widths of the specific heat decrease with the size as shown in Fig. 2(b). These features indicate that the phase transition is first order. However, there is another unusual feature. The pseudo-phase-transition temperatures are distributed in a wide range. The distribution width $\sigma_{T_w}(N)$ is $5.0(4) \times 10^{-2}, 4.7(3) \times 10^{-2}, 5.0(4) \times 10^{-2}, 5.2(4) \times 10^{-2}$ for $N = 80, 120, 160, 200$ respectively. It does not converge to zero as the size increases. If this feature remains as the system size increase to infinity, the wetting transition temperature is sample dependent.

Of course we can not guarantee the validity of the extrapolating to the infinite size since our calculations are carried on the finite size lattices. However we prove that the wetting transition temperature is sample dependent in the thermodynamic limit.

IV. COMPETITION BETWEEN THE GROUPS OF ADJACENT LINE DEFECTS

With $\alpha_n = 1$ for all $n$, the system is known as the Abraham’s model [12], which is solved exactly by Abraham. It undergoes a continuous wetting transition at a temperature $T_w$ below the critical temperature $T_c$ of the 2D Ising model. For $T_w < T < T_c$, the interface is depinned from the left wall and the interfacial free energy is obtained by Onsager [25]

$$f_O = 2k_BT(K - K^*)$$

where $K = J/k_BT$ and $\exp(-2K^*) = \tanh 2K$. For $T < T_w$, the interface is pinned by the the left wall and the interfacial free energy is obtained by Abraham [12]

$$f_A = -kB_T\ln(A - \sqrt{A^2 - 1})$$

with $A = \frac{1}{2}(B + \frac{1}{B}) + 1 - \frac{1}{2}(S + \frac{1}{S})$, and $B = \tanh K^* \coth K$, $S = \frac{\cosh 2K - \cosh 2\alpha_0 K}{\sinh 2K}$.

Forgacs et al. found that the wetting transition is the first order if one adds a line defect in the middle of the system [13], say the $N_{th}$ column bonds with $a_{N_k} < 1$ and $N_1 < N$. In the wetting phase, the interface is pinned at the line defect. The interfacial free energy is given by

$$f_{FSP} = -kB_T\ln| - x - \sqrt{x^2 - 1}|$$

where $x = \frac{c^* - c_2\sqrt{c^2 - 4}}{c^*_2 - 4}$ with $c = \cosh 2K, s = \sinh 2K, c^* = \cosh 2K^*, c_2 = \cosh 2(K_2^* - K^*), s_2 = \sinh 2(K_2^* - K^*)$ and $K_2 = a_{N_1}K$. Simply speaking, this first order wetting transition is a competition of two interface situations, one for the interface pinned at the left wall and one for the interface pinned at the line defect. For $T_1 < T < T_c$, where $T_1$ is the first order wetting transition temperature [13], it has $f_{FSP} < f_A, f_O$, the interface is pinned at the defect line and the free energy is given by $f_{FSP}$. On the contrary, for $T < T_1$, it has $f_{FSP} > f_A$, then the interface is pinned at the left wall and the interfacial free energy is given by $f_A$.
In a sense the present model is an extension of Forgacs et al.’s idea. We add many line defects into the system randomly. In order to understand the random bond case shown in Fig. 1 and 2, we calculate the following four cases with size $N = 120$

\[
\begin{align*}
S2 : & \quad a_n = 0.9 \quad \text{for} \quad n = 60, 61; \\
S4 : & \quad a_n = 0.9 \quad \text{for} \quad n = 59, 60, 61, 62. \\
D24 : & \quad a_n = 0.9 \quad \text{for} \quad n = 40, 41, 79, 80, 81, 82; \\
D42 : & \quad a_n = 0.9 \quad \text{for} \quad n = 39, 40, 41, 42, 80, 81;
\end{align*}
\]

and $a_n = 1.0$ for other $n$. In the case $S2$, there is a group of two adjacent line defects located about $n = 60$. In the case $S4$, there is a group of four adjacent line defects located about $n = 60$. In the case $D24$, both the two groups of adjacent line defects are present, one group is located about $n = 40$ and another one about $n = 80$. In the case $D42$, the two groups swap their positions.

We will show that the group of four adjacent line defects dominates the transition in the $D42$ and $D24$ cases. The first clue is $T_w$. As shown in Fig. 3(a), for the $S2$ case, it has $T_w \approx 2.022$ and for the $S4$ case, it has $T_w \approx 1.970$. For both the cases $D24$ and 42, it has $T_w \approx 1.970$.

The second clue is the interfacial free energy. In the Fig. 3(b), the solid line in black and red is given by Eq. (9) and (10) respectively. The solid line in green (and blue) is the interfacial free energy for $S2$ (and $S4$) case with $a_0 = 1$, in which the interface is always pinned at the adjacent line defects \[13\]. The interfacial free energy for $S2$ is divided into two parts by the pseudo-transition point (marked by the blue arrow): it coincides with the solid line in red for $T < T_w$ and with the green line for $T > T_w$. The interfacial free energy for both the cases $S24$ and $S42$ coincide with that one for $S4$. They are divided into two parts by the pseudo-transition point marked by the red arrow: they coincide with the solid line in red for $T < T_w$ and with the solid line in blue for $T > T_w$.

The third clue is the interface position. At the temperature $T = 1.961$, the system in the nonwet phase for both $D24$ and $D42$ and the interface is pinned at the left wall as shown in Fig. 3(c). At the temperature $T = 2.083$, the system is in the wet phase and the interface is pinned at the group of four adjacent line defects. For $D24$ and $D42$, the interface is pinned at about $n = 80$ and $n = 40$ respectively, where the group of four adjacent line defects is located. Fig. 3(d) shows that above the transition temperature the interface is always pinned at the group of four adjacent line defects and below the transition temperature the interface is pinned at the left wall.

Enlighten by this example, we know that the phase transition is the competition among the interface locations. See the Fig. 3(b), the interfacial free energy of the group of four adjacent line defects in $S4$ case is always lower than that of the two adjacent line defects in the $S2$ case above the transition temperature. In both $D24$ and $D42$ cases, the interfaces are pinned at the group of four adjacent line defects. Below the transition temperature the interfacial free energy at the left wall is lower, then the interfaces jump from the group of four line defects to the left wall.

V. TWO SEMI-RANDOM MODELS

Extending the above discussion, one can conjecture that the wetting transition in the random bond model Eq. (1) should be the competition among interface locations similarly. From the renormalization group theory, the adjacent line defects can be dealt as a single effective line defect. The more the adjacent line defects are, the weaker the bond of the effective line defect is. Therefore in the wet phase, the interface should be pinned at the group with the most adjacent line defects far from the left wall. The situations in the four samples shown in Fig. 1(b), (c), (d) are indeed so (see Fig 1(d)).

For an infinite system, one can find the group with an arbitrarily large number of adjacent line defects. The interfacial free energy for such a group should be given by that the interface is pinned at the group of infinite adjacent line defects. It can be obtained from the onusager exact result \[24\] and is given by $f = 2k_B T(0.9 K - K^*)$, where $0.9 K$ is the weak bond.

At the nonwet phase, the interface is pinned at the left wall. See Fig. 1(c) and 3(c), the absolute value of magnetization is depressed notably only near the left wall. Just these depression induce the interfacial free energy. The depression decays rapidly as the distance from the left wall increases, so the influence of the bonds to the interfacial free energy should decay rapidly similarly. Then the free energy of interface pinned at the left wall should spread in a range. This range will not decreases as the size of the system increases because it is only related to the configuration of the disorder near the left wall and not related to the disorder at other regions.

The intersection between the interfacial free energies at the left wall and at the group with the most adjacent line defects determines the phase transition temperature. As discussed above the spreading of the interfacial free energy at the left wall will not decreases even as the size of the system goes to infinity, so the distribution width $\delta T_w$ will not converge to be zero as the usual phase transition in the disordered systems.

To test this argument, we design two semi-random lattices. In the case SR1, we set that $a_n = 1.0$ for $n \leq 20$ and $a_n$ is random for $n > 20$. In the case SR2, we set that $a_n$ is random for $n \leq 20$, $a_n = 0.9$ for $N/2 < n \leq N/2 + 20$, and $a_n = 1.0$ for other $n$.

In the SR1 case, the interfacial free energy at the left wall is fixed. As the system size increases, the maximum of the number of the adjacent line defects increases. Then the interfacial free energy at the line defects will converge to a limit. Therefore the distribution width $\delta T_w(N)$ will decrease as the system size $N$ increases. In Fig. 4(a), the
distribution width $\delta T_w(N)$ is $2.0(1) \times 10^{-2}, 1.7(1) \times 10^{-2}, 1.6(1) \times 10^{-2}, 1.4(1) \times 10^{-2}$ for $N = 80, 120, 160, 200$ respectively. In the SR2 case, the interfacial free energy at the left wall will not converge as the system size increase, so the distribution width $\delta T_w(N)$ will not decrease. The numerical results for SR2 is shown in Fig. 4(b), in which the distribution width $\delta T_w(N)$ is $2.8(2) \times 10^{-2}, 3.4(2) \times 10^{-2}, 3.1(2) \times 10^{-2}, 3.2(2) \times 10^{-2}$ for $N = 80, 120, 160, 200$ respectively. The numerical results are consistent to our expectation.

VI. DISCUSSION

Why is the present model is unusual? The wetting transition in it is only related to the left wall and the group of the most adjacent line defects. For the usual phase transition, the free energy is related to the whole system. As first argued by Brout, we may divide the system into a large subsystems (much larger than the correlation length). If we assume that the coupling between neighboring subsystems is negligible, then the value of any density of an extensive quantity over the whole sample is equal to the average of the (independent) values of this quantity over the subsystems. The pseudo-phase-transition temperature fluctuates from sample to sample due to the finite-size effects. However as the system size goes to infinity, the pseudo-phase-transition temperatures should converge to a limit $T_C(\infty)$. Obviously, the present model can not be divided into two similar subsystems in the horizontal direction. If the left and right wall are separated, there is no wetting transition.

The groups of adjacent line defects are the so-called rare regions. Near the critical point of the McCoy-Wu model, the rare regions dominate the phase transition. In this wetting transition, the situation is more extreme. Only the largest rare region matters.

Because the McCoy-Wu model is equivalent to the one-dimensional random transverse field quantum Ising model, it is expected that a similar wetting transition exists in the one-dimensional random transverse field quantum Ising model. The quantum Ising chains with boundary fields has been studied by Campastrini et. al. There is a magnet-to-kink transition similar to the critical wetting transition in the Abraham model. The random quantum Ising chain with boundary filed is the quantum version of the wetting transition in the McCoy-Wu model.

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