Quantum phase transition of the transverse-field quantum Ising model on scale-free networks

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Abstract

I investigate the quantum phase transition of the transverse-field quantum Ising model in which nearest neighbors are defined according to the connectivity of scale-free networks. Using a continuous-time quantum Monte Carlo simulation method and the finite-size scaling analysis, I identify the quantum critical point and study its scaling characteristics. For the degree exponent $\lambda = 6$, I obtain results that are consistent with the mean-field theory. For $\lambda = 4.5$ and 4, however, the results suggest that the quantum critical point belongs to a non-mean-field universality class. The deviation from the mean-field theory becomes more pronounced for smaller $\lambda$.

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I. INTRODUCTION

Scale-free networks are a kind of complex networks whose degree distribution follows a power law, $P(k) \propto k^{-\lambda}$. They are observed in a variety of natural and man-made systems, such as the World Wide Web, the Internet, human social networks, ecological networks, and power grids. Due to their unique and remarkable characteristics, they have been a subject of many recent research works. In particular, when the nodes are occupied with dynamic objects that are interacting with nearest neighbors, the presence of hub nodes with a lot of connections tends to enhance the correlations substantially. For example, Ising models on scale-free networks have been widely studied and the properties of their magnetic phase transition have been well analyzed.

Recently, there have been efforts to extend the Ising model on scale-free networks to include quantum effects. As a magnetic field $\Delta$ is introduced in the direction perpendicular to the Ising spin direction, it gives rise to quantum fluctuations which tend to weaken the spin-spin correlation of the system. This effect is best manifested by the fact that the critical temperature $T_c$ decreases monotonically as $\Delta$ increases. If $T_c$ vanishes at a finite transverse field $\Delta_c$, this is a quantum critical point, at which rich and interesting phenomena of the quantum phase transition are observed. In general, the quantum critical point belongs to a different universality class from that of the classical critical point. In some cases, however, both kinds of critical points may belong to the same universality class. Most notably, if the dimensionality of the classical critical point is greater than or equal to the upper critical dimension, both the classical and quantum phase transitions are of the mean-field type.

The quantum critical point of the transverse-field quantum Ising model has been studied in various structures including the globally coupled network, Watts-Strogatz small-world networks, the Bethe lattice, and the Sierpinski carpet. One of the important properties of the quantum critical point is the dynamic critical exponent $z$. This quantity determines how the temporal dimension should scale compared to the spatial dimensions, in order to keep the action invariant under renormalization. In particular, it is known that $z = 1$ for the transverse-field Ising model in any integer dimensions. This theorem also applies to more complex systems such as Watts-Strogatz small-world networks whose quantum critical point belongs to the mean-field universality class.
upper critical dimension in this case is four and therefore is an integer. However, in other systems such as a fractal studied in Ref. 15, \( z \) may differ from one.

The transverse-field Ising model on scale-free networks is even more intriguing in the sense that the universality class of its classical critical point depends on the degree exponent \( \lambda \). \[3, 4, 7, 8\] For \( \lambda > 5 \), the finite-temperature phase transition is of the mean-field type. If \( 3 < \lambda < 5 \), however, the critical point does not belong to the mean-field universality class and its critical exponents depend on \( \lambda \). For \( \lambda < 3 \), there is no phase transition at finite temperatures. The critical behavior of the finite-temperature phase transition has been studied before, both in the mean-field, \[7\] and non-mean-field regimes, \[8\]. In those works, it was confirmed that the presence of the transverse magnetic field does not affect the universality class of the critical point, as far as \( \Delta < \Delta_c \) and \( T_c > 0 \). Although the quantum critical point of the model has not been studied, there are a few predictions we can make. First, the quantum critical point for \( \lambda > 5 \) is expected to be in the mean-field universality class, since the dimensionality of the classical critical point is already above the upper critical dimension. The properties of the quantum critical point for \( \lambda < 5 \) is, however, far from obvious. Yet we can think of two possible scenarios: Either the addition of the infinite temporal dimension would drive the critical point to the mean-field class, or it will still belong to a non-mean-field universality class, although it will be most likely different from that of the classical counterpart.

In this paper, I will study the behavior of the quantum critical point of the transverse quantum Ising model, for both cases in which \( \lambda > 5 \) and \( \lambda < 5 \). In order to investigate the properties of the system near zero temperature, I will employ a continuous-time quantum Monte Carlo simulation method. \[16\]. Performing a finite-size scaling analysis, I may identify the critical transverse field \( \Delta_c \) and test the critical exponents against the known values of the mean-field theory.

II. MODEL

The Hamiltonian of the transverse-field quantum Ising model is given by

\[
H = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z + \Delta \sum_i \sigma_i^x
\]  

(1)
where $\sigma^x_i$ and $\sigma^z_i$ are Pauli matrices representing the $x$ and $z$ components of the spin at site $i$. I will consider only the ferromagnetic case ($J > 0$), and use the unit in which $J = 1$ for simplicity. The first summation in the above equation runs over all nearest neighbor pairs, which are defined as the nodes that are connected in the scale-free network under consideration. Note that the second term does not commute with the first, hence causes quantum fluctuations to the energy eigenstates of the classical model.

The ensemble of the scale-free networks used in this research is defined by three parameters: the degree exponent $\lambda$, the total number of nodes $N$, and the average degree $k_{av}$. More specifically, the degree distribution probability is given by

$$P(k) = \begin{cases} 0, & \text{if } k < k_{\text{min}} \\ P_0, & \text{if } k = k_{\text{min}} \\ ck^{-\lambda}, & \text{if } k > k_{\text{min}}, \end{cases}$$

where $k_{\text{min}}$, $P_0$, and $c$ are determined by the conditions

$$\sum_{k=1}^{\infty} P(k) = 1 \quad \text{and} \quad \sum_{k=1}^{\infty} kP(k) = k_{av}. \quad (3)$$

Note that $k_{\text{min}}$ plays the role of the lower cutoff in the degree. In order to ensure that the average total number of connections is $Nk_{av}/2$, I have introduced a continuous parameter $P_0$, which is not greater than $ck_{\text{min}}^{-\lambda}$, but is as close as possible to it. Once the degree distribution is determined, actual networks are generated in the following way. First of all, each node is allotted "connecting arms", the number of which is probabilistically chosen according to the above distribution. Note that the total number of arms in the whole network is not fixed in this method, but its average will approach $Nk_{av}$ as the number of networks in the ensemble becomes large enough. Now, a random node is chosen as a seed of a cluster. Then we pick another random node unconnected to the cluster and join one of its arms to a randomly chosen unconnected arm in the cluster. This process is repeated until all nodes are connected to form one single cluster. Finally, all unconnected arms are randomly paired, without doubly connecting any two nodes.[17]

This model is most easily analyzed using the Suzuki-Trotter decomposition method.[18] If one writes the action as an integral in the imaginary time using the standard procedure, the temporal segments of world lines may be thought of as interacting with the nearest neighbors in the time direction. As usual, this allows us to map the quantum model into a
classical model with an additional dimension. The size of the imaginary time dimension is inversely proportional to $T$, and therefore becomes infinitely large at the quantum critical point. In order to deal with the infinite size of the system, I will resort to the finite-size scaling method for both spatial and temporal dimensions.

III. RESULTS

I developed a quantum Monte Carlo simulation program based on the Swendesen-Wang cluster algorithm. In order to handle the imaginary time, I adopted a continuous-time method\cite{16}. The critical transverse field $\Delta_c$ may be obtained using the fourth-order Binder cumulant\cite{19, 20}

$$U = 1 - \frac{\langle m^4 \rangle}{3 \langle m^2 \rangle^2} ,$$

where $m$ is the magnetization per spin, and $\langle \cdots \rangle$ and $[\cdots]$ denote the thermal and network average, respectively. In the vicinity of the quantum critical point, this quantity obeys a finite-size scaling form

$$U = \tilde{U} \left( (\Delta - \Delta_c) N^{1/\nu'}, T N^{z'/d'} \right).$$

Since the size of a scale-free network is characterized by the total number of nodes $N$, instead of a length, I will denote our critical exponents with primed letters to distinguish them from the usual exponents $\nu$ and $z$. In a system with $d$ spatial dimensions, they are related by $\nu' = d\nu$ and $z' = z/d$. Since the upper critical dimension of the quantum phase transition in our model is three, the mean-field values of these exponents become $\nu' = 3/2$ and $z' = 1/3$. If $\Delta = \Delta_c$, the first argument in Eq. (5) is zero and $\tilde{U}$ becomes a simple single-parameter scaling function. Since $\tilde{U}$ has a peak, I can identify $\Delta_c$ by demanding that the maximum of $\tilde{U}$ as a function of the second argument should not depend on the system size $N$. Then with an appropriate choice of $z'$, the curves for all system sizes should collapse onto a single curve within the scaling regime.

A. $\lambda > 5$ (mean-field regime)

Let us first investigate the case where $\lambda = 6$, for which the quantum critical point is expected to be in the mean-field class. The results of the Binder cumulant calculations are shown in Fig. 1. Since the middle plot shows the smallest dependence of the maximum of
FIG. 1. (Color online) The Binder cumulant $U$ as a function of $T$ at (a) $\Delta = 14.2$, (b) 14.35, and (c) 14.5 for $\lambda = 6$ and $k_{av} = 7$. Different symbols are used to represent different system sizes, as denoted in the plot. The dotted lines show the position of the mean-field value of the universal maximum $U^* \approx 0.270521$. The errorbars are omitted because they are negligible.

FIG. 2. (Color online) Data plots for $\lambda = 6$ and $k_{av} = 7$: (a) $U$ and (b) $\tilde{s}$ vs $TN^{1/3}$ at $\Delta = 14.35$. (c) $\tilde{s}$ vs $(\Delta - \Delta_c)N^{1/\nu'}$ at $TN^{1/3} = 5.848035$. I assumed $\Delta_c = 14.35$ and used the mean-field critical exponents $\nu' = 3/2$ and $\beta = 1/2$. The dotted line represents the mean-field universal maximum $U^* \approx 0.270521$.

$U$ on the system size $N$, I obtain $\Delta_c = 14.35 \pm 0.15$. Note that the maximum of $U$ is a little greater than the mean-field universal value $U^* \approx 0.270521$, but fairly close to it. Figure 2(a) shows a plot of the Binder cumulant $U$ as a function of $TN^{z'}$ using the mean-field dynamic critical exponent $z' = 1/3$. There are two things that call for special attention. First, the data for different system sizes collapse onto a single curve for small $T$, but they start to fall apart near $TN^{1/3} \sim 7$. This is the usual artifact of the finite-size effect. Note that this may also account for the fact that our maximum overshoot the universal value, albeit only by a little. Second, it is not easy to accurately estimate $z'$ because we cannot use the data with $TN^{1/3} \gtrsim 7$, especially those near the peak. Simply using the data in
the low temperature scaling regime does not provide us enough information to determine $z'$ decisively. Performing simulations with bigger systems may solve this problem, but it turns out to be very strenuous and time consuming with the current simulation method.

One of the ways to overcome this difficulty is to use a quantity that is not sensitive to the value of $z'$. Below, I will use a method that has been suggested in Ref. 12. Instead of magnetization $m$, they have used the instantaneous magnetization per spin

$$s = \frac{1}{N} \left[ \left\langle \sum_i \sigma_i^z(t) \right\rangle \right],$$

(6)
taken at a given time $t$. Due to the homogeneity in time, this quantity is actually independent of $t$. The advantage of using $s$ lies in the fact that it saturates to a finite expectation value of the ground state as $T \to 0$. As a consequence, it becomes independent of $T$ at low temperatures. Therefore, at low $T$, it is expected to follow a simple single-parameter scaling form

$$s = N^{-\beta/\nu'} \tilde{s} \left( (\Delta - \Delta_c) N^{1/\nu'} \right),$$

(7)

which does not require prior knowledge of $z'$. One can clearly see in Fig. 2(b) that indeed $\tilde{s}$ becomes independent of $T$ at low temperatures. Picking a point in the flat region and sweeping $\Delta$ in the vicinity of $\Delta_c$, one may test the scaling property described in Eq. (7). Below, I will use $TN^{1/3} = 5.848035$, which falls inside the flat region of the plot in Fig. 2(b).

Figure 2(c) shows a plot of the scaling function $\tilde{s} \left( (\Delta - \Delta_c) N^{1/\nu'} \right)$ where $TN^{1/3}$ is kept constant. I have used $\Delta_c = 14.35$ and the the mean-field critical exponents $\beta = 1/2$ and $\nu' = 3/2$. It appears that all data for different system sizes collapse nicely onto a single curve in the vicinity of the critical point, and it supports the previous conjecture that the quantum critical point for $\lambda = 6$ indeed belongs to the mean-field universality class.

B. $3 \leq \lambda < 5$ (non-mean-field regime)

If $3 < \lambda < 5$, the classical critical point is not in the mean-field universality class, and the critical exponents are given by

$$\alpha = \frac{\lambda - 5}{\lambda - 3}, \quad \beta = \frac{1}{\lambda - 3}, \quad \gamma = 1, \quad \nu' = \frac{\lambda - 1}{\lambda - 3}.$$ 

(8)

However, the value of these exponents for the quantum critical point are yet to be discovered. One interesting possibility is that the addition of the infinite temporal dimension to the
classical critical point might drive the quantum critical point to the mean-field universality class. In order to test it, a similar analysis as in the previous subsection has been performed for $\lambda = 4.5$. The results are presented in Fig. 3. First, we obtain the critical transverse field $\Delta_c = 16.3 \pm 0.1$ by carefully observing the maximum of $U$ as shown in Fig. 3(a). This is greater than the value obtained for $\lambda = 6$, which is a natural consequence of the fact that as $\lambda$ decreases, there are more hub nodes with very high degree, which can enhance correlations even more. The estimation of the dynamic critical exponent from $\tilde{s}$ is again inconclusive, and one cannot rule out the mean-field value $z' = 1/3$. [Fig. 3(a)] Notice, however, that the maximum of the Binder cumulant, which is estimated as $0.21 \pm 0.01$, is conspicuously smaller than the mean-field universal value. Just as I did for $\lambda = 6$, I will now assume the mean-field critical exponents and check its validity against the simulation data at a point.
in the flat region of $\tilde{s}$. One can clearly see that scaling function $\tilde{s}$ plotted in Fig. 3(b) does not quite collapse into a single curve, when the mean-field critical exponents are used.

Things get even worse for $\lambda = 4$. The critical transverse field in this case is estimated as $\Delta_c = 18.8 \pm 0.1$. As shown in Fig. 4(a), the Binder cumulant maximum is $0.15 \pm 0.01$, which is almost only one half of the universal value. One may also easily see that the scaling plot of $\tilde{s}$ using the mean-field critical exponents fail quite miserably. [Fig. 4(b)] We thus come to the conclusion that the quantum critical point does not belong to the mean-field universality class for $\lambda = 4.5$ and 4, and the deviation becomes more pronounced for the smaller value of $\lambda$.

C. $\lambda < 3$

In the classical Ising model with $\lambda < 3$, there is no ferromagnetic-paramagnetic phase transition and the system is ordered at all temperatures. How the quantum model is different from the classical counterpart is an interesting question in its own right. Especially, the possibility of a phase transition by the transverse magnetic field is quite intriguing. Yet this subject is beyond the scope of the current research, and it will be discussed elsewhere.

IV. SUMMARY AND DISCUSSIONS

In this paper, I examined the quantum critical point of the transverse-field quantum Ising model on scale-free networks. In order to check whether the quantum critical point belongs to the mean-field universality class, I assumed the mean-field values for the critical exponents and tested their validity. Using the continuous-time quantum Monte Carlo simulation method, I calculated the Binder cumulant $U$ and the instantaneous magnetization $s$, both for $\lambda > 5$ and $3 < \lambda < 5$. From the observation of the maximum of $U$, the critical transverse field $\Delta_c$ was obtained. While the estimation of the dynamic critical exponent $z'$ was problematic due to the finite-size effect, the use of the scaling behavior of $\tilde{s}$ allowed us to test the validity of the mean-field critical exponents. For $\lambda = 6$, I could confirm that the quantum critical point is in the mean-field universality class. For $\lambda = 4.5$ and 4, however, the peak value of $U$ was substantially smaller than the mean-field universal maximum and the finite-size scaling behavior was clearly incompatible with the mean-field theory. We also
noted that the deviation from the mean-field theory becomes more conspicuous for smaller \( \lambda \).

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