QMC study of the chiral Heisenberg Gross-Neveu universality class

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Abstract. We investigate a quantum criticality of an antiferromagnetic phase transition in the Hubbard model on a square lattice with a $d$-wave pairing field by large-scale auxiliary-field quantum Monte Carlo simulations. Since the $d$-wave pairing field induces Dirac cones in the non-interacting single-particle spectrum, the quantum criticality should correspond to the chiral Heisenberg universality class in terms of the Gross-Neveu theory, which is the same as those expected in the Hubbard model on the honeycomb lattice, despite the unit cells being different (e.g., they contain one and two sites, respectively). We show that both the two phase transitions, expected to occur on the square and on the honeycomb lattices, indeed have the same quantum criticality. We also argue that details of the models, i.e., the way of counting the total number $N$ of fermion components and the anisotropy of the Dirac cones, do not change the critical exponents.

1. Introduction

Accurate calculation of critical exponents of phase transitions to identify universality classes is one of the major issues in computational physics, especially for Monte Carlo simulations. There are many successful examples found in the studies of classical [1, 2, 3] and quantum [4, 5, 6, 7] spin systems. Recently, another family of the quantum phase transitions that involve fermionic degrees of freedom has attracted much attention in this context because sign-problem-free quantum Monte Carlo (QMC) methods as well as modern analytical techniques such as functional renormalization-group approach are applicable to investigate the fermionic quantum criticality.

The most well-studied example would be the Hubbard model on the honeycomb lattice (hereinafter referred to as the honeycomb lattice model), of which the antiferromagnetic (AF) semimetal(SM)-insulator phase transition was examined from the view point of the Mott...
transition [8, 9, 10, 11, 12]. Later, since the connection between the effective theory of the honeycomb lattice model and the Gross-Neveu (GN) model in high-energy physics was pointed out [13, 14], the focus has been shifted from the model-dependent quantum phase transitions to the universal nature of the quantum criticality because the existence of the universality classes for the interacting Dirac fermions had been well formulated by the GN model [15]. For the AF transition, which corresponds to the chiral-Heisenberg universality class in terms of the GN theory, reliable estimations of the critical exponents have been obtained employing the honeycomb lattice model [16, 17, 18] and the Hubbard model on the square lattice with $\pi$-flux [19, 20] (referred to as the $\pi$-flux model in the following).

In this paper, we revisit the chiral-Heisenberg universality class using another lattice model, the square-lattice Hubbard model with a $d$-wave pairing field [21], which we call the d-SC model. If we consider brick-wall square lattices [22, 23], it can be seen that the honeycomb lattice model and the $\pi$-flux model are smoothly connected to each other even without assuming the universality class. On the other hand, the present d-SC model is quite different from these two models as discussed in the next section, while the low-energy effective model is the same for all the three models, i.e., the GN model breaking the $SU(2)$ symmetry. Therefore, the examination of the critical exponents for the d-SC model is expected to serve as an independent and nontrivial check of the previous estimations.

2. Model and method
The Hamiltonian of the d-SC model reads as follows:

$$H = H_{\text{BCS}} + H_U,$$

where

$$H_{\text{BCS}} = \sum_{\langle i,j \rangle} \left\{ \left( c_{i\uparrow}^\dagger \ c_{i\downarrow} \right) \left( \begin{array}{cc} -t & \Delta_{ij} \\ \Delta_{ij}^* & \Delta \end{array} \right) \left( \begin{array}{c} c_{j\uparrow}^\dagger \\ c_{j\downarrow} \end{array} \right) + \text{h.c.} \right\}$$

and

$$H_U = U \sum_i n_{i\uparrow} n_{i\downarrow}.$$

Here, $t$ is the transfer integral between the nearest sites, chosen as an energy unit ($t=1$), and $\Delta_{ij}$ denotes the $d$-wave pairing field with its amplitude being uniform, i.e., $|\Delta_{ij}| = \Delta$. We consider the model at half filling. The Hubbard interaction denoted by $U$ triggers the AF transition at the strong coupling regime, where the mass gap opens. In the noninteracting limit ($U = 0$) for finite $\Delta$, the ground-state is the SM phase having four Dirac points at the Fermi level in the momentum space. This state is different from those of the honeycomb lattice or the $\pi$-flux model which has the two Dirac cones. In addition, the unit cell of the d-SC model has one site, whereas the honeycomb lattice or the $\pi$-flux model has two sublattices. Thus, at the level of the lattice model, they are indeed different. However, in the low energy continuum limit, these models should be described by the GN model with the same number of fermion components, $N = 8$, with the spin degrees of freedom considered. This is why we expect the same universality class for the different lattice models. Furthermore, the d-SC model has another unique feature that an anisotropy of the Dirac cone can be tuned by changing $\Delta$. It is isotropic as in the case of the honeycomb lattice or the $\pi$-flux model only at $\Delta = 1$, and otherwise the velocity at the Dirac point depends on the direction in the momentum space. Taking advantage of this feature, we also study whether the anisotropy affects the quantum criticality.

Since the square lattice is bipartite and the particle-hole symmetry holds at half filling, we investigate the d-SC model by the auxiliary-field QMC method without facing the negative-sign
Dirac points at \((\pi,\pi)\) boundary conditions for the isotropic \((\Delta = 1)\). Simulations are performed on finite-size clusters of \(L\) and chose \(\Delta\) with \(M\) \(\tau\) where \(\Delta\) is projection time and is divided by the Suzuki-Trotter decomposition into \(\tau/M = \Delta\tau\) with \(M\) being integer. We set \(\tau\) to be proportional to linear dimension of the square lattice \(L\) and chose \(\Delta\tau = 0.1\) to reduce the systematic errors compared to the stochastic errors. The simulations are performed on finite-size clusters of \(L=8, 12, 16, 20, 24, 32, 40\) with periodic boundary conditions for the isotropic \((\Delta = 1.0)\) and anisotropic \((\Delta = 0.5)\) cases. Therefore, the Dirac points at \((\pi,\pi)\) and other symmetry equivalent momenta are allowed in all these clusters.

### 3. Results

We calculate the spin structure factor \(S(k) = L^{-2} \sum_{i,j} e^{i k (r_i - r_j)} \langle S_i \cdot S_j \rangle\) in the standard notation and the quasiparticle weight \(Z(U,L) = D_s(U,L)/D_s(0,L)\) estimated from the equal-time Green’s function \(D_s(U,L) = L^{-2} \sum_i \langle c_i^\dagger c_i \rangle\) at the maximum distance \([27]\). Then, the obtained data are analyzed; by a conventional method to first extrapolate the results to the thermodynamics limit \((1/L \rightarrow 0)\); by a more sophisticated method called the crossing-point analysis \([6]\); and by a rather involved method of data collapse.

The critical point \(U_c\) dividing the SM and the AF insulator is in principle obtained as the value of \(U\) at which the order parameter sets in. In Figs. 1(a) and 1(b), we plot the staggered magnetization, that is, the AF order parameter, calculated as \(m_s = \lim_{1/L \rightarrow 0} \sqrt{S(\pi,\pi)}/L\) as a function of \(U\). From these plots, the critical points and the critical exponent \(\beta\) are estimated by fitting with the critical behavior \(m_s \sim (U/U_c - 1)^{\beta}\) as \(U_c = 7.8(2) [5.74(1)]\) and \(\beta = 0.7(2) [0.63(2)]\) for \(\Delta = 1.0\) \((0.5)\). Since the statistical errors are larger for the strong-coupling region, the error bars for \(\Delta = 1.0\) are large, which makes it difficult to safely conclude that the exponents are consistent between \(\Delta = 1.0\) and 0.5 or between the d-SC model and the honeycomb lattice or the \(\pi\)-flux model. We also find large error bars for the quasiparticle weight as shown in Figs. 1(c) and 1(d). In addition, it is not obvious which fitting function is suited both for the SM and the insulating phase to extrapolate \(Z(U,L)\) to the thermodynamics limit \(1/L = 0\) at each \(U\).

We are thus not able to plot the quasiparticle weight as the function of \(U\), although the rough estimates of \(U_c\) from Figs. 1(c) and 1(d) seem consistent with those obtained from \(m_s\).

Based on the previous studies of the honeycomb lattice model \([10, 11, 12]\), it is anticipated that the conventional method to deal directly with the order parameters discussed above tends to overestimate the critical points. Furthermore, it is not trivial to take into account a possible contribution from correction terms to the simplest scaling ansatz. Thus, here.
we take a more sophisticated approach. First, we calculate the correlation ratio defined as \( R_{mn}(U, L) = 1 - \frac{\langle \mathbf{S}(\mathbf{K}+b/L) \rangle}{\mathbf{S}(\mathbf{K})} \), where \( \mathbf{K} = (\pi, \pi) \) is the AF ordering momentum, and \( b \) is the smallest reciprocal-lattice vector [28]. Like the Binder ratio, this quantity has the advantage of being size-independent at the critical point when the correction terms are negligible. Conversely, we can know that the effects of the correction are non-negligible if we observe that curves of \( R_{mn}(U, L) \) as the function of \( U \) cross at different points of \( L \) for various \( L \). Since such a drift is indeed noticed in our results, we employ the crossing-point analysis: we determine the crossing points \( U^x(L, rL) \) at which the curves of \( L \) and \( rL \) cross and extrapolate them to \( 1/L = 0 \) assuming the critical behavior of \( U^x(L, rL) = U_c + cL^{-(\omega+1/\nu)} \), where \( c \) is a constant, \( \omega \) is an effective correction exponent, and \( \nu \) is the correlation-length exponent [6]. It turns out that this analysis yields reasonable estimates of the critical points and the exponents to confirm the expected universal nature of the quantum criticality [21]. Additionally, in Fig. 2, we show that \( R^x(L, rL) \), the values of \( R_{mn}(U, L) \) at the crossing points, also follow a similar universal behavior of \( R^x(L, rL) = R_{c}^x + dL^{-\omega} \) with \( R_{c}^x=0.33(10) \) \([0.40(7)]\) and \( \omega =0.43(13) \) \([0.46(11)]\) for \( \Delta=1.0 \) \((0.5)\).

Finally, we show details of the data-collapse fits of \( R_{mn}(U, L) \) in Fig. 3, where we collapse the data of \( L_{\text{min}} \leq L \leq L_{\text{max}}(= 40) \) changing \( L_{\text{min}} \). Since we utilize the simplest form of the finite-size-scaling ansatz without the correction terms, \( R_{mn}(U, L) = f_R(uL^{1/\nu}) \), where \( f_R(\cdot) \) denotes the scaling function, and \( u = (U - U_c)/U_c \), the non-negligible contribution from the correction terms are evident for smaller \( L_{\text{min}} \). The values of \( U_c \) and \( \nu \) estimated from the collapse fits for

**Figure 2.** \( 1/L \)-extrapolation of crossing points of \( R_{mn}(U, L) \) for (a) \( \Delta = 1.0 \) and (b) \( \Delta = 0.5 \).

**Figure 3.** Data-collapse fits of \( R_{mn}(U, L) \) for various \( L_{\text{min}} \); (a)-(d) \( \Delta = 1.0 \) and (e)-(f) \( \Delta = 0.5 \).
each \( L_{\text{min}} \) can be extrapolated to the thermodynamics limit by plotting the data as a function of \( 1/L_{\text{min}} \), and the results are consistent with those obtained by the crossing-point analysis within the error bars. Readers interested in more details of the critical exponents and comparison with analytical results are referred to Ref. [21].

4. Summary
We have investigated the square-lattice Hubbard model with a \( d \)-wave pairing field by large-scale auxiliary-field quantum Monte Carlo simulations with the aim to revisit the chiral-Heisenberg universality class. The critical exponents estimated by several ways are overall consistent with each other and also with those obtained in the previous studies of the Hubbard model on the honeycomb lattice and on the square lattice with \( \pi \)-flux, suggesting that all these models belong to the same chiral-Heisenberg universality class described by the Gross-Neveu model with the same number of the fermion components \( N = 8 \). We also confirm that the anisotropy of the Dirac cones does not affect the quantum criticality.

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