Quantum Monte Carlo Study on the Spin-1/2 Honeycomb Heisenberg Model with Mixing Antiferromagnetic and Ferromagnetic Interactions in External Magnetic Fields

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The continuous imaginary-time quantum Monte Carlo method with the worm update algorithm is applied to explore the ground state properties of the spin-1/2 Heisenberg model with antiferromagnetic (AF) coupling $J > 0$ and ferromagnetic (F) coupling $J' < 0$ along zigzag and armchair directions, respectively, on honeycomb lattice. It is found that by enhancing the F coupling $J'$ between zigzag AF chains, the system is smoothly crossover from one-dimensional zigzag spin chains to a two-dimensional magnetic ordered state. In absence of an external field, the system is in a stripe order phase. In presence of uniform and staggered fields, the uniform and staggered out-of-plane magnetizations appear while the stripe order keeps in xy plane, and a second-order quantum phase transition (QPT) at a critical staggered field is observed. The critical exponents of correlation length for QPTs induced by a staggered field for the cases with $J' > 0$, $J' < 0$ and $J < 0$, $J' > 0$ are obtained to be $\nu = 0.677(2)$ and $0.693(0)$, respectively, indicating that both cases belong to O(3) universality. The scaling behavior in a staggered field is analyzed, and the ground state phase diagrams in the plane of coupling ratio and staggered field are presented for two cases. The temperature dependence of susceptibility and specific heat of both systems in external magnetic fields is also discussed.

PACS numbers: 75.10.Jm, 75.40.Mg, 05.30.-d, 02.70.-c

I. INTRODUCTION

Since the spin-1/2 antiferromagnetic (AF) Heisenberg model is believed to be capable of describing the undoped precursors of high temperature superconducting cuprates, it has attracted intensive attention in condensed matter and statistical physics. Through extensive explorations both theoretically and experimentally in the past decades, many properties of this model have been exposed, and a great deal of advances have been achieved. However, as the complexity occurs intrinsically in many-body systems, there still remain a lot of ambiguities remaining to be investigated. For instance, by searching for exotic states of matter or studying quantum phase transitions (QPTs), people usually invoke this model with different interactions on various lattices as prototypes. To name but a few, quantum spin liquid is thought to exist in spin-1/2 AF Heisenberg models on lattices with geometrical frustrations, but its nature is still under active debate [1-8]; whether exotic phase transitions beyond the traditional Landau-Ginzburg-Wilson framework [9] exist or not were also discussed by introducing more complex interactions or by tuning the spatial anisotropy in coupling strength; and so on.

It has been shown that the spin-1/2 AF Heisenberg system on square lattice displays Néel order in ground state with the staggered magnetic moment per site $m_1 \approx 0.3075$ by quantum Monte Carlo (QMC) [10] and $m_2 \approx 0.3034$ by the spin-wave theory [11], while the one-dimensional (1D) AF spin chain is magnetically disordered with gapless excitations. The spin-1/2 AF Heisenberg chain is critical according to the exact result of Bethe ansatz or the results of, e.g., spin-wave theory with random phase approximation [12] and mean-field approaches [13], which is also confirmed by using the multi-chain mean-field method associated with SSE Monte Carlo algorithm [14]. The experiments on quasi-1D spin-1/2 AF chains such as Sr$_2$CuO$_3$ and Ca$_2$CuO$_3$ [15] trigger an interesting question: how does the AF long-range order in two-dimensional (2D) lattice (like square lattice) in ground state develop from coupled 1D spin chains with increasing inter-chain interactions? There are a number of studies to tackle this issue and determine the critical inter-chain coupling ratio $R_c = J_\perp/J$: the spin wave theory gives $R_c = 0.034$ [16], one-loop renormalization group analysis on an effectively spatially anisotropic nonlinear sigma model yields $R_c = 0.047$ [17], the series expansion numerical techniques bound $R_c$ upper to 0.02 [18]; whereas some self-consistent calculations [19] and exact diagonalization [20] predict it as high as 0.15 and 0.1 $\sim$ 0.2, respectively. Therefore, this question still calls on further more accurate explorations.

Alternatively, one can also study 2D anisotropic Heisenberg AF models with different bond interactions to observe crossover behaviors by tuning the bond interactions. For instance, such attempts were made on honeycomb lattice with the dimer pairs pinned on the armchair bonds by using the methods of tensor renormalization group [21] and QMC [22], where it is found that there is a QPT of classical O(3) universality from a disordered dimer phase to quantum Néel order at a critical inter-dimer AF interaction. In our previous work [23], we replaced the inter-dimer AF couplings by ferromagnetic (F) interactions along zigzag directions on honey-
comb lattice, and found that there is also a phase transition from a dimerized phase to a stripe phase. The scaling behaviors were analyzed, and the coupling parameters of two compounds were estimated by comparing our QMC calculated results.

In contrast to this previous work [23], where the interactions are supposed to be F along zigzag direction and AF along armchair direction, for the completeness of the study, in this paper we shall consider the spin-1/2 Heisenberg model with mixing AF interaction \( J \) along zigzag direction and F interaction \( J' \) along armchair direction on honeycomb lattice (Fig. 1) in magnetic fields. It should be remarked here that the present system (we refer to Case A later) is quite different from that considered in Ref. [23] (we refer to Case B later), and the two systems cannot be transformed mutually by simply using a unitary transformation. This observation is confirmed by our QMC studies, where we observe that a small inter-chain F interaction could make the 1D disordered state smoothly crossover to a 2D spin ordered state. In presence of uniform and staggered fields, the uniform and staggered magnetizations in \( \hat{z} \) direction appear while a stripe or ferromagnetic (F) rungs in \( m_2 \sim h \) curves [24], no zero magnetization plateau exists for both cases with \( J' = -J \) owing to the appearance of spin order. The phase diagram in a staggered field is also presented.

This paper is organized as follows. In Sec. II, we shall give the model Hamiltonian, calculational method and definitions of several physical quantities; the crossover behavior from 1D to 2D in absence of a magnetic field is discussed in Sec. III; the magnetization in presence of uniform and staggered external magnetic fields is presented in Sec. IV; the finite-size scaling analysis is given in Sec. V; Sec. VI shows the phase diagrams of two systems for a comparison; the temperature dependence of specific heat and susceptibility in magnetic fields is discussed in Sec. VII; and finally, a summary is given.

II. MODEL, METHOD AND DEFINITIONS

A. Model

By using the continuous imaginary time QMC with worm update algorithm, we shall study the spin-1/2 Heisenberg model on honeycomb lattice with coupling constants, \( h \) and \( h_s \), are the external uniform and staggered magnetic fields, respectively. We define the coupling ratio \( \alpha = \frac{J}{J'} \) for a later use. For convenience, we also mark the armchair and zigzag directions by \( x \) and \( y \) directions, respectively. The lattice size is \( N = L_x \times L_y \) with \( L_{x(y)} \) the length of \( x \) (\( y \)) direction.

From Sec. IV on, we shall also make comparisons between the present system and the system with \( J < 0 \) and \( J' > 0 \) in the previous work [23] in a staggered field, where the coupling ratio is defined as \( \alpha_2 = \frac{J}{J'} \).

B. Method

We shall use the continuous imaginary time QMC with worm update algorithm to study the system under consideration. This algorithm expands the partition function of system as a summation of path integrals with continuous loops under Fork states representation with \( \{S_{ij}^z\} \) as the basis in interaction picture by

\[
Z = Tr(e^{-\beta H}) = Tr(e^{-\beta H_0}) = \sum_{n=0}^{\infty} \int_0^{\beta} d\tau_n... \int_0^{\tau_1} d\tau_1(H_{1n}H_{2(n-1)1}...H_{11}),
\]

where \( \beta = \frac{1}{k_B T} \), the inverse temperature, acting as the length of the imaginary time in the simulation, \( k_B = 1 \) is the Boltzmann constant, \( H_0 \) stands for the interaction between spins along the \( z \) direction

\[
H_0 = J \sum_{(i,j)_{ZZ}} S_i^z S_j^z + J' \sum_{(i,j)_{AM}} S_i^z S_j^z - h \sum_{i=1}^{N} S_i^z - h_s \sum_{i=1}^{N} \langle -1 \rangle^k S_i^z \tag{3}
\]

and \( H_I \) is the hopping term in the \( xy \) plane of spin space

\[
H_I = J \sum_{(i,j)_{ZZ}} (S_i^+ S_j^- + S_i^- S_j^+) + J' \sum_{(i,j)_{AM}} (S_i^+ S_j^- + S_i^- S_j^+). \tag{4}
\]

In this framework, the object sampled during executing the algorithm is each term in Eq. (2), and the integration
is concretized to several configurations with special localizations of off-diagonal terms in the imaginary time axis. In lattice space and imaginary time coordination, such configurations are graphed as multiple worldlines with only continuous loops. By introducing the kink pair $S^+_{ir}$, $S^-_{ir}$, called a worm, a partition function configuration is switched into a Green function configuration. The hopping of the worm ends ($S^+_{ir}$ or $S^-_{ir}$) along the imaginary time or real space direction realizes the Green function configuration. The hopping of the worm ends (armchair bonds, otherwise) shows the size extrapolation of $\Omega$ [25].

The big difference between the partition function configuration and the Green function configuration is that the latter has an extra discontinuous worldline, i.e., the worm. This method extends the sampling space and could be used to calculate the winding number directly.

C. Definitions

Before we proceed further, we first give the definitions of relevant physical quantities that will be used later. As the calculations based on the QMC method are usually associated with the finite-size systems, where the spin O(3) rotational symmetry remains in a finite system, we should determine the order parameters by calculating the corresponding square values combined with a size extrapolation. The staggered magnetization per site is defined via the following expression

$$\langle m^z_i \rangle = \langle \frac{1}{N} \sum_j (\langle S^+_j \rangle^2 + \langle S^-_j \rangle^2 + \langle S^z_j \rangle^2) \rangle$$

$$= 3 \langle \frac{1}{N} \sum_j (\langle S^z_j \rangle^2) \rangle$$

$$= \frac{3}{2} \sum_0^N f(r) < S^+_0 S^-_r >,$$

where $f(r) = 1$ if $S^+_0$ and $S^-_r$ are both in the even or odd zigzag (armchair) bonds, otherwise $f(r) = -1$.

The staggered magnetization per site in the xy plane in presence of uniform or staggered field can be studied through

$$\langle m^z_i \rangle = \frac{N}{N^2} \sum_{n_1=0,n_2=0}^{N-N} f(r)(\langle S^z_{n_1} S^z_{n_2} + S^z_{n_1} S^z_{n_2} \rangle)$$

$$= \frac{1}{N} \sum_0^N f(r) \langle S^z_0 S^z_r \rangle.$$

The uniform magnetization per site is defined by

$$m_z = \langle \frac{1}{N^2} \sum_{i=1}^N \int_0^\theta d\tau_1 \int_0^\theta d\tau_2 S^z_{ir_1} S^z_{jr_2} \rangle$$

$$- \langle \int_0^\theta d\tau_1 S^z_{ir_1} \rangle \langle \int_0^\theta d\tau_2 S^z_{jr_2} \rangle.$$

The uniform magnetic susceptibility is given by

$$\chi_u = \frac{1}{N^2} \sum_{i,j} \int_0^\theta \int_0^\theta d\tau_1 d\tau_2 S^z_{ir_1} S^z_{jr_2} \rangle$$

$$- \langle \int_0^\theta d\tau_1 S^z_{ir_1} \rangle \langle \int_0^\theta d\tau_2 S^z_{jr_2} \rangle.$$

The staggered magnetization per site in z direction will be calculated by

$$m^z_i = \langle \frac{1}{N^2} \sum_{i,j} (\langle S^z_{ir_1} \rangle^2 - \langle S^z_{jr_1} \rangle^2) \rangle.$$

The spin stiffness $\rho$ is obtained by the fluctuation of winding numbers [32]

$$\rho^2 = \frac{\delta^2 \Omega}{\delta \Phi^2} = \frac{1}{\beta} \langle W^2 \rangle$$

$$= \frac{1}{\beta} \langle \langle (N^+ - N^-)^2 \rangle \rangle.$$

where $\Omega = \langle W \rangle$ is the free energy, $\Phi$, $W$, $N^+$ and $N^-$ are twisted angle at the boundaries, the winding number, number of sites for spin $\uparrow$ hopping along the positive and negative $\theta$ directions, respectively. It is noted that the spin stiffness $\rho$ in Eq. (10) has its counterpart in a boson system [26, 27], the superfluid density, which characterizes an off-diagonal long range order.

III. CROSSOVER FROM 1D TO 2D

Now let us consider the crossover behavior from 1D to 2D by altering the coupling ratios of the present system. During the calculations, the coupling ratio is changed to the value as low as $\alpha_1 = -0.010$.

We first take $L_x$ and $L_y$ to be equal and the inverse temperature to be size-dependent $\beta = 2 * \sqrt{N}/J$. Fig. 2(a) shows the size extrapolation of $m^z_i$ versus $1/\sqrt{N}$ for various coupling ratio $\alpha$. It is seen that as the system size increases, $\langle m^z_i \rangle$ first decreases and then increases, leaving a minimum at a finite size for each $\alpha$, and in this case, it shows a non-monotonic behavior, and therefore a size extrapolation is impossible. It is known that the finite size gap in the zigzag chain is $\Delta(L_x) \sim \frac{1}{L_x}$. When energy scales in the two directions are compatible, $\Delta(L_y) \sim \rho_x$, where $\rho_x$ scales the energy in the armchair direction, the system crossovers from 1D to 2D [14], and in this way, the size extrapolation for the order parameter square is meaningful. In order to make a reasonable size extrapolation, we should take $L_y \gg L_x$, for small $|\alpha|$.

We carry out simulations on lattices with $L_x = 8L_\pi$ for $\alpha_1$ from -0.04 to -0.18, where the inverse temperature is taken as $\beta = \sqrt{N}/J$. The size extrapolations to the square root of the total number of lattice sites $N = L_x * L_y$ are shown in Fig. 2(b). It can be observed that $\langle m^z_i \rangle$ decreases almost linearly against $1/\sqrt{N}$. By doing a polynomial fitting of order two to the data for $\alpha = -0.04$, the size extrapolation of $\langle m^z_i \rangle$ gives 0.0100(3), suggesting that the system is magnetically ordered.
where the two curves do not have crossings, implying that under interest.

generated fields on magnetization and susceptibility of the system to be calculated for \( \alpha \) and \( \beta = \sqrt{N}/J \) for (a) and \( \beta = \sqrt{N}/J \) for (b). In (a), \( \langle m^2 \rangle \) exhibits a minimum for every \( \alpha \). When \( L_x \gg L_y \), \( \langle m^2 \rangle \) decreases almost linearly against \( 1/\sqrt{N} \) in (b). The errors that are visible are of order \( 10^{-3} \) and the invisible ones are of \( 10^{-4} \) at least.

In Fig. 2(a), the fitting curves for \( \alpha_1 = -0.02 \) is very close to that for \( \alpha_1 = -0.01 \) till the thermodynamic limit is reached, where the two curves do not have crossings, implying that the system is in a spin ordered state when \( |\alpha_1| \) is larger than 0.01. The result \( \lim_{N \to \infty} \langle m^2 \rangle = 0.0100(3) \) for \( \alpha = -0.04 \), confirms the above observation. Therefore, upon tuning a very small inter-chain F interaction between the AF zigzag spin chains, the system immediately undergoes a crossover from a disordered 1D state to a 2D spin ordered state.

IV. MAGNETIZATION IN MAGNETIC FIELDS

We now consider the effects of external uniform and staggered fields on magnetization and susceptibility of the system under interest.

A. Presence of a uniform field

In the presence of a uniform field \( h \), the uniform magnetization \( m_z \), the staggered magnetization in \( xy \) plane \( m_z^x = \sqrt{\langle m^2 \rangle} \), and the uniform magnetic susceptibility \( \chi_u \), have been calculated for \( \alpha_1 = -0.3 \) on lattices with \( L_x = L_y = 32, 36 \), and \( \beta = 100/J \) for \( L_x = 32 \) and \( 108/J \) for \( L_x = 36 \).

Fig. 3 shows the field dependence of \( m_z \), \( m_z^x \), and \( \chi_u \) for \( \alpha_1 = -0.3 \). One may see that, in a weak field, \( m_z \) increases from zero slowly and goes to saturation when \( h/J \) approaches to 2.0, while \( m_z^x \) enhances from a finite value to a peak and then declines sharply around \( h/J = 2.0 \), and reaches zero when \( h/J > 2.0 \). The susceptibility \( \chi_u \) in the inset displays a sharp peak at \( h/J = 2.0 \), indicating a second-order in-plane phase transition, and being consistent with the observation in magnetic curves. When \( h \) is applied, the \( z \)-component (out of plane component) of magnetic moments begins to develop with the decay of the in-plane \( m_z^x \); when \( h/J \geq 2 \), the system is fully polarized and the transverse component is totally suppressed. We call such a phase before fully polarized the cantile phase, in which \( m_z^x > 0 \), and \( m_z < 0 \).

In contrast, for the system considered in Ref. 23 where \( J < 0 \) and \( J' > 0 \), there is a phase transition at \( J = J' = -0.93 \) from a disorder dimer phase to an ordered stripe phase, where the spin alignments are parallel along the same zigzag line and antiparallel along the armchair direction. \( m_z, \tilde{m}_z \) (the staggered magnetization in \( xy \) plane for the system explored in Ref. 23) and \( \chi \) for the ordered phase look like the ones of this present system. When it is in the dimer phase for \( \alpha_2 = -0.6 \), the zero magnetization plateau appears in \( m_z, \tilde{m}_z \) and \( \chi \). Since the present system has an in-plane long range order \( \langle m_z^x \rangle \neq 0 \) in the ground state, the excitation is gapless with Goldstone bosons, and there is no zero magnetization plateau in the magnetic curve (Fig. 3).

B. Presence of a staggered field

In this subsection, we shall investigate the magnetic curves the present system (we call Case A) and the system discussed in Ref. 23 (we call Case B) in a staggered field \( h_s \) (while keeping \( h = 0 \)). We study the staggered magnetization \( m_s \) (Eq. 9) and the magnetization square in the \( xy \) plane \( \langle m^2 \rangle \) under a field \( h_s \) for \( \alpha_1 = -1.0 \), and \( \langle m^2 \rangle \) for \( \alpha_2 = -1.0 \), respectively. The simulations are performed on lattices with \( L_x = L_y = 30, 36, 42, 48 \), and \( \beta = 100/J(J') \) for \( L_x < 30 \) and \( 3 \times L_x/J(J') \) for \( L_x > 30 \).

Fig. 4 presents the transverse staggered magnetization square \( \langle m^2_\perp \rangle \) and longitudinal staggered magnetization \( m_s^z \) as a function of staggered field \( h_s/J(J') \) of the system for...
while the staggered field \( h_s \) in the present system with coupling ratio \( \alpha_1 = -1.0 \) (Case A) and \( \alpha_2 = -1.0 \) (Case B). Here we take \( L_x = L_y = L \). Most of the data are as accurate as \( 10^{-4} \).

For Case B with \( \alpha_2 = -1.0 \), a staggered field \( h_s/J \) in [0.4145, 0.435] has been applied to the system on lattices \( L_x = L_y = 20, 24, 28, 32, 36, 40, 44 \) and 48 with \( \beta = 100/J \) for \( L_x < 34 \) and \( 3L_x/J > L_x > 34 \). Figs. 5(a) and (c) present the field dependence of \( \rho_s L_x \) and \( \rho_s L_y \), showing that the curves for different lattice sizes do intersect at about 0.424, which must be a critical point. To confirm this, we perform a finite-size scaling (FSS) by making data collapse analysis, as shown in Figs. 5(b) and (d), where all curves fall on a single almost straight line (see below for details).

For Case B with \( \alpha_2 = -1.0 \), we calculate \( \rho_s L_x \) and \( \rho_s L_y \) as function of staggered magnetic field on lattice sizes from \( L_x = 12 \) to \( L_x = 42 \) with \( \beta = 100/J' \) for \( L_x < 34 \) and \( 3L_x/J' > L_x > 34 \), as shown in Figs. 6(a) and (c), from which one may see that there is a crossing point at about 0.495, demonstrating that it may be a quantum critical point. The corresponding data collapses confirm this observation that all curves for different lattice sizes go to a single line [Figs. 6(b) and (d)]. It is also consistent with the vanishing points for \( \langle \hat{n}_z \rangle \) shown in Fig. 4 confirming the second-order QPT triggered by a staggered field. Here we would like to point out that in Ref. 23 we discussed the scaling behaviors of \( \rho_s L_x \) and \( \rho_s L_y \) against the coupling ratio (here \( |\alpha_2| \)), where the QPT occurs at a critical coupling ratio, and the transition induced by the staggered magnetic field is left for our present study.

In the framework of renormalization group, the finite-size scaling plays as an essential role in studying the critical be-

![FIG. 4. (Color online) The transverse staggered magnetization square \( \langle m^2_t \rangle \) and longitudinal staggered magnetization \( m^2_t \) versus the staggered field \( h_s \) in the present system with coupling ratio (a) \( \alpha_1 = -1.0 \) (Case A) and (b) \( \alpha_2 = -1.0 \) (Case B). Here we take \( L_x = L_y = L \). Most of the data are as accurate as \( 10^{-4} \).](image)

![FIG. 5. (Color online) (a) \( \rho_s L_x \) and (c) \( \rho_s L_y \) as function of \( h_s/J \) of the system with coupling ratio \( \alpha_1 = -1.0 \) near the critical point for various lattice sizes \( L_x = 20, 24, 28, 32, 36, 40, 44 \) and 48 ; (b) and (d) are the corresponding data collapses for the finite-size scaling, where the data fall on a line, respectively, giving a critical staggered field \( h_s/J \approx 0.42373(4) \) and an exponent \( \nu = 0.6772(2) \), which indicates that this is an O(3) universality transition. The errors for \( \rho_s \) are mostly of \( 10^{-4} \) and for \( \rho_s \) of \( 10^{-3} \).](image)
behavior near the transition point in finite-size systems [37, 40]. In the vicinity of a critical point, the correlation length $\xi$ is divergent and, as the lattice size obeys $L \leq \xi$, some quantities exhibit power-law divergent behaviors with $\xi$ and could be expressed by a scaling function of the form $Q(t, L) = L^{\nu(z)} g(t L^{1/\nu(z)})$, where $\nu$ is the critical exponent of $Q$ and $z$ of $\xi$, $t$ is the reduced phase transition tuning parameter and $g(x)$ is a smooth function which asymptotically behaves as $g(x) \sim x^{-\nu}$ for $x \to \infty$. Here for $\rho L$, $\nu$ is zero and $t = (h_s - h_{sc})/h_{sc}$.

In Case A, the intersection points for different pairs $[L, L']$, where $L' > L$, shift as $L$ enlarges, and a general scaling function under such conditions with extra corrections to $t L^{1/\nu(z)}$ and $Q(t, L)$ [41] can be taken

$$(1 + c L^{-\omega}) Q(t, L) = g(t L^{1/\nu(z)} + d L^{-\delta}).$$

The following scaling form will be more convenient

$$(1 + c L^{-\omega}) Q(t, L) = a_0 + a_1 t L^{1/\nu(z)} + a_2 (t L^{1/\nu(z)})^2,$$

where $c$, $\omega$, $a_0$, $a_1$ and $a_2$ are constants to be determined. For Case A only the correction $(1 + c L^{-\omega})$ [22] for $\rho_{z}(L_{0})$ are included in the scaling functions.

For Case B, the form $Q(t, L) = L^{x/\nu(z)} g(t L^{1/\nu(z)})$ works very well, and the scaling function is supposed to be polynomial of order two:

$$Q'(t, L) = a_0' + a_1' t L^{1/\nu(z)} + a_2' (t L^{1/\nu(z)})^2,$$

where $a_0'$, $a_1'$, $a_2'$ and $\nu$ are constants independent of $L$. The data are analyzed following the lines in Ref. 35. We take thousands of copies of bootstrap resamplings of the raw data as the fitting data, and prepare the same amount of sets of initial fitting parameters in above functions as the input in fitting procedures, which are based on the nonlinear Levenberg-Marquardt optimization algorithm (LMOA) [36].

Table I. The critical staggered magnetic field $h_{sc}$ and the exponent $\nu$ of correlation length determined from $\rho_{z}(L_{0})$ for the present system (Case A) and the system (Case B) considered in Ref. [23].

|        | Case A | Case B |
|--------|--------|--------|
| $h_{sc}/J(J')$ | $0.4233\,(1)$ | $0.42373\,(4)$ |
| $\rho_{L_{x}}$  | $0.51\,(1)$   | $0.49757\,(4)$ |
| $\rho_{L_{y}}$  | $0.51\,(1)$   | $0.49734\,(8)$ |
| $\nu$           | $0.686\,(3)$  | $0.677\,(2)$   |

For Case A, $h_{s}/J$ in the area of $[0.4230, 0.4245]$ for lattice sizes $L_x = L_y = 32, 36, 40, 44, 48$ are taken in the optimization procedure; while for Case B, all the data in Figs. 6(a) and (c) are included. The corresponding collapsed curves are shown in Figs. 5(b) and (d), and Figs. 6(b) and (d), respectively.

Table I presents the two sets of critical staggered magnetic field $h_{sc}$ and the exponent $\nu$ of correlation length for both cases. The values are determined by the lowest $\chi^2$/DOF [e.g., the weighted sum of squares residual per degree of freedom (DOF)] for each single LMOA fitting. For Case A, it gives $h_{sc}/J = 0.42373(4)$ and $\nu = 0.677(2)$; and for Case B, $h_{sc}/J = 0.49734(7)$ and $\nu = 0.693(0)$. Considering the calculation errors, both cases are close to $\nu = 0.7112(5)$ [42], showing that these QPTs belong to the classical Heisenberg O(3) universality.

VI. PHASE DIAGRAM IN A STAGGERED FIELD

As shown in Fig. 4 when $h_z < h_{sc}$ both systems exhibit a staggered magnetization in $z$ direction and keep the corresponding stripe order in $xy$ plane, that is, $m_z^1 > 0$ and $(m_z^2)(\langle \tilde{n}_z^2 \rangle) > 0$. We coin the so-defined phase for $h_z < h_{sc}$ as the canted phase $I$ for Case A and the canted phase $II$ for Case B. As $h_z > h_{sc}$, only the out-of-plane staggered magnetization remains in both cases, say, $m_z^1 > 0$, and $(m_z^2)(\langle \tilde{n}_z^2 \rangle) = 0$. We call such a phase for $h_z > h_{sc}$ as the Néel phase in a staggered field.

To draw a phase diagram, we inspect various coupling ratios for the two cases, and make use of the transition points in the curves of $m_z^1$, $(m_z^2)$, $(\tilde{n}_z^2)$, and $\rho L$ vs $h_z$ for each $\alpha_1$ or $\alpha_2$, forming the phase boundaries. In doing so, a schematic phase diagram in the plane of $h_z/J(J')$ vs $-\alpha_1(2)$ is thus depicted in Fig. 7.

For Case A, as shown in Fig. 7(a), there are three phases, the stripe phase $I$ (where $m_z^1 = 0$ but $(m_z^2) > 0$), the canted phase $I$, and the Néel phase. The stripe phase $I$ always remains in the absence of a staggered field. When $h_z$ is increasing, the system immediately first enters into the canted phase $I$, and then enters into the Néel phase when $h_z > h_{sc}$.

For Case B, as shown in Fig. 7(b), there are four phases, a dimerized phase, the stripe phase $II$, the canted phase $II$, and the Néel phase. Our previous study [23] shows that in the absence of a magnetic field, there is a phase transition at the
critical point \( \alpha_{2c} \approx -0.93 \) from a dimer phase to a stripe phase II with a nonvanishing \( \langle \tilde{m}^2 \rangle = \frac{1}{2} \langle \tilde{m}^2 \rangle \) but \( m_i^2 = 0 \). When the staggered field is increasing, the system in Case B immediately enters into the Néel phase for \( \alpha < \alpha_{2c} \), while for \( \alpha > \alpha_{2c} \), the system first enters into the canted phase II (where \( m_i^2 > 0 \) and \( \langle \tilde{m}^2 \rangle > 0 \) ), and then enters into the Néel phase \( (m_i^2 > 0 \) but \( \langle \tilde{m}^2 \rangle = 0 \) ) when \( h_i > h_{sc} \).

VII. TEMPERATURE DEPENDENCE OF SUSCEPTIBILITY AND SPECIFIC HEAT IN MAGNETIC FIELDS

In this section, we study the temperature dependence of the susceptibility \( \chi_u \) and specific heat \( C_v \) under different magnetic fields. The results are given in Figs. 8, 9 and 10 respectively.

In subsection IV A, it shows that for \( \alpha_1 = -0.3 \) the system is polarized when \( h/J \geq 2.0 \), and when \( h/J < 2.0 \), the system stays in a canted stripe state with \( m_i^2 > 0 \) and \( m_i > 0 \). In Fig. 8 one may see that for \( h/J < 2.0 \), \( \chi_u \) increases from a finite value with increasing temperature, which becomes larger with the increase of the magnetic field, and after undergoing a maximum it decreases quickly at low temperature; when \( h \) gets higher, the peak is sharper; as \( h \) is close to the critical point, \( \chi_u \) decays almost exponentially. When \( h/J = 2.0 \), \( \chi_u \) diverges as \( T \) decreases. For \( h/J > 2.0 \), \( \chi_u(T) \) is suppressed by the magnetic field, leading to all curves are below those of \( h/J \approx 2.0 \), showing the system enters into a different state. At high temperature, all curves coincide with each other owing to the domination of thermal fluctuations. At low temperature, when the system is partially polarized, \( \chi_u \) is influenced mainly by the transverse quantum fluctuations in \( xy \) plane, and closer to the critical point, stronger the quantum fluctuations and higher \( \chi_u \).

Fig. 8 shows temperature dependence of specific heat \( C_v \) of the system with \( \alpha_i = -0.3 \) under uniform fields. It can be observed that besides a round peak as that for \( h/J > 2.0 \), in the range of 1.4 < \( h/J < 2.0 \), \( C_v \) exhibits a sharp peak at lower temperature \( T_p \), as shown in the inset of Fig. 9. When \( h \) increases, \( T_p \) and \( C_v(T_p) \) decrease. This could be understood in the following way. As indicated in Fig. 1, the spins along the zigzag chain form a continuous antiferromagnetic arrangement, dividing the system into two sublattices and producing two sets of degenerate spin wave spectra: \( \omega_{\alpha k} = f(J, J', S, \gamma_k) \), where \( S \) is the spin on each site, and \( \gamma_k \) is the static structure factor. A uniform field \( h \) would split this overlapping spectra with a shift, \( \omega_{\alpha k}^h = f(J, J', S, \gamma_k) \pm h \), resulting in that two modes of low-lying excitations cause two minima in \( C_v \). The part of \( C_v \) contributed by lower frequency mode increases faster. \( h \) enlarges the difference of the increasing tendency between \( \omega_{\alpha k} \) and \( \omega_{\alpha k}^h \), making \( C_v \) steeper and \( T_p \) smaller for larger \( h < h_i \) at low temperature.

When \( h > h_i \), the system enters into the polarized state, and \( C_v \) versus \( T/J \) exhibit only one round peak at a relatively higher temperature.

In Fig. 10 it depicts the temperature dependence of susceptibility \( \chi_u \) for systems with \( \alpha_1 = -1.0 \) and \( \alpha_2 = -1.0 \) under different staggered magnetic fields, which differ from those in a uniform magnetic field. We showed that a staggered field can induce a quantum phase transition in Sec. V, which eliminates the off-diagonal long range order in the \( xy \) plane at \( h_{sc}/J \approx 0.423 \) for \( \alpha_1 = -1.0 \) and \( h_{sc}/J' \approx 0.5 \) for \( \alpha_2 = -1.0 \). Figs. 10(a) and (b) illustrate that, as \( h_i < h_{sc} \), \( \chi_u \) would start from a non-vanishing value, while as \( h_i \geq h_{sc} \), the susceptibility \( \chi_u \) goes to zero at \( T \rightarrow 0 \), revealing that the system in this situation enters into distinct phases under different staggered magnetic fields, consistent with the observation in
FIG. 10. (Color online) Temperature dependence of susceptibility of the system with (a) inset is the low temperature part. Before the system is polarized, $\chi_{\alpha}$ exhibits an extra peak at low temperature besides the round peak at relatively high temperature. Errors here are of $10^{-3}$.

FIG. 9. (Color online) Temperature dependence of specific heat $C_v$ for the system with $\alpha_1 = -0.3$ under different uniform fields. The inset is the low temperature part. Before the system is polarized, $C_v$ exhibits an extra peak at low temperature besides the round peak at relatively high temperature. Errors here are of $10^{-3}$.

VIII. SUMMARY

The spin-1/2 Heisenberg model with AF and F mixing interactions on honeycomb lattice has been studied by means of the continuous imaginary-time QMC with the worm update algorithm in uniform and staggered magnetic fields. It is found that so long as the F coupling on armchair bonds is tuned on, the system (Case A) is immediately crossover smoothly from 1D disordered AF zigzag spin chains to a stripe ordered 2D phase with $\langle m_z^2 \rangle > 0$. This is in contrast to the system considered in Ref. 23 where the F interactions are presumed on zigzag bonds and AF interactions on armchair bonds. In this latter system (Case B), upon tuning on the F interactions on zigzag bonds, the system is crossover smoothly from a disordered dimerized phase to a stripe ordered 2D phase.

In the presence of uniform or staggered magnetic fields, it is shown that for a given coupling ratio (e.g. $\alpha_1 = -0.3$ in a uniform field, and $\alpha_{1,2} = -1.0$ in a staggered field), with increasing the external magnetic fields, the system enters smoothly into a spin canted phase from a stripe order phase, and then undergoes a QPT into an out-of-plane polarized phase or Néel phase. This is also true for the system in Case B for the coupling ratio beyond a critical value (satisfying $-\alpha_2 > 0.93$). The whole phase diagrams in the plane of coupling ratio and staggered magnetic field for the systems in Case A and Case B are obtained. In Case A, there are three phases, including stripe order phase, canted phase and Néel phase, while in Case B, there are four phases, say, dimerized phase, stripe phase, canted phase and Néel phase.

In addition, by exploring the spin stiffness, the scaling behaviors in a staggered field for both systems are also discussed. The finite-size scaling analysis gives that the exponent $\nu$ of correlation length is $\nu = 0.677(2)$ and $0.693(0)$ for Case A and Case B, respectively, which is very close to $\nu = 0.7112$ of classical Heisenberg $O(3)$ universality, indicating that both systems fall into the $O(3)$ universality. Besides, the scaling functions are different from the two systems.

The temperature dependence of susceptibility $\chi_\alpha$ and specific heat $C_v$ have been studied for the system with $\alpha_1 = -0.3$ under various uniform fields. When the system stays in the canted stripe phase as $hJ < 2.0$, at low temperature the partially polarized spins have a nonzero value of $\chi_\alpha$ in the ground state and a sharp peak of $\chi_\alpha(T)$ appears at low temperature, and meanwhile, the specific heat $C_v$ also presents a sharp peak starting from a vanishing value when $T/J \rightarrow 0$. As $hJ \geq 2.0$, the polarized ferromagnetic state does not display such features because of nondegenerate spin wave spectra which could be separated by the uniform magnetic field. The behaviors of $\chi_\alpha$ versus $T/J(J')$ for $\alpha_1 = -1.0$ and $\alpha_2 = -1.0$ under different staggered fields are consistent with the phase diagram presented in Sec. V.

The present study shows that the competition among mixing interactions, external probes such as staggered magnetic field and temperature as well as the topology of the lattice, altogether, results in more complex phenomena in quantum many-body systems. Our results would also be helpful for further understanding the physical properties and scaling behaviors in 2D magnetic materials with mixing AF and F interactions.

ACKNOWLEDGMENTS

The authors acknowledge W. Li, B. Xin, X. Yan, and Z. C. Wang for helpful discussions. This work was supported in part by the MOST of China (Grant No. 2013CB933401), the NSFC (Grant No. 11474279), and the Strategic Priority Re-
[1] S. Yan, D. A. Huse, and S. R. White, Science 332, 1173 (2011).
[2] S. Depenbrock, I. P. McCulloch, and U. Schollwoeck, Phys. Rev. Lett. 109, 067201 (2012).
[3] T. -H. Han, J. S. Helton, S. Chu, D. G. Nocera, J. A. Rodriguez-Rivera, C. Broholm, Y. S. Lee, Nature 492, 406 (2012).
[4] Y. Iqbal, F. Becca, S. Sorella, and D. Poilblanc, Phys. Rev. B 87, 060405(R) (2013).
[5] Z. Y. Xie, J. Chen, J. F. Yu, X. Kong, B. Normand, and T. Xiang, Phys. Rev. X 4, 011025 (2014).
[6] T. Liu, W. Li, X. Yan, Y. Zhao, and G. Su, Phys. Rev. B 89, 054426 (2014).
[7] T. Liu, W. Li, A. Weichselbaum, J. von Delft, and G. Su, Phys. Rev. B 91, 060403(R) (2015).
[8] T. Liu, W. Li, and G. Su, Phys. Rev. E 94, 032114 (2016).
[9] A. W. Sandvik, Phys. Rev. Lett. 98, 227202 (2007).
[10] K. J. Runge, Phys. Rev. B 45, 7229 (1992); 45, 12292 (1992); N. Trivedi and D. M. Ceperley, Phys. Rev. B 41, 4552 (1990).
[11] T. Oguchi, Phys. Rev. 117, 117 (1960).
[12] N. Majlis, S. Selzer, and G. C. Strinati, Phys. Rev. B 45, 7872 (1992); 48, 957 (1993); H. Rosner, H. Eschrig, R. Hayn, S. -L. Drechsler, and J. Malek, Phys. Rev. B 56, 3402 (1997).
[13] H. J. Schulz, Phys. Rev. Lett. 77, 2790 (1996); Z. Wang, ibid. 78, 126 (1997).
[14] A. W. Sandvik, Phys. Rev. Lett. 83, 3069 (1999).
[15] K. Kojima, M. Larkin, B. Nachumi, Y. Uemura, H. Eisaki, M. Motoyama, S. Uchida, B. Sternlieb, and G. Shirane, Czech. J. Phys. 46 Suppl. S4, 1945 (1996); K. Yamada, J. Wada, S. Hosoya, Y. Endoh, S. Naguchi, S. Kawamura, and K. Okada, Physica C 253, 135 (1995); K. M. Kojima, Y. Fujimoto, M. Larkin, G. Luke, J. Merrin, B. Nachumi, Y. Uemura, N. Motoyama, H. Eisaki, S. Uchida, K. Yamada, Y. Endoh, S. Hosoya, B. Sternlieb, and G. Shirane, Rev. Phys. Rev. Lett. 78, 1787 (1997).
[16] T. Sakai abd M. Takahashi, J. Phys. Soc. Jpn. 58, 3131 (1989).
[17] A. H. Castro Néto and D. Hone, Phys. Rev. Lett. 76, 2165 (1996); D. Hone and A. H. Castro Néto, J. Suppercond. 10, 349 (1997).
[18] I. Affleck, M.P.Gelfand, and R. R. P. Singir, J.Phys. A 27, 7313 (1995).
[19] T. Aoki, J. Phys. Soc. Jpn. 64, 605 (1994).
[20] D. Ihle, C. Schindelin, A. Weisse, and H. Fehske, cond-mat/9904005; A. Parola, S. Sorella, and Q. F. Zhong, Phys. Rev. Lett. 71, 4393 (1993).
[21] W. Li, S.-S. Gong, Y.Zhao and G.Su, Phys. Rev. B 81, 184427 (2010).
[22] F. Jiang and U. Gerber, J. Stat. Mech.: Theory Exp. (2009), P09016.
[23] Y.-Z.Huang, B. Xi, X.Chen, W.Li, Z.-C.Wang, and G.Su, Phys. Rev. E. 93, 062110 (2016).
[24] Y. Zhao, W. Li, B. Xin, S-J. Ran, Y-Y. Zhu, B-W. Wang, S. Gao, and G. Su, EPL. 104, 54009 (2013).
[25] N.V. Prokof’ef , B.V. Svistunov, and I.S. Tupitsyn Sov. Phys.- JETP 87, p. 310 (1998).
[26] M. E. Fisher, M. N. Barber, and D. Jasnow, Phys. Rev. A 8, 1111 (1973).
[27] B. D. Josephson, Phys. Lett. 21, 608 (1966).
[28] B.Xi, S.-J.Hu, J.-Z.Zhao, G.Su, B.Normand and X.-Q.Wang Phys. Rev. B 84, 134407 (2011).
[29] K. Binder, Phys. Rev. Lett. 47, 693 (1981).
[30] K. Binder, Z.Phys.B: Condens. Matter 43, 119 (1981).
[31] K. Binder, D.P.Landau, Phys. Rev. B 30, 1477 (1984).
[32] A. W. Sandvik, AIP conf. Proc. 1297, 135 (2010).
[33] N. Schultka and E. Manousakis, Phys. Rev. B 49, 12071 (1994).
[34] N. Schultka and E. Manousakis, Phys. Rev. B 51, 11712 (1995).
[35] L. Wang, K. S. D. Beach, and A. W. Sandvik, Phys. Rev. B 73, 014431 (2006).
[36] P. R. Gill,W. Murray, and M. H. Wright, Practical Optimization (Academic Press, San Diego, 1988).
[37] M. E. Fisher and M. N. Barber, Phys. Rev. Lett. 28 1516 (1972).
[38] E. Br´ezin, J. Physique 43 15 (1982).
[39] M. N. Barber, Academic, in Phase Transitions and Critical Phenomena, C. Domb and J. L. Lebowitz (eds.) Press, New York, 1983), Vol. 8.
[40] L. Wang, K. S. D. Beach, and A. W. Sandvik, Phys. Rev. B 73, 0505194 (unpublished).
[41] M. Campostrini, M. Hasenbusch, A. Pelissetto, P. Rossi, and E. Vicari, Phys. Rev. B 65, 144520 (2002).
[42] A. Kl¨umper, Eur. Phys. J. B 5, 677 (1998).
[43] B. Gu, G. Su, S. Gao, Phys. Rev. B 73, 134427 (2006); S. S. Gong, S. Gao, G. Su, Phys. Rev. B 80, 014413 (2009).