Spin excitation spectra of two dimensional $S = 1/2$ Heisenberg model with checkerboard structures

Yining Xu,¹ Zijian Xiong,¹ Han-Qing Wu,¹ and Dao-Xin Yao¹,*

¹State Key Laboratory of Optoelectronic Materials and Technologies, School of Physics, Sun Yat-Sen University, Guangzhou 510275, China
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We study the spin excitation spectra of two-dimensional spin-$1/2$ Heisenberg model with checkerboard structures using stochastic analytic continuation of imaginary-time correlation function obtained from quantum Monte Carlo simulation. The checkerboard models have two different antiferromagnetic nearest-neighbor interactions $J_1$ and $J_2$, and the tuning parameter $g$ is defined as $J_2/J_1$. The dynamic spin structure factors are systematically calculated in all phases of the models as well as at the critical points. To give a full understanding of the dynamic spectra, spin wave theory is employed to explain some features of numerical results, especially for the low-energy part. When $g$ is close to 1, the features of the spin excitation spectra of each checkerboard model are roughly the same as those of the original square lattice antiferromagnetic Heisenberg model, and the high-energy continuum among them are discussed. In contrast to the other checkerboard structures investigated in this paper, the $3 \times 3$ checkerboard model has distinctive excitation features, like a gap between a low-energy gapless branch and a gapped high-energy part exists when $g$ is small. The gapless branch in this case can be regarded as spin wave in Néel order formed by "block spin" in each $3 \times 3$ plaquette with effective exchange interaction originated from renormalization. One finding is that the continuum also appears in this low-energy branch, which may originated from nearly deconfined process in "block spin".

I. INTRODUCTION

With the evolution of experimental measurement techniques, like the inelastic neutron scattering (INS), and the development of numerical calculation methods, the dynamic signatures of magnetic systems have attracted more attentions in recent years. For example, the high-energy portion of the spin excitation spectra of the spin-$1/2$ antiferromagnetic Heisenberg model predicted by the spin wave theory deviates from the experimental results [1–5], while the numerical results are well matched with the experiments[6, 7]. Meanwhile, two-magnon excitation spectra were measured in dimerized antiferromagnetic chain material [8], and two-triplon scattering of a cuprate ladder was quantitatively observed [9], and the structure of the magnetic excitation in a spin-$1/2$ antiferromagnetic triangular lattice Heisenberg system was also studied [10] which is significantly different from the theoretical expectation.

Furthermore, dynamical properties also have been studied for some exotic phenomena by using numerical methods, such as the deconfined quantum critical points [11, 12] and quantum spin liquids [13]. By studying the excitation spectra of magnetic materials and their related spin models, we can find some new features which can help us to gain a deeper insight of the mechanisms behind these physics.

Numerically, stochastic analytic continuation (SAC) [14–19] of imaginary-time correlation functions obtained from quantum Monte Carlo (QMC) simulations can be used to study the dynamic spin structure factor $S(q, \omega)$. The $S(q, \omega)$, which can reveal dynamical information of the system, can be accessed directly by INS and nuclear magnetic resonance (NMR) experiments. Moreover the $S(q, \omega)$ calculated by the QMC-SAC method has been confirmed to be consistent with the experimental results [19]. Recently, this method is used to study some exotic cases, such as random singlet state [20], quantum spin liquid [13], deconfined quantum critical point [12]. However, unlike the results given by analytical studies, the effects of various modes of spin excitation are intermingled in the results obtained by QMC-SAC. Therefore, the QMC-SAC results should be combined with theoretical explanations to gain further understanding.

Some materials, like SrCu$_2$(BO$_3$)$_2$, have found to exhibit like a plaquette phase under certain conditions[21, 22], in which the spins present a $2 \times 2$ periodic block structure. In theoretical studies, such periodic structures can be modeled by checkerboard models (also known as plaquette models in some literatures). The $2 \times 2$ checkerboard model is one of the well-studied spin models. Its ground state properties have been numerically calculated by series expansion [23, 24], quantum Monte Carlo [25–27], exact diagonalization [28, 29], real space renormalization group [30] and so on [27, 28, 31]. And some results also given through analytical studies like nonlinear $\sigma$ model [32–34], bond operator [35–38] and spin wave theory [33, 34]. Interestingly, some similar periodic structures are observed in other experimental materials, such as Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ [39, 40] and Ca$_{2-x}$Na$_x$CuO$_2$Cl$_2$ [41]. What is more, the antiferromagnetic clusters with $3 \times 3$ structure are realized in nanomagnets [42, 43]. In addition, a feasible method to implement the expected checkerboard models is constructed in the optical lattice[44–46] by cold atom experiment.

The checkerboard models investigated in this work include $2 \times 2$, $2 \times 3$, $2 \times 4$ and $3 \times 3$ structures. The structures of these checkerboard models are illustrated in FIG.1, and we refer to each spin block as a sublattice in this paper. In our recent work[47], the $O(3)$ universal quantum phase transitions of $2 \times 2$, $2 \times 3$ and $2 \times 4$ checkerboard models have been reported. The long-range Néel order is destroyed at the quantum critical point while the spin-rotation symmetry ($SU(2)$ symmetry) is restored [48]. For the disordered phase, i.e. plaquette phase, the lattice symmetry is not spontaneously broken.
FIG. 1. (Color online) Structures of different checkerboard lattices. (a) 2 × 2, (b) 2 × 3, (c) 2 × 4 and (d) 3 × 3. The intra-sublattice interactions $J_1$ and the inter-sublattice interactions $J_2$ are represented by thick red and thin blue lines respectively. Here we study the antiferromagnetic case, i.e. $J_1 > 0, J_2 > 0$. The tuning parameter $g$ is defined as $g = J_2 / J_1$, where $0 < g < 1$. In this paper, we refer to the spin blocks that make up the checkerboard lattice as sublattice.

but is destroyed by the designed model, which is very similar to the so-called dimer phase (or named coupled-dimer antiferromagnet) [12, 49].

Although there are some researches about 2 × 2 checkerboard lattice, the complete dynamical properties are still lacking. And we are interested in the signatures of the spin excitation spectra with different checkerboard models and the effect of the $O(3)$ quantum phase transition in $S(q, \omega)$. The $3 \times 3$ checkerboard model differs from the other three models in that the number of spins in its sublattice is odd and no quantum phase transition is observed by finite-size scaling of conventional physical quantities[47]. We suppose that in this case, the nine spins in a $3 \times 3$ sublattice would collectively appear as a "block spin" of spin-1/2. For the Néel phase of the checkerboard models, $SU(2)$ symmetry is broken simultaneously, and as expected, the Goldstone modes of all the checkerboard models can be described by using spin wave theory. However, the rest of the features that arise as the number of spins in the sublattice increases are equally noteworthy, and we also expect to interpret them from a theoretical perspective.

The rest of the paper is organized as follows: In Sec. II, we give the Hamiltonian of the models and briefly introduce the QMC-SAC method. In Sec. III, we present numerical results for dynamic spin structure factors of different checkerboard models in color plots and describe the features of them. In Sec. IV, the signatures of the low-energy excitation spectra are explained by using the spin wave theory, and the high-energy continuum is discussed in this section. The excitation spectra of the $3 \times 3$ model are considered separately due to its distinctive features. We summarize our findings in Sec. V.

II. MODEL AND NUMERICAL METHOD

A. Model

A two-dimensional antiferromagnetic Heisenberg Hamiltonian is considered on checkerboard lattices,

$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle i,j \rangle'} S_i \cdot S_j,$$

where $S_i$ denotes the spin-1/2 operator on each site $i$, $J_1$ and $J_2$ are antiferromagnetic nearest-neighbor interactions. The intra-sublattice interactions $J_1$ and the inter-sublattice interactions $J_2$ correspond to the thick red and the thin blue bonds in FIG. 1 respectively. The tuning parameter $g$ is defined as $g = J_2 / J_1$, where $g$ takes 0 to 1. For the case of $g = 1$, no matter which structure these are, they recover an original antiferromagnetic Heisenberg model with uniform interactions. When $g = 0$, the interactions between sublattices vanish and the sublattices are isolated from each other.

In all of these models, the intra-sublattice interaction $J_1$ takes a fixed value of $J_1 = 1$, and the inter-sublattice interaction $J_2$ varies according to $J_2 = g J_1$. The advantage of this setup is that the energy of high-energy excitation can be roughly estimated in spectrum when $g$ changes, and it is easier to analyze the effect of $g$ on the spectrum.

B. Numerical method

In the process of numerical calculation, the dynamic spin structure factor $S(q, \omega)$ cannot be directly calculated by QMC simulations. In order to obtain $S(q, \omega)$, the imaginary-time correlation function should be measured by using stochastic series expansion (SSE) [50, 51] QMC first. The imaginary-time correlation function $G_q(\tau)$ describes the dynamic spin-spin correlation of a given transferred momentum $q$ in momentum space, which is defined as

$$G_q(\tau) = \langle S_{-q}(\tau) \cdot S_{q}(0) \rangle.$$  

(2)

Here we consider the isotropic Heisenberg spin, so $G_q(\tau) = 3 \langle S_{-q}(\tau) \cdot S_{q}(0) \rangle$, where $S_{-q}$ is the Fourier transform of the spin. From the $G_q(\tau)$ for a series of imaginary-time points $\tau$, $S(q, \omega)$ can be reconstructed by the SAC method [14–19] using the relation between $G_q(\tau)$ and $S(q, \omega)$, which is given by

$$G_q(\tau) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega S(q, \omega) e^{-i\omega \tau}.$$  

(3)

In this process, the spectrum is parameterized as the sum of a large number of $\delta$ functions, and is sampled with a probability
distribution. The sampling weight for a given spectrum is
\[ P(S) \propto \exp(-\frac{\chi^2}{2\Theta}), \]
where \( \Theta \) is a fictitious temperature and \( \chi^2 \) is the goodness of fit between the SSE-computed result and the result obtained from the current spectrum by using Eq. (3). The technical details can be found in Ref. [18, 19].

III. NUMERICAL RESULTS

Here, we extract the \( S(q, \omega) \) for \( 2 \times 2, 2 \times 3, 2 \times 4 \) and \( 3 \times 3 \) checkerboard models, and display the results in color plots respectively, while the checkerboard models are classified into two classes based on whether a finite critical point can be measured by finite-size scaling of conventional physical quantities (like Binder ratio, uniform magnetic susceptibility and spin stiffness). In order to better present the spin excitation spectra, the color function of the \( S(q, \omega) \) shown in this section is a piecewise function, where the low-intensity portion of the result is represented by a linearly distributed color function and the divergent portion (which is less than 1% of the total amount of data) is treated with logarithm.

We use periodic boundary condition in the two dimensional \( L \times L \) checkerboard lattice with \( L = 48 \) and perform the numerical calculation. The QMC calculations are carried out at inverse temperature \( \beta = L \), which gives \( T = 0 \) results [18, 51] for \( G(q, \tau) \) at the momentum considered. The calculations are performed in all phases of the models as well as at the critical points.

A. checkerboard models with quantum phase transition

For the models with \( 2 \times 2, 2 \times 3 \) and \( 2 \times 4 \) checkerboard structure, the reduction of \( J_3 \) drives the long-range Néel order to the plaquette phase through quantum phase transition of the \( O(3) \) universality class at \( g = g_c \), where the \( O(3) \) transition is identified by the critical exponent of the finite-size scaling obtained in our recent work [47]. For \( 2 \times 2 \) structure, \( g_c = 0.548524(3) \), for \( 2 \times 3 \) structure, \( g_c = 0.4694(1) \), and for \( 2 \times 4 \) structure, \( g_c = 0.456978(2) \).

The \( S(q, \omega) \) results of \( 2 \times 2 \) checkerboard model are shown in FIG. 2 along the path \((0, 0) \rightarrow (\pi, 0) \rightarrow (\pi, \pi) \rightarrow (0, 0) \rightarrow (0, \pi) \rightarrow (\pi, \pi) \), and we analyze the salient features of the spin excitation spectra. In the Néel phase, the gapless Goldstone mode is observed at \((\pi, \pi)\) as shown in FIG. 2(a), where the spectral weight is well known divergent. And the gapless behavior appears at \((0, 0)\) also, but the spectral weight tends to vanish approach \((0, 0)\) as expected due to the conservation of total \( S_z \). For the case of \( g = g_r \) in FIG. 2(b), in addition to the two gapless points as in Néel phase, gapless excitation also occur at \((\pi, 0)\) and \((0, \pi)\), and they are ascribed to the effect of Brillouin zone folding. When \( g = 0.3 \), the spin system loses magnetic order due to the formation of spin singlets and is dominated by the disordered ground state with \( S U(2) \) symmetry. As shown in FIG. 2(c), all spin excitations are gapped and the spectral weight of the high-energy excitation partial increases, which implies that the spin system no longer has a magnetic order, and as \( g \) decreases, the excitations between the sublattices tend to disappear thus the spin excitations should be concentrated primarily in the sublattice.

For the models with \( 2 \times 3 \) and \( 2 \times 4 \) checkerboard structure, the results of \( S(q, \omega) \) are shown in FIG. 3. For these two models, in order to reflect the asymmetry of interaction between \( x \) and \( y \) directions in the spin excitation spectra, we choose the path: \((\pi, \pi) \rightarrow (0, 0) \rightarrow (\pi, 0) \rightarrow (\pi, \pi) \rightarrow (0, \pi) \rightarrow (\pi, 0)\). When \( g \) is no longer equal to 1, the ground state of these models are still in Néel phase and the features of \( S(q, \omega) \) in FIG. 3(a) and (d) are not significantly different from the results of \( 2 \times 2 \) checkerboard model, although the symmetry of the interactions changes from \( C_4 \) to \( C_2 \). But when \( g = g_c \), the difference becomes apparent. Along the path \((\pi, 0) \rightarrow (\pi, \pi)\) in FIG. 3(b) and (e), we can see that for the \( 2 \times 3 \) model, there is a gapless excitation at \((\pi, \pi/3)\), and for the \( 2 \times 4 \) model, gapless excitation appears at \((\pi, 0)\) and \((\pi, \pi/2)\), they are also from the effect of Brillouin zone folding. And in this path, the low-energy part of spin excitation spectra exhibits a folding feature. In addition, gapless excitations also appear at \((0, \pi)\) in FIG. 3(b) and (e). As \( g \) decreases, the ground state of the spin system becomes plaquette phase, and all spin excitations are gapped, but the periodic structures of \( S(q, \omega) \) survive, as shown in FIG. 3(c) and (f).

The periodic interactions of the designed model lead to the effect of Brillouin zone folding whether in the phase with a long-range order or at the critical point [33, 34]. This is illustrated by the spectrum in FIG. 2(b), FIG. 3(b) and (e), where the low-energy modes are not only appear at wave vectors \((\pi, \pi)\) and \((0, 0)\) but also at other wave vectors along the path \((\pi, 0) \rightarrow (\pi, \pi) \rightarrow (0, \pi)\) due to the folded \((\pi, \pi)\). \( S(q, \omega) \) at \((0, 0)\) is folded also but the low-energy mode can hardly observed along the path \((0, \pi) \rightarrow (0, 0) \rightarrow (\pi, 0)\) as a result of the negligible spectral weight around the Brillouin zone center. From the spin excitation spectra shown in FIG. 2(c), FIG. 3(c) and (f), we can find that the wave vectors of low-energy modes are the same as the corresponding critical spectra of each structure. Therefore, whether it means that the effect of Brillouin zone folding is also present in the plaquette phase. To answer this question, we should know the excitation inside the Brillouin zone, not just along the boundary. We calculate the \( S(q, \omega) \) on the path \((0, \pi) \rightarrow (\pi/2, 3\pi/4) \rightarrow (\pi, \pi)\) for \( 2 \times 4 \) checkerboard model with \( g = 0.25 \) and present it in FIG. 4, which shows the low-energy modes at \((\pi, \pi)\) and \((0, \pi)\). Thus, we can believe that although the plaquette phase is magnetically disordered, the effect of Brillouin zone folding still exists.

B. \( 3 \times 3 \) checkerboard model

The \( 3 \times 3 \) checkerboard model is very special, with 9 spins in each sublattice, which means that one spin is likely to be unpaired. When \( g \) changes, there is no quantum phase transition observed. We suspect this is due to the existence of...
FIG. 2. (Color online) Dynamic spin structure factor $S(q, \omega)$ obtained from QMC-SAC calculations for $2 \times 2$ checkerboard model in different $g$, where $g$ is 0.8 (a), $g_c(0.5485)$ (b) and 0.3 (c). When $g = 0.8$, the model is in the Néel phase. For $g = 0.3$, the model is in the plaquette phase, and the $SU(2)$ symmetry is restored, which appears as gapped spectra.

unpaired spins in each sublattice, more precisely, each $3 \times 3$ sublattice is "renormalized" to an effective "block spin" with spin-1/2. As discussed in the previous section, at the limits of $g = 1$ and $g = 0$, the ground states of the spin system are clearly different. In order to know how the change occurs when $g$ decreases, we calculate the $S(q, \omega)$ by taking $g = 0.7, 0.4$ and 0.1 to discuss the $3 \times 3$ checkerboard model from the perspective of dynamic signatures. The numerical results are shown in FIG. 5, in which wave vectors takes the path of $(0,0) \rightarrow (\pi,0) \rightarrow (\pi,\pi) \rightarrow (0,0) \rightarrow (0,\pi) \rightarrow (\pi,0)$.

When $g = 0.7$, $S(q, \omega)$ shown in FIG. 5(a) have the basic features in the spin excitation spectra as Néel phase obviously. When $g = 0.4$, the low-energy portion of the $S(q, \omega)$ shown in FIG. 5(b) exhibits a periodic structure, which is similar to

FIG. 3. (Color online) Dynamic spin structure factor $S(q, \omega)$ obtained from QMC-SAC calculations for $2 \times 3$ (a-c) and $2 \times 4$ (d-f) checkerboard model in different $g$. When $g \neq 1$, the symmetry changes from the original $C_4$ symmetry to the $C_2$ symmetry. The spectra of Néel phase are shown in (a) and (d), where $g$ is 0.75 and 0.7 for $2 \times 3$ and $2 \times 4$ model, respectively. In (b) and (e), $g$ takes a critical value $g_c$, $g_c = 0.4694$ for $2 \times 3$, and $g_c = 0.4569$ for $2 \times 4$. The gapped spectra of plaquette phase with $g = 0.25$ are shown in (c) and (f).
the \( S(q, \omega) \) of the \( 2 \times 3 \) model. Especially, the result along the path \((0, 0) \to (\pi, 0) \to (\pi, \pi) \) is almost the same as the corresponding result in FIG.3(b). But as \( g \) keep decreasing, when \( g = 0.1 \), we find that the spin excitation spectra become completely different from the previous results.

As shown in FIG.5(c), when \( g = 0.1 \), the gapless branch in the spectrum is totally separated from the high-energy part. It can be seen from the fact that the gapless branch has energy around \( J_2 \), which should be the excitation among the sublattices. And the existence of this gapless branch with a periodic structure prove our "block spin" guess. Since each \( 3 \times 3 \) sublattice is "renormalized" into a "block spin", we can regard it as an effective spin system with elongated lattice constant, and the Brillouin zone is reduced by three times in both the \( x \) and \( y \) directions correspondingly, so the results are repeated three times on all paths. Moreover, since the gapless branch has obvious character of the spin excitation spectrum in the Néel order, we can infer that the effective spin system has long-range Néel order.

The high-energy gapped part has energy around \( J_1 \), which should be the excitation inside the sublattice. Unlike the \( S(q, \omega) \) of \( g = 0.4 \) (FIG.5(b)), the high-energy part intersects the gapless branch, and they all have a gapless excitation at \( (\pi, \pi) \). When \( g = 0.1 \), there is a significant energy gap between the gapless branch and the gapped part, so it is obvious that the spin configuration within the sublattice must not be Néel order but is disordered to some extent. Therefore, we suspect that when \( g \) is small enough, the ground state of the \( 3 \times 3 \) checkerboard model may also have disordered valence bonds just similar as a checkerboard model with finite \( g_c \). Finally, a question can be raised, whether a different physical quantity can be defined to describe this kind of case, which simultaneously exhibits long-range ordered and disordered features.

### IV. ANALYSIS

In this section, we provide some account for the spectral features behaved in the numerical spectra. From the previously shown color plots, some common features in our numerical spectra can be identified:

a. When \( g \) is large the overall shape of spectra of checkerboard models (shown in FIG.2(a), FIG.3(a) and (d), FIG.5(a)) are almost the same as the well-known results in antiferromagnetic square lattice with Néel order (which is referred to bipartite case hereafter comparing with enlarged magnetic unit cell in checkerboard lattice). To be specific, the spectra behave as varying spectral weight along the dispersion curve \( \epsilon_k \propto \sqrt{1 - \gamma_k^2} \) with \( \gamma_k = (\cos k_x + \cos k_y)/2 \), and the spectral weight diverge at the \((\pi, \pi)\) due to the Néel order. Another noteworthy feature is the prominent high-energy continuum in all structures, and it is discussed in Sec. IV B.

b. As \( g \) decreases, some low-energy branches appear, which can be seen in FIG.2(b), FIG.3(b) and (e) and FIG.5(b). To have a qualitative understanding of these low-energy branches, the dispersions and transverse dynamic structure factors calculated by using linear spin wave theory are shown in Sec. IV A.

c. When \( g < g_c \), the spectra of \( 2 \times 2, 2 \times 3 \) and \( 2 \times 4 \) checkerboard models are gapped (as shown in FIG.2(c), FIG.3(c) and (f)), but the overall shape do not change a lot. However, the spectra of \( 3 \times 3 \) structure are gapless in all taken \( g \) owing to the persistent long range order, and they are discussed in Sec. IV C.

#### A. Low-energy excitation

To qualitatively study the low-energy branches, we use the linear spin wave theory (LSWT) outlined in the Appendix A to calculate theoretical transverse dynamic structure factor of \( 2 \times 2, 2 \times 3 \) and \( 2 \times 4 \) checkerboard models. It is well known that standard spin wave theory starts with the assumption of magnetic ordered phase and may not give the correct prediction about the critical behavior, so we use spin wave theory to study the ordered phase with \( g \) close to \( g_c \) and try to understand the spectra.

1. \( g \) close to \( g_c \)

When \( g \) close to \( g_c \), transverse dynamic structure factors (DSF) in linear spin wave level of models with \( 2 \times 2, 2 \times 3 \) and \( 2 \times 4 \) checkerboard structures are presented in FIG.6(b), FIG.7. Comparing them with corresponding numerical spectra in FIG.2(b), FIG.3(b) and (e), we find the shape of low-energy branches in LSWT match quite well with the numerical spectra. Concretely speaking:

In \( 2 \times 2 \) structure, there are two branches spin wave, namely optical and acoustic spin wave, and the magnon dispersions are shown in FIG.6(a). The features of "emergent" branch from \((\pi, 0)\) to \((\pi, \pi)\) and the DSF curve along \((\pi, 0) \to (\pi, \pi) \to (0, 0)\)
FIG. 5. (Color online) Dynamic spin structure factor $S(q, \omega)$ obtained from QMC-SAC calculations for $3 \times 3$ checkerboard model in different tuning parameter $g$, where $g$ is taken as 0.7 (a), 0.4 (b) and 0.1 (c). From these results, we can see that no matter how $g$ changes, the gapless mode at $(\pi, \pi)$ persists. The spectrum of $g = 0.1$ is different from the spectra of other structures, specially, the gapless branch is completely separated from the gapped part.

FIG. 6. (Color online) The linear spin wave results of the $2 \times 2$ checkerboard model. (a) White dashed lines are the linear spin wave dispersions with $g = 0.56$, which are shown here together with the results of FIG.2(b). (b) and (c) are the results of the zero temperature transverse dynamic structure factor with $g = 0.56$ and $g = 0.8$, respectively, which describe the excitation of a single magnon. Comparing (b) with (c), one may find that as $g$ decreases and approaches to $g_c$, the spectral weight of the acoustic branch increases and the low-energy branch becomes visible.

FIG. 7. (Color online) The linear spin wave results of the $2 \times 3$ checkerboard model with $g = 0.5$ are shown in (a) and (c), and the results of $2 \times 4$ with $g = 0.47$ are shown in (b) and (d). Here $g$ takes a value close to the critical point to ensure the system is in the ordered phase. In (a) and (b), the linear spin wave dispersions are represented by white dashed line with the color plots in FIG.3 (b) and (e) as background, and (c) and (d) are the corresponding zero temperature dynamic structure factors.

$(0,0)$ in FIG.2(b) are both captured by LSWT, so the low-energy excitation can be ascribed to the spin wave with no doubt.

One may wonder how the spectra evolve when tuning $g$ from 1 to $g_c$, or in other words, when the effect of reduction in Brillouin zone becomes visible. We find that when $g$ is large, for example $g = 0.8$, the LSWT spectra (as shown in FIG.6(c)) is very similar to bipartite case. The acoustic branch due to enlarged magnetic unit cell has small spectral weight when deviating from dispersion of antiferromagnetic square lattice, as $g$ decreases and approaches to $g_c$, this low-energy branch becomes visible.
For the spectra of 2 × 3 and 2 × 4 structures, there are many branches of spin wave since their magnetic unit cell contain many spins. For 2 × 3 structure, when \( \omega < 2 \), an asymmetric DSF curve with a shoulder peak along \((0, 0) \rightarrow (\pi, 0) \rightarrow (\pi, \pi/3)\) is observed in FIG.3(b), and it is formed by several branches of spin wave as in FIG.7(c). Moreover, for 2 × 4 structure, LSWT result in FIG.7(d) also matches the numerical spectra structure in FIG.5(c) from \((\pi, 0) \rightarrow (\pi, \pi)\) quite well when \( \omega < 1 \).

Comparing the theoretical spectra with corresponding numerics carefully, one may finds the energy of highest optical branches of spin wave since their magnetic unit cell contain continuum, this can be explained by the lack of renormalization factor from interaction. One may also finds spectral weight from interaction and phenomenologically introduce a chemical potential to the gap in the spectra.

We extract the energy dispersion curves from numerical results. (a) All the checkerboard models here reduce to the original square lattice antiferromagnetic Heisenberg model when \( g = 1 \), and the dispersion of \((\pi/2, \pi/2) \rightarrow (\pi, 0)\) is widely concerned in this case. (b) The dispersion curve of 2 × 2 checkerboard model with varying \( g \), where the high-energy dispersion curve shows a larger dip at \((\pi/2, \pi/2)\) as \( g \) decreases. (c) A comparison between the dispersion curves of the 2 × 2 and 3 × 3 checkerboard models in the Neél phase. When the structure of the model changes, the excitation of these two models at \((0, \pi)\) is different.

2. \( g < g_c \)

Spectra are gapped when \( g < g_c \), which mean that those systems are in disordered phase. But the overall shapes of spectra do not change a lot comparing with the critical spectra except the enhancement of spectra weight along some paths of momentum, for example the spectral weight are enhanced along \((0, 0) \rightarrow (\pi, 0) \) and \((\pi, 0) \rightarrow (\pi, \pi/2)\) in FIG.2(c).

To obtain the gapped spectra, one can use spin wave theory and phenomenologically introduce a chemical potential of the bosons and tune the chemical potential to open a gap, or use modified spin wave theory to calculate the gap self-consistently[33, 52, 53]. But as is known, low-energy excitations in these disordered phase are no longer gapless magnon, they are gapped spin-1 triplon which can be described by bond operator theory[35–38, 54]. For simplicity, we consider low-energy excitations in 2 × 2 structure (this picture should work for 2 × 3 and 2 × 4 also, except 3 × 3 which we discuss below separately). They can be understood as follow: when \( g = 0 \) the lattice decouples into isolated plaquettes, and the ground state of such a plaquette is a superposition state consisting of a pair of two-spin singlet along edges of plaquette (the explicit expression is given in Appendix.B). The first excited state is formed by breaking a bond, it is a direct product state of a singlet and a triplet. These excitations are localized, once \( g \) is switched on they can hop and lower the energy. But the energy required is still finite due to the confinement of spinons[49], this binding energy between a pair of confined spinons leads to the gap in the spectra.

B. High-energy continuum

From above comparisons, LSWT describes low-energy part of the spectra quite well. But it does not mean that the complete spectra of checkerboard lattices behave as single particle with slight modifications. Although LSWT can be improved by considering 1/S expansion and perform high-order perturbation to obtain multi-particle continuum[55–57], such as 3-magnon continuum in transverse DSF and 2-magnon continuum in longitudinal DSF, but the results are not satisfactory even in bipartite case. This standard perturbation method converges slowly[58], and cannot give a reasonable prediction for the energy difference between \((\pi, 0)\) and \((\pi/2, \pi/2)\) and spectral weight at these momenta in bipartite case. Many theories have been proposed to account for these anomalies, for example nearly deconfined spinon [19, 59], non-perturbative renormalization of magnon [60], singlon[61]. These mechanisms are quite different but they do not disprove each other and the nature of the high-energy excitation is still in debate. In this section, we study the high-energy part of the spectra in checkerboard model.

We extract the energy dispersion curves from numerical
data by collecting the energy of the local maximum in spectral weight along the selected momentum path shown above, but the energy extracted in this way will be slightly larger than the correct value owing to the finite width of "delta function". In spite of this, the behavior of the spectra should be correct up to a shift in energy. All of these lattice reduce to antiferromagnetic square lattice when \( g = 1 \), see FIG.8 (a), the roton-like dip at \((\pi, 0)\) is observed, and the energy difference between \((0, \pi)\) and \((\pi/2, \pi/2)\) is estimated to be 6.5% which has a good agreement with experiments in \( \text{Cu(DCOO)}_2 \cdot 4\text{D}_2\text{O} \) \[2, 3\]. But is should be noticed that these extracted energies are slightly larger than the experimental values as expected, the experimental values are \( \omega_{(\pi, 0)}/J = 2.19 \) and \( \omega_{(\pi/2, \pi/2)}/J = 2.38 \).

Firstly, we study the effect of structure on the anomaly in magnetic Brillouin zone (MBZ) boundary. When \( g \) is large, spectra of all structures seem like bipartite-case. The remarkable continuum in each structures (FIG.2 (a), FIG.3 (a) and (d), FIG.5 (a)) are around \((\pi, 0)\) and \((0, \pi)\), and they are extending from \( \omega \approx 1.8 \) to \( \omega \approx 3.5 \), which is close to the phenomenon observed in square lattice[2]. When \( g = g_c \), the low-energy branches appear which mean that the effect of reduction in MBZ become evident, we expect that the continuum should also appear around endpoints of the magnetic Brillouin zone boundary, for instance, \((\pi/2, \pi/2)\) in \( 2 \times 2 \) and \( 2 \times 3 \). But the numerical results deviate significantly from our expectation, the most prominent continuum are still around \((\pi, 0)\), \((0, \pi)\) (FIG.2(b), FIG.3(b) and (e), FIG.5(b) ). One may ascribe this to the nearly deconfined mechanism. To have a further look, we compare the extracted "dispersion" along \((0, 0) \rightarrow (0, \pi) \rightarrow (\pi/2, \pi/2) \rightarrow (0, 0)\) for \( 2 \times 2 \) and \( 3 \times 3 \) structure in ordered phase, i.e. in large \( g \) case, and they are shown in FIG.8(c). It should be noticed that they are not the true dispersion, the magnetic unit cell is enlarged when \( g < 1 \), so there should be much more branches of dispersion, though they can hardly be extracted from the spectra completely. Despite of this, we know the high-energy optical branches are nearly flat from spin wave calculation, thus it will make sense to study the high-energy part of the "dispersion". There are several extremums in the high-energy part of "dispersion", and anomaly at \((0, \pi)\) are found to be structure dependent. The energy at \((\pi, 0)\) is enhanced in \( 3 \times 3 \) structure compared with \((\pi/2, \pi/2)\), while it is reduced in \( 2 \times 2 \) structure.

Due to the similarity among these spectra of different checkerboard structures, we discuss the effect of \( g \) in \( 2 \times 2 \) structure for simplicity. Dispersions with different \( g \) are shown in FIG.8 (b), where the dip at \((0, \pi)\) persists in each phase and does not change so much. It is noteworthy that the variation in energy is much more prominent as \( g \) changes at \((\pi/2, \pi/2)\) than \((\pi, 0)\). At \( g = g_c \), the spectral weight at several momenta are shown in FIG.9, they all behave as asymmetric peak, the main contribution can be ascribed to a single optical magnon peak, and the remained part is from high-energy continuum.

Finally, we provide some potential account for the high-energy continuum in the checkerboard model investigated here with \( g \geq g_c \). Because of the complexity of these checkerboard structures, there are many mechanism may lead to these continuum. A) Energy are close for those optical modes, which means there are strong renormalization among these modes when considering interactions, then they span a larger high-energy range for multi-magnon continuum. B) Pairs of spin tend to form singlets due to checkerboard structure especially when \( g \) is small, then gapped excitation from these singlets may contribute to the high-energy part also[61]. C) Nearly deconfined spinon[19] may also exists in these models intrinsically, then a question can be raised: whether these spinons deconfined from different optical magnon modes are the same, or there are different modes of spinon. So these lattice provide a playground for studying high-energy continuum, and they also have close relation to the original square lattice. An open question is how to identify the intrinsic properties of excitations in these high-energy continuum.

C. \( 3 \times 3 \) model

As mentioned above, \( 3 \times 3 \) model is different from others. Firstly, no phase transition is observed based on finite-size scaling, i.e. we can not find any finite \( q \), because of the persistent long range order. Secondly, the ground state of an isolated sublattice is a doublet rather than singlet. From these perspectives, the spectrum is very unusual in this structure when \( g \) is small, it is consisted of a low-energy gapless branch and a gapped high-energy part as shown in FIG.5(c).

For a better understanding of the excitation in this case, the
spectrum of few $3 \times 3$ plaquettes is the key. But it is hard to write down the explicit wave functions for ground state and low-lying excited states even for such an isolated plaquette, so we adopt the exact diagonalization, the energy levels are given in Appendix B. According to the exact diagonalization result in Fig. 12(a), the ground state, the first excited state and the second excited state of the isolated $3 \times 3$ plaquette are $S = 1/2$ doublet, $S = 3/2$ quartet, and another $S = 1/2$ doublet, respectively. The gap between ground state and first excited state is quite large, and it equals $J_1$. Let us turn to small $g$ case, more precisely, $g \ll 1$, then $g$ can be considered as perturbation in this circumstance. Once $g$ is turned on, the original doublet ground state in isolated case will split into some lower energy states and some higher energy states. For example, let us consider two $3 \times 3$ plaquettes, the ground state of this system is a singlet, and the first excited state is a triplet, they are formed by original $S = 1/2$ ground state of each plaquette, and the energy differences between ground state and first excited state is around $g$. Following excited states are formed by combining an original $S = 1/2$ ground state and an original $S = 3/2$ first excited state, so they should be $S = 1$ and $S = 2$ states with energy around $J_1$. This picture is proved by exact diagonalization, see Fig. 12(b). For $2 \times 2$, $2 \times 3$ and $2 \times 4$ models, the ground states of the isolated plaquette are singlet, so their ground states will not split even $g$ is turned on. One more interesting thing is that: in small $g$ case, the ground state of $3 \times 3$ model depends on the size [62], the ground state is singlet or doublet depending on even or odd size, but this fact will not change the low-lying excitation.

As discussed above, the low-lying excited states splitting from original doublet are separated from the higher energy states by a gap with energy around $J_1$, and $\Delta S$ between ground state and first excited state should be 1. For this reason, we considered the $S = 1$ excitation from ground state to first excited state first. As a result of the existence of the low-energy gapless branch and $S = 1$ excitation, we find this gapless branch can be fitted by spin wave with enlarged lattice constant very well without other parameters, specifically, the dispersion is $g \sqrt{1 - \gamma_k^2}$, where $\gamma_k = (\cos 3k_x + \cos 3k_y)/2$, see Fig. 10. So this $S = 1$ excitation can be regarded as spin wave in Neél order formed by “block spin” in each $3 \times 3$ sublattice with effective exchange interaction originated from renormalization. The effective exchange interaction between these “block spin” is not that simple as only nearest neighbor interaction, next-nearest neighbor or even ring exchange interaction may exist also. What surprised us also is that the continuum centered at the endpoints of magnetic Brillouin zone boundary are still prominent, for example, at $(\pi, 0)$ and $(\pi, 2\pi/3)$. Then, a question is what mechanism leads to this low-energy continuum? Is the nearly deconfined account still works for such renormalized “block spin”? What is the contribution to the continuum from the “internal” structure of this “block spin”?

For the remaining part, namely gapped excitation, comparing to other structures, the low-energy features such as periodic structure and especially the shape around $(\pi, \pi)$ in ordered phase are almost lost when $g$ is small. Based on exact diagonalization result, this gapped continuum is from mixing multiplet states excitation, and they should be excitation mainly concentrated in sublattice as discussed in Sect. III, so it is hard to find well-defined dispersion behavior from the low-energy part of this continuum. It is noteworthy that we find such a system with coexistence of magnon and higher multiplet excitation and even nearly deconfined spinon, which is deserved to have further study for complete understanding of the anomaly high-energy continuum and nearly deconfined mechanism [63].

V. CONCLUSIONS

In this work, we have investigated dynamic spin structure factor of spin-1/2 antiferromagnetic Heisenberg model in several checkerboard structures, from ordered phase to disordered phase as well as at critical point by using QMC-SAC method. The models we studied can be classified into two classes according to whether there is a phase transition at finite $g_c$ or not, $2 \times 2$, $2 \times 3$ and $2 \times 4$ belong to the same class, while $3 \times 3$ is in other class.

For both classes of checkerboard models, when $g$ is large, the spectra of all structures behave as antiferromagnetic square lattice with prominent high-energy continuum around $(\pi, 0)$ and $(0, \pi)$. Due to the enlarged unit cell, the high-energy continuum may be contributed by different excitations, such as optical magnons and nearly deconfined spinons, some improved theory is needed to have a better understanding.

For models with a finite $g_c$, when approaching to $g_c$ from ordered phase, the low-energy branches due to enlarged magnetic unit cell become visible, and they can be described by linear spin wave theory quite well. When $g < g_c$, their spectra are gapped, but the overall shape do not change a lot comparing with corresponding critical spectra except enhancement of

FIG. 10. (Color online) Low-energy spectra extracted from Fig. 5(c), i.e. $3 \times 3$ checkerboard model with $g = 0.1$. Cyan dashed line is calculated by linear spin wave theory. A noteworthy feature is the prominent continuum centered at the endpoints of magnetic Brillouin zone boundary, for example, at $(\pi, 0)$ and $(\pi, 2\pi/3)$. For both classes of checkerboard models, when $g$ is large, the spectra of all structures behave as antiferromagnetic square lattice with prominent high-energy continuum around $(\pi, 0)$ and $(0, \pi)$. Due to the enlarged unit cell, the high-energy continuum may be contributed by different excitations, such as optical magnons and nearly deconfined spinons, some improved theory is needed to have a better understanding.

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spectra weight around some momenta.

There is no phase transition in $3 \times 3$ checkerboard model owing to the persistent long range order. The doublet ground state of an isolated $3 \times 3$ plaquette leads to the unusual spectra. A gap between gapless branch and high-energy part exists in this structure when $g$ is small. The high-energy continuum consists of mixed multiplet excitation. The gapless branch in this case can be regarded as spin wave in Néel order formed by "block spin" in each $3 \times 3$ plaquette with effective exchange interaction originated from renormalization. The effective exchange interaction between these "block spin" is not that simple as only nearest neighbor interaction, next-nearest neighbor or even ring exchange interaction may exist also. One noteworthy finding is that the continuum also appears in this low-energy branch, which may originated from nearly deconfined process in "block spin".

Finally, $2 \times 2$ plaquette-like lattice and $3 \times 3$ cluster have been realized in experiments, we would like to compare our theoretical results with further experimental spectra to gain insight into the understanding of these complicated excitations.

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Appendix A: Linear spin wave theory

There are many bosonization transformations for spin operator, Dyson-Maleev and Holstein-Primakoff transformation are widely used, they are the same in the linear spin wave level. The spin operators in linear spin wave level are expressed in terms of boson operators as:

$$S^z_i = -a_i^\dagger a_i, \quad S^z_j = \sqrt{2S}a_j, \quad S^+ = \sqrt{2S}a_j^\dagger,$$

$$S^- = b_j^\dagger b_j - S, \quad S^- = \sqrt{2S}b_j^\dagger, \quad S^- = \sqrt{2S}b_j,$$

(A1)

where $a_j^\dagger, a_i$ for up spin, $b_j^\dagger, b_j$ for down spin. The linear spin wave Hamiltonian $H_2$ ($H_2$ means quadratic form) can be obtained by using eqn.(A1) to express the original Hamiltonian eqn.(1) in terms of boson operators, then introducing Fourier transformation of boson operator. $H_2$ of the checkerboard lattices investigated in this paper are given as follow:

$$H_2 = \sum_k (2(1 + g)(a_k^\dagger a_k + b_k^\dagger b_k + c_k^\dagger c_k + d_k^\dagger d_k) + [\gamma(k_i)(a_k b_k + d_k^\dagger b_k^\dagger) + \gamma(k_o)(a_k c_k + d_k^\dagger c_k^\dagger)] + h.c).$$

(A2)

where $a_k, b_k, ...$ are boson operators for A,B,... sites as depicted in FIG.1(a), $\gamma(k) = e^{-ik} + g e^{ik}$, and h.c. means Hermitian conjugate. Then using the standard method[64] to diagonalize bosonic quadratic Hamiltonian equ.(A2) to obtain the linear spin wave dispersion, we have checked that our results are equivalent to Koga's results [33].

(2) $2 \times 3$:

$$H_2 = \sum_k (2(1 + g)(a_k^\dagger a_k + b_k^\dagger b_k + c_k^\dagger c_k + d_k^\dagger d_k) + h.c).$$

(A3)

with $\gamma(k_i) = e^{-ik} + g e^{ik}$ and $\gamma(k_o) = e^{-ik}$, there are 12 sites in a magnetic unit cell in this structure.

(3) $2 \times 4$:

$$H_2 = \sum_k (2(1 + g)(a_k^\dagger a_k + b_k^\dagger b_k + c_k^\dagger c_k + d_k^\dagger d_k) + h.c).$$

(A4)

with $\gamma(k_i) = e^{-ik} + g e^{ik}$ and $\gamma(k_o) = e^{-ik}$.

(4) $3 \times 3$:

$$H_2 = \sum_k (2(1 + g)(a_k^\dagger a_k + b_k^\dagger b_k + c_k^\dagger c_k + d_k^\dagger d_k) + h.c).$$

(A5)

where $\gamma(k) = e^{-ik}$, there are 18 sites in a magnetic unit cell in this structure.

Dynamic structure factor is defined by

$$S_{q}^{\beta}(q, \omega) = \sum_{-\infty}^{\infty} \frac{dt}{2\pi} S^{\beta}(t) S_{q}^{\beta}(0) e^{i\omega t},$$

(A6)
where $\alpha, \beta$ refer to $x, y, z$. Transverse part is $S^{xx}(q, \omega) + S^{yy}(q, \omega)$, longitudinal part is $S^{zz}(q, \omega)$.

Appendix B: isolated plaquette

1) $2 \times 2$ plaquette: In $g = 0$ limit, the lattice decomposes into isolated plaquette without inter-plaquette interaction. Consider an isolated plaquette (FIG.11), the Hamiltonian of this block is given by

$$H_p = J(S_1 \cdot S_2 + S_2 \cdot S_3 + S_3 \cdot S_4 + S_1 \cdot S_4), \quad (B1)$$

it can be easily solved[36–38] by introducing: $S_a = S_1 + S_3$ and $S_b = S_2 + S_4$, $S = S_a + S_b$, then the Hamiltonian can be written as

$$H_p = \frac{1}{2} J(S^2 - S_a^2 - S_b^2). \quad (B2)$$

the eigenvalues are given in Table I, the eigenstates can be labeled by quantum number $S, M, S_a, S_b, M$, corresponds to $S^z$. The ground state is a singlet with $S = 0, M = 0, S_a = 1, S_b = 1$, and energy $-2J_1$, the wave function is $(|1, 2| \otimes |4, 3| + |1, 4| \otimes |2, 3|)/\sqrt{3}$.

The first excited state is triplet with $S = 1, S_a = 1, S_b = 1$, and energy $-J_1$, the wave function are $|S = 1, M = 1⟩ \otimes |\uparrow, \uparrow⟩ + |1, 2⟩ \otimes |3, 4⟩ + |1, 2⟩ \otimes |3, 4⟩$ and $|S = 1, M = 0⟩ \otimes |\uparrow, \downarrow⟩ + |\downarrow, \uparrow⟩ \otimes |3, 4⟩$, where $[i, j] = ([\uparrow, \uparrow] - [\downarrow, \downarrow]) / \sqrt{2}, ([i, j] = ([\uparrow, \downarrow] + [\downarrow, \uparrow]) / \sqrt{2}$.

2) $3 \times 3$ plaquette

We calculated spectra of these 3 structure by exact diagonalization, the results are shown in FIG.12(a). The spectra of two $3 \times 3$ plaquette with different inter-plaquette interaction $g$ are shown in FIG.12(b).

![FIG. 11. (Color online) An isolated 2 $\times$ 2 plaquette.](image)

| $S_a$ | $S_b$ | $S$ | Eigenvalues | Degeneracy |
|------|-------|-----|-------------|------------|
| 0    | 0     | 0   | 0           | 1          |
| 0    | 1     | 1   | 0           | 3          |
| 1    | 0     | 1   | 0           | 3          |
| 1    | 1     | 0   | -2J         | 1          |
| 1    | 1     | 1   | -J          | 3          |
| 1    | 1     | 2   | J           | 5          |

The first excited state is triplet with $S = 1, S_a = 1, S_b = 1$, and energy $-2J_1$, the wave function is $(|1, 2| \otimes |4, 3| + |1, 4| \otimes |2, 3|)/\sqrt{3}$.

The first excited state is triplet with $S = 1, S_a = 1, S_b = 1$, and energy $-J_1$, the wave function are $|S = 1, M = 1⟩ \otimes |\uparrow, \uparrow⟩ + |1, 2⟩ \otimes |3, 4⟩ + |1, 2⟩ \otimes |3, 4⟩$ and $|S = 1, M = 0⟩ \otimes |\uparrow, \downarrow⟩ + |\downarrow, \uparrow⟩ \otimes |3, 4⟩$, where $[i, j] = ([\uparrow, \uparrow] - [\downarrow, \downarrow]) / \sqrt{2}, ([i, j] = ([\uparrow, \downarrow] + [\downarrow, \uparrow]) / \sqrt{2}$.

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![FIG. 12. (Color online) (a) Energy levels of isolated 2 $\times$ 3, 2 $\times$ 4 and 3 $\times$ 3 plaquette. (b) Energy levels of two 3 $\times$ 3 plaquette, inter- plaquette interaction is $g$.](image)

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