The numerical value for a universal quantity of a two-dimensional dimerized quantum antiferromagnet

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The numerical value for a universal quantity associated with the quantum critical regime, namely $\chi_u c^2 / T$, for a two-dimensional (2D) dimerized spin-1/2 antiferromagnet is calculated using the quantum Monte Carlo simulations (QMC). Here $\chi_u$, $c$, and $T$ are the uniform susceptibility, the spin-wave velocity, and the temperature, respectively. By simulating large lattices at moderately low temperatures, we find $\chi_u c^2 / T \sim 0.32$. Our estimation of $\chi_u c^2 / T$ deviates from the related analytic prediction but agrees with recent numerical calculations of other 2D dimerized spin-1/2 antiferromagnets.

I. INTRODUCTION

Spatial dimension two is special because of the famous Mermin–Wagner theorem [1]. Specifically, continuous symmetry cannot be broken spontaneously (at finite temperature $T$) in spatial dimension two. As a result, for two-dimensional (2D) quantum antiferromagnets, as $T$ rises from zero temperature, one encounters a crossover instead of a phase transition to a unique phase called the quantum critical regime (QCR).

Using the relevant field theory, properties of QCR are investigated [2]. In particular, several universal quantities are proposed. Among these quantities, we are especially interested in $\chi_u c^2 / T$ due to the recently found discrepancy between the analytic prediction and the numerical calculations. Here $\chi_u$ and $c$ are the uniform susceptibility and the spin-wave velocity, respectively.

Analytically, it is predicted that the numerical value of $\chi_u c^2 / T$ is given by (around) 0.27185. Although this prediction was confirmed by earlier Monte Carlo studies [2,4], recent investigations of 2D dimerized bilayer and plaquette spin-1/2 Heisenberg models conclude that $\chi_u c^2 / T \sim 0.32(0.33)$ [4,5]. Because of this discrepancy, it will be interesting to conduct a further examination on the numerical value of $\chi_u c^2 / T$.

In this study, we perform large-scale Monte Carlo simulations to determine the $\chi_u c^2 / T$ of a 2D dimerized quantum antiferromagnetic Heisenberg model. By simulating lattices as large as $L = 512$ ($L$ is the linear system size), we obtain $\chi_u c^2 / T \sim 0.32$ which matches quantitatively with recent outcomes claimed in Refs. [4,5]. Our result suggests that a refinement of analytic calculation is needed.

The rest of the paper is organized as follows. After the introduction, the model and the measured observables are described in Sec. II. We then present the obtained results in Sec. III. In particular, the numerical evidence to support $\chi_u c^2 / T \sim 0.32$ is demonstrated. We conclude our investigation in Sec. VI.

II. THE CONSIDERED MODEL AND OBSERVABLE

The Hamiltonian of the considered 2D spin-$\frac{1}{2}$ dimerized herringbone Heisenberg model takes the following expression

$$H = \sum_{\langle ij \rangle} J \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle i'j' \rangle} J' \mathbf{S}_{i'} \cdot \mathbf{S}_{j'},$$

where $J$ and $J'$ are the antiferromagnetic couplings connecting nearest neighbor spins $\langle ij \rangle$ and $\langle i'j' \rangle$, respectively, and $\mathbf{S}_i$ is the spin-$\frac{1}{2}$ operator at site $i$. A cartoon representation of the studied model is depicted in fig. 1. $J$ is set to 1 in our investigation. As the magnitude of $J'$ increases, a phase transition will occur for a particular value of $J' > J$. This special point $J'/J$ in the parameter space is denoted by $(J'/J)_c$ and is found to be $(J'/J)_c = 2.4981(2)$ in the literature [6]. The investigation presented in this study is conducted at the critical point $(J'/J)_c$.

To examine the universal quantity $\chi_u c^2 / T$ of QCR, the uniform susceptibility $\chi_u$ and the spin-wave velocity $c$ are measured. On a finite lattice of linear size $L$, the uniform susceptibility $\chi_u$ is defined by

$$\chi_u = \frac{\beta}{L^2} \left( \left\langle \sum_{i} S_{i}^z \right\rangle^2 \right).$$

The quantity $\beta$ appearing above is the inverse temperature. The spin-wave velocity $c$ for the investigated model is calculated through the temporal and spatial winding numbers squared ($\langle W_t^2 \rangle$ and $\langle W_i^2 \rangle$ with $i \in \{1, 2\}$).
III. NUMERICAL RESULTS

To conduct the proposed investigation, we have carried out large-scale quantum Monte Carlo calculations (QMC) using the stochastic series expansion algorithm (SSE) with efficient operate-loop update [7]. The obtained outcomes are described in the following subsections.

A. The determination of spin-wave velocity $c$

The observable spin-wave velocity $c$ is required to compute the numerical value of $\chi_u c^2 / T$. Therefore we have calculated this quantity first.

We compute the spin-wave velocity $c$ by the method of winding numbers squared [4, 8]. The procedure is as follows. For a given box size $L$ and a $J'/J$, the value of $\beta$ is tuned so that $\langle W_i^2 \rangle$ and $\langle W^2 \rangle = \frac{1}{2} \sum_{i=1,2} \langle W_i^2 \rangle$ match each other quantitatively. When this condition is fulfilled, the spin-wave velocity $c(L, J'/J)$ associated with this set of $L$ and $J'/J$ is given by $c(L, J'/J) = L/\beta$.

It should be pointed out that the existence of long-range antiferromagnetic order is essential to employ this method to calculate $c$. As a result, we conduct the related simulations at $J'/J = 2.4975$ which is close to the critical point $(J'/J)_c = 2.4981(2)$ and is in the antiferromagnetic phase.

The spin-wave velocity $c$ as a function of the linear system size $L$ is shown in fig. 2. The data in fig. 2 is fitted to the equation of $a_0 + a_1/L + a_2/L^2$. The determined $a_0$ is the bulk $c$ and is given by 1.952(5). The obtained $c$ will be used in estimating the numerical value of $\chi_u c^2 / T$.

B. $\chi_u c^2 / T$ as functions $\beta$

The simulations of calculating $\chi_u$ are done with $L = 128, 256$, and 512. In addition, the uncertainty of $(J'/J)_c$ is taken into account in these simulations. Using $c = 1.952(5)$, the $\chi_u c^2 / T$ of various $L$ and $(J'/J)_c$ as functions of $\beta$ are shown in fig. 3. The outcomes shown in the figure indicate that as $L$ and $\beta$ increase, the value of $\chi_u c^2 / T$ deviates from its analytic prediction of 0.27185 (the horizontal dashed line in the figure) and approaches 0.32 (the horizontal solid line in the figure). This result agrees with that of [4] and [5].

IV. DISCUSSIONS AND CONCLUSIONS

In this study, we calculate the numerical value of $\chi_u c^2 / T$ corresponding to the 2D dimerized quantum her-ringbone Heisenberg model using QMC. By simulating lattice as large as $L = 512$ at moderate low temperatures, we obtain $\chi_u c^2 / T \sim 0.32$. Our result deviates from the associated analytic prediction $\chi_u c^2 / T = 0.27185$ but agrees quantitatively with recent numerical calculations of 2D spin-1/2 bilayer and plaquette Heisenberg models. Based on the obtained outcomes in this study, it will be interesting to refine the relevant theoretical calculations.

Acknowledgement

Partial support from National Science and Technology Council (NSTC) of Taiwan is acknowledged (MOST 110-2112-M-003-015 and MOST 111-2112-M-003-011).

Author Contributions

F.J.J proposed the project, conducted the calculations, analyzed the data, and wrote up the manuscript.

Conflict of Interest

The author declares no conflict of interest.
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