Criticality of the low-frequency conductivity for the bilayer quantum Heisenberg model

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Abstract. The criticality of the low-frequency conductivity for the bilayer quantum Heisenberg model was investigated numerically. The dynamical conductivity (associated with the O(3) symmetry) displays the inductor \( \sigma(\omega) = (i\omega L)^{-1} \) and capacitor \( i\omega C \) behaviors for the ordered and disordered phases, respectively. Both constants, \( C \) and \( L \), have the same scaling dimension as that of the reciprocal paramagnetic gap \( \Delta^{-1} \). Then, there arose a question to fix the set of critical amplitude ratios among them. So far, the O(2) case has been investigated in the context of the boson-vortex duality. In this paper, we employ the exact diagonalization method, which allows us to calculate the paramagnetic gap \( \Delta \) directly. Thereby, the set of critical amplitude ratios as to \( C, L \) and \( \Delta \) are estimated with the finite-size-scaling analysis for the cluster with \( N \leq 34 \) spins.

PACS. 75.10.Jm Quantized spin models – 05.70.Jk Critical point phenomena – 75.40.Mg Numerical simulation studies – 05.50.+q Lattice theory and statistics (Ising, Potts, etc.)

1 Introduction

For the O(N)-symmetric (2 + 1)-dimensional system, the low-frequency conductivity (associated with the O(N) symmetry group) exhibits the inductor \( \sigma(\omega) = (i\omega L)^{-1} \) and capacitor \( i\omega C \) behaviors in the ordered and disordered phases, respectively [1]. In Fig. 1, a schematic drawing of \( L^{-1} \) and \( C^{-1} \) is presented for both ordered \( (J > J^*) \) and disordered \( (J < J^*) \) phases; here, the symbols, \( T \) and \( \sigma_q \), denote the helicity modulus and the quantum conductance \( \sigma_q = q^2/h \), respectively. A key ingredient is that the conductivity in two (spatial) dimensions is scale-invariant, and both constants, \( L^{-1} \) and \( C^{-1} \), have the same scaling dimension as that of the paramagnetic gap \( \Delta \); note that the angular velocity \( \omega \) has the same scaling dimension as that of the energy gap (reciprocal correlation length). Then, there arose a question to fix the set of amplitude ratios among \( L^{-1}, C^{-1} \) and \( \Delta \). These parameters govern the low-energy physics for both transport and spectral properties [2]. For generic values of \( N = 2, 3, \ldots \), these amplitude ratios were estimated with the non-perturbative renormalization-group method [3]; an overview is presented afterward. In Fig. 1, the Higgs mass gap \( m_H \) is shown as well. The critical amplitude ratio \( m_H/\Delta \) has been investigated rather extensively [4][5][6][7]. The Higgs particle may have a short life time for \( N \geq 3 \) [8]; the extended symmetry group O(N) leads to enhanced Goldstone-mode-mediated decay of the Higgs particle.

The underlying physics behind the amplitude ratio \( C/L \) would be elucidated by the duality theory for O(2) [9][10][11]. The case O(2) is relevant to the superfluid-insulator transition. According to the duality theory, the boson conductivity \( \sigma \) and its dual one (vortex conductivity) \( \sigma_v \) satisfy the reciprocal relation \( \sigma \sigma_v = q^2/h^2 \), resulting in the contrasting behaviors between the superfluid and insulator phases for the transport properties; see Fig. 1. Correspondingly, the superfluid and Mott-insulator phases are characterized by the superfluid density \( \rho_s (= T) \) and the vortex-condensation stiffness \( \rho_v \), respectively. These constants \( \rho_s, \rho_v \) are related to the reaction as \( \rho_s = h/(2\pi\sigma_q L) \) and \( \rho_v = \sigma_q h/(2\pi C) \), respectively [11]. Therefore, the amplitude ratio \( \rho_s/\rho_v = C/(L\sigma_q^2) \) admits a “quantitative measure” [12] of deviation from self-duality. As a matter of fact, the renormalization group method [3] yields \( \rho_s/\rho_v = 0.210 \) \((N = 2) \), which indicates marked deviation from self-duality \((\rho_s/\rho_v = 1) \). Although the duality idea does not apply to the O(3) case, the amplitude ratio \( C/L \) still makes sense, and worth considering [3]. Experimentally [13][14][15], the vortex-condensate stiffness \( \rho_v \) (equivalently, \( C \)) is an observable quantity [12], and hence, the amplitude ratio \( \rho_s/\rho_v \) is not a mere theoretical concept.

In this paper, we devote ourselves to the case O(3). For that purpose, we consider the bilayer Heisenberg model [11], which exhibits [16] the phase transition belonging to the O(3)-universality class [17][18]. We employed the exact diagonalization method, which allows us to calculate the dynamical quantities such as the paramagnetic gap \( \Delta \) without resorting to the inverse Laplace transformation.
In this section, we estimate the amplitude ratio $\Upsilon/\Delta$. The O(3) case has been investigated with the non-perturbative renormalization group [3,5,19] and Monte Carlo [1] methods.

The Hamiltonian for the bilayer Heisenberg model is given by

$$\mathcal{H} = -J \sum_{a=1}^{2} \sum_{\langle ij \rangle} S_{ai} \cdot S_{aj} - J_2 \sum_{a=1}^{2} \sum_{\langle \langle ij \rangle \rangle} S_{ai} \cdot S_{aj} + J' \sum_{i}^{N/2} S_{i1} \cdot S_{i2}. \quad (1)$$

Here, the quantum spin $S_{ai}$ is placed at each square-lattice point $i = 1, 2, \ldots, N/2$ within the layer specified by $a = 1, 2$. The summations, $\sum_{\langle ij \rangle}$ and $\sum_{\langle \langle ij \rangle \rangle}$, run over all possible nearest-neighbor and next-nearest-neighbor pairs, $\langle ij \rangle$ and $\langle \langle ij \rangle \rangle$, respectively, within each layer. The parameters $J$ and $J_2$ are the corresponding coupling constants. The variable $J'$ denotes the inter-layer antiferromagnetic interaction, which stabilizes the paramagnetic phase. According to the Monte Carlo simulation [14], a critical point

$$(J^*, J_2^*, J'^*) = (0.435, 0, 1), \quad (2)$$

was found. Our simulation was performed around this critical point.

It has to be mentioned that the conductivity for the Heisenberg model has been investigated extensively in the three-dimensional Heisenberg universality class. Hence, there is no adjustable fitting parameter involved in the scaling analysis. Rather satisfactorily, the scaled data obey the finite-size scaling for a considerably wide range of $\delta J$. In Fig. 2, it is notable that the paramagnetic gap closes (opens) in the (dis)ordered phase $\delta J > (\sim)$. In other words, the critical point $\nu = 0.7112$ [17,18] as well as the critical exponent $\nu = 0.7112$ [17,18] are supported by the present exact-diagonalization analysis. For such thermodynamic behavior, however, the Monte Carlo method is more advantageous than the exact-diagonalization approach. Hence, we do not pursue further details, and turn our attention to the analysis of the transport properties.

We turn to the analysis of the amplitude ratio $\mathcal{T}/\Delta$. In Fig. 3 we present the scaling plot, $\delta J \ell^{1/\nu} \cdot \mathcal{T}(\delta J)/\Delta(\delta J)$, for $N = 30$, $32$, and $34$. Here, the scaling parameter $\nu$ is the same as that of Fig. 2. The helicity modulus is calculated by the formula

$$\mathcal{T} = \frac{3}{2\ell^2} \langle 0 | K | 0 \rangle + \frac{3}{\ell^2} \left( \frac{P}{\mathcal{H} - E_0} \right) \langle 0 | j \cdot P | 0 \rangle. \quad (4)$$

Here, the symbols $E_0$, $P$, $K$ and $\delta J$ denote ground-state energy (eigenvalue), projection operator $P = 1 - |0\rangle \langle 0 |$, diamagnetic contribution, and current operator, respectively; in Appendix, the explicit formulas for $K$ and $J$ are presented. The overall prefactor $3/2$ is due to Ref. [20]. The resolvent term (the second term of Eq. (4)) was evaluated with the continued-fraction-expansion method [21]. The continued-fraction-expansion method is essentially the same as the Lanczos-tri-diagonalization sequence, and it is computationally less demanding.

In Fig. 3 we observe a plateau extending in a considerably wide range of parameter $\delta J \ell^{1/\nu} > 0.5$. This parameter indicates that the amplitude ratio takes a constant value $\mathcal{T}/\Delta \sim 0.4$. In a closer look, we found that the plateau takes an extremal point $\delta J \mathcal{T}(\delta J)/\Delta(\delta J)|_{\delta J = \delta J} = 0$ at $\delta J = \delta J$. The plateau height at this point may serve a good indicator for $\mathcal{T}/\Delta$.

In Fig. 4, we present the approximate amplitude ratio $\mathcal{T}/\Delta$ for $1/\ell^2$. The approximate amplitude ratio denotes the plateau height

$$\mathcal{T}/\Delta = \mathcal{T}(\delta J)/\Delta(\delta J)|_{\delta J = \delta J}. \quad (5)$$
for each system size. The least-squares fit to these data yields an estimate $T/\Delta = 0.434(64)$ in the thermodynamic limit $\ell \to \infty$. The data exhibit a wavy deviation; the bump at $1/\ell^2 \approx 0.082\ldots(=1/3.5^2)$ and depression at $\approx 0.049\ldots(= 4.5^2)$ are due to an artifact of the screw-boundary condition $[24]$. The wavy deviation amplitude appears to be $\sim 0.06$, which is bounded by the above-mentioned least-squares-fit error 0.064. Accepting the uppermost value 0.07 as an error margin, we estimate the amplitude ratio as

$$\frac{T}{\Delta} \approx \frac{h}{2\pi\sigma_l L/\Delta} = 0.43(7). \quad (6)$$

A comparison with the related studies is made in Sec. 2.2.4. Last, we address a remark as to the criticality of the bilayer Heisenberg model $[1]$ as well as the scaling analyses of Figs. 2 and 3. The imaginary time and the spatial distance have the same scaling dimension. Hence, the bilayer quantum model at the ground state belongs to the three-dimensional universality class. This mapping was confirmed by the analysis of Fig. 2. The correlation-length critical exponent $\nu$ is the same as that of Fig. 2. We observe a satellite peak of Figs. 2 and 3, where the abscissa scale is set to this scale-invariant parameter $\delta J(=0.55)$. In this section, we estimate the amplitude ratio $C/L\sigma_q^2(=T \cdot 2\pi C/\hbar\sigma_q)$. The capacitance $C$ is evaluated via the formula $C = \partial^2 \chi_c(k)/\partial k^2$ with the charge-density-wave susceptibility $\chi_c(k)$ (see Appendix). It is an advantage of the exact diagonalization method that the capacitance is calculated directly at the ground state; otherwise, the finite-temperature effect has to be assessed carefully.

### 2.2 Amplitude ratio $C/L\sigma_q^2(=T \cdot 2\pi C/\hbar\sigma_q)$

In this section, we estimate the amplitude ratio $C/L\sigma_q^2(=T \cdot 2\pi C/\hbar\sigma_q)$. The capacitance $C$ is evaluated via the formula $C = \partial^2 \chi_c(k)/\partial k^2$ with the charge-density-wave susceptibility $\chi_c(k)$ (see Appendix). It is an advantage of the exact diagonalization method that the capacitance is calculated directly at the ground state; otherwise, the finite-temperature effect has to be assessed carefully. In this section, we consider the interaction subspace $\delta J_2 = 0.15\delta J$.

In Fig. 3, we present the scaling plot, $\delta J L^{\nu/(\nu-2)} C(\delta J)/L(-\delta J)\sigma_q^2 |_{\delta J = \delta J}$, for $N = 30$ ($\times$), 32 ($\times$), and 34 ($\times$); here, the scaling parameter $\nu$ is the same as that of Fig. 2. We observe a plateau in the disordered phase $\delta J L^{\nu/(\nu-2)} < -2$. There appears an extremum point $\partial^2 \chi_c(k)/\partial k^2 |_{\delta J = \delta J}$, at $\delta J = \delta J$. The plateau height at this point may provide a good indicator for $C/L\sigma_q^2$.

In Fig. 4, we present the approximate amplitude ratio $C/L\sigma_q^2$ for $1/\ell^2$. Here, the approximate amplitude ratio denotes the plateau height $C/L\sigma_q^2 \approx C(\delta J)/L(-\delta J)\sigma_q^2 |_{\delta J = \delta J}$.

for each system size. The least-squares fit to these data yields an estimate $C/L\sigma_q^2 = 0.193(33)$ in the thermodynamic limit. The intermittent bump and shallow depression around $1/\ell^2 \approx 0.625(=1/4^2)$ and $\approx 0.111\ldots(=1/3^2)$, respectively, are due to an artifact of the screw boundary condition $[24]$. Such wavy deviation amplitude $\approx 0.03$ is bounded by the above-mentioned least-squares-fit error 0.033. Accepting the uppermost value 0.04 as an error margin, we estimate the amplitude ratio as

$$\frac{C}{L\sigma_q^2} \left(= \frac{T \cdot 2\pi C}{\hbar\sigma_q} \right) = 0.19(4). \quad (8)$$

### 2.3 Set of amplitude ratios ($T/\Delta, \hbar\sigma_q/2\pi C\Delta, C/L\sigma_q^2$): A brief overview

The amplitude ratios, Eqs. (6) and (9), immediately yield yet another one

$$\hbar\sigma_q/(2\pi C\Delta) = 2.3(6). \quad (9)$$

This amplitude ratio, in the O(2) case, reduces to $\rho_\sigma/\Delta$, which is dual to $\rho_\sigma/\Delta$. The above amplitude ratios, Eqs. (9) and (10), with $\hbar\sigma_q/2\pi C\Delta$ almost fix the low-energy physics of the O(3)-symmetric system in proximity to the critical point. The Higgs mode is hardly observable, because it is smeared out by the Goldstone modes $[29]$. Hence, it is significant to fix the amplitude ratio $\hbar\sigma_q/(2\pi C\Delta)$ quantitatively in order to search for the (putative) Higgs branch hidden by the Goldstone continuum.

This is a good position to address an overview on related studies; see Table 1. First, the amplitude ratio $T/\Delta$ was estimated with the Blaizot-Méndez-Galain-Wschebor (BMW) non-perturbative renormalization group (NPRG) method as $T/\Delta = 0.401$ $[5]$. Alternatively, with the derivative-expansion (DE) NPRG method, the estimates, $T/\Delta = 0.441$ $[3]$, and 0.3177 $[19]$ were obtained. According to the Monte Carlo simulation $[1]$, an estimate $T/\Delta = 0.34(1)$ was reported. Our result supports recent NPRG studies, $T/\Delta = 0.401$ $[5]$ and 0.441 $[3]$; as for the technical advantage of the former approach, namely, the NPRG-BMW method, we refer the reader to Ref. $[30]$. Second, for $\hbar\sigma_q/2\pi C\Delta$, the NPRG-DE analysis $[3]$ reported 1.98. Additionally, we draw reader’s attention to its O(2) counterpart 1.98 as well. The results for O(2) and O(3) seem to coincide with each other. As a matter of fact, according to the large-N analysis $[31]$, this amplitude ratio converges to $12/\pi = 1.909\ldots$ as $N \to \infty$. Hence, it is suggested that the $N \to \infty$ consideration almost suffices for the analysis of $\sigma_q/\sqrt{C}\Delta$. Last, we turn to $C/L\sigma_q^2$. Our result supports the NPRG-DE one 0.2226 $[3]$. These results indicate that a seemingly feasible relation $L/C\sigma_q^2 \approx 1$ is not quite validated. Hence, so as to fix this amplitude ratio quantitatively, it is desirable to carry out the non-perturbative analysis and the brute-force calculation.

### 3 Summary and discussions

The bilayer Heisenberg model $[1]$ was investigated with the exact diagonalization method, which enables us to
calculate the ground-state spectral and transport properties such as $\Delta$, $L$, and $C$ directly. Thereby, we shed light on its low-frequency conductivity beside the critical point (Fig. 1). So far, the $O(2)$ case has been investigated with the aide of the boson-vortex duality. By means of the finite-size-scaling analysis for the cluster with $N \leq 34$ spins, we obtained the amplitude ratios $(\Upsilon/\Delta, h\sigma/2\pi C\Delta, C/L\sigma^2) = (0.43(7), 2.3(6), 0.19(4))$. As for $\Upsilon/\Delta$, with the NPRG and Monte Carlo methods, there have been reported a number of estimates, $0.441$ [3], $0.401$ [5], and $0.3177$ [19], and $0.34(1)$ [4]. Our result supports the recent NPRG results $0.441$ [3] and $0.401$ [5]. Likewise, as for $h\sigma/2\pi C\Delta$ and $C/L\sigma^2$, our results agree with those of the recent NPRG study $3$, $1.98$ and $0.2226$, respectively. The latter suggests that a seemingly feasible relation $C/L\sigma^2 = 1$ is not validated quantitatively.

As a matter of fact, according to the proceeding computer simulation analyses [2,5,44], there was reported an estimate $m_H/\Delta \sim 2.2-2.7$, which differs significantly from the mean-field value $m_H/\Delta = \sqrt{2}$ [3]. The spectral and transport properties seem to acquire notable corrections with respect to those obtained through the hand-waving arguments. In this sense, so as to fix the low-energy phenomenology of the $O(N)$-symmetric spectral and transport properties [2], the non-perturbative and brute-force approaches may be desirable.

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**Table 1.** Preceding results for $O(3)$ are summarized. The non-perturbative renormalization group (NPRG) method has a number of variants. The abbreviations, DE and BMW, denote derivative expansion and Blaizot Méndez-Galain Wschebor, respectively.

| Amplitude ratios | $\Upsilon/\Delta$ | $h\sigma/2\pi C\Delta$ | $C/L\sigma^2$ |
|------------------|-------------------|------------------------|--------------|
| This work        | 0.43(7)           | 2.3(6)                 | 0.19(4)      |
| NPRG-DE [3]      | 0.441             |                        |              |
| NPRG-BMW [5]     |                   | 1.98                   | 0.2226       |
| NPRG-DE [19]     |                   |                        | 0.3177       |
| Monte Carlo [4]  |                   |                        | 0.34(1)      |
Fig. 5. The scaling plot of the amplitude ratio $Y/\Delta$, is plotted for $1/\ell^2$. The least-squares fit yields an estimate $Y/\Delta = 0.434(64)$ in the thermodynamic limit. A bump around $1/\ell^2 \approx 0.82 \ldots (= 3.5\%)$ and a depression around $\approx 0.49 \ldots (= 1/4.5\%)$ are due to an artifact of the screw-boundary condition \[24\]. A systematic error is considered in the text.

Fig. 6. The approximate amplitude ratio $C/L\sigma^2$, is plotted for $1/\ell^2$. The least-squares fit yields an estimate $C/L\sigma^2 = 0.193(33)$ in the thermodynamic limit. The intermittent bump and shallow depression around $1/\ell^2 \approx 0.625(= 1/4^2)$ and $0.111 \ldots (= 1/3^2)$, respectively, are due to an artifact of the screw-boundary condition \[24\]. A possible systematic error is considered in the text.

Simulation algorithm: Screw-boundary condition

In this paper, in order to implement the screw-boundary condition \[24\], we adopted the simulation algorithm as presented in Eq. (A.1) of Ref. \[7\]. The screw-boundary condition enables us to treat a variety of system sizes $N = 18, 20, \ldots, N$ in a systematic manner. The underlying idea behind this algorithm \[24\] is that an alignment of spins $S_i (i = 1, 2, \ldots)$ is wound up to form a toroidal coil, which is equivalent to a rectangular cluster under the screw-boundary condition. In the following, we present a number of extensions in order to cope with the $J_2$ interaction and transport properties. First, we need to incorporate the $J_2$ interaction. For that purpose, we added the term $-J_2 \sum_{n=1}^{N/2} \sum_{i=1}^{N/2} [S_{ai}(\ell + 1) \cdot S_{ai} - S_{ai}(\ell - 1) \cdot S_{ai}]$ with $\ell = \sqrt{N/2}$ to Eq. (A.1) of Ref. \[7\]. Here, the symbol $S_{ai}(\delta)$ denotes the $\delta$-shifted operator $S_{ai}(\delta) = P^{-\delta}a_i P^\delta$ with the translation operator $P$ \[24\]. Second, the current operator $\hat{J}$ in Eq. (11) is given by

$$\hat{J} = \frac{iJ}{2} \sum_{n=1}^{N/2} \sum_{i=1}^{N/2} (S_{ai}(1) S_{ai}^- - S_{ai}^-(1) S_{ai}^+)$$

$$+ \frac{iJ}{2} \sum_{n=1}^{N/2} \sum_{i=1}^{N/2} (S_{ai}(\ell + 1) S_{ai}^- - S_{ai}^-(\ell + 1) S_{ai}^+)$$

$$- \frac{iJ}{2} \sum_{n=1}^{N/2} \sum_{i=1}^{N/2} (S_{ai}(\ell - 1) S_{ai}^- - S_{ai}^-(\ell - 1) S_{ai}^+). (10)$$

Likewise, the diamagnetic part in Eq. (11) is given by

$$K = \frac{J}{2} \sum_{n=1}^{N/2} \sum_{i=1}^{N/2} (S_{ai}(1) S_{ai}^+ + S_{ai}^-(1) S_{ai}^-)$$

$$+ \frac{J_2}{2} \sum_{n=1}^{N/2} \sum_{i=1}^{N/2} (S_{ai}(\ell + 1) S_{ai}^+ + S_{ai}^-(\ell + 1) S_{ai}^-)$$

$$+ \frac{J_2}{2} \sum_{n=1}^{N/2} \sum_{i=1}^{N/2} (S_{ai}(\ell - 1) S_{ai}^+ + S_{ai}^-(\ell - 1) S_{ai}^+). (11)$$

Last, we calculated the capacitance $C$ via the formula $C = \frac{1}{2} \langle 0 | N_{k_1}^T (H-E_0)^{-1} N_k | 0 \rangle / k_l^2$ with $N_k = \sum_{n=1}^{N/2} \sum_{j=1}^{N/2} e^{ijk} S_{aj}^+$ and $k_1 = 2\pi / L \[12\].
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