Universality Class around the SU(3) Symmetric Point of the Dimer-Trimer Spin-1 Chain

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We numerically diagonalize the Dimer-Trimer (DT) spin-1 chain Hamiltonian in the vicinity of the SU(3) symmetric point, named the pure trimer (PT) point. We analyze our numerical results with the conformal field theory (CFT). First of all, we discover soft modes at the wave number $q = 0$ and $q = \pm \pi/3$ for the PT point, which means that the system is critical. Secondly, we find that the system at the PT point belongs to the CFT with the central charge $c = 2$ and the scaling dimension $x = 2/3$. Finally, by investigating the eigenvalues of the Hamiltonian in the vicinity of the PT point, we find that there is a phase transition at the PT point from a massive phase to a massless phase. From these numerical results, the phase transition at the PT point belongs to the Berezinskii-Kosterlitz-Thouless (BKT)-like universality class that is explained by the level-1 SU(3) Wess-Zumino-Witten (SU(3) WZW) model.

1 Introduction

Recently, there have been major achievements in the development of experiments and quantum simulations of ultracold alkaline earth metallic atoms in an optical lattice [11,13]. To illustrate these kinds of systems, the SU(ν) symmetric Hubbard model [4] (ν: integer) has especially attracted attentions, which is a generalization of the SU(2) spin-1/2 Fermi-Hubbard model. One can more deeply understand these kinds of systems by investigating SU(ν) symmetric Hamiltonians of spin chains.

In this paper, we investigate an example of spin chains, the Dimer-Trimer (DT) spin-1 chain [5], with SU(3) symmetry. The DT model Hamiltonian is defined [5] as

$$\hat{H}_{\text{DT}} = -\sum_{i=1}^{N} \left[ \cos \theta \hat{D}(i) + \sin \theta \hat{T}(i) \right],$$

(1)

competing dimer and trimer interactions. The operators $\hat{D}(i)$ and $\hat{T}(i)$ are defined as follows. To begin with, we let $\hat{S}_i$ denote the spin-1 operator at site $i$. We then introduce $\hat{S}_{ij} \equiv \hat{S}_i + \hat{S}_j$ for a pair of adjacent sites ($j \equiv i + 1$), and $\hat{S}_{ijk} \equiv \hat{S}_i + \hat{S}_j + \hat{S}_k$ for a set of three adjacent sites ($k \equiv i + 2$). Then, we define the dimer projection operator $\hat{P}_D(i)$ and the trimer projection operator $\hat{P}_T(i)$ as [5]

$$\hat{P}_D(i) \equiv \frac{1}{12} \left( \hat{S}_{ij}^2 - 2 \right) \left( \hat{S}_{ij}^2 - 6 \right),$$

(2)

$$\hat{P}_T(i) \equiv -\frac{1}{144} \left( \hat{S}_{ijk}^2 - 2 \right) \left( \hat{S}_{ijk}^2 - 6 \right) \left( \hat{S}_{ijk}^2 - 12 \right).$$

(3)

Each projection operator gives an eigenvalue +1 for spin singlets, and 0 for all other spin multiplets. The operators used in Eq. (1) are expressed [5] as

$$\hat{D}(i) \equiv 3\hat{P}_D(i),$$

(4)

$$\hat{T}(i) \equiv 6\hat{P}_T(i).$$

(5)

The DT model was originally proposed [5] for the sake of explaining the characteristics of a trimer liquid (TL). It has been so far hard to write down a microscopic spin-1 Hamiltonian describing the TL phase. This is due to the lack of the orthogonality of different trimer configurations. Oh et al. carried out [5] numerical calculations employing the density-matrix renormalization group (DMRG), which tried to identify the phases of the DT model according to the parameter $\theta$. The region $\pi/8 < \theta < \pi/4$ is the symmetry-protected topological (SPT) phase. The phase is translationally symmetric and a massive phase. The region $\pi/4 < \theta < \pi$, the TL phase, is a massless phase and has soft modes at the wave number $q = 0, \pm \pi/3$. The point $\theta = \pi/2$, called the PT point, is SU(3) symmetric. In Ref. [5], it was argued that the PT point lies in the TL phase.

Here, we review other theories of SU(3) symmetric systems of spin chains. The issue has drawn significant attention in a spin-1 chain, whose Hamiltonian is

$$\hat{H}_{\text{BLBQ}} = \sum_{i=1}^{N} \left[ \cos \theta \left( \hat{S}_i \cdot \hat{S}_{i+1} \right) + \sin \theta \left( \hat{S}_i \cdot \hat{S}_{i+1} \right)^2 \right].$$

(6)

named the bilinear-biquadratic (BLBQ) Hamiltonian. The region $-\pi/4 < \theta < \pi/4$ has the ground state illustrated by the Haldane phase, in which there is the spin-1 antiferromagnetic Heisenberg model [6] at $\theta = 0$, and several exact results were obtained [7,8] at $\theta = \tan^{-1}(1/3)$. The phase is translationally invariant and a massive phase [10,11]. The region $\pi/4 < \theta < \pi/2$ is the massless trimerized (spin quadrupolar) phase, which was investigated by several numerical works [12,13]. The massless trimerized phase has soft modes at $q = 0, \pm 2\pi/3$ [13]. The point $\theta = \pi/4$, which is SU(3) symmetric, is known as the Uimin-Lai-Sutherland (ULS) point [15,16], which is exactly solvable by the Bethe ansatz. The system at the ULS point is critical, whose universality class is explained by the level-1 SU(3) Wess-Zumino-Witten (SU(3) WZW) model [19,21]. The SU(3) WZW model reproduces several exact results [22,23] gained from the Bethe ansatz. Around the ULS point, numerical studies were carried out [14] to calculate the central charge $c$, which is utilized to determine the universality class of the system. Itoi and Kato analyzed [24] systems around the ULS point with renormalization group (RG). They found [25] that the phase transition at the ULS point belongs to the Berezinskii-Kosterlitz-Thouless (BKT)-like universality...
class, which we explain in the next paragraph. Additionally, at the ULS point, they observed several non-trivial behaviors as in the conformal field theory (CFT) formulated by marginal operators [25,30,32].

In a system that belongs to the BKT or BKT-like universality classes, the correlation length $\xi$ behaves as [29]

$$\xi \sim \begin{cases} \exp \left[ C(\theta_C - \theta)^{-\sigma} \right], & (\text{for } \theta < \theta_C) \\ \infty, & (\text{for } \theta \geq \theta_C) \end{cases}$$

(7)

where $C$ is a constant positive, $\theta_C$ is a phase transition point, and $\sigma$ is a critical exponent. In a system with the U(1) symmetry, such as the 2D classical XY model, it is known that the exponent $\sigma = 1/2$ and the central charge $c = 1$. This kind of phase transition is generally called the BKT transition. On the other hand, if the system has symmetries higher than U(1), it can be $\sigma \neq 1/2$ and $c \neq 1$. In this paper, we will call this kind of phase transition the BKT-like transition.

In this paper, we numerically study the Hamiltonian of the DT model under periodic boundary condition (PBC), $S_{N+i} = S_i$, to investigate critical behaviors near the PT point. The DT model Hamiltonian at the PT point is composed only of exchange operators

$$\hat{P}_{ij}$$

In this theory, in the case of the ULS point of the BLBQ model, the ground-state energy is the lowest energy at $q = 0$, and $S_T = 0$, $E_g = E(0) = E_0(0)$. Moreover, soft modes appear at $q = 0, \pm 2\pi/3$ for all the system sizes as shown in Fig. 1. These results are consistent with the theory of Sutherland [15].

3 The PT Point

In this section, we show the results of our numerical calculations of the DT model Hamiltonian at the PT point, utilizing the conservation of the number of each spin, $N_1$, $N_0$, $N_{-1}$, and the translational symmetry. Then, we investigate several physical quantities, mainly the scaling dimension $x$ and the central charge $c$, to specify the universality class of the system.

To begin with, we let $\hat{T}$ be a translational operator, which shifts spins in the system by one site. $\hat{T}$ has an eigenvalue written as

$$\hat{T}|\cdots\rangle = \exp(\imath q)|\cdots\rangle,$$

(13)

where $q$ is the wave number. Under PBC, $\hat{T}^N$ is an identity operator. Therefore, the wave number should be $q = 2\pi n/N$ ($n$: integer).

The energy eigenvalue $E$ is a function of the wave number $q$ and the total spin quantum number of the system $S_T$. So, we let $E_{S_T}(q)$ denote the lowest energy at certain $q$ and $S_T$. We define the difference between $E_{S_T}(q)$ and the ground-state energy $E_g$ as

$$\Delta E_{S_T}(q) \equiv E_{S_T}(q) - E_g.$$ 

(14)

Then, we let $E(q)$ be the lowest energy at a certain $q$ and define the difference between $E(q)$ and $E_g$ as

$$\Delta E(q) \equiv E(q) - E_g.$$ 

(15)

3.1 Dispersion curves

Figure 1 shows dispersion curves at the PT point with $N = 9 \sim 21$ as a function of the wave number $q$. We find that the ground-state energy is the lowest energy at $q = 0$ and $S_T = 0$, $E_g = E(0) = E_0(0)$. Moreover, soft modes appear at $q = 0, \pm 2\pi/3$ for all the system sizes as shown in Fig. 1. These results are consistent with the theory of Sutherland [15].

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The spin wave velocity is a function of $N$, $v_0(N)$. In the numerical calculations, we investigate the slope of the spectrum shown in Fig. 1 in order to obtain the velocity written as

$$v_0(N) = \frac{E(2\pi/N) - E(0)}{2\pi/N}. \tag{20}$$

The values of the velocity are plotted in Fig. 3. We are interested in the behavior of systems near the ground state, therefore we choose $q_0 = 0$.

### 3.3 Scaling dimension

In this subsection, we show our numerical results of the scaling dimension. The scaling dimension is one of the critical exponents, which specify a universality class. The elementary excitation at a certain $S_T$ follows the equation \[29\]

$$\Delta E_{S_T}(\pm \frac{2\pi}{3}) = \frac{2\pi v_0}{N} \left(x_{S_T} + \frac{d_{S_T}}{\ln N}\right), \tag{21}$$

where $x_{S_T}$ is the scaling dimension at $S_T$ and $d_{S_T}$ is a coefficient depending on $S_T$. The $x_{S_T}$ and $d_{S_T}$ take the values \[29\] shown in Table. 1 at the point illustrated by the SU(3) WZW model corresponding to the line $g_1 < 0$, $g_2 = 0$ in Fig. 4. We apply these values to Eq. \[21\] and then remove the logarithmic correction in Eq. \[21\] by considering

$$\frac{1}{9} \left[ \Delta E_0 \left( \pm \frac{2\pi}{3} \right) + 3\Delta E_1 \left( \pm \frac{2\pi}{3} \right) + 5\Delta E_2 \left( \pm \frac{2\pi}{3} \right) \right] = \frac{2\pi v_0(N)}{N} r(N), \tag{22}$$

where we rewrite $v_0$ to $v_0(N)$ defined in Eq. \[20\]. We can acquire the effective scaling dimension at the system size $N$,

| $S_T = 0$ | $S_T = 1$ | $S_T = 2$ |
|-----------|-----------|-----------|
| $x_{S_T}$ | 2/3       | 2/3       | 2/3       |
| $d_{S_T}$ | 8/9       | -1/9      | -1/9      |

### 3.2 Spin wave velocity

In this subsection, we show our numerical results of the spin wave velocity, which is utilized for later calculations of the scaling dimension and the central charge. The spin wave velocity $v$ at a certain wave number $q_0$ is defined as

$$v_{q_0} = \frac{dE(q)}{dq} \bigg|_{q=q_0}. \tag{19}$$
where the effective central charge \( c(N, N-3) \) is determined by using Eq. (25) in combination with energy eigenvalues at two different system sizes \( N \) and \( N - 3 \). Also, the effective central charge \( c(N, N-3) \) converges as \( c(N, N-3) \to c \) shown in Eq. (25) in the thermodynamical limit \( N \to \infty \).

Additionally, similarly as Eq. (24), we extrapolate the effectivecentral charge \( c(N, N-3) \) as

\[
c(N, N-3) = c + D_1 (N-3/2)^{-2} + D_2 (N-3/2)^{-4} + O ((N-3/2)^{-6}),
\]

where \( D_1 \) and \( D_2 \) are constants. Note that although the central charge has a logarithmic correction as a form \( O ((\ln N)^{-3}) \) in the \( c = 2 \) CFT, we neglect it since it is small enough.

### 3.4 Central charge

In this subsection, we investigate the central charge, which is also one of the critical exponents, characterizes the quantum anomaly, and specifies the universality class of the system. At the critical point of one-dimensional quantum systems, the ground-state energy density at \( N \) should converge \[28,29\] as

\[
\frac{E_g(N)}{N} = \epsilon_{\infty} - \frac{\pi v_0 e}{6 N^2},
\]

where \( \epsilon_{\infty} \) is the ground-state energy density in the thermodynamic limit \( N \to \infty \) and \( c \) is the central charge. The ground-state energy densities are plotted in Fig. 5 at the PT point.

**FIG. 4:** The effective scaling dimension \( x(N) \) at the PT point as a function of \( N^{-2} \).

**FIG. 5:** The ground-state energy density \( E_g/N \) vs \( N^{-2} \) at the PT point.

**FIG. 6:** The effective central charge \( c(N, N-3) \) as a function of \((N-3/2)^{-2} \) at the PT point.
If we choose a function of the form $c(N, N - 3) = c + D_1(N - 3/2)^{-2}$ for extrapolating the effective central charge, and then we obtain $c = 2.0085 \pm 0.0026$ when we fit the $c(N, N - 3)$ with three points, $N = 15 \sim 21$. If we choose a function of the form $c(N, N - 3) = c + D_1(N - 3/2)^{-2} + D_2(N - 3/2)^{-4}$ as a fitting function, we obtain $c = 1.9677 \pm 0.0001$ when we fit the $c(N, N - 3)$ with four points, $N = 12 \sim 21$. From these results, we conclude that the system at PT point belongs to the CFT with $c = 2$.

4 Around the PT Point

In this section, we investigate the DT model Hamiltonian in the vicinity of the PT point to specify a phase transition and the universality classes of the systems, making use of the conservation of the magnetization, $M = \sum_i S_i^z$, and the translational symmetry. The reduction of the Hilbert space, mentioned in Sect. 2, is not so efficient except at the PT point. Thus, we deal with only smaller systems up to $N = 18$.

To begin with, we investigate the elementary excitations around the PT point to specify details of phases. In Fig. 7 we plot the excitation gaps at $q = \pm 2\pi/3$ of the singlet state ($S_T = 0$), the triplet state ($S_T = 1$), and the quintuplet state ($S_T = 2$) for varied $\theta$ with $N = 15, 18$. According to Fig. 7, the system lies in a massless phase, corresponding to the second quadrant $g_1 < 0, g_2 > 0$ and the line of $g_1 < 0, g_2 = 0$ in Fig. 8. They also found that if the energy excitations have an order other than Eq. (28), the system lies in a massive phase. Collating our numerical results in Fig. 7 with the theory [29], we find that the region $\theta \leq \pi/2$ in Fig. 7 is a massless phase. We also find that the region $\theta < \pi/2$ in Fig. 7 is a massive phase.

In summary, from Figs. 7 and 8 with the CFT plus the RG method, they found that if the order of the energy excitations is

$$\Delta E_0(\pm 2\pi/3) > \Delta E_1(\pm 2\pi/3) \geq \Delta E_2(\pm 2\pi/3),$$

the system lies in a massless phase, corresponding to the second quadrant $g_1 < 0, g_2 > 0$ and the line of $g_1 < 0, g_2 = 0$ in Fig. 8. They also found that if the energy excitations have an order other than Eq. (28), the system lies in a massive phase. Collating our numerical results in Fig. 7 with the theory [29], we find that the region $\theta \leq \pi/2$ in Fig. 7 is a massless phase. We also find that the region $\theta < \pi/2$ in Fig. 7 is a massive phase.
5 Conclusions

We have investigated the DT model to clarify the critical behavior around the PT point, by numerically diagonalizing the DT model Hamiltonian. We summarize our findings as follows. First of all, soft modes appear at the wave number $q = 1/2, \pi/3$ for the PT point, and the system is critical. Secondly, the PT point belongs to the SU(3) WZW universality class [19–21]. Finally, there occurs a phase transition at the PT point, unlike the results of Oh et al. [5] mentioned in Sect. 1. The discrepancy between our results and those of Oh et al. comes from the fact that the energy gap is too small for the DMRG to detect in the vicinity of the PT point. Thus, with the DMRG, one cannot properly discuss the critical phenomena that belongs to the BKT-like universality class. By contrast, numerical diagonalizations combined with the conformal field theory are suitable to study the critical phenomena, since one can use not only the energy eigenvalues but also the symmetric eigenvalues such as the wave-number.

We also believe that numerical results of the DT model can be applied to experiments and quantum simulations illustrated by SU($\nu$) symmetric Hubbard model [3], written in Sect. 11.

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APPENDIX:A

In this section, we review the RG calculation by Itoi and Kato [29] to investigate the critical behavior around the system of spin-1 chains illustrated by the SU(3) WZW model [19–21].

To begin with, we let $x_0$ be the time in the system and $z_1$ be the position of the field. We then put $z$ and $\bar{z}$ as follows

$$z \equiv x_0 + ix_1, \quad \bar{z} \equiv x_0 - ix_1.$$

(29)

We define the action $\hat{A}$ as

$$\hat{A} \equiv \hat{A}_{\text{SU}(3)_1} + \sum_{i=1}^{2} g_i \int \frac{d^2z}{2\pi} \hat{\Phi}^{(i)}(z, \bar{z}),$$

(30)

where $\hat{A}_{\text{SU}(3)_1}$ is the action of the free fields in the SU(3) WZW model [19–21]. Both $\hat{\Phi}^{(1)}$ and $\hat{\Phi}^{(2)}$ are operators of the marginal or relevant field with rotational symmetry and chiral $\mathbb{Z}_3$ symmetry. Especially, $\hat{\Phi}^{(1)}$ is SU(3) symmetric, $\hat{\Phi}^{(2)}$ is SU(3) asymmetric and U(1) symmetric. The scaling variables $g_1$ and $g_2$ are perturbational parameters. If $g_2 = 0$, the system remains SU(3) symmetric regardless of the value of $g_1$. If $g_2 \neq 0$, the SU(3) symmetry of the system is broken. According to Itoi and Kato [29], the renormalization-group equations for the scaling variables become

$$\begin{align*}
\frac{dg_1}{dl} &= \frac{1}{\sqrt{2}} \left( \frac{3}{2} g_1^2 + 3 g_1 g_2 \right), \\
\frac{dg_2}{dl} &= \frac{1}{\sqrt{2}} \left( \frac{3}{2} g_2^2 + 3 g_1 g_2 \right),
\end{align*}$$

(31)

(32)

From Eqs. 31 and 32, there is a fixed point at $g_1 = g_2 = 0$. Moreover, in the case of $g_1 = 0$, it remains 0 after the renormalization, and $g_2$ diverges or converges as follows

$$(g_1, g_2) \to \begin{cases} (0, 0), & \text{(for } g_2 > 0) \\
(0, -\infty), & \text{(for } g_2 < 0) \end{cases}$$

Also, in the case of $g_2 = 0$, it remains 0 after the renormalization, and $g_1$ diverges or converges as below

$$(g_1, g_2) \to \begin{cases} (\infty, 0), & \text{(for } g_1 > 0) \\
(0, 0), & \text{(for } g_1 < 0) \end{cases}$$

Here, we put $X \equiv g_1 - g_2$ and $Y \equiv -g_1 + g_2$. From Eqs. 31 and 32, we obtain two equations as

$$\begin{align*}
\frac{d}{dl} (X^2 - Y^2) &= \frac{\sqrt{2}}{1} (X^2 - Y^2) X, \\
\frac{d}{dl} |Y| &= -\frac{3}{2\sqrt{2}} |Y| X.
\end{align*}$$

(33)

(34)

Making use of these equations, we acquire

$$\frac{d}{dl} \left( \frac{X^2 - Y^2}{|Y|^{1/3}} \right) = 0.$$ 

(35)

In conclusion, a solution of the renormalization-group equations is found to be

$$X^2 - Y^2 = C |Y|^{1/3},$$

(36)

where $C$ is a constant.

From Eq. 36, flows [29] of the RG can be drawn, as shown in Fig. 9. Then, we can discuss critical behaviors around the system illustrated by the SU(3) WZW model [19–21], by analyzing the convergence and the divergence of the perturbational parameters, $g_1$ and $g_2$. The graph can be divided into six regions according to the values of $g_1$ and $g_2$. The parameters

![Figure 9: The trajectory gained from the solution of renormalization-group equations, Eq. 36.](image)
diverge or converge differently depending on the regions they belong to. After repeating the renormalization infinite times, they diverge or converge as shown below:

\[(g_1, g_2) \to \begin{cases} 
  (\infty, 0), & \text{for } g_1 > 0, g_2 > 0 \\
  (0, 0), & \text{for } g_1 < 0, g_2 > 0 \\
  (0, -\infty), & \text{for } g_1 < 0, g_2 < 0 \\
  (\infty, 0), & \text{for } g_1 > 0, g_2 < 0, g_1 + g_2 > 0 \\
  (\infty, -\infty), & \text{for } g_1 > 0, g_2 < 0, g_1 + g_2 = 0 \\
\end{cases}\]

Therefore, the region \(g_1 < 0, g_2 > 0\) is correspond to a massless phase, and the other regions are correspond to different massive phases. The transition point which we deal with in this paper corresponds to the line of \(g_1 < 0, g_2 = 0\), named SU(3) BKT-like line. According to Itoi and Kato \[29\], the order of the energy Eq. \[28\] holds only in the case where the parameters belong to the second quadrant, \(g_1 < 0, g_2 > 0\). Also, according to Fig. \[3\] the region \(\theta < \pi/2\) in Figs. \[7\] and \[8\] corresponds to the case where the parameters belong to the third quadrant, \(g_1 < 0, g_2 < 0\). In other words, the BKT-like transition in this paper corresponds to the transition between the second quadrant and the third quadrant.

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