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Degenerate States in Nonlinear Sigma Model with U(1) Symmetry

—For Study on Violation of Cluster Property

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Abstract

Entanglement in quantum theory is a concept that has confused many scientists. This concept implies that the cluster property, which means no relations between sufficiently separated two events, is non-trivial. In the works for some quantum spin systems, which have been recently published by the author, extensive and quantitative examinations were made about the violation of cluster property in the correlation function of the spin operator. The previous study of these quantum antiferromagnets showed that this violation is induced by the degenerate states in the systems where the continuous symmetry spontaneously breaks. Since this breaking is found in many materials such as the high temperature superconductors and the superfluidity, it is an important question whether we can observe the violation of the cluster property in them. As a step to answer this question we study a quantum nonlinear sigma model with U(1) symmetry in this paper. It is well known that this model, which has been derived as an effective model of the quantum spin systems, can also be applied to investigations of many materials. Notifying that the existence of the degenerate states is essential for the violation, we made numerical calculations in addition to theoretical arguments to find these states in the nonlinear sigma model. Then, successfully finding the degenerate states in the model, we came to a conclusion that there is a chance to observe the violation of cluster property in many materials to which the nonlinear sigma model applies.

Keywords

Quantum Nonlinear Sigma Model, U(1) Symmetry, Cluster Property, Spontaneous Symmetry Breaking, Degenerate States

1. Introduction

Entanglement [1] [2] [3] is quite difficult concept even for researchers [4], because it contradicts the classical concept on the locality [5]. This difficulty has not been reduced when a huge number of researchers apply entanglement to quantum information [6] [7] [8] after the birth of the concept of quantum computer [9] that originates from Deutsch [10]. Entanglement is the correlation of quantum objects, which can not be explained by the classical statistics. When the entangled correlation is found at the infinitely large distance, it leads to violation of the cluster decomposition [11], or the cluster property [12], which is a fundamental concept of physics that there is no relation between two events occurring infinitely apart from each other. Since this violation was found in toy models or in the academic models [12], there are active studies on the cluster property in the many-body systems [13] [14] [15] and in quantum field theory [16] [17] including QCD [18] [19].

In previous researches [20] [21] [22] we studied two-dimensional antiferromagnetic quantum spin systems on the square lattice with U(1) or SU(2) symmetry. We presented the methods to observe the violation of the cluster property on the system where the continuous symmetry breaks spontaneously [11] [23]. In the case of U(1) symmetry [20], we introduced, in order to make the ground state unique, an explicitly symmetry breaking interaction whose strength is g. Then we pointed out that the violation is the order of $1/\left(\sqrt{g}N_s\right)$ on the finite lattice with N_s sites. For the quantum spin system with SU(2) symmetry [21], we discussed the observation of the violation introducing two kinds of explicitly symmetry breaking interactions. Our results there also indicated the possibility to observe the violation, although the effect of the violation contains the factor $1/N_s$ so that fine experiments would be necessary. In the following work [22], however, we found this situation changes when the spin system couples with another spin system. We showed that the Hamiltonian in this work includes Curie-Weiss model [24] [25] [26] induced by the violation of the cluster property. Then we found that the effective Hamiltonian has the factor $1/N_s$, which is needed for the thermodynamical properties to be well-defined. We concluded that it is possible to find the effect from the violation of the cluster property through observing the thermodynamical properties given by Curie-Weiss model.

In these studies where our models are quantum antiferromagnets, we recognized that the degenerate states due to the spontaneous symmetry breaking induce this violation. As is well known this breaking is found in many materials [27] [28] [29], including the high temperature superconductor. It is quite important to examine whether we can observe the violation of the cluster property in such materials. Therefore we are sure that to observe the violation of the cluster property is not only a theoretical concern but also a subject to be experimentally investigated in many systems.

In order to make quantitative discussions, we need to find a model which effectively helps us to study the low energy behaviors in many systems. Keeping this purpose in mind we now study a quantum nonlinear sigma model, which has been derived as the effective model for two-dimensional Heisenberg antiferromagnets [30] [31] [32] and has been applied to various spin systems [33] [34] [35] [36]. We also find many applications of this model in particle physics [37] [38] [39], since the chiral Lagrangian that contains it has given fruitful results on hadron physics [40]. The reason for such wide applications is that this model realizes the symmetry by the minimum degrees of freedom when the continuous symmetry is spontaneously broken.

In our study of the cluster property with spontaneous symmetry breaking in the system on a lattice with N_s sites, the key observation is the quasi-degenerated states $\left|n_Q\right\rangle$ whose energy E_{n_Q} is the lowest one for a quantum number n_Q related to the symmetry. In the spin systems, it has been well known that the energy gap $E_{n_Q}-E_0$ is proportional to n_Q^2/N_s [27]. In our work on the nonlinear sigma model, we will reveal the existence of the quasi-degenerated states. We then show that the energy gap in this model is also proportional to n_Q^2/N_s.

Let us describe the plan of this paper.

In the next section, we describe our quantum nonlinear sigma model on the square lattice with U(1) symmetry. The first subsection is devoted to comments on the model which has the continuous symmetry. Then we clarify the quantum property of our model with the discrete symmetry in the second subsection. The third subsection discusses relations between these two models.

In many researches, the nonlinear sigma model is defined by the effective action [30] [34], where the local field is given by the finite and continuous variable called the angle variable. This effective action is given by the path integral so that it is defined by the classical variables, not by the quantum operators. In this work, on the contrary, we introduce the quantum theory of the discrete symmetry using a discrete and finite variable instead of the angle variable. The reason for it is that in numerical approaches we need to fix the quantum number to calculate the lowest energy with this number. We then introduce a state $\left|n\right\rangle_q$, where $n=0,1,\cdots,(L_d-1)$ with the degree of the discrete variable L_d. We expect that the discrete variable is close to the angle variable when L_d is large enough. In order to justify the model with the discrete variable, our discussion starts from the Weyl relation [41] [42] [43] where the basic operators are not hermitian but unitary. We replace the basic operators $\hat{q},\hat{p}$ by two kinds of unitary operators, $\hat{U}_q(t)=\exp(it\hat{q})$ and $\hat{U}_p(s)=\exp(is\hat{p})$. In other words, we have the Weyl relation $\hat{U}_q(t)\hat{U}_p(s)=\hat{U}_p(s)\hat{U}_q(t)\mathrm{e}^{ist}$ instead of the commutation relation $[\hat{q},\hat{p}]=i$. Note that the commutation relation on $\hat{q}$ and $\hat{p}$ can not be represented by finite dimensional matrices, while the Weyl relation on $\hat{U}_q(t)$ and $\hat{U}_p(s)$ can be extended to the operators $\hat{U}_q$ and $\hat{U}_p$ which are represented by finite dimensional matrices. A brief description for $\hat{U}_q(t)$ and $\hat{U}_p(s)$ as well as for $\hat{U}_q$ and $\hat{U}_p$ will be found in **Appendix**.

In the second subsection, we define our model on the square lattice where the unitary operators $\hat{U}_{qi}$ and $\hat{U}_{pi}$ are defined at each site *i*. The Hamiltonian of the model has two terms named *A*-term and *B*-term, which correspond with the kinetic term and the potential term in the ordinary nonlinear sigma model respectively. Here we introduce *q*-representation where the *B*-term of the Hamiltonian is diagonalized, and *p*-representation where the *A*-term is diagonalized. The Hamiltonian introduced in [31] has the symmetry that it does not change when we increase the angle variables at every site by the same magnitude. To this symmetry, we have the generator for which the quantum number is defined. Therefore we impose that our Hamiltonian is invariant under increment of the discrete variables, which correspond to the angles in the continuous symmetry, at every site by the same magnitude. By this invariance, we can define the unitary operator for the increment transformation. Furthermore, we can introduce the hermitian operator $\hat{n}_Q$ whose quantum number is denoted by the integer n_Q. One of features of our model is that $\hat{n}_Q$ is diagonalized in *p*-representation.

When L_d is quite large, we suppose the variable of our model becomes the angle variable. Discussing the *A*-term of our Hamiltonian in the large L_d case, we show that this term becomes the kinetic term which is the differential operators in *q*-representation. It means that *A*-term $\sum_i \left(\hat{U}_{pi} + \hat{U}_{pi}^{\dagger}\right)$ becomes $\sum_i \partial^2 / \partial\theta_i^2$ in the large L_d limit, where $2\pi n / L_d$ becomes θ.

Sections 3 is devoted to the theoretical discussion for the lowest energy $E_{n_Q}\left(L_d, N_s\right)$ with a fixed value of n_Q, while Sections 4 is to the numerical investigation for this energy. Our purpose of our work is to show that the energy gap $E_{n_Q}\left(L_d, N_s\right) - E_{n_Q=0}\left(L_d, N_s\right)$ is proportional to n_Q^2 / N_s. In section 3, we give the theoretical arguments for this form, neglecting the effect due to the *B*-term. Through this discussion, we find correction terms for the energy gap which would be observed on small lattices. Section 4 is to show our numerical results on lattices with $N_s = 5$, 9, 16, 36 and 64 sites. In the first subsection, the results of $N_s = 5$ and 9 are presented. For the $N_s = 5$ lattice we employ the diagonalization so that we are not bothered by the numerical error. The results on the $N_s = 9$ lattice are obtained by stochastic state selection method [44]-[51], where we could make the numerical errors quite small. We extensively examine the energy gap including the contribution from the correction terms. The results on both lattices support our discussion in section 3. Calculations for $N_s = 16$, 36 and 64 lattices are carried out by quantum Monte Carlo methods [52] [53] [54]. The results, which are also in good agreement to our theoretical predictions, are presented in the second subsection. There we show that we successfully observe the effect from the correction terms on the $N_s = 16$ lattice beyond the statistical errors. On $N_s = 36$ and 64 lattices, on the other hand, part of the correction effect turned out to be too small to observe.

In the last section, we conclude that the quasi-degenerate states exist in the quantum nonlinear sigma model by summarizing the theoretical studies and the extensive examinations by numerical approaches. Also we make comments on the dependence of the interaction strength on our conclusion, as well as those on future studies on the violation of the cluster property and the extension of our work to the model with SU(2) symmetry.

2. Quantum Nonlinear Sigma Model

2.1. Continuous Model

In many literatures, the quantum nonlinear sigma model has been defined in the form of the effective action. In this work, however, we define it in the form of Hamiltonian following to [31]. Instead of SU(2) symmetry which is supposed in [31] we employ U(1) symmetry for simplicity.

First we introduce a variable $\hat{\omega}$ for which the eigenvalue is ω and the eigenstate is $|\omega\rangle$.

$$\hat{\omega}|\omega\rangle = |\omega\rangle\omega, \ \langle\omega|\omega'\rangle = \delta(\omega-\omega'). \tag{1}$$

The value of ω is continuous and is limited to the range $[0,2\pi]$, since $\hat{\omega}$ expresses U(1) symmetry.

We also introduce a conjugate operator of $\hat{\omega}$, which we denote $\hat{p}_\omega$.

$$[\hat{\omega},\hat{p}_\omega] = i. \tag{2}$$

This commutation relation implies that

$$\langle\omega|\psi\rangle = \psi(\omega), \ \langle\omega|\hat{p}_\omega|\psi\rangle = -i\frac{\mathrm{d}}{\mathrm{d}\omega}\psi(\omega). \tag{3}$$

The eigenvalue of $\hat{p}_\omega$ should be discrete because, for the eigenstate $|p_\omega\rangle$ of $\hat{p}_\omega$, the inner product $\langle\omega|p_\omega\rangle = \exp(i\omega p_\omega)$ has the same value at $\omega=0$ and $\omega=2\pi$. Therefore we denote $|p_\omega\rangle = |n\rangle$ hereafter,

$$\hat{p}_\omega|n\rangle = |n\rangle n, \ n = 0,\pm1,\pm2,\cdots. \tag{4}$$

For models on the lattice, we introduce operators $\hat{\omega}_j$ and $\hat{p}_{\omega j}$ at each site *j*, where $j = 0,1,\cdots,N_s-1$ for the lattice size N_s. They satisfy the following commutation relations.

$$[\hat{\omega}_j,\hat{p}_{\omega l}] = i\delta_{jl}, \ [\hat{\omega}_j,\hat{\omega}_l] = 0, \ [\hat{p}_{\omega j},\hat{p}_{\omega l}] = 0. \tag{5}$$

Using these operators given at every site, we define the Hamiltonian for a nonlinear sigma model on the square lattice by

$$\hat{H}_{Lattice} \equiv f\sum_{j=0}^{N_s-1}(\hat{p}_{\omega j})^2 - g\sum_{(l,n)}\cos(\hat{\omega}_l-\hat{\omega}_n). \tag{6}$$

Here *j* denotes the site number, while (l,n) denotes the nearest neighbor on the square lattice. For this Hamiltonian, we can introduce the generator $\hat{Q}_{lattice}$ defined by

$$\hat{Q}_{Lattice} \equiv \sum_{j=0}^{N_s-1}\hat{p}_{\omega j}. \tag{7}$$

Using Equations (5) and (6) it is easy to see that

$$\left[\hat{H}_{Lattice},\hat{Q}_{Lattice}\right] = -g\sum_{(l,n)}\left[\cos\left(\hat{\omega}_l-\hat{\omega}_n\right),\hat{Q}_{Lattice}\right]$$
$$= -g\sum_{(l,n)}\left[\cos\left(\hat{\omega}_l-\hat{\omega}_n\right),\hat{p}_{\omega l}+\hat{p}_{\omega n}\right] \tag{8}$$
$$= -ig\sum_{(l,n)}\left\{\sin\left(\hat{\omega}_l-\hat{\omega}_n\right)-\sin\left(\hat{\omega}_l-\hat{\omega}_n\right)\right\} = 0.$$

2.2. Discrete Model

We would like to obtain the energy for the quantum number of the generator $\hat{Q}_{Lattice}$ in numerical calculations by the diagonalization or quantum Monte Carlo methods. Since these methods are formulated through a finitely dimensional linear algebra, we employ the discrete variable instead of the continuous one. For this purpose, the commutation relation (5) is not suitable, because it can not apply to the quantum theory of the discrete variable. In order to make a model that has the discrete variable and that is a good approximation to the model with $\hat{H}_{Lattice}$ of the angle variable ω, we would like to make our model to satisfy the Weyl relation.

Based on the discussion in **Appendix A2**, we introduce two kinds of unitary operators $\hat{U}_{pj}$ and $\hat{U}_{qj}$ at each lattice site *j*, and impose the following Weyl relation to them.

$$\hat{U}_{pj}\hat{U}_{qj} = \hat{U}_{qj}\hat{U}_{pj}\exp\left(i\delta_d\right),\ \ \delta_d \equiv 2\pi/L_d,$$
$$\left[\hat{U}_{qj},\hat{U}_{ql}\right]=0,\ \left[\hat{U}_{pj},\hat{U}_{pl}\right]=0,\ \left[\hat{U}_{pj},\hat{U}_{ql}\right]=0,\quad \text{for } j\neq l. \tag{9}$$

Assuming the existence of an eigenstate $|0\rangle_{qj}$ of $\hat{U}_{qj}$ and the relation (9) we obtain, for $n=0,1,\cdots,L_d-1$, the eigenstates of $\hat{U}_{qj}$ or $\hat{U}_{pj}$.

$$|n\rangle_{qj} \equiv \left(\hat{U}_{pj}\right)^n|0\rangle_{qj},\ \hat{U}_{qj}|n\rangle_{qj} = |n\rangle_{qj}\exp\left(-in\delta_d\right),$$
$$|n\rangle_{pj} \equiv \left(\hat{U}_{qj}\right)^n|0\rangle_{pj},\ \hat{U}_{pj}|n\rangle_{pj} = |n\rangle_{pj}\exp\left(in\delta_d\right). \tag{10}$$

Here $|0\rangle_{pj}$ is defined by $|0\rangle_{qj}$ following Equation (63) in **Appendix**. We also obtain

$$\hat{U}_{pj}|n\rangle_{qj} = \left(\hat{U}_{pj}\right)^{n+1}|0\rangle_{qj} = |n+1\rangle_{qj},\ \ \hat{U}_{qj}|n\rangle_{pj} = \left(\hat{U}_{qj}\right)^{n+1}|0\rangle_{pj} = |n+1\rangle_{pj}. \tag{11}$$

Here $|L_d\rangle_{qj}=|0\rangle_{qj}$ and $|L_d\rangle_{pj}=|0\rangle_{pj}$, as is shown in **Appendix**. Also the inner product ${}_{qj}\langle n|m\rangle_{pj}$ is given by

$${}_{qj}\langle n|m\rangle_{pj} = \left({}_{pj}\langle m|n\rangle_{qj}\right)^* = \frac{1}{\sqrt{L_d}}\exp\left(-inm\delta_d\right). \tag{12}$$

The state in *q*-representation on the lattice is defined by

$$|n_0,n_1,\cdots,n_{N_s-1}\rangle_q \equiv |n_0\rangle_{q0}\otimes|n_1\rangle_{q1}\otimes\cdots\otimes|n_{N_s-1}\rangle_{qN_s-1}. \tag{13}$$

Similarly the state in *p*-representation on the lattice is defined by

$$|n_0,n_1,\cdots,n_{N_s-1}\rangle_p \equiv |n_0\rangle_{p0}\otimes|n_1\rangle_{p1}\otimes\cdots\otimes|n_{N_s-1}\rangle_{pN_s-1}. \tag{14}$$

We then define a Hamiltonian $\hat{H}_D$ for the discrete variables on the lattice by

$$\hat{H}_D \equiv \hat{H}_A + \hat{H}_B,$$
$$\hat{H}_A \equiv -A\sum_l \left(\hat{U}_{pl} + \hat{U}_{pl}^\dagger - 2\right),\ \hat{H}_B \equiv -B\sum_{(l,n)} \left(\hat{U}_{ql}^\dagger \hat{U}_{qn} + \hat{U}_{qn}^\dagger \hat{U}_{ql}\right). \tag{15}$$

For $\hat{H}_D$ we can introduce an increment operator $\hat{Q}_D$ defined by

$$\hat{Q}_D \equiv \prod_l \hat{U}_{pl},\ \hat{Q}_D \hat{U}_{qj} \hat{Q}_D^\dagger = \hat{U}_{qj} \exp(i\delta_d). \tag{16}$$

We can obtain the eigenstate which is common to $\hat{H}_D$ and $\hat{Q}_D$, because

$$\begin{aligned}\left[\hat{H}_D, \hat{Q}_D\right] &= -B\sum_{(l,n)} \left[\left(\hat{U}_{ql}^\dagger \hat{U}_{qn} + \hat{U}_{qn}^\dagger \hat{U}_{ql}\right), \hat{Q}_D\right] \\ &= -B\sum_{(l,n)} \left[\left(\hat{U}_{ql}^\dagger \hat{U}_{qn} + \hat{U}_{qn}^\dagger \hat{U}_{ql}\right), \hat{U}_{pl}\hat{U}_{pn}\right] \prod_{j\neq l,n} \hat{U}_{pj} = 0.\end{aligned} \tag{17}$$

In the last equation of Equation (17), note that, for $l \neq n$, we have

$$\begin{aligned}\hat{U}_{ql}^\dagger \hat{U}_{qn} \hat{U}_{pl} \hat{U}_{pn} &= \hat{U}_{ql}^\dagger \hat{U}_{pl} \hat{U}_{qn} \hat{U}_{pn} = \left\{\hat{U}_{pl} \hat{U}_{ql}^\dagger \exp(i\delta_d)\right\}\left\{\hat{U}_{pn} \hat{U}_{qn} \exp(-i\delta_d)\right\} \\ &= \hat{U}_{pl} \hat{U}_{ql}^\dagger \hat{U}_{pn} \hat{U}_{qn} = \hat{U}_{pl} \hat{U}_{pn} \hat{U}_{ql}^\dagger \hat{U}_{qn},\end{aligned}$$
$$\hat{U}_{qn}^\dagger \hat{U}_{ql} \hat{U}_{pl} \hat{U}_{pn} = \hat{U}_{qn}^\dagger \hat{U}_{ql} \hat{U}_{pn} \hat{U}_{pl} = \hat{U}_{pn} \hat{U}_{pl} \hat{U}_{qn}^\dagger \hat{U}_{ql} = \hat{U}_{pl} \hat{U}_{pn} \hat{U}_{qn}^\dagger \hat{U}_{ql}. \tag{18}$$

Operating $\hat{Q}_D$ to the state $\left|n_0, n_1, \cdots, n_{N_s-1}\right\rangle_p$ given by the definition (14) we obtain

$$\begin{aligned}\hat{Q}_D \left|n_0, n_1, \cdots, n_{N_s-1}\right\rangle_p &= \prod_{j=0}^{N_s-1} \hat{U}_{pj} \left|n_0, n_1, \cdots, n_{N_s-1}\right\rangle_p \\ &= \left|n_0, n_1, \cdots, n_{N_s-1}\right\rangle_p \prod_{j=0}^{N_s-1} \exp\left(i\delta_d n_j\right) \\ &= \left|n_0, n_1, \cdots, n_{N_s-1}\right\rangle_p \exp\left(i\delta_d \sum_{j=0}^{N_s-1} n_j\right).\end{aligned} \tag{19}$$

2.3. Hamiltonian for Large L_d

As described in the previous section, the eigenvalue of $\hat{U}_{qj}$ is discrete. When L_d is quite large, however, the continuous eigenvalue of $\hat{U}_{qj}$ would be realized so that the physical quantities of our model become good approximations to those of $\hat{H}_{Lattice}$. Consider the case $\delta_d = 2\pi/L_d \ll 1$. If we introduce a notation $\theta = \delta_d n = 2\pi n/L_d$, we can replace $|n\rangle_{qj}$ by $|\theta\rangle_{qj}$. Then we have

$$\hat{U}_{qj} |\theta\rangle_{qj} = |\theta\rangle_{qj} \exp(-i\theta). \tag{20}$$

Let us operate $\left(\hat{U}_{pj} + \hat{U}_{pj}^\dagger - 2\right)$ to a state of $|\Psi\rangle_{qj} \equiv \sum_\theta |\theta\rangle_{qj} \psi(\theta)$ at a site j of the lattice. Then

$$\begin{aligned}\left(\hat{U}_{pj} + \hat{U}_{pj}^\dagger - 2\right)|\Psi\rangle_{qj} &= \sum_\theta \left(\hat{U}_{pj} + \hat{U}_{pj}^\dagger - 2\right)|\theta\rangle_{qj} \psi(\theta) \\ &= \sum_\theta \left(|\theta + \delta_d\rangle_{qj} + |\theta - \delta_d\rangle_{qj} - 2|\theta\rangle_{qj}\right)\psi(\theta) \\ &= \sum_\theta |\theta\rangle_{qj} \left\{\psi(\theta - \delta_d) + \psi(\theta + \delta_d) - 2\psi(\theta)\right\} \\ &\sim \sum_\theta |\theta\rangle_{qj}\, \delta_d^2 \left\{\frac{\mathrm{d}^2\psi(\theta)}{\mathrm{d}\theta^2}\right\}.\end{aligned} \tag{21}$$

We apply this discussion to the whole state $\left|\theta_0,\theta_1,\cdots,\theta_{N_s-1}\right\rangle_q$ (13). The state $\left|\Phi\right\rangle_q$ is given by

$$\left|\Phi\right\rangle_q \equiv \sum_{\{\theta_j\}}\left|\theta_0,\theta_1,\cdots,\theta_{N_s-1}\right\rangle_q \phi_q\left(\theta_0,\theta_1,\cdots,\theta_{N_s-1}\right). \tag{22}$$

Hereafter we abbreviate $\phi_q\left(\theta_0,\theta_1,\cdots,\theta_{N_s-1}\right)$ as $\phi_q\left(\left\{\theta_j\right\}\right)$. Operating $\hat{H}_A$ in Equation (15) to this state we obtain

$$\hat{H}_A\left|\Phi\right\rangle_q \sim -A\sum_{\{\theta_j\}}\left|\theta_0,\theta_2,\cdots,\theta_{N_s-1}\right\rangle_q \sum_{l=0}^{N_s-1}\delta_d^2\frac{\partial^2\phi_q\left(\left\{\theta_j\right\}\right)}{\partial\theta_l^2}. \tag{23}$$

As for $\hat{H}_B$ note that, for one nearest neighbor pair (l,n),

$$\begin{aligned}&\left(\hat{U}_{ql}^{\dagger}\hat{U}_{qn}+\hat{U}_{qn}^{\dagger}\hat{U}_{ql}\right)\left|\theta_0,\theta_2,\cdots,\theta_{N_s-1}\right\rangle_q\\&=\left\{\exp\left(i\theta_l\right)\exp\left(-i\theta_n\right)+\exp\left(i\theta_n\right)\exp\left(-i\theta_l\right)\right\}\left|\theta_0,\theta_2,\cdots,\theta_{N_s-1}\right\rangle_q\\&=2\cos\left(\theta_l-\theta_n\right)\left|\theta_0,\theta_2,\cdots,\theta_{N_s-1}\right\rangle_q.\end{aligned} \tag{24}$$

Therefore

$$\hat{H}_B\left|\Phi\right\rangle_q = \sum_{\{\theta_j\}}\left|\theta_0,\theta_2,\cdots,\theta_{N_s-1}\right\rangle_q \phi_q\left(\left\{\theta_j\right\}\right)\left\{-2B\sum_{(l,n)}\cos\left(\theta_l-\theta_n\right)\right\}. \tag{25}$$

With Equations (23) and (25) we obtain

$$\begin{aligned}\hat{H}_D\left|\Phi\right\rangle_q \sim &\sum_{\{\theta_j\}}\left|\theta_0,\theta_2,\cdots,\theta_{N_s-1}\right\rangle_q\\&\times\left\{-A\delta_d^2\sum_{l=0}^{N_s-1}\frac{\partial^2\phi_q\left(\left\{\theta_j\right\}\right)}{\partial\theta_l^2}-2B\phi_q\left(\left\{\theta_j\right\}\right)\sum_{(l,n)}\cos\left(\theta_l-\theta_n\right)\right\}.\end{aligned} \tag{26}$$

3. Energy with a Fixed Number n_Q

In this section, we present a theoretical argument about the lowest energy with a fixed number n_Q. In the first subsection, we discuss the effective Hamiltonian where the operator $\hat{n}_Q$ is clearly separated. The second subsection is to estimate the energy gap using this effective Hamiltonian.

3.1. Effective Hamiltonian

Here we use new operators $\hat{V}_{ql}$ and $\hat{V}_{pl}$ instead of $\hat{U}_{qj}$ and $\hat{U}_{pj}$. We will show that we can express the increment operator $\hat{Q}_D$ (16) by the single operator $\hat{V}_{p0}$. In addition, we express $\hat{H}_B$ in Equation (15) by $\hat{V}_{ql}$ ($l \geq 1$). As for $\hat{H}_A$ in Equation (15) we present an expression where $\hat{Q}_D$ is included in an explicit form.

First we consider an operator $\hat{m}_j$ which is defined by $\hat{U}_{pj}$ as

$$\exp\left(i\delta_d\hat{m}_j\right)\equiv\hat{U}_{pj}. \tag{27}$$

Note that $\hat{m}_j$ is hermitian. For a set of operators $\left\{\hat{m}_j\right\}$ ($j=0,1,\cdots,N_s-1$) we can introduce a set of new operators $\left\{\hat{\zeta}_l\right\}$.

$$\hat{\zeta}_l \equiv \sum_{j=0}^{N_s-1} a_{lj}\hat{m}_j,\ \hat{m}_j = \sum_{l=0}^{N_s-1} b_{jl}\hat{\zeta}_l,\ \sum_{l=0}^{N_s-1} b_{jl}a_{lk} = \delta_{jk},\ \sum_{j=0}^{N_s-1} a_{lj}b_{jn} = \delta_{ln}. \tag{28}$$

Let us assume that the matrix $\left[a_{lj}\right]$ is orthonormal, *i.e.* $b_{jl} = a_{lj}$ and they are real. Therefore $\sum_j a_{lj}a_{nj} = \delta_{ln}$ and $\sum_l a_{lj}a_{lk} = \delta_{jk}$. Also we assume $a_{0j} = 1/\sqrt{N_s}$ for any *j*, which means that $b_{j0} = a_{0j} = 1/\sqrt{N_s}$ and $\sum_j a_{0j}b_{j0} = \sum_j (1/N_s) = 1$. Using a_{lj} and b_{jl} we define unitary operators $\hat{V}_{pl}$ and $\hat{V}_{ql}$,

$$\hat{V}_{ql} \equiv \prod_{j=0}^{N_s-1}\left(\hat{U}_{qj}\right)^{b_{jl}},\ \hat{V}_{pl} \equiv \prod_{j=0}^{N_s-1}\left(\hat{U}_{pj}\right)^{a_{lj}}. \tag{29}$$

Then we express $\hat{U}_{qj}$ and $\hat{U}_{pj}$ by $\hat{V}_{ql}$ and $\hat{V}_{pl}$.

$$\begin{aligned}
\prod_{l=0}^{N_s-1}\left(\hat{V}_{ql}\right)^{a_{lj}} &= \prod_{l=0}^{N_s-1}\left\{\prod_{k=0}^{N_s-1}\left(\hat{U}_{qk}\right)^{b_{kl}}\right\}^{a_{lj}} = \prod_{k=0}^{N_s-1}\left(\hat{U}_{qk}\right)^{\sum_{l=0}^{N_s-1} b_{kl}a_{lj}} \\
&= \prod_{k=0}^{N_s-1}\left(\hat{U}_{qk}\right)^{\delta_{kj}} = \hat{U}_{qj}, \\
\prod_{l=0}^{N_s-1}\left(\hat{V}_{pl}\right)^{b_{jl}} &= \prod_{l=0}^{N_s-1}\left\{\prod_{k=0}^{N_s-1}\left(\hat{U}_{pk}\right)^{a_{lk}}\right\}^{b_{jl}} = \prod_{k=0}^{N_s-1}\left(\hat{U}_{pk}\right)^{\sum_{l=0}^{N_s-1} a_{lk}b_{jl}} \\
&= \prod_{k=0}^{N_s-1}\left(\hat{U}_{pk}\right)^{\delta_{kj}} = \hat{U}_{pj}.
\end{aligned} \tag{30}$$

Next we show that a set of operators $\left\{\hat{V}_{pl},\hat{V}_{ql}\right\}$ has the same Weyl relations as those of $\left\{\hat{U}_{pj},\hat{U}_{qj}\right\}$ given by Equation (9). Namely,

$$\begin{gathered}
\hat{V}_{pl}\hat{V}_{ql} = \hat{V}_{ql}\hat{V}_{pl}\exp\left(i\delta_d\right), \\
\left[\hat{V}_{ql},\hat{V}_{qn}\right] = 0,\ \left[\hat{V}_{pl},\hat{V}_{pn}\right] = 0,\ \left[\hat{V}_{pl},\hat{V}_{qn}\right] = 0,\quad \text{for } l \neq n.
\end{gathered} \tag{31}$$

The first Weyl relation is verified by notifying

$$\begin{aligned}
\hat{V}_{pl}\hat{V}_{qn} &= \prod_{j=0}^{N_s-1}\left(\hat{U}_{pj}\right)^{a_{lj}}\prod_{k=0}^{N_s-1}\left(\hat{U}_{qk}\right)^{b_{kn}} = \prod_{j=0}^{N_s-1}\left(\hat{U}_{pj}\right)^{a_{lj}}\left(\hat{U}_{qj}\right)^{b_{jn}} \\
&= \prod_{j=0}^{N_s-1}\left(\hat{U}_{qj}\right)^{b_{jn}}\left(\hat{U}_{pj}\right)^{a_{lj}}\exp\left(i\delta_d a_{lj}b_{jn}\right) \\
&= \hat{V}_{qn}\hat{V}_{pl}\exp\left(i\delta_d\sum_j a_{lj}b_{jn}\right) = \hat{V}_{qn}\hat{V}_{pl}\exp\left(i\delta_d\delta_{ln}\right).
\end{aligned} \tag{32}$$

The rest of relations are trivial from Equations (9) and (29). By this proof we confirm that the set of $\left\{\hat{V}_{pl},\hat{V}_{ql}\right\}$ is independent and complete.

Then we will express $\hat{H}_B$ in Equation (15) by $\hat{V}_{ql}$. For this purpose, we calculate $\hat{U}_{ql}\hat{U}^{\dagger}_{qn}$, noting $\hat{U}^{\dagger}_{qn} = \hat{U}^{-1}_{qn}$ and $a_{0l} = a_{0n} = 1/\sqrt{N_s}$,

$$\hat{U}_{ql}\hat{U}^{\dagger}_{qn} = \prod_{j=0}^{N_s-1}\left(\hat{V}_{qj}\right)^{a_{jl}}\prod_{k=0}^{N_s-1}\left(\hat{V}_{qk}\right)^{-a_{kn}} = \prod_{j=0}^{N_s-1}\left(\hat{V}_{qj}\right)^{a_{jl}-a_{jn}} = \prod_{j=1}^{N_s-1}\left(\hat{V}_{qj}\right)^{a_{jl}-a_{jn}}. \tag{33}$$

It should be noted that $\hat{U}_{ql}\hat{U}^{\dagger}_{qn}$ contains no $\hat{V}_{q0}$. Therefore we can express $\hat{H}_B$ by $\left(N_s-1\right)$ operators $\hat{V}_{qj}$ $(j \geq 1)$.

$$\hat{H}_B = -B\sum_{(l,n)}\left\{\prod_{j=1}^{N_s-1}\left(\hat{V}_{qj}\right)^{a_{jl}-a_{jn}} + \prod_{j=1}^{N_s-1}\left(\hat{V}_{qj}\right)^{a_{jn}-a_{jl}}\right\}. \tag{34}$$

Next we express $\hat{H}_A$ in Equation (15) by means of new operators $\hat{\zeta}_l$ defined in Equation (28). It should be noted that, from Equations (27) and (28), we obtain

$$\hat{\zeta}_0 = \frac{\hat{n}_Q}{\sqrt{N_s}}, \quad \hat{Q}_D = \prod_{j=0}^{N_s-1} \hat{U}_{pj} = \exp\left(i\delta_d \hat{n}_Q\right), \quad \hat{n}_Q \equiv \sum_{j=0}^{N_s-1} \hat{m}_j. \tag{35}$$

Then we can express $\hat{H}_A$ in Equation (15) using $\hat{n}_Q$ and $\hat{\zeta}_l$ ($l \geq 1$) because

$$\begin{aligned}\hat{U}_{pl} &= \exp\left(i\delta_d \hat{m}_l\right) = \exp\left\{ i\delta_d \left(\sum_{n=1}^{N_s-1} b_{ln}\hat{\zeta}_n + \frac{\hat{\zeta}_0}{\sqrt{N_s}} \right) \right\} \\ &= \exp\left\{ i\delta_d \left(\sum_{n=1}^{N_s-1} b_{ln}\hat{\zeta}_n + \frac{\hat{n}_Q}{N_s} \right) \right\} \\ \hat{U}_{pl}^{\dagger} &= \exp\left\{ -i\delta_d \left(\sum_{n=1}^{N_s-1} b_{ln}\hat{\zeta}_n + \frac{\hat{n}_Q}{N_s} \right) \right\}.\end{aligned} \tag{36}$$

The result is, with $\hat{\eta}_l \equiv \sum_{n=1}^{N_s-1} b_{ln}\hat{\zeta}_n$,

$$\begin{aligned}\hat{H}_A &= -A\sum_{l=0}^{N_s-1}\left\{ \exp\left[i\delta_d \left(\hat{\eta}_l + \frac{\hat{n}_Q}{N_s} \right) \right] + \exp\left[-i\delta_d \left(\hat{\eta}_l + \frac{\hat{n}_Q}{N_s} \right) \right] - 2 \right\} \\ &= -2A\sum_{l=0}^{N_s-1}\left\{ \cos\left[\delta_d \left(\hat{\eta}_l + \frac{\hat{n}_Q}{N_s} \right) \right] - 1 \right\}.\end{aligned} \tag{37}$$

Now consider the case $\delta_d \ll 1$, where we expand $\hat{H}_A$ by δ_d.

$$\begin{aligned}\hat{H}_A &= \sum_{k=0}^{\infty} \hat{h}_A^{(k)}\delta_d^k = -2A\sum_{l=0}^{N_s-1}\left\{ \sum_{k=0}^{\infty}\left[\delta_d \left(\hat{\eta}_l + \frac{\hat{n}_Q}{N_s} \right) \right]^{2k} \frac{(-1)^k}{(2k)!} - 1 \right\} \\ &= -2A\left\{ \sum_{k=1}^{\infty} \delta_d^{2k} \frac{(-1)^k}{(2k)!} \sum_{l=0}^{N_s-1}\left(\hat{\eta}_l + \frac{\hat{n}_Q}{N_s} \right)^{2k} \right\}.\end{aligned} \tag{38}$$

It should be noted that $\hat{h}_A^{(0)} = 0$ due to the definition of $\hat{H}_A$ and $\hat{h}_A^{(2k+1)} = 0$ because $\hat{H}_A$ is hermitian. In the second order of δ_d we obtain $\hat{H}_A^{(2)}$,

$$\begin{aligned}\hat{H}_A^{(2)} &\equiv \hat{h}_A^{(2)}\delta_d^2 = -2A\delta_d^2 \frac{(-1)}{2!}\sum_{l=0}^{N_s-1}\left(\hat{\eta}_l + \frac{\hat{n}_Q}{N_s} \right)^2 \\ &= A\delta_d^2 \sum_{l=0}^{N_s-1}\left\{ \hat{\eta}_l^2 + 2\hat{\eta}_l \frac{\hat{n}_Q}{N_s} + \left(\frac{\hat{n}_Q}{N_s} \right)^2 \right\} \\ &= A\delta_d^2 \left(\sum_{l=0}^{N_s-1} \hat{\eta}_l^2 + \frac{\hat{n}_Q^2}{N_s} \right).\end{aligned} \tag{39}$$

Here note that

$$\begin{aligned}\sum_{l=0}^{N_s-1}\hat{\eta}_l &= \sum_{l=0}^{N_s-1}\sum_{n=1}^{N_s-1} b_{ln}\hat{\zeta}_n = \sum_{n=1}^{N_s-1}\left(\sum_{l=0}^{N_s-1} b_{ln} \right)\hat{\zeta}_n = \sqrt{N_s}\sum_{n=1}^{N_s-1}\left(\sum_{l=0}^{N_s-1} b_{ln}\frac{1}{\sqrt{N_s}} \right)\hat{\zeta}_n \\ &= \sqrt{N_s}\sum_{n=1}^{N_s-1}\left(\sum_{l=0}^{N_s-1} b_{ln}b_{l0} \right)\hat{\zeta}_n = \sqrt{N_s}\sum_{n=1}^{N_s-1}\delta_{0n}\hat{\zeta}_n = 0.\end{aligned} \tag{40}$$

For later use we also calculate $\hat{H}_A^{(4)} \equiv \hat{h}_A^{(2)}\delta_d^2 + \hat{h}_A^{(4)}\delta_d^4$. We obtain

$$\begin{aligned}
\hat{H}_A^{(4)} &= \hat{H}_A^{(2)} - 2A\delta_d^4 \frac{1}{4!}\sum_{l=0}^{N_s-1}\left(\hat{\eta}_l + \frac{\hat{n}_Q}{N_s}\right)^4 \\
&= \hat{H}_A^{(2)} - \frac{A}{12}\delta_d^4 \sum_{l=0}^{N_s-1}\left\{\hat{\eta}_l^4 + 4\hat{\eta}_l^3\frac{\hat{n}_Q}{N_s} + 6\hat{\eta}_l^2\left(\frac{\hat{n}_Q}{N_s}\right)^2 + 4\hat{\eta}_l\left(\frac{\hat{n}_Q}{N_s}\right)^3 + \left(\frac{\hat{n}_Q}{N_s}\right)^4\right\} \\
&= \hat{H}_A^{(2)} - A\delta_d^4 \sum_{l=0}^{N_s-1}\left\{\frac{1}{12}\sum_{l=0}^{N_s-1}\hat{\eta}_l^4 + \frac{\hat{n}_Q}{3N_s}\sum_{l=0}^{N_s-1}\hat{\eta}_l^3 + \frac{\hat{n}_Q^2}{2N_s^2}\sum_{l=0}^{N_s-1}\hat{\eta}_l^2 + \frac{\hat{n}_Q^4}{12N_s^3}\right\}.
\end{aligned} \tag{41}$$

In Equation (41) we dropped the term of $\sum_l \hat{\eta}_l$ because of Equation (40).

3.2. Energy with a Fixed Value of n_Q

In order of δ_d^2 the Hamiltonian $\hat{H}_D^{(2)}$ is given by

$$\hat{H}_D^{(2)} \equiv \hat{H}_A^{(2)} + \hat{H}_B = \hat{H}_{D0}^{(2)} + A\delta_d^2\frac{\hat{n}_Q^2}{N_s},$$

$$\hat{H}_{D0}^{(2)} \equiv A\delta_d^2\sum_{l=0}^{N_s-1}\hat{\eta}_l^2 - B\sum_{(l,n)}\left\{\prod_{j=1}^{N_s-1}\left(\hat{V}_{qj}\right)^{a_{jl}-a_{jn}} + \prod_{j=1}^{N_s-1}\left(\hat{V}_{qj}\right)^{a_{jn}-a_{jl}}\right\}. \tag{42}$$

When we calculate the energy in p-representation, where the basic state is $\left|m_0, m_1, m_2, \cdots, m_{N_s-1}\right\rangle_p$ (14), the eigenvalue of the operator $\hat{n}_Q$ is $n_Q = \sum_j m_j$. Therefore the lowest energy with a fixed value of n_Q is given by

$$E_{n_Q}^{(2)} = E_0^{(2)} + A\delta_d^2\frac{n_Q^2}{N_s}. \tag{43}$$

Here $E_0^{(2)}$ is the lowest energy from $\hat{H}_{D0}^{(2)}$. We conclude that the energy gap $\Delta_{n_Q}^{th,2}$ with a fixed value of n_Q is given by

$$\Delta_{n_Q}^{th,2} \equiv E_{n_Q}^{(2)} - E_0^{(2)} = A\delta_d^2\frac{n_Q^2}{N_s}. \tag{44}$$

Then let us discuss energy up to δ_d^4. The effective Hamiltonian $\hat{H}_D^{(4)}$ is given by

$$\hat{H}_D^{(4)} \equiv \hat{H}_A^{(4)} + \hat{H}_B = \hat{H}_{D0}^{(2)} + A\delta_d^2\frac{\hat{n}_Q^2}{N_s} - A\delta_d^4\left\{\hat{e}_0 + \hat{e}_1\hat{n}_Q + \hat{e}_2\hat{n}_Q^2 + \hat{e}_4\hat{n}_Q^4\right\},$$

$$\hat{e}_0 \equiv \frac{1}{12}\sum_{l=0}^{N_s-1}\hat{\eta}_l^4,\ \hat{e}_1 \equiv \frac{1}{3N_s}\sum_{l=0}^{N_s-1}\hat{\eta}_l^3,\ \hat{e}_2 \equiv \frac{1}{2N_s^2}\sum_{l=0}^{N_s-1}\hat{\eta}_l^2,\ \hat{e}_4 \equiv \frac{1}{12N_s^3}. \tag{45}$$

As for terms with $\hat{e}_k$ we estimate their contributions by the first-order perturbation theory. When the eigenstate of $\hat{H}_{D0}^{(2)}$ with the eigen energy $E_0^{(2)}$ is $|E_0^{(2)}\rangle$, the energy is given by

$$\begin{aligned}
E_{n_Q}^{(4)} &\equiv E_{n_Q}^{(2)} + \left\langle E_0^{(2)}\right|\left\{\hat{H}_D^{(1)} - \hat{H}_D^{(2)}\right\}\left|E_0^{(2)}\right\rangle \\
&= \left(E_0^{(2)} + A\delta_d^2\frac{n_Q^2}{N_s}\right) - A\delta_d^4\left(\frac{N_s}{12}\overline{\eta}^4 + \frac{n_Q}{3}\overline{\eta}^3 + \frac{n_Q^2}{2N_s}\overline{\eta}^2 + \frac{n_Q^4}{12N_s^3}\right),
\end{aligned}$$

$$\overline{\eta}^k \equiv \frac{1}{N_s}\left\langle E_0^{(2)} \left| \sum_{l=0}^{N_s-1} \hat{\eta}_l^k \right| E_0^{(2)} \right\rangle. \quad (46)$$

Here we see that $\overline{\eta}^3$ vanishes. The reason is that $\hat{H}_D$ is invariant under the exchange of $\hat{U}_{ql}$ and $\hat{U}_{ql}^\dagger$ as well as the exchange of $\hat{U}_{pl}$ and $\hat{U}_{pl}^\dagger$, which means to replace $\hat{\eta}_l$ by $-\hat{\eta}_l$. In conclusion, the energy gap up to δ_d^4 is given by

$$\Delta_{n_Q}^{th,4} \equiv E_{n_Q}^{(4)} - E_0^{(4)} = A\delta_d^2 a_{sq}^{th,2} \frac{n_Q^2}{N_s} - A\delta_d^4 \frac{n_Q^4}{12N_s^3},$$

$$E_0^{(4)} = E_0^{(2)} - A\delta_d^4 \frac{N_s}{12}\overline{\eta}^4,\ a_{sq}^{th,2} \equiv 1 - \frac{1}{2}\delta_d^2 \overline{\eta}^2. \quad (47)$$

Note that the value of $a_{sq}^{th,2}$ depends on not only $\hat{H}_A$ but also $\hat{H}_B$.

4. Numerical Results

Now we present our numerical results of the lowest energy from the Hamiltonian $\hat{H}_D$ (15) with a fixed value of n_Q, which we denote $E_{n_Q}(L_d, N_s)$, for several values of L_d on the square lattice whose size is N_s. In order to obtain the energy for each value of n_Q we employ the basis states in *p*-representation, which consist of $\left| m_0, m_1, \cdots, m_{N_s-1} \right\rangle_p$ (14) with $\sum_l m_l = n_Q$. We examine the numerically obtained energy gap defined by

$$\Delta_{n_Q}(L_d, N_s) \equiv E_{n_Q}(L_d, N_s) - E_0(L_d, N_s). \quad (48)$$

Throughout this section we fix A in $\hat{H}_D$ to be $\delta_d^{-2} = (2\pi/L_d)^{-2}$, so that $A\delta_d^2 = 1$, and $B = 1$. Note that the energy gap scarcely depends on *B*. Our study is carried out on $N_s = 5$, 9, 16, 36 and 64 lattices with $L_d = 32$, 36 or 64. The fixed value ranges from $n_Q = 0$ to $n_Q = L_d/2$. Note that the result for $L_d - n_Q$, which means the result for $-n_Q$, is the same as the result for n_Q because of the periodicity of the operators.

We will show that $\Delta_{n_Q}(L_d, N_s)$ is well described by $\Delta_{n_Q}^{th,2}$ (44) or $\Delta_{n_Q}^{th,4}$ (47) which we discussed in the previous section. For this purpose, we introduce three ratios,

$$D1_{n_Q}(L_d, N_s) \equiv \left\{ \Delta_{n_Q}(L_d, N_s) - \frac{n_Q^2}{N_s} \right\} \Big/ \Delta_{n_Q}(L_d, N_s),$$

$$D2_{n_Q}(L_d, N_s) \equiv \left\{ \Delta_{n_Q}(L_d, N_s) - a_{sq}^{th,2} \frac{n_Q^2}{N_s} \right\} \Big/ \Delta_{n_Q}(L_d, N_s),$$

$$D3_{n_Q}(L_d, N_s) \equiv \left\{ \Delta_{n_Q}(L_d, N_s) - \Delta_{n_Q}^{th,4} \right\} \Big/ \Delta_{n_Q}(L_d, N_s). \quad (49)$$

Here $D1_{n_Q}(L_d, N_s)$ is useful to compare numerical results with $\Delta_{n_Q}^{th,2}$, while $D2_{n_Q}(L_d, N_s)$ is for the comparison with the first term of $\Delta_{n_Q}^{th,4}$. Since $\overline{\eta}^2 = \left\langle E_0^{(2)} \left| \sum_l \hat{\eta}_l^2 \right| E_0^{(2)} \right\rangle \Big/ N_s$ in $a_{sq}^{th,2}$ of the expression (47) is beyond analytical arguments, we numerically estimate this expectation value by $\left\langle E_0 \left| \sum_l \hat{\eta}_l^2 \right| E_0 \right\rangle \Big/ N_s$, where $\left|E_0\right\rangle$ is the state of the lowest energy with $n_Q = 0$.

4.1. Results on N_s = 5, 9 Lattices

In this subsection, we present the numerical results of $\Delta_{n_Q}\left(L_d = 32, N_s = 5\right)$ and $\Delta_{n_Q}\left(L_d = 32, N_s = 9\right)$.

The edge vectors for the $N_s = 5$ lattice are $(2,1)$ and $(-1,2)$. On this lattice we calculate the lowest energy with $n_Q = 0$ to 16 by means of the diagonalization so that we can obtain precise results to start with. The number of the states we should consider amounts to $32^5 = 2^{25} \sim 3.4\times10^7$. For the $N_s = 9$ lattice, which is already too large to apply the diagonalization, we employ stochastic state selection method [44]-[51] to obtain $\Delta_{n_Q}\left(L_d = 32, N_s = 9\right)$.

Figure 1 shows our results $\Delta_{n_Q}\left(L_d = 32, N_s = 5\right)$ and $\Delta_{n_Q}\left(L_d = 32, N_s = 9\right)$ plotted as a function of n_Q^2. We also plot $\Delta_{n_Q}^{th,2} = n_Q^2 / N_s$ in the figure. We see the data agree with $\Delta_{n_Q}^{th,2}$ when n_Q is small. For large values of n_Q, on the contrary, we observe a little discrepancy between the data and $\Delta_{n_Q}^{th,2}$. Then in Figure 2 we plot $D2_{n_Q}\left(L_d, N_s\right)$ and $D3_{n_Q}\left(L_d, N_s\right)$ together with $D1_{n_Q}\left(L_d, N_s\right)$ for $L_d = 32$ and $N_s = 5$, where $a_{sq}^{th,2}$ has been calculated to be 0.98984. Here we can see that the theoretical prediction up to δ_d^4 agrees well with the numerical results because $D3_{n_Q}\left(L_d, N_s\right)$ is almost zero in all range of n_Q. As for $D2_{n_Q}\left(L_d, N_s\right)$, on the other hand, they differ from zero in most range of n_Q. These results tell us that the second term of $\Delta_{n_Q}^{th,4}$ is important except for very small values of n_Q. In Figure 3 we compare our numerical results for $N_s = 9$ using $Dk_{n_Q}\left(L_d, N_s\right)$ $(k = 1,2,3)$. We employ two values of L_d, $L_d = 32$ and $L_d = 36$, for which the estimated $a_{sq}^{th,2}$ is 0.98431 and 0.98764, respectively. Here we plot the data with $n_Q \geq 2$ only, because $\Delta_{n_Q=1}\left(L_d, N_s\right)$ is too small to avoid large statistical errors in $Dk_{n_Q=1}\left(L_d, N_s\right)$s $(k = 1,2,3)$. For large values of n_Q we observe large discrepancies between Δ_{n_Q} s and $\Delta_{n_Q}^{th,2}$ s as well as Δ_{n_Q} s and $a_{sq}^{th,2}$ s, while $\Delta_{n_Q}^{th,4}$ s are consistent with Δ_{n_Q} s.

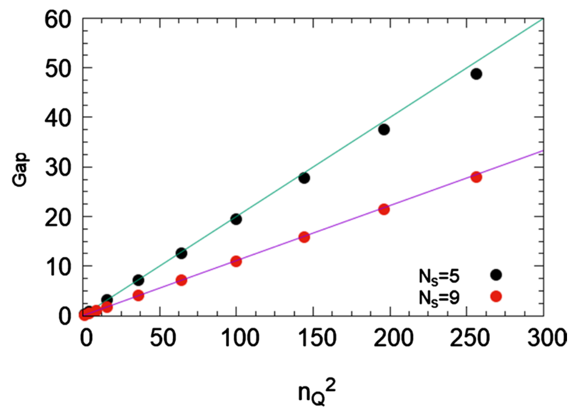

Figure 1. Energy gap $\Delta_{n_Q}\left(L_d = 32, N_s\right)$ defined by Equation (48) for $N_s = 5$ and 9 as a function of n_Q^2.

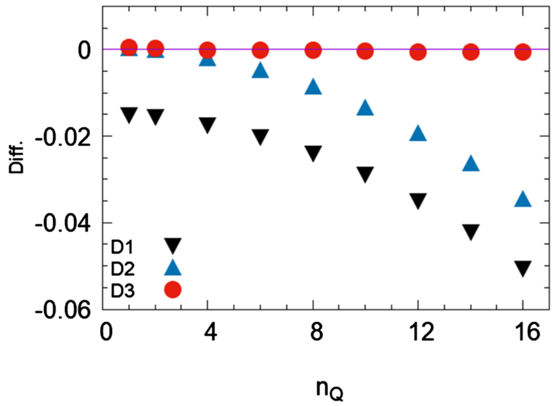

Figure 2. $Dk_{n_Q}(L_d = 32, N_s = 5)$ ($k = 1,2,3$) defined by Equation (49), which measure differences between numerically obtained energy gaps and theoretical estimations, versus n_Q. Black down triangles, blue up triangles and red circles are results for $k = 1,2$ and 3, respectively.

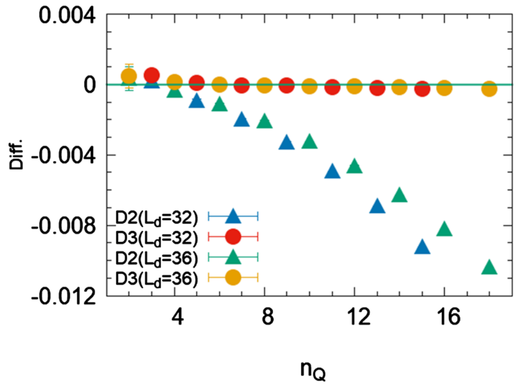

Figure 3. $Dk_{n_Q}(L_d, N_s = 9)$ ($k = 2,3$) defined by Equation (49) for $L_d = 32$ and 36 versus n_Q. Blue triangles ($k = 2$) and red circles ($k = 3$) are results for $L_d = 32$, while green triangles ($k = 2$) and yellow circles ($k = 3$) are results for $L_d = 36$.

4.2. Results on N_s = 16, 36, 64 Lattices

For larger lattices with $N_s = 16,36,64$ we estimate the energy gaps by means of quantum Monte Carlo methods [52] [53] [54]. The reasons why we employ these methods are that we can easily apply them to the study on these lattices and that we can obtain reliable results on the energy. In quantum Monte Carlo methods we have two technical parameters, which are inverse temperature β and Trotter number l_t. For the lowest energy, we need large β as well as large l_t. Since our concern is the energy gap, we judge that β and l_t are large enough if the gap calculated with some values of β and l_t does not change for slightly smaller or larger values of β and l_t. Table 1 shows the results for $\Delta_{n_Q=16}(L_d = 32, N_s = 16)$ with several values of β and l_t. We observe the gaps coincide within the statistical errors for $\beta \geq 3.5$ and $l_t \geq 112$. We also calculate the energy gap using stochastic state selection method to obtain $\Delta_{n_Q=16}(L_d = 32, N_s = 16) = 15.71 \pm 0.03$. Based on these results we use values $\beta = 3.5$ and $l_t = 148$ in our Monte Carlo study.

What we want to examine is whether our results agree with $\Delta^{th,4}_{n_Q}$ within the statistical error, which we will denote ε_{N_s} hereafter. It should be noted that ε_{N_s} is scarcely dependent on values of n_Q. Then we need to estimate values of n_Q for which we can see the effect of the correction terms in $\Delta^{th,4}_{n_Q}$. From discussions in the previous section we see that, with $A\delta_d^2 = 1$,

$$\Delta^{th,4}_{n_Q} - \Delta^{th,2}_{n_Q} = -\delta_d^2\left(c_1\overline{\eta}^2 + c_2\right),\ c_1 \equiv \frac{n_Q^2}{2N_s},\ c_2 \equiv \frac{n_Q^4}{12N_s^3}. \tag{50}$$

Note that the first correction term in Equation (50), which enables us to distinguish $D2_{n_Q}\left(L_d, N_s\right)$ from $D1_{n_Q}\left(L_d, N_s\right)$, is observable in the range of n_Q to satisfy $\delta_d^2 c_1\overline{\eta}^2 \ge \varepsilon_{N_s}$. Similarly we should search for values of n_Q which satisfy the condition $\delta_d^2 c_2 \ge \varepsilon_{N_s}$ in order to find difference between $D3_{n_Q}\left(L_d, N_s\right)$ and $D2_{n_Q}\left(L_d, N_s\right)$.

Now let us first present our results on the $N_s = 16$ lattice. **Figure 4** plots $Dk_{n_Q}\left(L_d, N_s\right)$ ($k = 1,2,3$) with $L_d = 32$ and $L_d = 64$ as a function of n_Q. Instead of $a^{th,2}_{sq}$ in the expression (47) we use

$$a^{MC,2}_{sq} \equiv 1 - \frac{\delta_d^2}{2N_s}\left\langle E_0 \middle| \sum_l \hat{\eta}_l^2 \middle| E_0 \right\rangle. \tag{51}$$

Table 1. Results of the energy gap $\Delta_{n_Q=16}\left(L_d = 32, N_s = 16\right)$ given by Equation (48) obtained by means of the quantum Monte Carlo method.

β	l_t	$\Delta_{n_Q=16}$
3.8	164	15.70 ± 0.02
3.8	140	15.70 ± 0.02
3.8	120	15.70 ± 0.02
3.5	152	15.69 ± 0.02
3.5	132	15.70 ± 0.02
3.5	112	15.70 ± 0.02

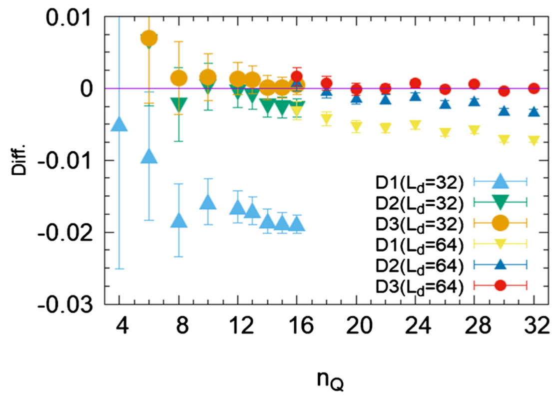

Figure 4. $Dk_{n_Q}\left(L_d, N_s = 16\right)$ ($k = 1,2,3$) defined by Equation (49) for $L_d = 32$ and 64 versus n_Q. The results for $L_d = 32$ are plotted by pale blue up triangles ($k = 1$), green down triangles ($k = 2$) and orange circles ($k = 3$), while the results for $L_d = 64$ by yellow down triangles ($k = 1$), blue up triangles ($k = 2$) and red circles ($k = 3$).

[Table 2](#) shows numerical results on $\langle E_0 | \sum_l \hat{\eta}_l^2 | E_0 \rangle$ and $a_{sq}^{MC,2}$ as well as ε_{N_s} and $\delta_d^2 c_j$ ($j = 1,2$). Since the statistical error is $\varepsilon_{N_s=16} \simeq 0.02$ for both $L_d = 32$ and $L_d = 64$ we need, with $L_d = 32\,(64)$, $n_Q \geq 5\,(10)$ to see the effect of the first correction term and $n_Q \geq 13\,(18)$ to see the effect of the second correction term. In Figure 4 we observe that only $D3_{n_Q}(L_d, N_s)$s are consistent with zero.

Next we present results of $Dk_{n_Q}(L_d = 64, N_s = 36)$ ($k = 1,2$) in Figure 5. Since the statistical error turns out $\varepsilon_{N_s=36} \sim 0.03$, we see that the minimum n_Q to find the correction from the c_1 term is 17. In this figure we did not plot $D3_{n_Q}(L_d, N_s)$ because, as we can see in Table 2, the correction from the c_2 term on this lattice is too small to distinguish $D3_{n_Q}(L_d, N_s)$ from $D2_{n_Q}(L_d, N_s)$. As is shown in Figure 5 the difference $D1_{n_Q}(L_d, N_s)$s are consistent with zero until $n_Q \leq 18$ but, even taking account of the statistical error, they clearly differ from zero when $n_Q \geq 19$. On the other hand, we see that the difference $D2_{n_Q}(L_d, N_s)$ is consistent with zero for all values of n_Q. These results support our argument on $a_{sq}^{th,2}$ in the expression (47).

Finally Figure 6 plots our results on $Dk_{n_Q}(L_d = 64, N_s = 64)$ ($k = 1,2$). We observe that $D1_{n_Q}(L_d, N_s)$s differ from zero when $n_Q \geq 24$, while $D2_{n_Q}(L_d, N_s)$ is consistent with zero for all values of n_Q.

Conclusively speaking, therefore, numerical results presented in this section on $N_s = 5, 9, 16, 32$ and 64 lattices strongly support our discussions on the energy gap in section 3.

Table 2. Values obtained from our Monte Carlo study on $N_s \geq 16$ lattices.

L_d	N_s	$\max(\delta_d^2 c_1)$	$\max(\delta_d^2 c_2)$	ε_{N_s}	$\langle E_0 \lvert \sum_l \hat{\eta}_l^2 \rvert E_0 \rangle / N_s$	$a_{sq}^{MC,2}$
32	16	0.31	0.05	0.02	0.818	0.98423
64	16	0.31	0.21	0.02	0.814	0.99606
64	36	0.14	0.03	0.03	0.820	0.99605
64	64	0.08	0.003	0.03	0.820	0.99605

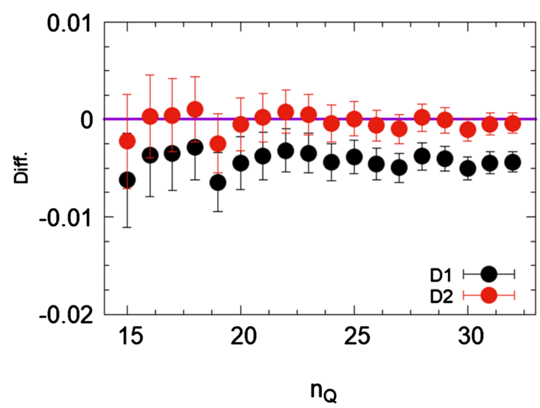

Figure 5. $Dk_{n_Q}(L_d = 64, N_s = 36)$ ($k = 1,2$) defined by Equation (49) versus n_Q. Black circles and red circles are results for $k = 1$ and 2, respectively.

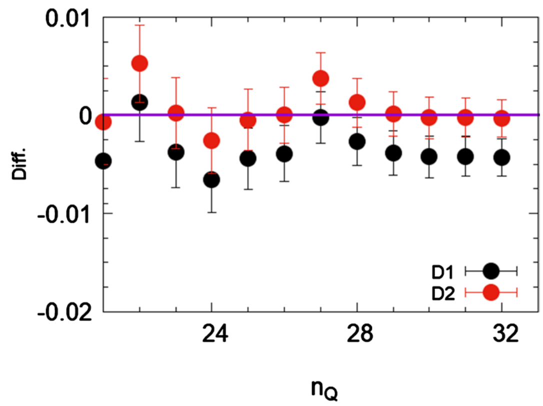

Figure 6. $Dk_{n_Q}(L_d = 64, N_s = 64)$ ($k = 1, 2$) defined by Equation (49) versus n_Q. Black circles and red circles are results for $k = 1$ and 2, respectively.

5. Conclusions and Comment to Future Study

In this paper, we studied the quasi-degenerate states, which is essential on the violation of the cluster property, in the quantum nonlinear sigma model with U(1) symmetry. Here we present our conclusion on the quasi-degenerate states by summarizing previous sections. Also in addition to the influence of the interaction strength on these states, we comment on the observation of the violation and the extension to the model with SU(2) symmetry.

In previous researches [20] [21] [22] we have shown that it is possible to observe the violation of the cluster property in spin systems when the continuous symmetry breaks spontaneously. The quite important question is whether we can observe the violation in other systems. It is specially interesting to examine whether the nonlinear sigma model shows the violation or not, because this model can be used as the effective model in the low energy region for the system with the spontaneous symmetry breaking. The study on the spin system showed that the existence of the quasi-degenerate states is the key for the violation. If there exist the quasi-degenerate states whose energies are proportional to the squared value of the quantum number, we can apply the same discussion as that in the spin system to the nonlinear sigma model. Therefore in this paper, we have presented the extensive study on the energy of this model.

In this work we have considered a quantum model defined on a lattice, introducing discrete and finite variables instead of the continuous angle variables. In order to justify these discrete variables, our discussion has started from the Weyl relation [41] [42] [43] for the basic unitary, not hermitian, operators. Based on this model we have defined the increment operator of the discrete variable $\hat{Q}_D$. Then we have introduced the quantum number n_Q and calculated the energy with the fixed value of n_Q adopting theoretical and numerical approaches. Through discussions in section 3 we have theoretically calculated the energy gap which includes n_Q^2/N_s and the correction terms. Our numerical results in section 4, which we have obtained by the diagonalization on the $N_s = 5$ lattice, by stochastic state selection method [44]-[51] on the $N_s = 9$ lattice and by quantum

Monte Carlo methods [52] [53] [54] on the $N_s = 16$, 36 and 64 lattices, showed good agreement with the theoretical estimations. By these numerical examinations as well as the theoretical studies we conclude that the quasi-degenerate states exist in the quantum nonlinear sigma model with U(1) symmetry.

A few comments are in order now.

First let us comment on the parameter B in our Hamiltonian $\hat{H}_D$ (15), which we chose to be 1 in section 4. Although the estimated value of $\bar{\eta}^2$ increases as B becomes large, the second term $\delta_d^2 \bar{\eta}^2 / 2$ in $a_{sq}^{th,2}$ in the expression (47) will still stay small compared to the first term 1. We therefore expect that our numerical results in this paper will not be largely changed even if we use larger values of B. In order to confirm this expectation, we carried out several additional calculations on the $N_s = 5$ lattice with $L_d = 32$, increasing the value of B up to 50. The result is $\langle E_0 | \sum_l \hat{\eta}_l^2 | E_0 \rangle / N_s = 0.79$ (6.2) when $B = 1$ (50). Then the difference $D3_{n_Q=1}(L_d, N_s)$ in Equation (49) becomes ~3 × 10^{-3} for $B = 50$, which should be compared with the value ~4 × 10^{-4} for $B = 1$. Summarizing the results for $B = 50$, we confirmed that $D3_{n_Q}(L_d, N_s) \le 0.015$ for all values of N_Q.

The next comment is on the violation of the cluster property in the nonlinear sigma model with U(1) symmetry. Based on discussions in the previous work [20], where we studied an antiferromagnetic spin system with U(1) symmetry, we would need an additional interaction such as $-ig \sum_i \{ \hat{U}_{qi} - \hat{U}_{qi}^\dagger \}$ in the Hamiltonian to explicitly break the symmetry. Then the model would have the unique ground state and the violation would be observed with the magnitude $1 / (g \sqrt{N_s})$ when we measure a correlation function in the ground state at the large distance. More quantitative studies will be made in future works.

The final comment is on an extension of our work to the nonlinear sigma model with SU(2) symmetry. The essential element of our present work is founded on the formulation of the model in p-representation, where we can fix the quantum number n_Q. In addition, we introduced discrete variables so that we can calculate the energy using the finite dimensional matrices for the Hamiltonian. Can we apply our ideas to the study of the model with SU(2) symmetry? The answer is perhaps yes, but more technical improvement would be required. The reason is the following. The nonlinear sigma model has been defined by fixing the magnitude of the scalar field whose Hamiltonian is the same as that of the free field. Then we have the variables with SU(2) symmetry only, which are the angles in the polar coordinate. It is difficult, however, to define the conjugate operators corresponding to these angle variables. Therefore we have no naive method to construct the nonlinear sigma model in p-representation. The technical improvement to solve this problem is under study now.

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Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

References

[1] Bell, J.S. (1964) On the Einstein-Podolsky-Rosen Paradox. *Physics Physique Fizika*, **1**, 195-200. https://doi.org/10.1103/PhysicsPhysiqueFizika.1.195

[2] Kochen, S. and Specker, E.P. (1967) The Problem of Hidden Variables in Quantum Mechanics. *Journal of Mathematics and Mechanics*, **17**, 59-87. https://doi.org/10.1512/iumj.1968.17.17004

[3] Hardy, L. (1993) Nonlocality of Two Particles without Inequalities for Almost All Entangled States. *Physics Review Letters*, **71**, 1665-1668. https://doi.org/10.1103/PhysRevLett.71.1665

[4] Horodecki, R., Horodecki, P., Horodecki, M. and Horodecki, K. (2003) Quantum Entanglement. *Review of Modern Physics*, **81**, 865-942. https://doi.org/10.1103/RevModPhys.81.865

[5] 't Hooft, G. (2006) The Mathematical Basis for Deterministic Quantum Mechanics. In: Nieuwenhuizen, T.M., Mehmani, B., Špička, V., Aghdami, M.J. and Khrennikov, A.Y., Eds., *Beyond the Quantum*, World Scientific, Singapore, 3-19. https://doi.org/10.1142/9789812771186_0001

[6] Gühne, O. and Tóth, G. (2009) Entanglement Detection. *Physics Reports*, **474**, 1-75. https://doi.org/10.1016/j.physrep.2009.02.004

[7] Ekert, A., Alves, C., Oi, D., Horodecki, M., Horodecki, P. and Kwek, L. (2002) Direct Estimations of Linear and Nonlinear Functionals of a Quantum State. *Physical Review Letters*, **88**, Article ID: 217901. https://doi.org/10.1103/PhysRevLett.88.217901

[8] Napoli, C., Bromley, T.R., Cianciaruso, M., Piani, M., Johnston, N. and Adesso, G. (2016) Robustness of Coherence: An Operational and Observable Measure of Quantum Coherence. *Physical Review Letters*, **116**, Article ID: 150502. https://doi.org/10.1103/PhysRevLett.116.150502

[9] Nielsen, M.A. and Chuang, I.L. (2000) Quantum Computation and Quantum Information. Cambridge University, Cambridge.

[10] Deutsch, D. (1985) Quantum Theory, the Church-Turing Principle and the Universal Quantum Computer. *Proceedings of the Royal Society of London. Series A*, **400**, 97-117. https://doi.org/10.1098/rspa.1985.0070

[11] Weinberg, S. (1995) The Quantum Theory of Fields. Vol. 2, Cambridge University, Cambridge.

[12] Strocchi, F. (2008) Symmetry Breaking. Vol. 732, Springer, Berlin. https://doi.org/10.1007/978-3-540-73593-9

[13] Dell'Anna, L., Salberger, O., Barbiero, L., Trombettoni, A. and Korepin, V. (2016) Violation of Cluster Decomposition and Absence of Light Cones in Local Integer and Half-Integer Spin Chains. *Physical Review B*, **94**, Article ID: 155140. https://doi.org/10.1103/PhysRevB.94.155140

[14] Shimizu, A. and Miyadera, T. (2002) Cluster Property and Robustness of Ground States of Interacting Many Bosons. *Journal of the Physical Society of Japan*, **71**,

56-59. https://doi.org/10.1143/JPSJ.71.56

[15] Shimizu, A. and Miyadera, T. (2002) Stability of Quantum States of Finite Macroscopic Systems against Classical Noises. *Perturbations from Environments, and Local Measurements*, **89**, Article ID: 270403. https://doi.org/10.1103/PhysRevLett.89.270403

[16] Xu, S. and Fan, S. (2017) Generalized C Luster Decomposition Principle Illustrated in Waveguide Quantum Electrodynamics. *Physical Review A*, **95**, Article ID: 063809. https://doi.org/10.1103/PhysRevA.95.063809

[17] Fröhlich, J. and Rodríguez, P. (2017) On Cluster Properties of Classical Ferromagnets in an External Magnetic Field. *Journal of Statistical Physics*, **166**, 828-840. https://doi.org/10.1007/s10955-016-1556-2

[18] Strocchi, F. (1978) Local and Covariant Gauge Quantum Field Theories. Cluster Property, Superselection Rules, and the Infrared Problem. *Physics Review D*, **17**, 2010-2021. https://doi.org/10.1103/PhysRevD.17.2010

[19] Lowdon, P (2016) Conditions on the Violation of the Cluster Decomposition Property in QCD. *Journal of Mathematical Physics*, **57**, Article ID: 102302. https://doi.org/10.1063/1.4965715

[20] Munehisa, T. (2018) Violation of Cluster Property in Quantum Antiferromagnet. *World Journal of Condensed Matter Physics*, **8**, 1-22. https://doi.org/10.4236/wjcmp.2018.81001

[21] Munehisa, T. (2018) Violation of Cluster Property in Heisenberg Antiferromagnet. *World Journal of Condensed Matter Physics*, **8**, 203-229. https://doi.org/10.4236/wjcmp.2018.84015

[22] Munehisa, T. (2020) Quantum Curie-Weiss Magnet Induced by Violation of Cluster Property. *World Journal of Condensed Matter Physics*, **10**, 27-52. https://doi.org/10.4236/wjcmp.2020.102003

[23] Anderson, P.W. (1984) Basic Notions of Condensed Matter Physics. Benjamin/ Cummings, Menlo Park.

[24] Kochmanski, M., Paszkiewicz, T. and Wolski, S. (2013) Curie-Weiss Magnet?—A Simple Model of Phase Transition. *European Journal of Physics*, **34**, Article No. 1555. https://doi.org/10.1088/0143-0807/34/6/1555

[25] Chayes, L., Crawford, N., Ioffe, D. and Levit. A. (2008) The Phase Diagram of the Quantum Curie-Weiss Model. *Journal of Statistical Physics*, **133**, Article No. 131. https://doi.org/10.1007/s10955-008-9608-x

[26] Carneiro, C. and Pellegrino, G. (2018) Analysis of Quantum Phase Transition in Some Different Curie-Weiss Models: A Unified Approach.

[27] Richter, J., Schulenburg, J. and Honecker, A. (2004) Quantum Magnetism in Two Dimensions: From Semi-Classical Néel Order to Magnetic Disorder. In: Schollwöck, U., Richter, J., Farnell, D.J.J. and Bishop, R.F., Eds., *Quantum Magnetism*, Vol. 645, Springer-Verlag, Berlin, 85-153. https://doi.org/10.1007/BFb0119592

[28] Manousakis, E (1991) The Spin 1/2 Heisenberg Antiferromagnet on a Square Lattice and Its Application to the Cuprous Oxides. *Review Modern of Physics*, **63**, 1-62. https://doi.org/10.1103/RevModPhys.63.1

[29] Landee, C. and Turnbull, M. (2013) Recent Developments in Low-Dimensional Copper(II) Molecular Magnets. *European Journal of Inorganic Chemistry*, **2013**, 2266-2285. https://doi.org/10.1002/ejic.201390053

[30] Haldane, F. (1983) Nonlinear Field Theory of Large-Spin Heisenberg Antiferromagnets: Semiclassically Quantized Solitons of the One-Dimensional Easy-Axis

Néel State. *Physical Review Letters*, **50**, 1153-1156.
https://doi.org/10.1103/PhysRevLett.50.1153

[31] Chakravarty, S., Halperin, B, and Nelson, S. (1989) Two-Dimensional Quantum Heisenberg Antiferromagnet at Low Temperatures. *Physical Review B*, **39**, 2344-2371.
https://doi.org/10.1103/PhysRevB.39.2344

[32] Chubukov, A., Sachdev, S. and Ye, J. (1994) Theory of Two-Dimensional Quantum Heisenberg Antiferromagnets with a Nearly Critical Ground State. *Physical Review B*, **49**, 11919-11961. https://doi.org/10.1103/PhysRevB.49.11919

[33] Auerbach, A. (1994) Interacting Electrons and Quantum Magnetism. Springer-Verlag, New York. https://doi.org/10.1007/978-1-4612-0869-3

[34] Chen, Y. and Neto, A. (2000) Effective Field Theory for Layered Quantum Antiferromagnets with Nonmagnetic Impurities. *Physical Review B*, **61**, Article No. R3772-R3775. https://doi.org/10.1103/PhysRevB.61.R3772

[35] Dupre, T. (1996) Localization Transition in Three Dimensions: Monte Carlo Simulation of a Nonlinear Sigma Model. *Physical Review B*, **54**, 12763-12774.
https://doi.org/10.1103/PhysRevB.54.12763

[36] Schaefer, L. and Wegner, F. (1980) Disordered System with N Orbitals Per Site: Lagrange Formulation, Hyperbolic Symmetry, and Goldstone Modes. *Zeitschrift für Physik B Condensed Matter*, **38**, 113-126. https://doi.org/10.1007/BF01598751

[37] Bulgadaev, S. (2000) D-Dimensional Conformal Sigma-Models and Their Topological Excitation. arXiv:hep-th/0008017v1.

[38] Alles, B., Borisenko, O. and Papa, A. (2018) Finite Density 2D $O(3)$ Sigma Model: Dualization and Numerical Simulations. *Physics Review D*, **98**, Article ID: 114508.
https://doi.org/10.1103/PhysRevD.98.114508

[39] Abanov, A. and Wiegmann, P. (2000) Chiral Non-Linear Sigma-Models as Models for Topological Superconductivity.

[40] Scherer, S. (2002) Introduction to Chiral Perturbation Theory.

[41] Schmudgen, K. (1983) On the Heisenberg Commutation Relation. I. *Journal of Functional Analysis*, **50**, 8-49. https://doi.org/10.1016/0022-1236(83)90058-7

[42] Albeverio, S. and Sengupta, A. (2016) Complex Phase Space and Weyl's Commutation Relations. *Expositiones Mathematicae*, **34**, 249-286.
https://doi.org/10.1016/j.exmath.2015.12.006

[43] Arai, A. (2016) A Family of Inequivalent Weyl Representations of Canonical Commutation Relations with Applications to Quantum Field Theory. *Reviews in Mathematical Physics*, **28**, Article ID: 1650007.
https://doi.org/10.1142/S0129055X16500070

[44] Munehisa, T. and Munehisa, Y. (2003) A New Approach to Stochastic State Selections in Quantum Spin Systems. *Journal of the Physical Society of Japan*, **72**, 2759-2765.
https://doi.org/10.1143/JPSJ.72.2759

[45] Munehisa, T. and Munehisa, Y. (2004) The Stochastic State Selection Method for Energy Eigenvalues in the Shastry-Sutherland Model. *Journal of the Physical Society of Japan*, **73**, 340-347. https://doi.org/10.1143/JPSJ.73.340

[46] Munehisa, T. and Munehisa, Y. (2004) Numerical Study for an Equilibrium in the Recursive Stochastic State Selection Method.

[47] Munehisa, T. and Munehisa, Y. (2004) A Recursive Method of the Stochastic State Selection for Quantum Spin Systems. *Journal of the Physical Society of Japan*, **73**, 2245-2251. https://doi.org/10.1143/JPSJ.73.2245

[48] Munehisa, T. and Munehisa, Y. (2006) The Stochastic State Selection Method Com-

bined with the Lanczos Approach to Eigenvalues in Quantum Spin Systems. *Journal of Physics*: *Condensed Matter*, **18**, 2327-2335.
https://doi.org/10.1088/0953-8984/18/7/018

[49] Munehisa, T. and Munehisa, Y. (2007) An Equilibrium for Frustrated Quantum Spin Systems in the Stochastic State Selection Method. *Journal of Physics*: *Condensed Matter*, **19**, 196202-196220. https://doi.org/10.1088/0953-8984/19/19/196202

[50] Munehisa, T. and Munehisa, Y. (2009) A Constrained Stochastic State Selection Method Applied to Frustrated Quantum Spin Systems. *Journal of Physics*: *Condensed Matter*, **21**, 236008-236019. https://doi.org/10.1088/0953-8984/21/23/236008

[51] Munehisa, T. and Munehisa, Y. (2010) Numerical Study of the Spin-1/2 Heisenberg Antiferromagnet on a 48-Site Triangular Lattice Using the Stochastic State Selection Method.

[52] Hatano, N. and Suzuki, M. (1993) Quantum Monte Carlo and Related Methods: Recent Developments. In: Suzuki, M., Ed., *Quantum Monte Carlo Methods in Condensed Matter Physics*, World Scientific, Singapore, 13-47.
https://doi.org/10.1142/9789814503815_0002

[53] De Raedt, H. and von der Linden, W. (1995) The Monte Carlo Method in Condensed Matter Physics. Springer-Verlag, Berlin, Heidelberg, 249-284.

[54] Kawashima, N. (2002) Quantum Monte Carlo Methods. *Progress of Theoretical Physics Supplement*, **145**, 138-148. https://doi.org/10.1143/PTPS.145.138

Appendix

A1. Weyl Relation

Here we present a brief description for the Weyl relation. In quantum mechanics for one particle the commutation relation of the hermite operator of the position $\hat{q}$ and the operator of the momentum $\hat{p}$ is a starting point.

$$[\hat{q},\hat{p}]=i,\ \hat{q}|q\rangle=|q\rangle q,\ \hat{p}|p\rangle=|p\rangle p,\ \langle p|q\rangle=\exp(-ipq). \tag{52}$$

In the Weyl relation, we introduce unitary operators defined by

$$\hat{U}_q(t)\equiv\exp(i\hat{q}t),\ \hat{U}_p(s)\equiv\exp(i\hat{p}s). \tag{53}$$

Here s and t are real numbers. In this representation, we define the Weyl relation by

$$\hat{U}_q(t)\hat{U}_p(s)=\hat{U}_p(s)\hat{U}_q(t)\exp(-ist),\ \hat{U}_p(s)\hat{U}_q(t)=\hat{U}_q(t)\hat{U}_p(s)\exp(ist). \tag{54}$$

Using these operators we have

$$\begin{gathered}\hat{U}_q(t)|q\rangle=|q\rangle\exp(itq),\quad \hat{U}_p(s)|p\rangle=|p\rangle\exp(isp),\\ \hat{U}_p(s)|q\rangle=|q-s\rangle,\ \hat{U}_q(t)|p\rangle=|p+t\rangle.\end{gathered} \tag{55}$$

The third equation is led by

$$\begin{aligned}\hat{U}_p(s)|q\rangle&=\int\mathrm{d}p\frac{1}{2\pi}\hat{U}_p(s)|p\rangle\langle p|q\rangle\\ &=\int\mathrm{d}p\frac{1}{2\pi}|p\rangle\exp(isp)\exp(-ipq)=|q-s\rangle.\end{aligned} \tag{56}$$

A2. Wely Relation for Discrete Variable

In our work, we introduce an unitary operator $\hat{U}_q$ with a discrete value n where $n=0,1,\cdots,L_d-1$ for a finite integer L_d. We then introduce another unitary operator $\hat{U}_p$ which satisfies the following Weyl relation.

$$\hat{U}_p\hat{U}_q=\hat{U}_q\hat{U}_p\exp(i\delta_d),\ \delta_d\equiv 2\pi/L_d. \tag{57}$$

Note that

$$\begin{aligned}\hat{U}_q\left(\hat{U}_p\right)^n&=\hat{U}_q\hat{U}_p\left(\hat{U}_p\right)^{n-1}=\hat{U}_p\hat{U}_q\left(\hat{U}_p\right)^{n-1}\exp(-i\delta_d)\\ &=\cdots=\left(\hat{U}_p\right)^m\hat{U}_q\left(\hat{U}_p\right)^{n-m}\exp(-im\delta_d)\\ &=\cdots=\left(\hat{U}_p\right)^n\hat{U}_q\exp(-in\delta_d).\end{aligned} \tag{58}$$

We suppose that $\hat{U}_q$ has an eigenstate $|n_0\rangle_q$ whose eigenvalue is $\lambda_0=\exp(i\gamma)$ with a real number γ.

$$\hat{U}_q|n_0\rangle_q=|n_0\rangle_q\lambda_0. \tag{59}$$

Here we can make $\lambda_0=1$ by using $\hat{U}_q\exp(-i\gamma)$ instead of $\hat{U}_q$. Then, with this re-defined $\hat{U}_q$, we obtain

$$\hat{U}_q|0\rangle_q=|0\rangle_q,$$

$$\hat{U}_q\left(\hat{U}_p\right)^n|0\rangle_q = \left(\hat{U}_p\right)^n\hat{U}_q|0\rangle_q \exp\left(-in\delta_d\right) = \left(\hat{U}_p\right)^n|0\rangle_q \exp\left(-in\delta_d\right). \quad (60)$$

The state $|n\rangle_q \equiv \left(\hat{U}_p\right)^n|0\rangle_q$ is therefore the eigenstate of the unitary operator $\hat{U}_q$ with the eigenvalue $\lambda_n \equiv \exp\left(-in\delta_d\right)$.

Let us consider the state $|L_d\rangle_q \equiv \hat{U}_p|L_d-1\rangle_q$. Then

$$\begin{aligned}\hat{U}_q|L_d\rangle_q &= \hat{U}_q\hat{U}_p|L_d-1\rangle_q = \hat{U}_p\hat{U}_q\exp\left(-i\delta_d\right)|L_d-1\rangle_q \\ &= \hat{U}_p|L_d-1\rangle_q\exp\left(-i\delta_d\right)\exp\left\{-i\left(L_d-1\right)\delta_d\right\} = |L_d\rangle_q\cdot 1.\end{aligned} \quad (61)$$

Therefore $|L_d\rangle_q$ is the eigenstate of $\hat{U}_q$ with the eigenvalue 1 so that $|L_d\rangle_q = |0\rangle_q\,\mathrm{e}^{i\beta}$ holds for a real number β. Re-defining $\hat{U}_p\mathrm{e}^{-i\beta/L_d}$ as $\hat{U}_p$ we obtain

$$|L_d\rangle_q = |0\rangle_q. \quad (62)$$

Let us next make a new state $|0\rangle_p$ defined by

$$|0\rangle_p \equiv \frac{1}{\sqrt{L_d}}\sum_{k=0}^{L_d-1}\left(\hat{U}_p\right)^k|0\rangle_q = \frac{1}{\sqrt{L_d}}\sum_{k=0}^{L_d-1}|k\rangle_q. \quad (63)$$

This state is the eigenstate of $\hat{U}_p$ with the eigenvalue 1, because

$$\begin{aligned}\hat{U}_p|0\rangle_p &= \frac{1}{\sqrt{L_d}}\sum_{k=0}^{L_d-1}\left(\hat{U}_p\right)^{k+1}|0\rangle_q = \frac{1}{\sqrt{L_d}}\sum_{k=1}^{L_d}\left(\hat{U}_p\right)^k|0\rangle_q \\ &= \frac{1}{\sqrt{L_d}}\left\{\sum_{k=1}^{L_d-1}\left(\hat{U}_p\right)^k + \left(\hat{U}_p\right)^{L_d}\right\}|0\rangle_q \\ &= \frac{1}{\sqrt{L_d}}\left\{\sum_{k=1}^{L_d-1}\left(\hat{U}_p\right)^k + \hat{I}\right\}|0\rangle_q = |0\rangle_p.\end{aligned} \quad (64)$$

We then see that $|m\rangle_p \equiv \left(\hat{U}_q\right)^m|0\rangle_p$ is the eigenstate of $\hat{U}_p$ with the eigenvalue $\exp\left(im\delta_d\right)$, since

$$\begin{aligned}\hat{U}_p|m\rangle_p &= \hat{U}_p\left(\hat{U}_q\right)^m|0\rangle_p = \left(\hat{U}_q\right)^m\hat{U}_p|0\rangle_p\exp\left(im\delta_d\right) \\ &= \left(\hat{U}_q\right)^m|0\rangle_p\exp\left(im\delta_d\right) = |m\rangle_p\exp\left(im\delta_d\right).\end{aligned} \quad (65)$$

Finally we calculate the inner product ${}_q\langle n|m\rangle_p$. Note that

$$\begin{aligned}\hat{U}_p^\dagger\hat{U}_q &= \left\{\hat{U}_p^\dagger\hat{U}_q\right\}\left\{\hat{U}_p\hat{U}_p^\dagger\right\} = \hat{U}_p^\dagger\left\{\hat{U}_q\hat{U}_p\right\}\hat{U}_p^\dagger = \hat{U}_p^\dagger\left\{\hat{U}_p\hat{U}_q\exp\left(-i\delta_d\right)\right\}\hat{U}_p^\dagger \\ &= \left\{\hat{U}_p^\dagger\hat{U}_p\right\}\left\{\hat{U}_q\hat{U}_p^\dagger\right\}\exp\left(-i\delta_d\right) = \hat{U}_q\hat{U}_p^\dagger\exp\left(-i\delta_d\right).\end{aligned} \quad (66)$$

Using (64) and (66) we obtain

$$\begin{aligned}{}_q\langle n|m\rangle_p &= {}_q\langle 0|\left(\hat{U}_p^\dagger\right)^n\left(\hat{U}_q\right)^m|0\rangle_p = {}_q\langle 0|\left(\hat{U}_q\right)^m\left(\hat{U}_p^\dagger\right)^n|0\rangle_p\exp\left(-inm\delta_d\right) \\ &= {}_q\langle 0|0\rangle_p\exp\left(inm\delta_d\right) = {}_q\langle 0|\frac{1}{\sqrt{L_d}}\left(\sum_{k=0}^{L_d-1}|k\rangle_q\right)\exp\left(-inm\delta_d\right) \\ &= {}_q\langle 0|\frac{1}{\sqrt{L_d}}|0\rangle_q\exp\left(-inm\delta_d\right) = \frac{1}{\sqrt{L_d}}\exp\left(-inm\delta_d\right).\end{aligned} \quad (67)$$