Fermionic theory for quantum antiferromagnets with spin $S > \frac{1}{2}$

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The fermion representation for $S = \frac{1}{2}$ spins is generalized to spins with arbitrary magnitudes. The symmetry properties of the representation is analyzed where we find that the particle-hole symmetry in the spinon Hilbert space of $S = \frac{1}{2}$ fermion representation is absent for $S > \frac{1}{2}$. As a result, different path-integral representations and mean-field theories can be formulated for spin models. In particular, we construct a Lagrangian with restored particle-hole symmetry, and apply the corresponding mean-field theory to one-dimensional (1D) $S=1$ and $S=3/2$ antiferromagnetic (AFM) Heisenberg models, with results that agree with Haldane's conjecture. For a $S=1$ open chain, we show that Majorana fermion edge states exist in our mean-field theory. The generalization to spins with arbitrary magnitude S is discussed. Our approach can be applied to higher dimensional spin systems. As an example, we study the geometrically frustrated $S=1$ AFM on triangular lattice. Two spin liquids with different pairing symmetries are discussed: the gapped $p_x + ip_y$ -wave spin liquid and the gapless f -wave spin liquid. We compare our mean-field result with the experiment on NiGa_2S_4 , which remains disordered at low temperature and was proposed to be in a spin-liquid state. Our fermionic mean-field theory provide a framework to study $S > \frac{1}{2}$ spin liquids with fermionic spinon excitations.

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I. INTRODUCTION

Quantum magnetism is one of the oldest central problems in condensed matter and many body physics. Few exact results are known except at one dimension (1D) or when long-range spin order is established at low temperature. In the later case, Landau's symmetry-breaking paradigm is applicable, and the long-range spin order determines the low-energy physics of the system. The low-energy spin excitations are spin waves or magnons.¹ Systematic corrections to spin-wave theory can be obtained through semiclassical approach ($1/S$ expansion²) and/or nonlinear σ model.³ However, it was suggested that for some antiferromagnetic materials, strong quantum fluctuations due to small spin magnitude and low dimensionality combined with geometric frustration may lead to quantum coherent, spin disordered ground states.^{4,5} In such cases, a quantum fluid approach⁶ is probably a better starting point to describe the low-energy physics instead of usual spin-wave or semiclassical approach.

There exist at present two common quantum fluid approaches based on different "particle" representations of spins. In the "bosonic" approach^{6,7} spins are represented by spin up and down Schwinger bosons with the constraint that total boson number at each site is $2S$. A spin-disordered state is obtained in a mean-field theory as long as Bose condensation does not occur. The low-lying excitations coming from this theory are bosonic. The other possibility is to represent spins by fermions. Up to now, the fermionic approach is mainly restricted to $S = \frac{1}{2}$ spin systems.^{6,8} Because of the Pauli exclusion principle, we cannot put more than two spin up or down fermions on a site to form $S > \frac{1}{2}$ objects as in bosonic approach. One way out is to introduce more species of fermions. It was proposed in Ref. 9, that $(2S+1)$ species of boson/fermions can be used to construct the spin- S swapping operators. Later, it is shown that the fermionic representation

can be used to describe a $S=1$ valence bond solid state.¹⁰

In this paper, we systematically study the fermionic representation for arbitrary spins. To construct a spin operator with spin magnitude S , we follow Ref. 9 and introduce different fermion operators for different S_z states. We find that for half-odd-integer spins, the spin operator thus constructed is invariant under a $SU(2)$ transformations,⁸ i.e., the symmetry group is $SU(2)$ group whereas for integer spins the symmetry group is $U(1) \otimes \mathbb{Z}_2$. Fermionic path-integral formulations for spin systems with arbitrary spin S can then be formulated and the corresponding mean-field theories can be studied. We shall see that one of the mean-field theories applied to 1D antiferromagnetic (AFM) Heisenberg model produces mean-field excitation spectrums which agrees with Haldane's conjecture.³ Moreover, there exist zero-energy Majorana edge modes for open integer spin chains. We also apply our approach to two-dimensional (2D) antiferromagnetic Heisenberg models on triangular lattices where we obtain two translational and rotational invariant spin-liquid solutions, one (with $p_x + ip_y$ -wave pairing symmetry) is gapped and the other one (with f -wave pairing symmetry) has nodes at the spinon Fermi level. Comparing with experiments on NiGa_2S_4 , we argue that the f -wave pairing spin liquid is a plausible ground state.

It should be noted that rather different fermionic/bosonic spinon approaches have also been applied to $SU(N)$ spin models where the dynamic symmetry is generalized from $SU(2)$ to $SU(N)$, and the Hamiltonian is composed of $SU(N)$ generators.^{6,11,12} In these approaches, N species of particles are introduced to construct the $SU(N)$ -spin operator and Hamiltonians.¹² The major difference between our approach and the $SU(N)$ approaches is that $(2S+1)$ species of fermions are introduced to form a $SU(2)$ spin [or irreducible representation of $SU(2)$ group] in our approach. Unlike the $SU(N)$ models,¹² our approach is not limited to bipartite lattices.

The paper is organized as follows. In Sec. II, we introduce the general fermionic spinon representation for arbitrary spin S and discuss the symmetry properties associated with the representation. In Sec. III, we introduce the path-integral formalism where different ways of imposing particle number constraints are presented. A particle-hole symmetric way of imposing constraint is discussed. In Secs. IV A and IV B, we focus on 1D Heisenberg models for spin-1 and spin-3/2, respectively, and study two versions of the mean-field theories. The cases for general spin S are discussed in Sec. IV C. In Sec. V we study 2D AFM models on triangular lattice. Our paper is summarized and concluded in Sec. VI.

II. GENERAL FERMIONIC SPIN REPRESENTATION

We begin with the fermionic representation for spins. For spin $S = \frac{1}{2}$, two species of fermions $c_\uparrow$ and $c_\downarrow$ are introduced to construct the three spin operators $S^{x,y,z}$. To generalize this fermionic representation to arbitrary spin S , we introduce $2S+1$ species of fermionic operators c_m satisfying anticommutation relations,

$$\{c_m, c_n^\dagger\} = \delta_{mn}, \quad (1)$$

where $m, n = S, S-1, \dots, -S$. The spin operator can be expressed in terms of c_m and $c_n^\dagger$ s,

$$\hat{S} = C^\dagger \mathbf{I} C,$$

where $C = (c_S, c_{S-1}, \dots, c_{-S})^T$ and I^a ($a = x, y, z$) is a $(2S+1) \times (2S+1)$ matrix whose matrix elements are given by

$$I_{mn}^a = \langle S, m | S^a | S, n \rangle.$$

It is easy to see that the operators $\hat{S}^a$ satisfy the $SU(2)$ angular momentum algebra, $[\hat{S}^a, \hat{S}^b] = i\epsilon^{abc}\hat{S}^c$. Under a rotational operation, C is a spin- S “spinor” transforming as $C_m \rightarrow D_{mn}^S C_n$ and $\hat{S}$ is a vector transforming as $S^a \rightarrow R_{ab} S^b$, here D^S is the $2S+1$ -dimensional irreducible representation of $SU(2)$ group generated by $\mathbf{I}$ and R is the adjoint representation.

As in the $S=1/2$ case, a constraint that there is only one fermion per site is needed to project the fermionic system into the proper Hilbert space representing spins, i.e.,

$$(\hat{N}_i - N_f)|\text{phy}\rangle = 0, \quad (2)$$

where i is the site index and $N_f=1$ (the particle representation, one fermion per site). Alternatively, it is straightforward to show that the constraint $N_f=2S$ (the hole representation, a single hole per site) represents a spin equally. The $N_f=1$ representation can be mapped to the $N_f=2S$ representation via a *particle-hole transformation*. For $S=\frac{1}{2}$, the particle picture and the hole picture are identical, reflecting an intrinsic particle-hole symmetry of the underlying Hilbert space which is absent for $S \geq 1$.

Following Affleck *et al.*,⁸ we introduce another spinor $\bar{C} = [c_{-S}^\dagger, -c_{-S+1}^\dagger, c_{-S+2}^\dagger, \dots, (-1)^{2S} c_S^\dagger]^T$, whose components can be written as $\bar{C}_m = (-1)^{S-m} c_{-m}^\dagger$, where the index m runs from S to $-S$ as in C . To examine whether $\bar{C}$ is really a spinor, we

construct a spin singlet state for two spins at site i and j , $\frac{C_i^\dagger \bar{C}_j}{\sqrt{2S+1}} |\text{vac}\rangle = \frac{1}{\sqrt{2S+1}} \sum_{m=-S}^S (-1)^{S-m} |S, m\rangle_i |S, -m\rangle_j$. Therefore $C_i^\dagger \bar{C}_j$ is a scalar operator as $C_i^\dagger C_j$, meaning that $\bar{C}$ and C must behave identically under spin rotation. Consequently, the spin operators can also be written in terms of $\bar{C}$,

$$\hat{S} = \bar{C}^\dagger \mathbf{I} \bar{C}.$$

Combining C and $\bar{C}$ into a $(2S+1) \times 2$ matrix $\psi = (C, \bar{C})$,⁸ we can reexpress the spin operators as

$$\hat{S} = \frac{1}{2} \text{Tr}(\psi^\dagger \mathbf{I} \psi) \quad (3)$$

and the constraint can be expressed as

$$\text{Tr}(\psi \sigma_z \psi^\dagger) = 2S + 1 - 2N_f = \pm (2S - 1), \quad (4)$$

where the $+$ sign implies $N_f=1$ and $-$ sign implies $N_f=2S$.

We are interested in two kinds of operations (or groups) acting on ψ . The first kind belongs to a $(2S+1)$ -dimensional irreducible representation of $SU(2)$ group, acting on the left of ψ . Suppose G is an element of this irreducible representation, then $G^\dagger I^a G = R^{ab} I^b$ [R belongs to the adjoint irreducible representation of $SU(2)$ group, which is a $SO(3)$ matrix]. Under transformation $\psi \rightarrow G\psi$, the spin operator $\hat{S}^a = \frac{1}{2} \text{Tr}(\psi^\dagger I^a \psi)$ becomes $\hat{S}^a \rightarrow R^{ab} \hat{S}^b$, which means a *rotation of the spin*. It is obvious that the particle number constraint Eq. (4) remains unchanged under the action of G .

The other kind belongs to a 2×2 unitary group acting on the right of ψ which keeps the spin operator Eq. (3) and the fermionic statistics Eq. (1) invariant. This group reflects the symmetry properties of the underlying Hilbert space structure in the fermionic representation. We call it an *internal symmetry group*. The internal symmetry group is different for integer and half-integer spins. It is $U(1) \bar{\otimes} Z_2 = \{e^{i\sigma_z \theta}, \sigma_x e^{i\sigma_z \theta} = e^{-i\sigma_z \theta} \sigma_x; \theta \in \mathbb{R}\}$ for the former and $SU(2)$ for the latter. We leave the rigorous proof in Appendix A, and shall explain qualitatively the reason behind here. Notice that C and $\bar{C}$ are not independent. The operators in the internal symmetry group will “mix” the two fermion operators in the same row of C and $\bar{C}$, i.e., c_S and $c_{-S}^\dagger$, c_{S-1} and $-c_{-S+1}^\dagger$, etc. For integer spins, c_0 and $(-1)^S c_0^\dagger$ will be “mixed.” To keep the relation $\{c_0, c_0^\dagger\} = 1$ invariant, there are only two methods of “mixing:” one is an $U(1)$ transformation, the other is interchanging the two operators. These operations form the $U(1) \bar{\otimes} Z_2$ group. For half-odd-integer spins, the pair $[c_0, (-1)^S c_0^\dagger]$ do not exist, and the symmetry group is the maximum group $SU(2)$. The difference between integer and half-integer spins is a fundamental property of the fermionic representation as we shall see more later.

Now let us see how the constraints Eq. (4) transform under the symmetry group. For $S=\frac{1}{2}$, the constraint Eq. (4) is invariant under the transformation $\psi \rightarrow \psi W$ because the right hand side vanishes (due to the particle-hole symmetry of the Hilbert space). For integer spins, if $W = e^{i\sigma_z \theta}$, then $W \sigma_z W^\dagger = \sigma_z$, and Eq. (4) is invariant. If $W = \sigma_x e^{i\sigma_z \theta}$, then $W \sigma_z W^\dagger$

$= -\sigma_z$, meaning that the particle picture [+ sign in Eq. (4)] and the “hole” picture [− sign in Eq. (4)] are transformed to each other.

For a half-odd-integer spin with $S \geq 3/2$, $W \in SU(2)$ is a rotation and we need to extend the constraint into a vector form similar to $S = \frac{1}{2}$ case⁸ so that Eq. (4) becomes

$$\text{Tr}(\psi \sigma \psi^\dagger) = [0, 0, \pm (2S - 1)]^T. \quad (5)$$

Under the group transformation $\psi \rightarrow \psi W$,

$$\text{Tr}(\psi \sigma \psi^\dagger) \rightarrow (R^{-1})[0, 0, \pm (2S - 1)]^T, \quad (6)$$

where $W \sigma^a W^\dagger = R_{ab} \sigma^b$, $a, b = x, y, z$, i.e., R is a 3×3 matrix representing a three-dimensional rotation in the internal Hilbert space. The transformed constraint represents a new Hilbert subspace which is still a $(2N+1)$ -dimensional irreducible representation of the spin $SU(2)$ algebra. Any measurable physical quantity such as the spin $\mathbf{S}$ remains unchanged in the new Hilbert space. Therefore, for half-odd-integer spins ($S \geq 3/2$), there exists infinitely many ways of imposing the constraint that gives rise to a Hilbert subspace representing a spin. However, for integer spins, there exists only two possible constraint representations.

The different representations of constraints for $S > \frac{1}{2}$ systems result in different path-integral representations and different mean-field theories. These mean-field theories are equivalent in the sense that they can be transformed to each other by the internal symmetry group. In the next section, we shall study the Heisenberg model in different representations and shall construct a mixed path-integral representation which restored particle-hole symmetry, and the internal symmetry group becomes “almost” a gauge symmetry.⁸ The mixed representation is studied in Sec. IV where a distinct mean-field theory is proposed which recovers Haldane conjecture at 1D for the Heisenberg model.

III. PATH-INTEGRAL FORMALISM AND MEAN-FIELD THEORY FOR HEISENBERG MODEL

We shall focus on the antiferromagnetic Heisenberg model $H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$ with $J > 0$ in the rest of the paper. We start by presenting some useful algebraic manipulations of the Hamiltonian, and then discuss the general path-integral formalism. The different ways of handling constraints and how they affect the symmetry of the Lagrangian will be discussed in the process.

A. Heisenberg model and an effective Hamiltonian

It is known that for spin- $\frac{1}{2}$ the Heisenberg interaction can be written as⁸

$$\begin{aligned} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j &= -\frac{1}{8} \text{Tr}(\psi_i^\dagger \psi_j \psi_j^\dagger \psi_i) \\ &= -\frac{1}{4} :(\chi_{ij}^\dagger \chi_{ij} + \Delta_{ij}^\dagger \Delta_{ij}):, \end{aligned} \quad (7)$$

where

$$\chi_{ij} = C_i^\dagger C_j, \quad \Delta_{ij} = \bar{C}_i^\dagger C_j \quad (8)$$

are spin-singlet operators. χ_{ij} and Δ_{ij} will be extended to arbitrary spin magnitudes with the above definition and will be used in the following discussions. Interestingly, an expression almost the same as Eq. (7) holds for $S=1$, but this is no longer true for larger spins. We shall present precise formula for $S=3/2$ and $S=2$, and provide a general discussion for higher spins.

For $S=1$, the three spin matrices are

$$I_+ = (I_-)^\dagger = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}, \quad I_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

where $I_\pm = I_x \pm iI_y$. The matrix operator ψ is given by

$$\psi = (C \bar{C}) = \begin{pmatrix} c_1 & c_{-1}^\dagger \\ c_0 & -c_0^\dagger \\ c_{-1} & c_1^\dagger \end{pmatrix}.$$

The spin operator can be written in form of Eq. (3), and it can be shown after some straightforward algebra that the Hamiltonian can be written as

$$\begin{aligned} H &= J \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j = -\frac{J}{2} \sum_{\langle i,j \rangle} \text{Tr}(\psi_i^\dagger \psi_j \psi_j^\dagger \psi_i) \\ &= -J \sum_{\langle i,j \rangle} :(\chi_{ij}^\dagger \chi_{ij} + \Delta_{ij}^\dagger \Delta_{ij}):. \end{aligned} \quad (9)$$

For $S=3/2$, the three spin matrices are

$$I_+ = (I_-)^\dagger = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad I_z = \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}.$$

and the matrix operator ψ is given by $\psi = (C \bar{C})$, where $C = (c_{3/2}, c_{1/2}, c_{-1/2}, c_{-3/2})^T$ and $\bar{C} = (c_{-3/2}^\dagger, -c_{-1/2}^\dagger, c_{1/2}^\dagger, -c_{3/2}^\dagger)^T$. In this case the singlet operators χ_{ij} and Δ_{ij} alone are not enough to represent the Heisenberg Hamiltonian, and triplet hoping and pairing terms are necessary. After some straightforward but tedious algebra, we find that the Hamiltonian for spin $S=3/2$ Heisenberg model can be written as

$$\begin{aligned} H &= J \sum_{i,j} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \\ &= -\frac{J}{4} \sum_{i,j} :[\text{Tr}(\psi_i^\dagger \mathbf{I} \psi_j \cdot \psi_j^\dagger \mathbf{I} \psi_i) + S^2 \text{Tr}(\psi_i^\dagger \psi_j \psi_j^\dagger \psi_i)]:. \end{aligned} \quad (10)$$

It is interesting to note that the above form holds also for $S=1$.¹³ However, for $S=1$, the two terms in the square bracket

can be transformed from one to another, which does not hold for $S=3/2$. This suggests that $S=\frac{1}{2}, 1$ Heisenberg models have a higher “hidden symmetry” compared with $S=3/2$. Actually, there is another hidden symmetry for the spin $S=\frac{1}{2}$ systems which is absent for spin-1,

$$:\chi_{ij}^\dagger \chi_{ij}: = :\Delta_{ij}^\dagger \Delta_{ij}: - \hat{N}_i \hat{N}_j,$$

where $\hat{N}_i = C_i^\dagger C_i$ is the particle number on site i . Our analysis suggests that smaller spins have higher symmetry when the spin interaction is expressed in the fermionic representation.

For $S=2$, the Heisenberg Hamiltonian can be written as

$$H = J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j = -\frac{J}{2} \sum_{\langle i,j \rangle} \text{Tr}:(\psi_i^\dagger \mathbf{I} \psi_j \cdot \psi_j^\dagger \mathbf{I} \psi_i):.$$

As in the case of lower spins, the terms $\text{Tr}:(\psi_i^\dagger \mathbf{I} \psi_j \cdot \psi_j^\dagger \mathbf{I} \psi_i):$ and $\text{Tr}:(\psi_i^\dagger \psi_j \psi_j^\dagger \psi_i):$ have finite overlaps and are not completely independent of each other. For $S > 2$, it is not possible to represent the Hamiltonian in the above two terms alone. Quintet and higher multipolar hopping and pairing operators are needed to represent the Heisenberg Hamiltonian and we are not able to obtain any general expression.

Summarizing, the Heisenberg model can be written in the fermionic representation as

$$H = -\frac{J}{2} \sum_{\langle i,j \rangle} [a(S) \text{Tr}:(\psi_i^\dagger \psi_j \psi_j^\dagger \psi_i): + b(S) \text{Tr}:(\psi_i^\dagger \mathbf{I} \psi_j \cdot \psi_j^\dagger \mathbf{I} \psi_i): + \dots], \quad (11)$$

where $a(S), b(S), \dots$ are parameters dependent on the spin magnitude S and $\dots$ represents quintet and higher multiplet terms. In the following, we shall study in detail a Hamiltonian which keeps the first two terms only. The Hamiltonian can be considered as an effective Hamiltonian for constructing trial ground-state wave functions in a variational calculation. Notice that the effective Hamiltonian is in fact “exact” up to $S=2$ if $a(S)$ and $b(S)$ are chosen properly.

B. Path-integral formalism and constraints

In imaginary time path-integral formalism, the partition function is given by

$$Z = \text{Tr}(e^{-\beta H}) = \int D\psi D\psi^\dagger D\lambda e^{-\int_0^\beta L(\psi, \psi^\dagger, \lambda) d\tau},$$

$$L = \sum_i \frac{1}{2} [\text{Tr} \psi_i (\partial_\tau - i\lambda_i \sigma_z) \psi_i^\dagger \pm i(2S-1)\lambda_i] + H, \quad (12)$$

where λ_i is the Lagrange multiplier field introduced to impose the constraint Eq. (4). The $+$ ($-$) sign corresponds to the particle ($\hat{N}=1$) and hole ($\hat{N}=2S$) representations. The Grassmann number ψ satisfy the antiperiodic boundary condition $\psi(0) = -\psi(\beta)$.

Notice that Lagrangian (12) is not invariant under the action of the internal symmetry group because of the noninvariant particle number constraint Eq. (4), i.e., the internal symmetry group of the spin operator is not a symmetry

group of the Lagrangian. In the following we will employ a trick to restore the symmetry of the Lagrangian. The integer- and half-odd-integer spin models will be discussed separately because of the intrinsic difference in their internal symmetry groups.

1. Integer spins

Our trick is to consider an average of all the partition functions with different particle-number constraint representations. In the integer spin case, the average is given by

$$\begin{aligned} Z &= \int D\psi D\psi^\dagger e^{-\int_0^\beta (\sum_i 1/2 \text{Tr}[\psi_i \partial_\tau \psi_i^\dagger] + H) d\tau} \\ &\times \prod_{\{i,\tau\}} \frac{1}{2} [\delta(\hat{N}_i - 1) + \delta(\hat{N}_i - 2S)] \\ &= \int D\psi D\psi^\dagger D\lambda e^{-\int_0^\beta (\sum_i (1/2) \text{Tr}[\psi_i \partial_\tau \psi_i^\dagger] + H) d\tau} \\ &\times \prod_{\{i,\tau\}} \frac{1}{2} (e^{i\lambda_i/2 [\text{Tr}(\psi_i \sigma_z \psi_i^\dagger) - 2S + 1]} + e^{i\lambda_i/2 [\text{Tr}(\psi_i \sigma_z \psi_i^\dagger) + 2S - 1]}). \end{aligned} \quad (13)$$

Notice that we do not make any approximations in deriving Eq. (13) from Eq. (12) and the partition function is a faithful representation of Heisenberg model except that it averages over all possible particle and hole representations of constraints locally. Similar ideas have been applied to generate the supersymmetric representation¹⁴ and the $SU(2)$ representation of the t - J model.¹⁵ The fermion particle-hole symmetry is restored in this representation. The Lagrangian corresponding to Eq. (13) is

$$L = \frac{1}{2} \sum_i \left[\text{Tr}[\psi_i (\partial_\tau - i\lambda_i \sigma_z) \psi_i^\dagger] - 2 \ln \cos \frac{(2S-1)\lambda_i}{2} \right] + H.$$

This form of Lagrangian is invariant under the internal symmetry group $U(1) \otimes Z_2$ and the symmetry group becomes almost a “gauge symmetry” of the new Lagrangian as we shall see in the following. We note that the Lagrangian is complex because of the multiplier λ . This problem can be solved by lifting the contour of integration over λ into complex plane via analytic continuation to find a saddle point in the imaginary axis.¹⁶ For convenience, we write $\tilde{\lambda}_i = i\lambda_i$, and integrate $\tilde{\lambda}_i$ from $-i\infty$ to $i\infty$ (the saddle point of $\tilde{\lambda}_i$ is real). Then the Lagrangian becomes

$$L = \frac{1}{2} \sum_i \left\{ \text{Tr}[\psi_i (\partial_\tau - \tilde{\lambda}_i \sigma_z) \psi_i^\dagger] - 2 \ln \cosh \frac{(2S-1)\tilde{\lambda}_i}{2} \right\} + H. \quad (14)$$

We shall now consider the path-integral representation in terms of the effective Hamiltonian (11) keeping only the first two terms. The effective Hamiltonian can be decoupled by a Hubbard-Stratonovich matrix field (see Appendix B)

$$\hat{U}_{ij} = \psi_i^\dagger \psi_j = \begin{pmatrix} \chi_{ij} & -\Delta_{ij}^\dagger \\ \Delta_{ij} & -\chi_{ij}^\dagger \end{pmatrix},$$

$$\hat{\mathbf{V}}_{ij} = \psi_i^\dagger \mathbf{I} \psi_j = \begin{pmatrix} \mathbf{v}_{ij} & \mathbf{u}_{ij}^\dagger \\ \mathbf{u}_{ij} & \mathbf{v}_{ij}^\dagger \end{pmatrix},$$

where $\mathbf{u}_{ij} = C_i^\dagger \mathbf{I} C_j$, and $\mathbf{v}_{ij} = \bar{C}_i^\dagger \mathbf{I} C_j$. Note that $\mathbf{u}_{ij}$ and $\mathbf{v}_{ij}$ form two sets of spin triplet operators, respectively. The Hamiltonian becomes

$$H = \frac{J}{2} \sum_{\langle i,j \rangle} \{ a(S) \text{Tr}[\hat{U}_{ij}^\dagger \hat{U}_{ij} - (\hat{U}_{ij}^\dagger \psi_i^\dagger \psi_j + \text{H.c.})] + b(S) \text{Tr}[\hat{\mathbf{V}}_{ij}^\dagger \cdot \hat{\mathbf{V}}_{ij} - (\hat{\mathbf{V}}_{ij}^\dagger \psi_i^\dagger \psi_j + \text{H.c.})] \}. \quad (15)$$

The $\hat{U}_{ij}$, $\hat{\mathbf{V}}_{ij}$, and $\tilde{\lambda}_i$ fields define $U(1) \bar{\otimes} Z_2$ lattice gauge fields coupling to the fermionic particles which we shall call spinons in the following. Under the local gauge transformation $\psi_i \rightarrow \psi_i W_i$, the temporal component and the spacial component of the gauge fields transform as

$$\begin{aligned} \tilde{\lambda}_i \sigma_z &\rightarrow W_i^\dagger \left(\tilde{\lambda}_i \sigma_z - \frac{d}{d\tau} \right) W_i, \\ \hat{U}_{ij} &\rightarrow W_i^\dagger \hat{U}_{ij} W_j, \\ \hat{\mathbf{V}}_{ij} &\rightarrow W_i^\dagger \hat{\mathbf{V}}_{ij} W_j. \end{aligned} \quad (16)$$

Notice that λ_i changes sign under a uniform Z_2 gauge transformation, and χ_{ij} , Δ_{ij} exchange their roles under a “staggered” Z_2 transformation where we have σ_x on one sublattice and $\mathbf{I}$ on the other sublattice. Notice also that the Lagrangian is not invariant under a time-dependent gauge transformation, because the term $2 \ln \cosh \frac{(2S-1)\tilde{\lambda}_i}{2}$ is not invariant. A similar situation occurs in the supersymmetric representation of Heisenberg model.¹⁴ Because of this restriction the internal symmetry group does not generate a complete “gauge symmetry” in the path-integral formalism.

Integrating out the fermion fields, we get an effective action in terms of the U_{ij} , $\hat{\mathbf{V}}_{ij}$, and λ_i fields. The mean-field values of the these fields are given by the saddle point of the effective action determined by the self-consistent equations $U = \langle \hat{U}_{ij} \rangle$, $\mathbf{V} = \langle \hat{\mathbf{V}}_{ij} \rangle$ with the mean-field Hamiltonian

$$\begin{aligned} H_m = J \sum_{\langle i,j \rangle} [&a(S) [- (\chi^* C_i^\dagger C_j + \Delta^* \bar{C}_i^\dagger C_j + \text{H.c.}) + |\chi|^2 + |\Delta|^2] \\ &+ b(S) [- (\mathbf{v}^* \cdot C_i^\dagger \mathbf{I} C_j + \mathbf{u}^* \cdot \bar{C}_i^\dagger \mathbf{I} C_j + \text{H.c.}) + |\mathbf{u}|^2 + |\mathbf{v}|^2] \\ &+ \sum_i \left[\tilde{\lambda} \left(\hat{N}_i - \frac{2S+1}{2} \right) - \ln \cosh \frac{(2S-1)\tilde{\lambda}}{2} \right], \end{aligned} \quad (17)$$

where $\chi = \langle C_i^\dagger C_j \rangle$, $\Delta = \langle \bar{C}_i^\dagger C_j \rangle$, $\mathbf{u} = \langle \bar{C}_i^\dagger \mathbf{I} C_j \rangle$, $\mathbf{v} = \langle C_i^\dagger \mathbf{I} C_j \rangle$, and $\tilde{\lambda}$ is determined by the condition

$$\langle \hat{N}_i \rangle - \frac{2S+1}{2} = \frac{2S-1}{2} \tanh \frac{(2S-1)\tilde{\lambda}}{2}.$$

Notice that the averaged particle number satisfies $1 < \langle \hat{N}_i \rangle < 2S$ because we are mixing the particle and hole pictures in the constraint. If the ground state does not break the particle-

hole symmetry, then $\tilde{\lambda} = 0$ and we get the half-filling condition $\langle \hat{N}_i \rangle = (2S+1)/2$.

2. Half odd integer spins

We first examine how the two particle number constraints $\text{Tr}(\psi \sigma_z \psi^\dagger) = \pm (2S-1)$ are transformed into each other by the $SU(2)$ internal symmetry group. We consider the vector constraint Eq. (5) for $S \geq \frac{1}{2}$

$$\hat{\mathbf{M}} = \frac{1}{2S-1} \text{Tr}(\psi \boldsymbol{\sigma} \psi^\dagger) = (0, 0, 1)^T,$$

where

$$\hat{M}_x = \frac{1}{2S-1} \text{Tr}(\bar{C} C^\dagger + C \bar{C}^\dagger),$$

$$\hat{M}_y = \frac{i}{2S-1} \text{Tr}(\bar{C} C^\dagger - C \bar{C}^\dagger),$$

$$\hat{M}_z = \frac{1}{2S-1} \text{Tr}(C C^\dagger - \bar{C} \bar{C}^\dagger).$$

The M_x and M_y components indicate that the one-site pairings $c_S c_{-S}, \dots$ and $c_{1/2} c_{-1/2}$ are equal to 0 and the M_z component imposes the constraint that there is exactly one fermion per site. Notice that the first two components of the constraint is automatically satisfied if the third component is satisfied rigorously. Under the $SU(2)$ transformation $\psi \rightarrow \psi W$, the constraint becomes $\frac{1}{2S-1} \text{Tr}(\psi \boldsymbol{\sigma} \psi^\dagger) = R^{-1}(0, 0, 1)^T$, where $W \sigma_a W^\dagger = R_{ab} \sigma_b$, R is an $SO(3)$ rotation. Since the constraint is invariant under an $U(1)$ gauge transformation generated by σ_z , the continuum space formed by different constraints is the surface of a sphere $SU(2)/U(1) = S^2$. In particular, for $W = e^{i\sigma_x \pi/2}$, the north pole of the sphere which corresponds to the positive sign in Eq. (4) is transformed to the south pole, $R^{-1}(0, 0, 1)^T = (0, 0, -1)^T$, corresponding to the negative sign in Eq. (4).

Now we construct a Lagrangian which is invariant under the $SU(2)$ internal symmetry group. In the path-integral formalism, the particle number constraint $\frac{1}{2S-1} \text{Tr}(\psi_i \boldsymbol{\sigma} \psi_i^\dagger) = (\hat{M}_i^x, \hat{M}_i^y, \hat{M}_i^z)^T = (0, 0, 1)^T$ can be realized by introducing a vector Lagrange multiplier field $\boldsymbol{\lambda}_i$

$$\begin{aligned} &\delta(\hat{M}_i^x) \delta(\hat{M}_i^y) \delta(\hat{M}_i^z - 1) \\ &= \left(\frac{1}{2\pi} \right)^3 \int d\lambda_i^x d\lambda_i^y d\lambda_i^z \\ &\quad \times \exp\{i[\lambda_i^x \hat{M}_i^x + \lambda_i^y \hat{M}_i^y + \lambda_i^z (\hat{M}_i^z - 1)]\}. \end{aligned} \quad (18)$$

The vector $(0, 0, 1)^T$ changes into $R^{-1}(0, 0, 1)^T = (n^x, n^y, n^z)^T = \hat{\mathbf{n}}$ under $SU(2)$ gauge transformation, where $\hat{\mathbf{n}}$ is a unit vector on the surface of the sphere S^2 . As in the integer spin case, a $SU(2)$ invariant path-integral formalism can be obtained by averaging over all possible particle number constraints

$$\begin{aligned}
& \langle \delta(\hat{M}_i^x - n^x) \delta(\hat{M}_i^y - n^y) \delta(\hat{M}_i^z - n^z) \rangle_{\{\hat{n}\}} \\
&= \frac{1}{4\pi} \left(\frac{1}{2\pi} \right)^3 \int d^2 \hat{n} \int d^3 \lambda_i \exp\{i \boldsymbol{\lambda}_i \cdot (\hat{\mathbf{M}}_i - \hat{\mathbf{n}})\} \\
&= \left(\frac{1}{2\pi} \right)^3 \int d^3 \lambda_i \exp\left\{i \left(\boldsymbol{\lambda}_i \cdot \hat{\mathbf{M}}_i - i \ln \frac{\sin \lambda_i}{\lambda_i} \right)\right\}, \quad (19)
\end{aligned}$$

where $\lambda_i = \sqrt{(\lambda_i^x)^2 + (\lambda_i^y)^2 + (\lambda_i^z)^2}$. Introducing $\tilde{\boldsymbol{\lambda}}_i = i \boldsymbol{\lambda}_i$, we obtain a Lagrangian with “almost” $SU(2)$ gauge symmetry

$$L = \frac{1}{2} \sum_i \left[\text{Tr}[\psi_i (\partial_\tau - \tilde{\boldsymbol{\lambda}}_i \cdot \boldsymbol{\sigma}) \psi_i^\dagger] - (2S-1) \ln \frac{\sinh \tilde{\lambda}_i}{\tilde{\lambda}_i} \right] + H. \quad (20)$$

As in the case of integer spins, we replace H by the effective Hamiltonian Eq. (11) with only the first two terms. Introducing the Hubbard Stratonovich field as in the integer spin case (see Appendix B for details),

$$\begin{aligned}
\hat{U}_{ij} &= \psi_i^\dagger \psi_j = \begin{pmatrix} \chi_{ij} & \Delta_{ij}^\dagger \\ \Delta_{ij} & -\chi_{ij}^\dagger \end{pmatrix}, \\
\hat{\mathbf{V}}_{ij} &= \psi_i^\dagger \mathbf{I} \psi_j = \begin{pmatrix} \mathbf{v}_{ij} & -\mathbf{u}_{ij}^\dagger \\ \mathbf{u}_{ij} & \mathbf{v}_{ij}^\dagger \end{pmatrix},
\end{aligned}$$

then $\hat{U}_{ij}$, $\hat{\mathbf{V}}_{ij}$, and $\tilde{\boldsymbol{\lambda}}_i$ form an $SU(2)$ lattice gauge field coupling to the spinons. (Notice the sign difference in the matrix elements of U and $\hat{\mathbf{V}}$ between integer and half-odd-integer spins.) Under gauge transformation $\psi_i \rightarrow \psi_i W_i$ ($W_i \in SU(2)$) the gauge fields transform as,

$$\tilde{\boldsymbol{\lambda}}_i \cdot \boldsymbol{\sigma} \rightarrow W_i^\dagger \left(\tilde{\boldsymbol{\lambda}}_i \cdot \boldsymbol{\sigma} - \frac{d}{d\tau} \right) W_i,$$

$$\hat{U}_{ij} \rightarrow W_i^\dagger \hat{U}_{ij} W_j$$

$$\hat{\mathbf{V}}_{ij} \rightarrow W_i^\dagger \hat{\mathbf{V}}_{ij} W_j,$$

and the Lagrangian Eq. (20) is invariant only under time-independent gauge transformations as in the integer spin case because of the noninvariant term $(2S-1) \ln \frac{\sinh \tilde{\lambda}_i}{\tilde{\lambda}_i}$. This is different from the $S=\frac{1}{2}$ case, where the Lagrangian is invariant under time-dependent gauge transformations. The mean-field effective Hamiltonian corresponding to Eq. (20) is

$$\begin{aligned}
H_m &= J \sum_{\langle i,j \rangle} [a(S) [-(\chi^* C_i^\dagger C_j + \Delta^* \bar{C}_i^\dagger C_j + \text{H.c.}) + |\chi|^2 + |\Delta|^2] \\
&+ b(S) [-(\mathbf{v}^* \cdot C_i^\dagger \mathbf{I} C_j + \mathbf{u}^* \cdot \bar{C}_i^\dagger \mathbf{I} C_j + \text{H.c.}) + |\mathbf{u}|^2 + |\mathbf{v}|^2]] \\
&- \sum_i \frac{2S-1}{2} \left(\tilde{\boldsymbol{\lambda}} \cdot \hat{\mathbf{M}}_i + \ln \frac{\sinh \tilde{\lambda}}{\tilde{\lambda}} \right) \quad (21)
\end{aligned}$$

where the parameters $\chi, \Delta, \mathbf{u}, \mathbf{v}$ are solved self-consistently by the mean-field equations $U = \langle \hat{U}_{ij} \rangle$, $\mathbf{V} = \langle \hat{\mathbf{V}}_{ij} \rangle$, and $\tilde{\boldsymbol{\lambda}}$ is determined by

$$\langle \hat{\mathbf{M}}_i \rangle + \frac{\tilde{\boldsymbol{\lambda}}}{\tilde{\lambda}^2} (\tilde{\lambda} \coth \tilde{\lambda} - 1) = 0.$$

The averaged particle number per site is again given by $\langle \hat{N}_i \rangle = (2S+1)/2$ if the ground state respects particle-hole symmetry ($\tilde{\lambda}=0$).

C. An important difference between integer and half-odd-integer spins

It can be proved (see Appendix B) that for integer spins, $\chi_{ji} = \chi_{ij}^\dagger$, $\Delta_{ji} = -\Delta_{ij}$, $\mathbf{u}_{ji} = \mathbf{u}_{ij}$, and $\mathbf{v}_{ji} = \mathbf{v}_{ij}^\dagger$ whereas for half-odd-integer spins, $\chi_{ji} = \chi_{ij}$, $\Delta_{ji} = \Delta_{ij}$, $\mathbf{u}_{ji} = -\mathbf{u}_{ij}$, and $\mathbf{v}_{ji} = \mathbf{v}_{ij}^\dagger$. Notice that the parity of the pairing terms Δ_{ij} and $\mathbf{u}_{ij}$ are different for integer and half-odd-integer spins. These operators are central to the mean-field theory, because the ground states are completely determined by their expectation values. In particular, for a mean-field theory with $\Delta, \chi \neq 0$ and $\mathbf{u}, \mathbf{v} = 0$, the mean-field ground state is a BCS spin-singlet pairing state where the order parameter $\langle \Delta_{ij} \rangle$ has even parity for half-odd-integer spins, but has odd parity for integer spins. We shall see how this important difference leads to different excitation spectrums between integer and half-odd-integer spin systems in the fermionic mean-field theory. Similar result exists for states with $\Delta, \chi = 0$ and $\mathbf{u}, \mathbf{v} \neq 0$. In this case the mean-field ground state is a BCS spin-triplet pairing state and the parity of the order parameters are reversed.

We note that as in the $S=\frac{1}{2}$ case, the mean-field Hamiltonian should be viewed as a trial Hamiltonian for the ground-state wave function of the spin systems after Gutzwiller projection. For the mean-field theory with particle-hole symmetry the Gutzwiller projection is rather nontrivial. The state is a coherent superposition of states which allows sites with both one fermion and with $2S$ fermions. The numerical analysis of such a state is complicated and we shall not go into details in this paper.

IV. FERMIONIC MEAN-FIELD THEORY IN 1D AND HALDANE CONJECTURE

In this section we apply our mean-field theory to the antiferromagnetic Heisenberg model in one dimension. We first consider the cases of spin $S=1$ and $S=3/2$ where two versions of mean-field theories based on different methods of implementing the constraints will be discussed. The mean-field results are summarized in Sec. IV C where the case of general spin S and Haldane conjecture will be discussed.

To simplify our analysis we make use of the Wagner-Mermin theorem which asserts that a continuous symmetry cannot spontaneously break in one dimension.¹⁷ Therefore we assume in our mean-field theory that the ground state is a spin singlet (spin-liquid state) and the expectation values of $\langle \mathbf{u}_{ij} \rangle$ and $\langle \mathbf{v}_{ij} \rangle$ are zero, since the rotational symmetry will be broken otherwise. As a result, we keep only the $a(S)$ term in the trial Hamiltonian. For simplicity we shall also restrict ourselves to translational invariant solutions of the mean-field theory in this paper.

TABLE I. Solutions of two versions of mean fields for spin-1 AFM Heisenberg chain. E is the ground-state energy per site and E_{gap} is the excitation gap.

$\langle N_i \rangle$	χ	Δ	$\tilde{\lambda}$	$E(J)$	$E_{gap}(J)$	$\langle \mathbf{S}_i \cdot \mathbf{S}_i \rangle$
3/2	3/4	3/4	0	-9/8	3/2	3/2
1	0.7625	0.5671	0.7709	-0.9032	0.3634	4/3

A. Integer spin: $S=1$

We choose H_{tr} to be the same as Eq. (9), i.e., $a(1)=-1$ and $b(1)=0$. For convenience of discussion, we introduce two different fermions c_s, c_a which are the symmetric and antisymmetric combinations of c_1 and c_{-1} ,

$$\begin{aligned} c_{si} &= (c_{1i} + c_{-1i})/\sqrt{2}, \\ c_{ai} &= (c_{1i} - c_{-1i})/\sqrt{2}. \end{aligned} \quad (22)$$

The mean-field Hamiltonian Eq. (17) becomes completely decoupled in terms of c_s, c_a , and c_0 . In Fourier space, it can be written as

$$\begin{aligned} H_m &= \sum_k \chi_k (c_{sk}^\dagger c_{sk} + c_{ak}^\dagger c_{ak} + c_{0k}^\dagger c_{0k}) \\ &\quad - \sum_k \left[\frac{\Delta_k^*}{2} (c_{s-k} c_{sk} - c_{a-k} c_{ak} - c_{0-k} c_{0k}) + \text{H.c.} \right] \\ &\quad + JN(|\chi|^2 + |\Delta|^2) - N \left(\frac{3}{2} \tilde{\lambda} + \ln \cosh \frac{\tilde{\lambda}}{2} \right), \end{aligned} \quad (23)$$

where $\chi_k = \tilde{\lambda} - 2J\chi \cos k$, $\Delta_k^* = 2iJ\Delta \sin k$ (since the phases of χ and Δ are unimportant in 1D, we choose χ and Δ to be real numbers) and N is the length of the chain. The mean-field Hamiltonian can be diagonalized by a Bogoliubov transformation

$$\begin{aligned} \gamma_{sk} &= u_k c_{sk} + v_k c_{s-k}^\dagger, \\ \gamma_{ak} &= u_k c_{ak} - v_k c_{a-k}^\dagger, \\ \gamma_{0k} &= u_k c_{0k} - v_k c_{0-k}^\dagger. \end{aligned} \quad (24)$$

The coefficients u_k, v_k satisfy the Bogoliubov-de Gennes (BdG) equations,

$$\begin{aligned} E_k u_k &= \chi_k u_k - \Delta_k^* v_k \\ E_k v_k &= -\Delta_k u_k - \chi_k v_k. \end{aligned} \quad (25)$$

Solving the equations we obtain

$$E_k = \sqrt{(\lambda - 2J\chi \cos k)^2 + (2J\Delta \sin k)^2}, \quad (26a)$$

$$u_k = \cos \frac{\theta_k}{2}, \quad v_k = i \sin \frac{\theta_k}{2}, \quad (26b)$$

where θ_k is given by $\tan \theta_k = \frac{\Delta_k^*}{i\chi_k}$ and the diagonalized Hamiltonian is

$$H_m = \sum_{k>0} E_k (\gamma_{sk}^\dagger \gamma_{sk} + \gamma_{ak}^\dagger \gamma_{ak} + \gamma_{0k}^\dagger \gamma_{0k}) + E_0,$$

where $E_0 = \sum_k (\chi_k - E_k) + JN(\chi^2 + \Delta^2) - N(\frac{3}{2}\tilde{\lambda} + \ln \cosh \frac{\tilde{\lambda}}{2})$ is the ground-state energy. Minimizing E_0 , we obtain the self-consistent mean-field equations at zero temperature,

$$\chi = \frac{2S+1}{2N} \sum_k \cos k \left(1 - \frac{\chi_k}{E_k} \right), \quad (27a)$$

$$\Delta = \frac{2S+1}{2N} \sum_k \sin k \frac{\Delta_k}{E_k}, \quad (27b)$$

$$\left\langle \frac{2S+1}{2} - \hat{N}_i \right\rangle = \frac{2S+1}{2N} \sum_k \frac{\chi_k}{E_k} = -\frac{2S-1}{2} \tanh \frac{(2S-1)\tilde{\lambda}}{2} \quad (27c)$$

with $S=1$. The above equations are solved numerically where we obtain $\chi=\Delta=3/4$ and $\tilde{\lambda}=0$ as shown in the first row of Table I. The averaged particle number of the spinons per site is 3/2, indicating that the ground state respects particle-hole symmetry. The ground-state energy is $E_0 = -J(\chi^2 + \Delta^2)$, and the excitation spectrum is flat (i.e., k independent) with a finite energy gap $3J/2$. The spin-spin correlation function is

$$\langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle = \frac{3}{2N^2} \sum_{p,q} e^{i(q-p)r} \left[\left(1 + \frac{\chi_p}{E_p} \right) \left(1 - \frac{\chi_q}{E_q} \right) - \frac{\Delta_p^* \Delta_q}{E_p E_q} \right]$$

and is nonzero only for $r=0$ and $r=1$, with $\langle \mathbf{S}_i \cdot \mathbf{S}_i \rangle = 3/2$ and $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle = 3/4$. The correlation function is zero for $r \geq 2$, indicating that the mean-field theory describes a short-ranged valence-bond-solid state.

We have also studied the mean-field theory based on the Lagrangian Eq. (12) for comparison. It gives rise to a dual of mean-field theories with particle number constraints $\langle \hat{N}_i \rangle = 1$ and $\langle \hat{N}_i \rangle = 2$, respectively. There is a one-to-one correspondence between the solutions of the two mean-field theories and we will only consider the particle representation $\langle \hat{N}_i \rangle = 1$. The mean-field equations are the same as Eq. (27) except that Eq. (27c) becomes

$$\langle \hat{N}_i \rangle = \frac{3}{2N} \left(1 - \sum_k \frac{\chi_k}{E_k} \right) = 1.$$

The solution is also summarized in Table I. The excitation spectrum is gapped but no longer dispersionless. We note that the mean-field solution Eq. (27) with particle-hole symmetry has a better ground-state energy.

TABLE II. Solutions of two versions of mean fields for spin-3/2 Heisenberg chain. In the first row (χ, Δ) means the real combinations satisfying $\sqrt{\chi^2 + |\Delta|^2} = 1.2732$.

$\langle N_i \rangle$	χ	Δ	$\tilde{\lambda}_z$	$E(J)$	$E_{gap}(J)$	$\langle \mathbf{S}_i \cdot \mathbf{S}_i \rangle$
2	χ	Δ	0	-1.5198	0	15/4
1	0	1.1490	0.7181	-1.2377	0.6732	45/16

B. Half-odd-integer spin: $S=3/2$

For the spin-3/2 Heisenberg chain, we consider the effective Hamiltonian (21) with $b(\frac{3}{2})=0$ such that the ground state is a singlet state. We shall also take $a(\frac{3}{2})=\frac{15}{16}$ for reason we shall see later. In momentum space, the effective Hamiltonian becomes

$$H_m = \sum_k \chi_k (c_{3/2k}^\dagger c_{3/2k} + c_{1/2k}^\dagger c_{1/2k} + c_{-1/2k}^\dagger c_{-1/2k} + c_{-3/2k}^\dagger c_{-3/2k}) + \sum_k [\Delta_k^* (c_{-3/2-k} c_{3/2k} - c_{-1/2-k} c_{1/2k}) + \text{H.c.}] + \text{const},$$

where $\chi_k = \tilde{\lambda}_z - \frac{15}{8} J \chi \cos k$ and $\Delta_k^* = \tilde{\lambda}_x - i \tilde{\lambda}_y - \frac{15}{8} J \Delta^* \cos k$. We shall set χ and Δ to be real numbers in the following.

As in the $S=1$ case, the Hamiltonian can be diagonalized by Bogoliubov transformations and lead to the self consistent mean-field equations at zero temperature,

$$\begin{aligned} \chi &= \frac{2S+1}{2N} \sum_k \cos k \left(1 - \frac{\chi_k}{E_k} \right), \\ \Delta &= \frac{2S+1}{2N} \sum_k \cos k \frac{\Delta_k}{E_k}, \\ \langle M_+ \rangle &= \frac{2S+1}{N(2S-1)} \sum_k \frac{\Delta_k}{E_k} = \frac{(1 - \tilde{\lambda} \coth \tilde{\lambda}) \tilde{\lambda}_+}{\tilde{\lambda}^2}, \\ \langle \hat{M}_z \rangle &= \frac{2S+1}{N(2S-1)} \sum_k \frac{\chi_k}{E_k} = \frac{(1 - \tilde{\lambda} \coth \tilde{\lambda}) \tilde{\lambda}_z}{\tilde{\lambda}^2}, \end{aligned} \quad (28)$$

where $S=3/2$, $\hat{M}_+ = \hat{M}_x + i \hat{M}_y$, $\tilde{\lambda}_+ = \tilde{\lambda}_x + i \tilde{\lambda}_y$, and

$$E_k = \sqrt{\left(\tilde{\lambda}_z - \frac{15}{8} J \chi \cos k \right)^2 + \left| \tilde{\lambda}_+ - \frac{15}{8} J \Delta \cos k \right|^2} \quad (29)$$

is the spinon dispersion.

Solving the equations we find that $\tilde{\lambda}=0$ (i.e., the ground state does not break particle-hole symmetry) and there exists infinite degenerate solutions for χ and Δ satisfying $\sqrt{\chi^2 + |\Delta|^2} = 1.2732$ (see Table II). This is a direct consequence of the $SU(2)$ gauge symmetry for half-odd integer spins we mentioned in Sec. III B 2, and all these solutions are equivalent. Notice that the ground-state energy $E_0 = -\frac{15NJ}{16}(\chi^2 + |\Delta|^2)$ is the same as the expectation value of Heisenberg Hamiltonian (10), which is why we should choose $a(\frac{3}{2})=\frac{15}{16}$ in the effective Hamiltonian. As a result of the particle-hole symmetry ($\tilde{\lambda}=0$), the spinon energy disper-

sion Eq. (29) is gapless at Fermi points $k = \pm \pi/2$. The spin-spin correlation is given by

$$\langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle = \frac{15}{4N^2} \sum_{p,q} e^{i(q-p)r} \left[\left(1 + \frac{\chi_p}{E_p} \right) \left(1 - \frac{\chi_q}{E_q} \right) - \frac{\Delta_p^* \Delta_q}{E_p E_q} \right]$$

and decays at large distance as $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle \propto r^{-2}$ because of linearized spectrum around Fermi surface. This is also confirmed directly by numerical calculation.

Similar to the $S=1$ case, we have also solved the mean-field theory with particle number constraint $\langle \hat{N}_i \rangle = 1$ or equivalently $\langle \hat{\mathbf{M}} \rangle = (0, 0, 1)^T$. The solution is listed in Table II. Since $\tilde{\lambda}_z \neq 0$ in this case, the spinon dispersion $E_k = \frac{15J}{8} \sqrt{(\tilde{\lambda}_z/2 - \chi \cos k)^2 + |\Delta \cos k|^2}$ breaks particle-hole symmetry and has a finite gap over the whole Brillouin zone. The particle-hole symmetric solution is also found to have a lower mean-field ground-state energy.

C. Haldane's conjecture and edge states

Comparing the mean-field energy dispersion Eqs. (26a) and (29), we find that the excitation spectrum of spin-1 Heisenberg model is gapped whereas the excitation spectrum for the spin-3/2 Heisenberg model is gapless in the mean-field formulation with particle-hole symmetry. This difference between integer spin and half-odd-integer spin persists for any spin S , if we consider the trial Hamiltonian (17) or (21) with $a(S) \neq 0$, $b(S)=0$, i.e., if we consider BCS spin-singlet ground-state wave functions. The mean-field equations for arbitrary S are the same as Eq. (27) or Eq. (28) for arbitrary S , and the dispersion is qualitatively the same as Eq. (26a) or Eq. (29), as long as we consider particle-hole symmetric mean-field solutions which do not break translational invariance. The main effect of changing S in mean-field theory is to change the number of fermionic spinon species. This result is consistent with the Haldane conjecture,³ which asserts that the integer spin Heisenberg chains have singlet ground state with finite excitation gaps and exponentially decaying spin-spin correlation functions, while half-odd-integer spin chains have singlet ground states with gapless excitation spectrums and power law decaying correlations. Our particle-hole symmetric mean-field results agree well with Haldane conjecture.

Haldane noticed that the time-reversal operator satisfies $T^2=1$ for integer spin and $T^2=-1$ for half-odd-integer spin, and this results in different Berry phase contributions from the topological excitations (skyrmion or instanton) in the path-integral formulation given by $e^{i2\pi S Q}$, where

$$Q = \int dt dx \frac{1}{4\pi} \mathbf{n} \cdot (\partial_t \mathbf{n} \times \partial_x \mathbf{n}) \quad (30)$$

is the Skyrmion number. For Q =odd integer, the Berry phase $(e^{i2\pi S})^Q$ is $1^Q=1$ for integer spins and $(-1)^Q=-1$ for half-odd-integer spins. The difference in the ± 1 factor between integer spin and half-odd-integer spin is the origin of Haldane's conjecture. The situation is quite similar in our mean-field theory. Noticing that $\Delta_{ij} = \bar{C}_i^\dagger C_j$ is a singlet formed by two spin- S particles. The Clebsch-Gordan coefficients implies that $\Delta_{ji} = -\Delta_{ij}$ for integer S and $\Delta_{ji} = \Delta_{ij}$ for half-odd-integer S (see Appendix B). This sign or parity difference results in appearance of $\Delta \sin k$ in Eq. (26a) for $S=1$ and $\Delta \cos k$ in Eq. (29) for $S=3/2$, which leads to different symmetries of ground-state wave functions and different excitation spectrums between integer and half-odd-integer spin chains.

The topological term Eq. (30) leads to exponentially localized edge states for open integer spin chains which is absent for half-odd-integer spin chains.¹⁸ This important difference between integer spin and half-odd-integer spin chains is also reflected in our mean-field theory where zero-energy Majorana edge fermions exist at the open boundaries for integer spin chains which are absent for half-odd-integer spin chains. The existence of Majorana edge fermions for integer spin chains is a direct consequence of the odd-pairing symmetry for integer spin chains.¹⁹ The details of the Majorana edge fermions is discussed in Appendix C.

V. 2D: $S=1$ SPIN LIQUIDS ON TRIANGULAR LATTICE

We show in the previous section that our mean-field theory is able to capture the essential physics of spin-liquid states in 1D antiferromagnetic quantum spin chains. In this section we shall apply our mean-field theory to the 2D $J_1 - J_3$ Heisenberg model on triangular lattice. We shall show that our mean-field theory admits spin-liquid solutions not explored before. Some results of this model have been reported in a previous paper,²⁰ where particle number constraint is treated in the ‘‘particle representation’’ ($\langle \hat{N}_i \rangle = 1$). In this paper, we shall revisit this model with the particle-hole symmetric constraint. The Hamiltonian of the $J_1 - J_3$ model is

$$H = \sum_{\langle i,j \rangle} J_1 \mathbf{S}_i \cdot \mathbf{S}_j + J_3 \sum_{[i,j]} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (31)$$

where $\langle i,j \rangle$ denotes nearest neighbor (NN) and $[i,j]$ the next-next-nearest neighbors (NNNN). For $S=1$, there are two channels of decoupling the spin interaction, namely, $\mathbf{S}_i \cdot \mathbf{S}_j = -\frac{1}{2} : \text{Tr}(\psi_i^\dagger \psi_j \psi_j^\dagger \psi_i) :$ or $\mathbf{S}_i \cdot \mathbf{S}_j = -\frac{1}{2} : \text{Tr}(\psi_i^\dagger \mathbf{I} \psi_j \cdot \psi_j^\dagger \mathbf{I} \psi_i) :$. Since there is no Mermin-Wigner theorem to protect us at zero temperature at 2D, we have to keep both terms in the effective Hamiltonian Eq. (17). We shall choose $b=1-a$, with the weight a determined by minimizing the ground-state energy.

Next we introduce the mean-field parameters χ_1 , Δ_1 , $\mathbf{u}_1$, and $\mathbf{v}_1$ (for NN) and χ_3 , Δ_3 , $\mathbf{u}_3$, and $\mathbf{v}_3$ (for NNNN) to decouple the Hamiltonian. We assume that $\mathbf{u}$ and $\mathbf{v}$ are parallel so we only keep the z component of these vectors, and note them simply as $u_{1,3}$ and $v_{1,3}$ (which are set as real numbers).

FIG. 1. (Color online) The first Brillouin zone of the triangular lattice. $\mathbf{b}_1 = (2\pi, \frac{2\pi}{\sqrt{3}})$ and $\mathbf{b}_2 = (0, \frac{4\pi}{\sqrt{3}})$ are two reciprocal vectors. The Brillouin zone is divided into three regular pieces by the three new bases $\mathbf{u}$, $\mathbf{v}$, and $\mathbf{w}$.

As in 1D case we consider here only spin-liquid solutions that respect translation and rotational symmetries. Since the pairings have odd parity $\langle \Delta_{ij} \rangle = -\langle \Delta_{ji} \rangle$, only p -wave and f -wave like pairings are allowed. Solving the mean-field equations we find two kinds of solutions (see Fig. 2), which have f -wave and $p_x + ip_y$ -wave pairing symmetries, respectively. We shall concentrate on these two kinds of solutions in the following.

In momentum space (Fig. 1), the mean-field Hamiltonian Eq. (17) can be written as

$$\begin{aligned} H_m = & \sum_{\mathbf{k}} \chi_k (c_{1k}^\dagger c_{1k} + c_{0k}^\dagger c_{0k} + c_{-1k}^\dagger c_{-1k}) \\ & - \sum_{\mathbf{k}} \left[\Delta_k^* \left(c_{-1-k} c_{1k} - \frac{1}{2} c_{0-k} c_{0k} \right) + \text{H.c.} \right] \\ & + \sum_{\mathbf{k}} v_k (c_{1k}^\dagger c_{1k} - c_{-1k}^\dagger c_{-1k}) - \sum_{\mathbf{k}} u_k^* (c_{-1-k} c_{1k} + \text{H.c.}) \end{aligned} \quad (32)$$

with

$$\chi_k = \tilde{\lambda} - aZ(J_1 \chi_1 \gamma_k + J_3 \chi_3 \gamma_{2k}),$$

$$\Delta_k^* = iaZ(J_1 \Delta_1 \psi_k + J_3 \Delta_3 \psi_{2k}),$$

$$v_k = -(1-a)Z(J_1 \gamma_k v_1 + J_3 \gamma_{2k} v_3),$$

$$u_k^* = (1-a)Z(J_1 \gamma_k u_1 + J_3 \gamma_{2k} u_3),$$

where $\tilde{\lambda}$ is the Lagrange multiplier and

$$\gamma_k = \frac{1}{3} \left[\cos k_x + \cos \left(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2} \right) + \cos \left(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2} \right) \right],$$

$$\psi_k^f = \frac{1}{3} \left[\sin k_x + \sin \left(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2} \right) + \sin \left(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2} \right) \right],$$

FIG. 2. (Color online) Two different pairing symmetries for the singlet pairing Δ_{ij} . We indicate the relative phase of the nearest-neighbor pairing $\langle \Delta_{ij} \rangle = \Delta_1 e^{i\varphi_{ij}}$. (a) f -wave pairing. The dashed lines are the zero lines of the pairing function (in lattice space or momentum space). (b) $p_x + ip_y$ -wave pairing. There are no zero lines, the pairing function vanishes only at the Γ point.

$$\psi_k^{p+ip} = \frac{1}{3} \left[\sin k_x + e^{i\pi/3} \sin \left(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2} \right) + e^{i2\pi/3} \sin \left(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2} \right) \right].$$

The pairing symmetries can be verified easily by expanding the pairing terms at small k : $\Delta_k^f \propto k_x(k_x^2 - 3k_y^2)$ and $\Delta_k^{p_x+ip_y} \propto k_x + ik_y$. There are three lines of zeros for the f -wave pairing function as shown in Fig. 2.

Introducing a vector $C_k = (c_{1k}, c_{-1-k}^\dagger, c_{0k}, c_{0-k}^\dagger)^T$, the Hamiltonian Eq. (32) can be written in a matrix form

$$H_m = \sum_{\mathbf{k}} C_k^\dagger H_k C_k + \sum_{\mathbf{k}} \left(\frac{3}{2} \chi_k - v_k \right), \quad (33)$$

where

$$H_k = \begin{pmatrix} \chi_k + v_k & -u_k - \Delta_k & 0 & 0 \\ -u_k^* - \Delta_k^* & -\chi_k + v_k & 0 & 0 \\ 0 & 0 & \frac{\chi_k}{2} & \frac{\Delta_k}{2} \\ 0 & 0 & \frac{\Delta_k^*}{2} & -\frac{\chi_k}{2} \end{pmatrix}.$$

H_k can be diagonalized by the Bogoliubov transformation,

$$\begin{aligned} A_k &= \cos \frac{\theta_k}{2} c_{1k} - \sin \frac{\theta_k}{2} e^{i\eta_k} c_{-1-k}^\dagger, \\ B_{-k}^\dagger &= \sin \frac{\theta_k}{2} e^{-i\eta_k} c_{1k} + \cos \frac{\theta_k}{2} c_{-1-k}^\dagger, \\ D_k &= \cos \frac{\Theta_k}{2} c_{0k} + \sin \frac{\Theta_k}{2} e^{i\phi_k} c_{0-k}^\dagger, \end{aligned} \quad (34)$$

where $\tan \theta_k = \frac{|u_k + \Delta_k|}{\chi_k}$, $e^{i\eta_k} = \frac{u_k + \Delta_k}{|u_k + \Delta_k|}$, $\tan \Theta_k = \frac{|\Delta_k|}{\chi_k}$, and $e^{i\phi_k} = \frac{\Delta_k}{|\Delta_k|}$. The corresponding eigenvalues are given by $v_k \pm E_{1k}$ and $\pm E_{0k}$, where

FIG. 3. (Color online) Phase diagram for the J_1 - J_3 Heisenberg model with $J_1 + J_3 = 1$. We use the constraint $\langle \hat{N}_i - \frac{3}{2} \rangle = \frac{1}{2} \tanh \frac{\tilde{\lambda}}{2}$. The red dotted line indicate energy per site for the $p_x + ip_y$ state and the black square line is for the f -wave state. Dirac nodes exist for the f -wave state. The number of nodes is 6 when J_1 is dominating and 24 when J_3 is dominating.

$$E_{1k} = \sqrt{\chi_k^2 + |\Delta_k|^2 + u_k^2}, \quad E_{0k} = \sqrt{\chi_k^2 + |\Delta_k|^2},$$

and the self-consistent mean-field equations are

$$\bar{\chi}_{1,3} = \frac{1}{N} \sum_{\mathbf{k}} \gamma_{k,2k} \left[\frac{3}{2} - \frac{\chi_k}{E_{1k}} - \frac{\chi_k}{2E_{0k}} \right],$$

$$\bar{\Delta}_{1,3} = \frac{1}{N} \sum_{\mathbf{k}} \psi_{k,2k} \left[\frac{|\Delta_k|}{E_{1k}} + \frac{|\Delta_k|}{2E_{0k}} \right],$$

$$\bar{u}_{1,3} = \frac{1}{N} \sum_{\mathbf{k}} \gamma_{k,2k} \frac{u_k}{E_{1k}},$$

$$\bar{v}_{1,3} = 0,$$

$$\left\langle \hat{N}_i - \frac{3}{2} \right\rangle = \frac{1}{2} \tanh \frac{\tilde{\lambda}}{2}, \quad (35)$$

where we have adopted the particle-hole symmetric constraint in writing down the mean-field equations. We have also checked the mean-field solutions with constraint $\langle \hat{N}_i \rangle = 1$ (Ref. 20) and found that the excitation spectrums are qualitatively the same as those in the particle-hole symmetric theory. The ground-state energy is lowest for vanishing $u_{1,3}, v_{1,3}$, i.e., $a=1$, $u_k=v_k=0$ and the ground state is a spin singlet. The excitations are characterized by three branches of fermionic spinons with $S_z=0, \pm 1$ and identical dispersion $E_k = \sqrt{\chi_k^2 + |\Delta_k|^2}$.

Our mean-field theory for the J_1 - J_3 model contains two regimes of spin-liquid states for both f and $p_x + ip_y$ pairing symmetries as a function of J_1/J_3 . A first-order phase transition occurs between the two regimes at $J_1/J_3 \sim 1$ (see Fig. 3). When J_1 dominates, the spin-liquid state is characterized by $\chi_{1,3} \neq 0$ and $\Delta_{1,3} \neq 0$ (consequently $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle < 0$ and $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+2} \rangle < 0$); while when J_3 dominates, $\chi_1 = \Delta_1 = 0$ and $\chi_3 \neq 0$, $\Delta_3 \neq 0$ (consequently $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle = 0$, $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+2} \rangle < 0$). The $p_x + ip_y$ states remain lower in energy in both regimes.

FIG. 4. (Color online) The spinon dispersion the f -wave pairing state with constraint $\langle \hat{N}_i - \frac{3}{2} \rangle = \frac{1}{2} \tanh \frac{\tilde{\lambda}}{2}$ for $J_1=0.6$ and $J_3=0.4$. The figure on the right shows the dispersion along the line linking two K points of the Brillouin zone (see the blue lines on the left). The negative energy part is filled and the excitation is gapless with six Dirac nodes in the first Brillouin zone. The dispersion for the mean-field solution with $\langle \hat{N}_i \rangle = 1$ is similar to the above one except that the locations of the nodes are shifted a little bit.

The f -wave pairing solution respects particle-hole symmetry and has $\langle \hat{N}_i \rangle = \frac{3}{2}$. The excitation is gapless with several Dirac cones in the first Brillouin zone. A cut of the spinon dispersion is shown in Fig. 4 where the particle-hole symmetry is obvious. The mean-field solution with $\langle \hat{N}_i \rangle = 1$ has similar properties, except that the particle-hole symmetry is lost and the position of the Dirac nodes are shifted.²⁰

For the $p_x + ip_y$ -wave pairing, we find that the ground state breaks particle-hole symmetry and $\tilde{\lambda} \neq 0$. The excitation spectrum is fully gapped. Similar to integer spin chains, we find that the $p_x + ip_y$ -wave state is topologically nontrivial (see also Appendix C). The solution has $|\tilde{\lambda}| < Z|J_1\chi_1 + J_3\chi_3|$ so that χ_k can be either positive or negative, depending on $\mathbf{k}$. Therefore the Bogoliubov spinor space described by the vector $(\frac{Im\Delta_k}{E_k}, \frac{Re\Delta_k}{E_k}, \frac{\chi_k}{E_k})^T$ (which is S^2) covers the Brillouin zone ($\mathbf{k}$ space, which is also S^2) at least once. In other words, the topological (Skyrmion) number of mapping from the $\mathbf{k}$ space to the spinor space is nonzero $m \neq 0$. However, in the vacuum where the spinon density is zero, $\tilde{\lambda}$ is very big and χ_k can only take positive values, which gives a zero topological number.¹⁹ Since the bulk and vacuum belong to different topological sectors, the boundary defines a domain wall between the two phases, and there should exist gapless (chiral) Majorana edge states in the $p_x + ip_y$ state following the analysis of Read and Green.¹⁹ In this sense, the $p_x + ip_y$ -state describes a time-reversal symmetry-breaking topological spin liquid.

Next we consider the specific heat and spin susceptibility for the f and $p_x + ip_y$ states. For the $p_x + ip_y$ -wave pairing states, since the excitations are fully gapped as in BCS superconductors, the specific heat and spin susceptibility will show exponential behavior²¹ at low temperature. For the f -wave pairing states, both the specific heat and the spin susceptibility show power law behavior due to the Dirac cone structure (see Fig. 4). The energy for the system is $E = 3 \sum_k \frac{E_k}{e^{\beta E_k} + 1}$ in mean-field theory. At low temperature, the specific heat is dominated by the low-energy excitations near the nodes of the Fermi surface, which is given approximately by

$E_k = v_F k$, where v_F is the Fermi velocity (the anisotropy of the dispersion can be removed by a rescaling of momentum and will not affect the result qualitatively). The magnetic specific heat is given by

$$\begin{aligned} C_M &= \frac{\partial E}{\partial T} \\ &= 3 \frac{\partial}{\partial T} \int_0^{k_\Lambda} \frac{v_F k}{e^{v_F k/T} + 1} 2\pi k dk \\ &= 3 \frac{\partial}{\partial T} \int_0^{v_F k_\Lambda/T \rightarrow \infty} \frac{1}{e^x + 1} 2\pi x^2 \frac{T^3}{v_F^2} dx \propto n \pi T^2 / v_F^2, \end{aligned} \quad (36)$$

where n is the number of Dirac cones. The magnetic susceptibility can be calculated from the linear response theory with

$$\begin{aligned} \chi_z(k, i\omega) &= \int d^2r \int d\tau T_\tau \langle S_z(r, \tau) S_z(0, 0) \rangle e^{i(\omega\tau - kr)} \\ &= \frac{2}{N^2} \int d^2r \int d\tau e^{i(\omega\tau - kr)} \sum_{q, q', p, p'} e^{i(q' - q)r} \\ &\quad \times [T_\tau \langle c_1^\dagger(q, \tau) c_1(q', \tau) c_1^\dagger(p, 0) c_1(p', 0) \rangle \\ &\quad - T_\tau \langle c_1^\dagger(q, \tau) c_1(q', \tau) c_{-1}^\dagger(p, 0) c_{-1}(p', 0) \rangle]. \end{aligned} \quad (37)$$

The static susceptibility is given by $\chi_z = \lim_{k \rightarrow 0} \chi_z(k, 0) \propto \frac{T}{v_F^2}$. The detailed calculation is given in Appendix D.

Recently, a spin-1 material NiGa_2S_4 was discovered, where the $S=1\text{Ni}^{2+}$ ions form a triangular lattice with antiferromagnetic (AFM) interaction. The system has a Curie-Weiss temperature ~ 80 K, and is found to exhibit no conventional magnetic order down to 0.35 K. Several plausible ground states have been proposed for this system,^{22–28} including an antiferromagnetic state,²⁴ a ferronematic state,²³ and a KT phase driven by vortices.²⁸ Spin liquid is also proposed to be a plausible ground state. In our mean-field theory, the f -wave pairing spin liquid has coherent gapless excitation with specific heat scaling as T^2 at low temperature which is consistent with the experimental result.²² Furthermore, the Knight shift data in Ref. 23 shows that the intrinsic susceptibility decreases with decreasing temperature (but the very low-temperature data are missing.²³) This matches qualitatively with our mean-field result Eq. (37). We therefore proposed that the f -wave pairing spin-liquid state is a plausible ground state for the material.

VI. COMMENTS AND CONCLUSION

Summarizing, we show in this paper how the fermionic representation for spin $S=\frac{1}{2}$ systems can be generalized to spin systems with $S > \frac{1}{2}$. The symmetry group of the spin operator is $SU(2)$ group for integer spin and $U(1) \bar{\otimes} Z_2$ group for half-odd-integer spin. Different path-integral formulations and mean-field theories are developed corresponding to different ways of handling the constraints. In 1D, we show that the particle-hole symmetric mean-field theory for $S=1$ and $S=3/2$ spin chains are consistent with Haldane's con-

ture, and we argue that the difference reflects a fundamental difference between integer and half-odd-integer spin chains. We also study 2D spin-1 AFM on triangular lattice where we find two spin-liquid states, one is a gapless f -wave spin liquid and the other is a topological $p_x + ip_y$ spin-liquid state. We propose that the gapless f -wave spin liquid is a plausible ground state for the material NiGa_2S_4 . Our approach can be applied to any other spin models and provides a distinct approach to spin-liquid states for $S > \frac{1}{2}$ spin systems.

We note that because of limitation in scope we have addressed only a very limited number of issues in the study of spin-liquid states in this paper. Within the mean-field theory we have restricted ourselves to spin-liquids solutions of Hamiltonian (31) with spin rotational symmetry (1D) and lattice translational symmetry (1D and 2D). We note that solutions which break spin rotational symmetry exist in our theory which may serve as ground states of Hamiltonian (31).²⁰ For example, we show in Ref. 20 that state with long-ranged magnetic order exists as lowest energy state of the mean-field theory of the $J_1 - J_3$ model and antiferromagnetic order may exist when the biquadratic $[K(\mathbf{S}_i \cdot \mathbf{S}_j)^2]$ spin-spin interaction exists in the Hamiltonian. For simplicity we only considered the mean-field states without breaking the translational symmetry. We note that states that break translational symmetry (such as dimerized states) are believed to be ground states of some 1D or 2D spin models.²⁹

Another very important issue is whether the spin-liquid states we find are stable against gauge fluctuations. In 1D, the gauge fluctuations can be removed by a time-dependent Read-Newns gauge transformation and thus have no effect to the low-energy properties.⁶ The situation is very different in two or higher dimensions where the stability of the mean-field state depends on dimensionality and the (gauge) structure of the gauge field fluctuations. For instance, Z_2 spin liquid is believed to be stable at 2D (Ref. 30) and gapless $U(1)$ Dirac fermionic spin liquids is stable at 2D in the large- N limit.³¹ In our case of spin-liquid solutions for the $S=1$ Heisenberg model, the $U(1)$ gauge fluctuation is gapped by the spinon-pairing term via the Anderson-Higgs mechanism. The ground state is stable against the low-energy gauge fluctuations which is described by an effective Z_2 gauge theory. We note that the emergence of gauge-field structure is a direct consequences of particle number constraints and a reliable answer to the question of stability of spin-liquid states can be obtained only if we can handle the particle number constraint reliably. Gauge field theory can only handle long distance, low-energy gauge fluctuations and a more satisfactory answer to the question of stability of the spin-liquid states can be obtained only after the Gutzwiller Projection wave functions are studied carefully.

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APPENDIX A: SYMMETRY GROUP OF THE SPIN OPERATORS AND THE PAIRING PARITY

We shall look for allowed transformations $\psi \rightarrow \psi W$, which keep the spin operator Eq. (3) invariant. At first glance, this condition is satisfied as long as $W \in U(2)$. However, it is *not true* because c_m 's and $c_m^\dagger$'s are not independent. By checking each row of ψ directly, it is easy to see that $[c_m, (-1)^{S-m} c_{-m}^\dagger]$ transforms to $[c_m, (-1)^{S-m} c_{-m}^\dagger] W$ and $[c_m^\dagger, (-1)^{S-m} c_{-m}] \rightarrow [c_m^\dagger, (-1)^{S-m} c_{-m}] W^*$. Noticing that $[c_m^\dagger, (-1)^{S-m} c_{-m}] = (-1)^{S-m} [c_{-m}, (-1)^{S-m} c_m^\dagger] \sigma_x$, we obtain

$$(-1)^{S-m} [c_{-m}, (-1)^{S-m} c_m^\dagger] \sigma_x \rightarrow (-1)^{S-m} [c_{-m}, (-1)^{S-m} c_m^\dagger] \sigma_x W^*$$

or

$$[c_{-m}, (-1)^{S-m} c_m^\dagger] \rightarrow [c_{-m}, (-1)^{S-m} c_m^\dagger] \sigma_x W^* \sigma_x. \quad (\text{A1a})$$

On the other hand, $[c_{-m}, (-1)^{S+m} c_m^\dagger]$ transforms to

$$[c_{-m}, (-1)^{S+m} c_m^\dagger] W.$$

Noticing that

$$\begin{aligned} [c_{-m}, (-1)^{S+m} c_m^\dagger] &= [c_{-m}, (-1)^{-S-m} c_m^\dagger] \\ &= [c_{-m}, (-1)^{S-m} c_m^\dagger] (\sigma_z)^{-2S} \end{aligned}$$

and $(\sigma_z)^{-2S} = (\sigma_z)^{2S}$, we obtain

$$[c_{-m}, (-1)^{S-m} c_m^\dagger] (\sigma_z)^{2S} \rightarrow [c_{-m}, (-1)^{S-m} c_m^\dagger] (\sigma_z)^{2S} W$$

or

$$[c_{-m}, (-1)^{S-m} c_m^\dagger] \rightarrow [c_{-m}, (-1)^{S-m} c_m^\dagger] (\sigma_z)^{2S} W (\sigma_z)^{2S}. \quad (\text{A1b})$$

Equations (A1a) and (A1b) impose the condition

$$\sigma_x W^* \sigma_x = (\sigma_z)^{2S} W (\sigma_z)^{2S}. \quad (\text{A2})$$

For integer spin, Eq. (A2) becomes $W^* = \sigma_x W \sigma_x$, which results in $W = e^{i\theta \sigma_z}$ or $W = e^{i\theta \sigma_z} \sigma_x$, i.e., $W \in U(1) \otimes Z_2$, where $U(1) = \{e^{i\sigma_z \theta}\}$ is the usual gauge symmetry group and $Z_2 = \{I, \sigma_x\}$ is the particle-hole symmetry group. Notice that the two groups don't commute, thus the total symmetry group is a semidirect product of the $U(1)$ group and the Z_2 group $U(1) \otimes Z_2 = \{e^{i\sigma_z \theta}, \sigma_x e^{i\sigma_z \theta} = e^{-i\sigma_z \theta} \sigma_x; \theta \in \mathbb{R}\}$. For half-odd-integer spin, Eq. (A2) implies $W^* = \sigma_y W \sigma_y$, which is equivalent to $\det W = 1$ since $W^\dagger W = 1$. This indicate that $W \in SU(2)$. Thus the symmetry group is $SU(2)$ group.

APPENDIX B: PROOF OF SOME ALGEBRAIC RELATIONS

First we introduce a $(2S+1) \times (2S+1)$ matrix B , which is essential in our proof

$$B = \begin{pmatrix} & & & 1 \\ & & -1 & \\ & 1 & & \\ \dots & & & \end{pmatrix}. \quad (\text{B1})$$

The matrix is the CG coefficients combining two spin S to a spin-singlet state, i.e., $|0,0\rangle = B_{mm'}|S,m\rangle_1|S,m'\rangle_2 = C^\dagger \bar{C}|\text{vac}\rangle$. Thus $\bar{C}$ can be expressed as $\bar{C} = BC^* = B(c_S^\dagger, c_{S-1}^\dagger, \dots, c_{-S}^\dagger)^T$. Notice that for integer spin $B^{-1} = B$ while for half-odd-integer spin $B^{-1} = -B$.

The following are some common properties of the B matrix. Suppose $\hat{R}$ is an rotation operation, and $D(R)$ is its $(2S+1) \times (2S+1)$ -dimensional matrix representation, then we have $\hat{R}C = D(R)C$, and

$$\hat{R}\bar{C} = D(R)\bar{C} = D(R)BC^*.$$

On the other hand, $\hat{R}C^* = D(R)^*C^*$ so

$$\hat{R}\bar{C} = \hat{R}(BC^*) = B\hat{R}C^* = BD(R)^*C^*.$$

Comparing these two, we have $D(R)B = BD(R)^*$ or

$$B^{-1}D(R)B = D(R)^*. \quad (\text{B2})$$

This means that B is the transformation matrix which transfers the representation matrix of a rotational operator to its complex conjugate. In general, $D(R)$ can be written as $D(R) = e^{i\mathbf{R}}$, where $\mathbf{R}$ are the $SU(2)$ group parameters (real numbers) for the operator $\hat{R}$, and consequently $D(R)^* = e^{-i\mathbf{R}}$. From Eq. (B2) we have

$$B^{-1}D(R)B = B^{-1}e^{i\mathbf{R}}B = e^{iB^{-1}\mathbf{R}} = D(R)^* = e^{-i\mathbf{R}}.$$

So we have

$$B^{-1}\mathbf{I}B = -\mathbf{I}^* = -\mathbf{I}^T.$$

Noticing $B^{-1} = \pm B$, above equation is equivalent to $B\mathbf{I}B^{-1} = -\mathbf{I}^* = -\mathbf{I}^T$.

Now let us consider the spin algebra. The spin interaction is decomposed by the following two operators:

$$\psi_i^\dagger \psi_j = \begin{pmatrix} C_i^\dagger C_j & C_i^\dagger \bar{C}_j \\ \bar{C}_i^\dagger C_j & \bar{C}_i^\dagger \bar{C}_j \end{pmatrix}, \quad (\text{B3})$$

$$\psi_i^\dagger \mathbf{I} \psi_j = \begin{pmatrix} C_i^\dagger \mathbf{I} C_j & C_i^\dagger \mathbf{I} \bar{C}_j \\ \bar{C}_i^\dagger \mathbf{I} C_j & \bar{C}_i^\dagger \mathbf{I} \bar{C}_j \end{pmatrix}. \quad (\text{B4})$$

We define $\chi_{ij} = C_i^\dagger C_j$, $\Delta_{ij} = \bar{C}_i^\dagger C_j$ and $\mathbf{u}_{ij} = \bar{C}_i^\dagger \mathbf{I} C_j$, $\mathbf{v}_{ji} = C_i^\dagger \mathbf{I} C_j$. The following discussions distinguish integer- and half-odd-integer spins and prove the results in Sec. III C.

1. Integer spins ($B^\dagger = B^T = B^{-1} = B$)

The second term on the first row of Eq. (B3) can be written as

$$C_i^\dagger \bar{C}_j = C_i^\dagger B C_j^* = -(C_i^\dagger B C_j^*)^T = -C_j^\dagger B C_i^* = -C_j^\dagger \bar{C}_i = -\Delta_{ij}^\dagger$$

In second step, we have used the fact that the transverse of a scalar operator is equivalent to reversing the order of the constituting components. Commuting two fermionic operators we obtain a minus sign. On the other hand, $\Delta_{ji}^\dagger = (\bar{C}_j^\dagger C_i)^\dagger = C_i^\dagger \bar{C}_j$, so $\Delta_{ji} = -\Delta_{ij}$.

The second term on the second row of Eq. (B3) is

$$\bar{C}_i^\dagger \bar{C}_j = C_i^T B B C_j^* = -(C_i^T B C_j^*)^T = -C_j^\dagger C_i = -\chi_{ij}^\dagger.$$

It is obvious that $\chi_{ji} = \chi_{ij}^\dagger$.

To simplify Eq. (B4), we will use the following relations: $B\mathbf{I}B = -\mathbf{I}^T$, $B\mathbf{I} = -\mathbf{I}^T B$, and $\mathbf{I}B = -B\mathbf{I}^T$. The second term on the first row of Eq. (B4) is

$$\begin{aligned} C_i^\dagger \mathbf{I} \bar{C}_j &= C_i^\dagger \mathbf{I} B C_j^* = -C_i^\dagger B \mathbf{I}^T C_j = (C_i^\dagger B \mathbf{I}^T C_j^*)^T \\ &= C_j^\dagger \mathbf{I} B C_i^* = C_j^\dagger \mathbf{I} \bar{C}_i = (\bar{C}_i^\dagger \mathbf{I} C_j)^\dagger = \mathbf{u}_{ij}^\dagger. \end{aligned} \quad (\text{B5})$$

On the other hand, above operator can be written into another form, $C_i^\dagger \mathbf{I} \bar{C}_j = (\bar{C}_j^\dagger \mathbf{I} C_i)^\dagger = \mathbf{u}_{ji}^\dagger$. Comparing with Eq. (B5) we get $\mathbf{u}_{ij} = \mathbf{u}_{ji}$.

The second term on the second row of Eq. (B4) is

$$\bar{C}_i^\dagger \mathbf{I} \bar{C}_j = C_i^T B \mathbf{I} B C_j^* = -C_i^T B \mathbf{I}^T C_j^* = (C_i^T B \mathbf{I}^T C_j^*)^T = C_j^\dagger \mathbf{I} C_i = \chi_{ij}^\dagger. \quad (\text{B6})$$

And the relation $\mathbf{v}_{ji}^\dagger = \mathbf{v}_{ij}$ manifests itself.

2. Half-odd-integer spins ($B^\dagger = B^T = B^{-1} = -B$)

Repeating the above procedures, it is straightforward to show that

$$C_i^\dagger \bar{C}_j = \Delta_{ij}^\dagger, \bar{C}_i^\dagger \bar{C}_j = -\chi_{ij}^\dagger,$$

$$C_i^\dagger \mathbf{I} \bar{C}_j = -\mathbf{u}_{ij}^\dagger, \bar{C}_i^\dagger \mathbf{I} \bar{C}_j = \mathbf{v}_{ij}^\dagger \quad (\text{B7})$$

with $\chi_{ji} = \chi_{ij}^\dagger$, $\Delta_{ji} = \Delta_{ij}$, $\mathbf{u}_{ji} = -\mathbf{u}_{ij}$, $\mathbf{v}_{ji} = \mathbf{v}_{ij}$.

APPENDIX C: EDGE STATES IN OPEN INTEGER SPIN CHAINS

It is known that integer spin antiferromagnetic Heisenberg model has free edge states with spin magnitude $S/2$.¹⁸ Majorana fermion edge states also exist in our mean-field theory under open boundary condition. Our discussion will follow the argument of Ref. 19 for 2D pairing fermions. First, we point out the existence of two topologically distinct phases under periodic boundary condition and then we discuss the zero-energy edge state solution at an open boundary.

In our mean-field theory, all the properties of the ground state are completely determined by u_k and v_k (or χ_k and Δ_k). Noticing that u_k and v_k obey $|u_k|^2 + |v_k|^2 = 1$ so they can be viewed as a spinor. This spinor is equivalent to a vector $(u^*, v^*) \boldsymbol{\sigma} (u, v)^T = (0, \sin \theta_k, \cos \theta_k)^T = (0, \frac{\Delta_k^*}{iE_k}, \frac{\chi_k}{E_k})^T$ where we have used Eq. (26b). Obviously, the spinor (u, v) spans a S^1 space. Recalling that the first Brillouin zone is also S^1 , the functions u_k, v_k describe a mapping from S^1 (k space) to S^1

(spinor space). The mapping degree is characterized by the first homotopy group $\pi_1(S^1) = \mathbb{Z}$. When $-2J\chi < \lambda < 2J\chi$ (which is the case for our mean-field theory), the map is nontrivial because every point of the spinor S^1 is covered once, in other words, the mapping degree is $m=1$. This topological number defines a phase, we call it A phase. When $|\lambda| > 2J\chi$, the mapping is topologically trivial since χ_k is always positive (or negative) and the lower half circle (or upper circle) of the spinor S^1 is never covered so the mapping degree is $m=0$. We call this region B phase. Since the mapping cannot be smoothly deformed from $m=0$ to $m=1$, a topological phase transition occurs at $|\lambda|=2J\chi$. We will see that the existence of zero-energy edge states is tied with a phase boundary between the bulk (A phase) and the vacuum (B phase).

Next we consider an infinite chain with a single edge. We assume that the edge is located at $x=0$, and $x<0$ is the vacuum where the spinon density is zero. The boundary can be described by a potential $V(x)$ that is large and positive at $x<0$ so that the wave function of the spinon vanishes exponentially at $x<0$. Equivalently, we can assume a position-dependent Lagrange multiplier term $\lambda(x)$ which becomes very large and positive (so that the condition $|\lambda| > 2J\chi$ is satisfied) at $x<0$. This implies that the vacuum belongs to the B phase and the boundary is a domain wall between A phase and B phase.

We now study the edge states in the continuum approximation. It is convenient to introduce $\mu(x) = 2J\chi - \lambda(x)$ such that μ is positive in the bulk, becomes zero near the edge and turns negative outside the edge. Expanding χ_k and Δ_k to first order in k near $k=0$, we obtain $\chi_k \sim -\mu$ and $\Delta_k \sim 2iJ\Delta k$. To see the effects of the domain wall, we consider the BdG equation Eq. (25), which can be written in position space as

$$\begin{aligned} i\frac{\partial u}{\partial t} &= -\mu u - 2J\Delta \frac{\partial v}{\partial x}, \\ i\frac{\partial v}{\partial t} &= \mu v + 2J\Delta \frac{\partial u}{\partial x}, \end{aligned} \quad (\text{C1})$$

where we have replaced E and k by $i\frac{\partial}{\partial t}$ and $-i\frac{\partial}{\partial x}$, respectively. The BdG equation is compatible with $u(x,t) = v(x,t)^*$, the spinor (u,v) satisfying this relation describes Majorana fermions. There is a normalizable zero-energy solution for the above equations. Putting $u=v$, then

$$2J\Delta \frac{\partial u}{\partial x} = -\mu u,$$

and the solution is

$$u(x) = v(x) = \propto e^{-1/2J\Delta \int^x \mu(x) dx}.$$

Notice that the BdG equation Eq. (C1)

$$\begin{aligned} Eu &= -\mu u - 2J\Delta \frac{\partial v}{\partial x}, \\ Ev &= \mu v + 2J\Delta \frac{\partial u}{\partial x} \end{aligned}$$

at $E \neq 0$ admits *no* normalizable bound solutions. This shows that the zero mode is the only plausible bound state solution.

In the case of a pair of boundaries at $x=0$ and $x=W$, we can replace the two first-order equations by a second-order equation,

$$E^2(u \pm v) = \left[\mu^2 - (2J\Delta)^2 \frac{\partial^2}{\partial x^2} \mp (2J\Delta) \frac{\partial \mu}{\partial x} \right] (u \pm v),$$

and the energy E is not zero for finite W . However, two bound state solutions with energy going to zero exponentially with increasing W exist. The solution $u+v$ is centered at $x=0$ and $u-v$ is centered at $x=W$. Notice that there is only one solution for the above BdG equations, and the two modes $u \pm v$ are Majorana fermions.

The above discussion is applicable to our mean-field theory for $S=1$ open antiferromagnetic chain. The discussion can be generalized to larger integer spins $S>1$ if we adopt the effective Hamiltonian (23).

Unlike the $S=1$ case, our $S=3/2$ mean-field theory produces a mapping from k -space S^1 to the (u,v) space S^1 which is topologically trivial (essentially because of the even parity of the pairing term), and the Majorana edge states don't exist anymore. This is in agreement with the result that no exponentially localized edge state exists for open half-odd-integer spin chains. The existence of power-law localized edge states in half-odd-integer spin chains¹⁸ is more subtle and is not produced by our mean-field theory.

APPENDIX D: CALCULATION OF THE SUSCEPTIBILITY

Substituting the Bogoliubov transformation Eq. (34) into the Kubo formula Eq. (37), we obtain

$$\begin{aligned} \chi_z(k, i\omega) &= \frac{2}{V} \int d\tau e^{i\omega\tau} \sum_q \{ [C_q^2 G_A(q, -\tau) - S_q^2 G_B(-q, \tau)] \\ &\quad \times [-C_{q+k}^2 G_A(q+k, \tau) + S_{q+k}^2 G_B(-q-k, -\tau)] \\ &\quad - C_q S_q [G_A(q, -\tau) + G_B(-q, \tau)] \\ &\quad \times C_{q+k} S_{q+k} [G_A(q+k, \tau) + G_B(-q-k, -\tau)] \} \\ &= \frac{2}{\beta V} \sum_{q, i\Omega} \{ [C_q^2 G_A(q, i\Omega) - S_q^2 G_B(-q, -i\Omega)] \\ &\quad \times [-C_{q+k}^2 G_A(q+k, i\Omega + i\omega) + S_{q+k}^2 G_B(-q-k, \\ &\quad -i\Omega - i\omega)] - C_q S_q C_{q+k} S_{q+k} [G_A(q, i\Omega) + G_B(-q, \\ &\quad -i\Omega)] [G_A(q+k, i\Omega + i\omega) + G_B(-q-k, -i\Omega \\ &\quad -i\omega)] \} \end{aligned}$$

with the notations $C_q = \cos \frac{\theta_q}{2}$ and $S_q = \sin \frac{\theta_q}{2}$. Using the results $G_A(k, i\omega) = G_B(k, i\omega) = G(k, i\omega)$ and $G(-k, i\omega) = G(k, i\omega) = \frac{1}{i\omega - E_k}$, we get the static susceptibility

$$\begin{aligned} \chi_z &= \lim_{k \rightarrow 0} \chi_z(k, 0) \\ &= \lim_{k \rightarrow 0} \frac{2}{\beta V} \sum_{q, i\Omega} [- (C_q C_{q+k} + S_q S_{q+k})^2 G(q, i\Omega) G(q+k, i\Omega) \\ &\quad + (C_q S_{q+k} - S_q C_{q+k})^2 G(q, i\Omega) G(q+k, -i\Omega)] \end{aligned}$$

$$\begin{aligned}
&= \lim_{k \rightarrow 0} \frac{2}{V} \sum_q \left[- (C_q \mathcal{C}_{q+k} + \mathcal{S}_q \mathcal{S}_{q+k})^2 \frac{n_f(\epsilon_{q+k}) - n_f(\epsilon_q)}{\epsilon_{q+k} - \epsilon_q} \right] \\
&= -2 \int d^2 q \frac{\partial n_f(\epsilon_q)}{\partial \epsilon_q} \quad (D1)
\end{aligned}$$

which is the Pauli susceptibility for free fermions. At low

temperature, the excitation spectrum can be approximated by Dirac cones so we have

$$\chi_z \doteq -2 \int_0^\infty 2\pi q \frac{\partial n_f(\epsilon_q)}{v_F \partial q} dq = \frac{4\pi}{v_F} \int_0^\infty n_f(\epsilon_q) dq \propto \frac{T}{v_F^2}. \quad (D2)$$

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respectively. This is because that the elementary excitations in both situations are spin-1 magnons which can be viewed as bound states of two spin- $\frac{1}{2}$ spinons. However, for 1D half-odd-integer antiferromagnetic spin chains, elementary excitations are spin- $\frac{1}{2}$ spinons. So far we do not know how this modified spin-wave theory can be generalized to deal with this situation.

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