Fermionic theory for quantum antiferromagnets with spin $S > 1/2$

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The fermion representation for $S = 1/2$ 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 $S = 1/2$ fermion representation is absent for $S > 1/2$. 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 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$_2$S$_4$, 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 $S > 1/2$ 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 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. Systematic corrections to spin wave theory can be obtained through semiclassical approach (1/S expansion) and/or nonlinear $\sigma$ model. However, it was suggested that for some anti-ferromagnetic 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. In such cases, a quantum fluid approach 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, 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 $S = 1/2$ spin systems. Because of the Pauli exclusion principle, we cannot put more than two spin up or down fermions on a site to form $S > 1/2$ objects as in bosonic approach. One way out is to introduce more species of fermions. It was proposed in Ref. [11], 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.

In this paper, we systematically study the fermionic representation for arbitrary spins. To construct a spin operator with spin magnitude $S$, we follow Ref. [11] and introduce different fermion operators for different $S$ states. We find that for half-odd-integer spins, the spin operator thus constructed is invariant under a $SU(2)$ transformations, i.e. the symmetry group is $SU(2)$ group whereas for integer spins the symmetry group is $U(1) \otimes Z_2$. 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 Heisenberg model produces mean field excitation spectrums which agrees with Haldane’s conjecture. 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 paring symmetry) is gapped and the other one (with $f$-wave pairing symmetry) has nodes at the spinon Fermi level. Comparing with experiments on NiGa$_2$S$_4$, 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. In these approaches, $N$-species of particles are introduced to construct the $SU(N)$-spin operator and
II. GENERAL FERMIonic SPIN REPRESENTATION

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

$$\{c_m, c_n^\dagger\} = \delta_{mn},$$

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

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

where $C = (c_S, c_{S-1}, \cdots, c_{-S})^T$ 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 $\mathcal{I}$ 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.

$$\langle \hat{N}_i - N_f | \text{phy} \rangle = 0,$$

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 $S = 1/2$, 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., we introduce another “spinor” $C = (c_\downarrow, -c_{\downarrow+1}, c_{\downarrow+2}, \cdots, (-1)^S c_{\downarrow+1})^T$, whose components can be written as $\bar{C}_m = (-1)^{S-m} c_{\downarrow-m}$, 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 $j$,

$$\frac{C_i^\dagger \bar{C}_j}{\sqrt{2S+1}} | \text{vac} \rangle = \frac{1}{\sqrt{2S+1}} \sum_{m=-S}^S (-1)^{S-m} | S, m \rangle | S, -m \rangle.$$ 

Therefore $C_i^\dagger \bar{C}_j$ is a scalar operator as $C_i^\dagger C_j$, meaning that $C$ and $\bar{C}$ must behave identically under spin rotation. Consequently, the spin operators can also be written in terms of $C$,

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

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

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

and the constraint can be expressed as

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

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 $\psi$. The first kind belongs to a $(2S+1)$-dimensional irreducible representation of $SU(2)$ group, acting on the left of $\psi$. 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 $SO(3)$ 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 $2 \times 2$ unitary group acting on the right of $\psi$ which keeps the spin operator Eq. (3) and the fermionic statistics Eq. (11) 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 $U(1) \otimes Z_2 = \{ e^{i\pi \delta_\theta} \sigma_z, e^{i\pi \sigma_z} \theta = e^{-i\pi \sigma_z} \sigma_z | \theta \in \mathbb{R} \}$ 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 $c_{S+1}^\dagger$, $c_{S-1}$ and $-c_{-S+1}^\dagger$, etc. For integer spins, $c_0$ and $(-1)^Sc_0^\dagger$ 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 $U(1)\otimes Z_2$ group. For half-integer spins, the pair $(-1)^Sc_0^\dagger$ 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 $S = 1/2$, 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 $W = e^{i\sigma_3 \theta}$, then $W_\sigma_2 W_\dagger^\tau = \sigma_z$, and Eq. (4) is invariant. If $W = \sigma_x e^{i\sigma_3 \theta}$, then $W_\sigma_2 W_\dagger^\tau = -\sigma_z$, 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 $S = 1/2$ case\(^8\) so that Eq. (4) becomes

\[
\text{Tr}(\psi_\sigma \psi_\dagger^\tau) = (0, 0, \pm(2S - 1))^T. \tag{5}
\]

Under the group transformation $\psi \rightarrow \psi W$, \[
\text{Tr}(\psi_\sigma \psi_\dagger^\tau) \rightarrow (R^{-1})(0, 0, \pm(2S - 1))^T. \tag{6}
\]

where $W_\sigma_2 W_\dagger^\tau = R_{ab} \sigma_b$, $a, b = x, y, z$, i.e. $R$ is a 3 by 3 matrix representing a 3D 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 $SU(2)$ 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 $S > 1/2$ 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 section IV where a new 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 $H = J \sum_{(i,j)} \hat{S}_i \cdot \hat{S}_j$ 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-1/2 the Heisenberg interaction can be written as\(^8\)

\[
\hat{S}_i \cdot \hat{S}_j = -\frac{1}{8} \text{Tr} : (\psi_i^\dagger \psi_j \psi_j^\dagger \psi_i) :
\]

\[
= -\frac{1}{4} : (\chi_{ij} \chi_{ij} + \Delta_{ij}^\dagger \Delta_{ij}) :, \tag{7}
\]

where \[
\chi_{ij} = C_{ij}^\dagger C_{ij}, \quad \Delta_{ij} = \bar{C}_{ij}^\dagger C_{ij}. \tag{8}
\]

are spin-singlet operators, $\chi_{ij}$ and $\Delta_{ij}$ 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 $\psi$ 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

\[
H = J \sum_{(i,j)} \hat{S}_i \cdot \hat{S}_j = -\frac{J}{2} \sum_{(i,j)} \text{Tr} : (\psi_i^\dagger \psi_j \psi_j^\dagger \psi_i) :
\]

\[
= -J \sum_{(i,j)} : (\chi_{ij} \chi_{ij} + \Delta_{ij}^\dagger \Delta_{ij}) :. \tag{9}
\]

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

\[
I_+ = (I_-)^\dagger = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad I_z = \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}
\]
and the matrix operator $\psi$ is given by $\psi = (C \, C)^T$ where $C = (c^+_x, c^+_y, c^+_z, c^+_\bar{z}, c^-_x, c^-_y, c^-_z, c^-_\bar{z})^T$ and $C = (e^+_x, e^+_y, e^+_z, e^+_\bar{z}, e^-_x, e^-_y, e^-_z, e^-_\bar{z})^T$. In this case the singlet operators $\chi_{ij}$ and $\Delta_{ij}$ alone are not enough to represent the Heisenberg Hamiltonian, and triplet hoping and pairing terms are necessary. After some straightforward but tedious analysis suggests that smaller spins have higher symmetry functions with different particle-number constraint representations. In the integer spin case, the average is given by

$$Z \approx Tr(\bar{\psi}N_{i=1}^N \bar{\psi})$$

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

where $\hat{N}_i = C^+_i C_i$ 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

$$H = J \sum_{(i,j)} \hat{S}_i \cdot \hat{S}_j = -\frac{J}{2} \sum_{(i,j)} Tr(\psi^+_i I \psi^+_j \cdot \psi^+_j I \psi^+_i) : .$$

As in the case of lower spins, the terms $Tr(\psi^+_i I \psi^+_j \cdot \psi^+_j I \psi^+_i)$ and $Tr(\psi^+_i I \psi^+_j \cdot \psi^+_j I \psi^+_i)$ 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

$$H = -\frac{J}{2} \sum_{(i,j)} \left[ a(S) Tr(\psi^+_i I \psi^+_j \cdot \psi^+_j I \psi^+_i) : + b(S) Tr(\psi^+_i I \psi^+_j \cdot \psi^+_j I \psi^+_i) : + \cdots \right]$$

(11)

where $a(S), b(S), \cdots$ are parameters dependent on the spin magnitude $S$ and $\cdots$ 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 wavefunctions 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

$$Z = Tr(e^{-\beta H}) = \int D\psi D\psi^+ e^{-\int_0^\beta \psi^+ \left[ \sum_i \left( \frac{\delta}{\delta \psi^+_{\sigma_z} \psi^+_{\sigma_z} \psi^+_{\sigma_z}} \right) + H \right] \overline{d\tau}}$$

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

(12)

where $\lambda_i$ is the Lagrange multiplier field introduced to impose the constraint Eq. (11). The $(-)$ sign corresponds to the particle ($\hat{N}_i = 1$) and hole ($\hat{N}_i = 2S$) representations. The Grassmann number $\psi$ satisfy the antiperiodic boundary condition $\psi(0) = -\psi(\beta)$.

Notice that the Lagrangian Eq. (12) is not invariant under the action of the internal symmetry group because of the non-invariant 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

$$Z = \int D\psi D\psi^+ e^{-\int_0^\beta \sum_i \left( \frac{\delta}{\delta \psi^+_{\sigma_z} \psi^+_{\sigma_z} \psi^+_{\sigma_z}} \right) + H} \overline{d\tau} \times$$

$$\prod_{\langle i,\tau \rangle} \frac{1}{2} \left[ \delta(\hat{N}_i - 1) + \delta(\hat{N}_i - 2S) \right]$$

$$= \int D\psi D\psi^+ e^{-\int_0^\beta \sum_i \left( \frac{\delta}{\delta \psi^+_{\sigma_z} \psi^+_{\sigma_z} \psi^+_{\sigma_z}} \right) + H} \overline{d\tau} \times$$

$$\prod_{\langle i,\tau \rangle} \frac{1}{2} \left( e^{\frac{i}{2}\int_0^\beta \left[ Tr(\psi_i (\sigma_z \psi_i) + 2S+1) \right] + \int_0^\beta \psi_i^+ (\sigma_z \psi_i) + 2S-1 \right) \right.$$}

(13)

Notice that we do not make any approximations in deriving Eq. (13) from Eq. (12) and the “new” 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 representation and the SU(2) representation of the t-J model. The fermion particle-hole symmetry is restored in this representation. The Lagrangian corresponding to Eq. (13) is

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

This form of Lagrangian is invariant under the internal symmetry group U(1)⊗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 \( \lambda_i \). This problem can be solved by lifting the contour of integration over \( \lambda \) into complex plane via analytic continuation to find a saddle point in the imaginary axis. We write \( \lambda_i = i\lambda_i \), and integrate \( \lambda_i \) from \(-i\infty\) to \(i\infty\) (the saddle point of \( \lambda_i \) is real). Then the Lagrangian becomes

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

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

\[ \hat{U}_{ij} = \psi_i^\dagger \psi_j = \left( \begin{array}{cc} \chi_{ij} & -\Delta_{ij}^\dagger \\ \Delta_{ij} & -\chi_{ij} \end{array} \right), \]

\[ \hat{V}_{ij} = \psi_i^\dagger I \psi_j = \left( \begin{array}{cc} v_{ij} & u_{ij}^\dagger \\ u_{ij} & v_{ij} \end{array} \right), \]

where \( u_{ij} = C_i^\dagger IC_j \), and \( v_{ij} = \tilde{C}_i^\dagger IC_j \). Note that \( u_{ij} \) and \( v_{ij} \) form two sets of spin triplet operators, respectively. The Hamiltonian becomes

\[ H = \sum_{(i,j)} \left\{ a(S)\text{Tr}[\hat{U}_{ij} \hat{U}_{ij} - (\hat{U}_{ij})^\dagger \psi_i^\dagger \psi_j + h.c.] \right\} + b(S)\text{Tr}[\hat{V}_{ij}^\dagger \hat{V}_{ij} - (\hat{V}_{ij})^\dagger \psi_i \psi_i + h.c.]. \]

The \( \hat{U}_{ij} \) and \( \hat{V}_{ij} \) have fields define U(1)⊗Z_2 lattice gauge fields coupling to the fermionic particles which we shall call spinons in the following. Under the local gauge transformation the temporal component and the spacial component of the gauge fields transform as

\[ \hat{\lambda}_i \sigma_z \rightarrow W_i^\dagger (\hat{\lambda}_i \sigma_z - \frac{d}{dt}) W_i, \]

\[ \hat{U}_{ij} \rightarrow W_i^\dagger \hat{U}_{ij} W_j, \]

\[ \hat{V}_{ij} \rightarrow W_i^\dagger \hat{V}_{ij} W_j. \] (16)

Notice that \( \lambda_i \) changes sign under an uniform Z_2 gauge transformation, and \( \chi_{ij} \), \( \Delta_{ij} \) exchange their roles under a “staggered” Z_2 transformation where we have \( \sigma_x \) on one sublattice and \( \sigma_z \) on the other sublattice. Notice also that the Lagrangian is not invariant under a time-dependent gauge transformation, because the term \( 2 \ln \cosh \left( \frac{2(S-1)\lambda_i}{2} \right) \)

is not invariant. A similar situation occurs in the supersymmetric representation of Heisenberg model. 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 \( U_{ij} \), \( \hat{V}_{ij} \) and \( \lambda_i \) 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 \( U = \langle \hat{U}_{ij} \rangle, \hat{V} = \langle \hat{V}_{ij} \rangle \) with the mean field Hamiltonian

\[ H_m = J \sum_{(i,j)} \left[ a(S)\langle \chi C_i^\dagger C_j + \Delta^\dagger \tilde{C}_i^\dagger IC_j + h.c. \rangle \right] + |\chi|^2 \]

\[ + |\Delta|^2 + b(S)\langle -v^\dagger C_i^\dagger IC_j + u^\dagger \tilde{C}_i^\dagger IC_j + h.c. \rangle \]

\[ + |u|^2 + |v|^2 \right] + \sum_i \langle \lambda (\hat{N}_i - \frac{2S+1}{2}) \rangle, \quad (17) \]

where \( \chi = \langle C_i^\dagger C_j \rangle, \Delta = \langle \tilde{C}_i^\dagger IC_j \rangle, u = \langle \tilde{C}_i^\dagger IC_j \rangle, v = \langle C_i^\dagger IC_j \rangle, \) and \( \lambda \) is determined by the condition

\[ \langle \hat{N}_i \rangle = \frac{2S+1}{2} = \frac{2S-1}{2} \tanh \left( \frac{2(S-1)\lambda}{2} \right). \]

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 doesn’t break the particle-hole symmetry, then \( \lambda = 0 \) 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 \( \text{Tr}[\psi^\dagger \sigma \psi^\dagger] = \pm (2S-1) \) are transformed into each other by the SU(2) internal symmetry group. We consider the vector constraint Eq. (15) for \( S \geq 1/2 \)

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

where

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

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

\[ \hat{M}_z = \frac{1}{2S-1}\text{Tr}(\hat{C} \hat{C}^\dagger - \hat{C} \hat{C}^\dagger). \]
The $M_x$ and $M_y$ components indicate that the one-site pairings $c_{c\cdots c}.\cdots, c_{\tilde{c}\cdots \tilde{c}}.$ 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 $\frac{1}{2\pi} \text{Tr}(\hat{\psi} \sigma \hat{\psi}^\dagger) = R^{-1}(0,0,1)^T$, where $W_M W^\dagger = R_{ab} g_{b}$. $R$ is an $SO(3)$ rotation. Since the constraint is invariant under an $U(1)$ gauge transformation generated by $g_z$, the continuum space formed by different constraints is the surface of a sphere $SU(2)/U(1) = S^2$. In particular, for $W = e^{ia_\pi/2}$, the north pole of the space which corresponds to the positive sign in Eq. (4) is transformed 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 $\sum_{i\in n} \lambda_i$ is realized by introducing a vector Lagrange multiplier field $\lambda_i$.

$$\delta(M^x_i) \delta(M^y_i) \delta(M^z_i - 1) = \frac{1}{2\pi} \int d\lambda^\dagger_i d\lambda^\dagger_i \lambda_i \exp \left( i \frac{\lambda^\dagger_i \lambda_i}{\lambda_i} \right) \left( \sum_{i\in n} \lambda_i \right)$$

The vector $(0,0,1)^T$ changes into $R^{-1}(0,0,1)^T = (n^x,n^y,n^z)^T = n$ under $SU(2)$ gauge transformation, where $n$ 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:

$$\langle \delta(M^x_i - n^x) \delta(M^y_i - n^y) \delta(M^z_i - n^z) \rangle_{\hat{n}}$$

$$= \frac{1}{2\pi} \int d\hat{n} \int d\lambda \exp \left\{ i \lambda_i \cdot (\hat{M}_i - \hat{n}) \right\}$$

$$= \frac{1}{2\pi} \int d\lambda \exp \left\{ i \lambda_i \cdot (\hat{M}_i - \hat{n}) - i \ln \frac{\sinh \lambda_i}{\lambda_i} \right\}$$

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

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

It can be proved (see Appendix B) that for integer spins, $\chi_{ij} = \chi^\dagger_{ij}$, $\Delta_{ij} = -\Delta_{ij}$, $u_{ij} = u_{ij}$ and $v_{ij} = v^\dagger_{ij}$, whereas for half-odd-integer spins, $\chi_{ij} = \chi^\dagger_{ij}$, $\Delta_{ij} = \Delta_{ij}$, $u_{ij} = -u_{ij}$ and $v_{ij} = v^\dagger_{ij}$. Notice that the parity of the pairing terms $\Delta_{ij}$ and $u_{ij}$ 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 $u, v = 0$, 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 $u,v \neq 0$. 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 $S = 1/2$ case, the mean field Hamiltonian should be viewed as a trial Hamiltonian for the ground state wavefunction of the spin systems after Gutzwiller projection. For the mean field theory with particle-hole symmetry the Gutzwiller projection is rather non-trivial. The state is a coherent superposition of states which allows sites with both one fermion and with 2$S$ 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 section 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. Therefore we assume in our mean-field theory that the ground state is a spin singlet (spin liquid state) and the expectation values of $\langle u_{ij}\rangle$ and $\langle v_{ij}\rangle$ 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.

A. integer spin: $S = 1$

We choose $H_{tr}$ to be the same as Eq. (19), i.e., $a(1) = -1, b(1) = 0$. For convenience of discussion, we introduce two new fermions $c_s, c_a$ which are the symmetric and antisymmetric combinations of $c_1$ and $c_{-1}$,

$$
c_{si} = (c_{1i} + c_{-1i})/\sqrt{2},
$$

$$
c_{ai} = (c_{1i} - c_{-1i})/\sqrt{2}.
$$

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

$$
H_m = \sum_k \chi_k (c_{sk}^\dagger c_{sk} + c_{ak}^\dagger c_{ak} + c_{0k}^\dagger c_{0k})
$$

$$
- \sum_k [\Delta_k^* (c_{sk} - c_{-k} c_{sk} - c_a - c_{sk} c_{ak} - c_{0k} - c_{0k} c_{0k})] + h.c.
$$

$$
+ J N (|\chi|^2 + |\Delta|^2) - N (\frac{3}{2} \tilde{\lambda} + \ln \cosh \frac{\tilde{\lambda}}{2}),
$$

(23)

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

$$
\gamma_{sk} = u_k c_{sk} + v_k c_{-sk}^\dagger, \quad \gamma_{ak} = u_k c_{ak} - v_k c_{a-k}^\dagger, \quad \gamma_{0k} = u_k c_{0k} - v_k c_{0-k}^\dagger.
$$

(24)

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

$$
E_k u_k = \chi_k u_k - \Delta_k v_k, \quad E_k v_k = -\Delta_k^* u_k - \chi_k v_k.
$$

(25)

Solving the equations we obtain

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

(26a)

$$
u_k = \cos \frac{\theta_k}{2}, \quad v_k = i \sin \frac{\theta_k}{2},
$$

(26b)

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

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

(27a)

$$
\Delta = \frac{2S + 1}{2N} \sum_k \sin k \frac{\Delta_k}{E_k},
$$

(27b)

$$
\langle \frac{2S + 1}{2} - \hat{N}\rangle = \frac{2S + 1}{2N} \sum_k \frac{\chi_k}{E_k}
$$

(27c)

$$
= -\frac{2S - 1}{2} \tanh (\frac{2S - 1}{2} \tilde{\lambda}),
$$

with $S = 1$. The above equations are solved numerically where we obtain $\chi = \frac{\Delta}{\Delta} = 3/4$ 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

$$\langle S_i \cdot S_{i+r} \rangle = \frac{3}{2N} \sum_{p,q} e^{i(p-q)r} \left[ (1 + \frac{\chi_p}{E_p})(1 - \frac{\chi_q}{E_q}) \right]$$

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

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

For the spin-3/2 Heisenberg chain, we consider the effective Hamiltonian Eq. (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

$$H_m = \sum_k \chi_k (c_{\frac{3}{2}+k} c_{\frac{3}{2}+k}^\dagger + c_{\frac{3}{2}-k} c_{\frac{3}{2}-k}^\dagger + c_{\frac{3}{2}+k} c_{\frac{3}{2}-k}^\dagger + c_{\frac{3}{2}-k} c_{\frac{3}{2}+k}^\dagger)$$

$$+ \sum_k \Delta^*_k (c_{\frac{3}{2}+k} c_{\frac{3}{2}+k}^\dagger - c_{\frac{3}{2}-k} c_{\frac{3}{2}-k}^\dagger) + h.c. + \text{const.},$$

where $\chi_k = \tilde{\lambda}_z - \frac{15}{8} J \chi \cos k$ and $\Delta^*_k = \tilde{\lambda}_x - i \tilde{\lambda}_y - \frac{15}{2} J \Delta^* \cos k$. We shall set $\chi$ and $\Delta$ 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,

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

$$\Delta = \frac{2S + 1}{2N} \sum_k \cos k \Delta_k E_k,$$

$$\langle \hat{M}_+ \rangle = \frac{2S + 1}{N(2S - 1)} \sum_k \Delta_k \frac{E_k}{E_k} = \frac{(1 - \tilde{\lambda} \coth \tilde{\lambda}) \tilde{\lambda}_+}{\lambda^2},$$

$$\langle \hat{M}_0 \rangle = \frac{2S + 1}{N(2S - 1)} \sum_k \chi_k \frac{E_k}{E_k} = \frac{(1 - \tilde{\lambda} \coth \tilde{\lambda}) \tilde{\lambda}_z}{\lambda^2}$$

(28)

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

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

(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 $\chi$ and $\Delta$ 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 Section III.B.2. and all these solutions are equivalent. Notice that the ground state energy $E_0 = -\frac{15N\lambda}{8}(\chi^2 + |\Delta|^2)$ is the same as the expectation value of the Heisenberg Hamiltonian Eq. (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 dispersion Eq. (29) is gapless at Fermi points $k = \pm \pi/2$. The spin-spin correlation is given by

$$\langle S_i \cdot S_{i+r} \rangle = \frac{15}{4N^2} \sum_{p,q} e^{i(p-q)r} \left[ (1 + \frac{\chi_p}{E_p})(1 - \frac{\chi_q}{E_q}) \right]$$

$$- \left[ \frac{\Delta^*_p \Delta_q}{E_p E_q} \right]$$

and decays at large distance as $\langle S_i \cdot S_{i+r} \rangle \propto r^{-2}$ 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 ($\hat{M}_0 = (0, 0, 1)^T$. The solution is listed in Table II. Since $\tilde{\lambda}_z \neq 0$ in this case, the spinon dispersion $E_k = \frac{15}{8} \sqrt{(\tilde{\lambda}_x^2 / 2 - \chi \cos k)^2 + |\Delta \cos k|^2}$ breaks particle-hole symmetry and has a finite gap over the whole Brillouin zone. The particle-hole symmetric solution is also found to has a lower mean field ground state energy.

**C. Haldane’s conjecture and Edge states**

Comparing the mean field energy dispersion Eq. (26a) and Eq. (29), we find that the excitation spectrum of
TABLE II: Solutions of two versions of mean fields for spin-3/2 Heisenberg chain. In the first row \(\langle \chi, \Delta \rangle\) means the real combinations satisfying \(\sqrt{\chi^2 + \Delta^2} = 1.2732\).

| \(\langle N_i \rangle\) | \(\chi\) | \(\Delta\) | \(\lambda_s\) | \(E(J)\) | \(E_{\text{prop}}(J)\) | \(\langle S_i \cdot S_j \rangle\) |
|----------------------|--------|--------|----------|--------|----------------|--------------------|
| 2                    | \(x\)  | \(\Delta\) | 0        | -1.5198 | 0             | 15/4               |
| 1                    | 0      | 1.1490 | 0.7181   | -1.2977 | 0.6732         | 45/16              |

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 Eq. (14) or Eq. (21) with \(a(S) = 0\), \(b(S) = 0\), i.e., if we consider BCS spin-singlet ground state wavefunctions. 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\[^{26}\] 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

\[
Q = \int dtdx \frac{1}{4\pi} \mathbf{n} \cdot (\partial t \mathbf{n} \times \partial x \mathbf{n})
\]

is the Skyrmion number. For \(Q = 0\) odd phase, 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 \pm 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 \(\Delta_{ij} = C_i^j C_j\) is a singlet formed by two spin-\(S\) particles. The Clebsch-Gordan coefficients implies that \(\Delta_{ij} = -\Delta_{ji}\) 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 \(\sin k\) in Eq. (26a) for \(S = 1\) and \(\cos k\) in Eq. (29) for \(S = 3/2\), which leads to different symmetries of ground state wavefunctions and different excitation spectrums between integer and half-odd-integer spin chains.

The topological term Eq. (20) leads to exponentially localized edge states for open integer spin chains which is absent for half-odd-integer spin chains\[^{26}\]. 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\[^{26}\]. 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 new spin liquid solutions not explored before. Some results of this model have been reported in a previous paper\[^{27}\], where particle number constraint is treated in the “particle representation” \((\langle N_i \rangle = 1\) ). In this paper, we shall revisit this model with the particle-hole symmetric constraint. The Hamiltonian of the \(J_1-J_3\) model is

\[
H = \sum_{\langle i,j \rangle} J_1 S_i \cdot S_j + J_3 \sum_{\langle i,j \rangle} S_i \cdot S_j,
\]

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, \(S_i \cdot S_j = -\frac{1}{2} \text{Tr}(\psi_i^\dagger \psi_j \psi_j^\dagger \psi_i)\) or \(S_i \cdot S_j = -\frac{1}{2} \text{Tr}(\psi_i^\dagger \psi_j \psi_i \psi_j)\). 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.

\[
\begin{align*}
\tilde{\Delta}_k &= \lambda - aZ(J_1 \chi \gamma_k + J_3 \chi^3 \gamma_{2k}), \\
\Delta_k^x &= i a Z(J_1 \Delta \psi_k + J_3 \Delta \psi_{2k}), \\
v_k &= -(1 - a) Z(J_1 \gamma_v u_1 + J_3 \gamma_v u_3), \\
u_k^* &= (1 - a) Z(J_1 \gamma_v u_1 + J_3 \gamma_v u_3),
\end{align*}
\]

where $\lambda$ is the Lagrange multiplier and
\[
\gamma_k = \frac{1}{3} \left[ \cos k_x + \cos \left( - \frac{k_x}{2} + \frac{\sqrt{3} n_y}{2} \right) + \cos \left( - \frac{k_x}{2} - \frac{\sqrt{3} n_y}{2} \right) \right],
\]
\[
\psi_k^f = \frac{1}{3} \left[ \sin k_x + \sin \left( - \frac{k_x}{2} - \frac{\sqrt{3} n_y}{2} \right) - \sin \left( - \frac{k_x}{2} + \frac{\sqrt{3} n_y}{2} \right) \right],
\]
\[
\psi_k^{p+i} = \frac{1}{3} \left[ \sin k_x + e^{i \omega} \sin \left( k_x \frac{3}{2} \right) + e^{-i \omega} \sin \left( - k_x \frac{3}{2} \right) \right].
\]

The pairing symmetries can be verified easily by expanding
the pairing terms at small $k$: $\Delta_1^f \propto k_x (k_x^2 - 3 k_y^2)$, and
$\Delta_{p+i}^{+} \propto k_x + i k_y$. There are three lines of zeros for the
$j$-wave pairing function as shown in Fig. [2].

Introducing a vector $C_k = (c_{1k}, c_{\perp 1-k}, c_{3k}, c_{\perp 3k})^T$, the
Hamiltonian Eq. (32) can be written in a matrix form:

\[
H_m = \sum_k \frac{3}{2} \chi_k - v_k, \quad (33)
\]

where
\[
H_k = \begin{pmatrix}
\chi_k + v_k & -u_k - \Delta_k & 0 & 0 \\
0 & -u_k - \Delta_k & 0 & 0 \\
0 & 0 & \Delta_k & \Delta_k \\
0 & 0 & \Delta_k & \Delta_k
\end{pmatrix}.
\]

$H_k$ can be diagonalized by the Bogoliubov transformation,
\[
A_k = \frac{\theta_k}{2} c_{1k} - \frac{\theta_k}{2} e^{i \varphi_k} c_{\perp 1-k},
\]
\[
B_k = \frac{\theta_k}{2} e^{-i \varphi_k} c_{1k} + \frac{\theta_k}{2} c_{\perp 1-k},
\]
\[
D_k = \frac{\Theta_k}{2} c_{3k} + \frac{\Theta_k}{2} e^{i \varphi_k} c_{\perp 3k},
\]

where $\tan \theta_k = \frac{|a_k + \Delta_1|}{\chi_k}$, $\tan \Theta_k = \frac{|\Delta_1|}{\chi_k}$
and $\tan \varphi_k = \frac{\Delta_1}{\chi_k}$. The corresponding eigenvalues are given
by $v_k \pm E_{1k}$ and $\pm E_{0k}$, where
\[
E_{1k} = \sqrt{\chi_k^2 + |\Delta_k|^2}, \quad E_{0k} = \sqrt{\chi_k^2 + |\Delta_k|^2},
\]
and the self-consistent mean field equations are
\[
\tilde{\chi}_{1,3} = \frac{1}{N} \sum_k \gamma_{k,2k} \left[ \frac{3}{2} - \frac{\chi_k}{E_{1k}} - \frac{\chi_k}{E_{0k}} \right],
\]
\[
\tilde{\Delta}_{1,3} = \frac{1}{N} \sum_k \psi_{k,2k} \left[ \frac{|\Delta_k|}{E_{1k}} + \frac{|\Delta_k|}{E_{0k}} \right],
\]
\[
\tilde{u}_{1,3} = \frac{1}{N} \sum_k \gamma_{k,2k} \frac{u_k}{E_{1k}},
\]
\[
\tilde{v}_{1,3} = 0,
\]
\[
\langle \tilde{N}_1 \rangle \frac{3}{2} = \frac{1}{2} \tanh \frac{\tilde{\lambda}}{2}, \quad (35)
\]
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 \( \langle N_i \rangle = \frac{1}{2} \) and found that the excitation spectra 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 \( E_k = \sqrt{\lambda_k^2 + |\Delta_k|^2} \) (which is \( S^2 \)) covers the Brillouin zone (\( k \) space, which is also \( S^2 \)) at least once. In other words, the topological (Skyrmion) number of mapping from the \( k \) space to the spinor space is nonzero \( m \neq 0 \). However in the vacuum where the spinon density is zero, \( \lambda \) is very big and \( \chi_k \) can only take positive values, which gives a zero topological number\(^{27} \). Since the bulk and vacuum belong to different topological sectors, the boundary defines a domain wall between the two phases, and there should exists gapless (chiral) Majorana edge states in the \( p_x + ip_y \) state following the analysis of Read and Green\(^{27} \). In this sense, the \( p_x + ip_y \)-state describes a time-reversal symmetry breaking topological spin liquid.

```
FIG. 3: (Color online) Phase diagram for the \( J_1-J_3 \) Heisenberg model with \( J_1 + J_3 = 1 \). We use the constraint \( \langle N_i \rangle = \frac{1}{2} \). The red dot 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.
```

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 \( \langle S_i \cdot S_{i+1} \rangle < 0 \) and \( \langle S_i \cdot S_{i+2} \rangle < 0 \)); while when \( J_3 \) dominates, \( \chi_1 = \Delta_1 = 0 \) and \( \chi_3 \neq 0, \Delta_3 \neq 0 \) (consequently \( \langle S_i \cdot S_{i+1} \rangle = 0, \langle S_i \cdot S_{i+2} \rangle < 0 \)). The \( p_x + ip_y \) states remain lower in energy in both regimes.

The f-wave pairing solution respects particle-hole symmetry and has \( \langle N_i \rangle = \frac{1}{2} \). 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 \( \langle N_i \rangle = 1 \) has similar properties, except that the particle-hole symmetry is lost and the position of the Dirac nodes are shifted\(^{22} \).

For the \( p_x + ip_y \)-wave pairing, we find that the ground state breaks particle-hole symmetry and \( \lambda \neq 0 \). 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 \( |\lambda| < Z|J_1\chi_1 + J_3\chi_3| \), so that \( \chi_k \) can be either positive or negative, depending on \( k \). Therefore the Bogoliubov spinor space described by the vector \( \left( \frac{E_k}{E_k}, \frac{\chi_k}{E_k}, \frac{\chi_k}{E_k} \right)^T \) (see also Appendix C). The solution has \( |\lambda| < Z|J_1\chi_1 + J_3\chi_3| \), so that \( \chi_k \) can be either positive or negative, depending on \( k \). Therefore the Bogoliubov spinor space described by the vector \( \left( \frac{E_k}{E_k}, \frac{\chi_k}{E_k}, \frac{\chi_k}{E_k} \right)^T \) (which is \( S^2 \)) covers the Brillouin zone (\( k \) space, which is also \( S^2 \)) at least once. In other words, the topological (Skyrmion) number of mapping from the \( k \) space to the spinor space is nonzero \( m \neq 0 \). However in the vacuum where the spinon density is zero, \( \lambda \) is very big and \( \chi_k \) can only take positive values, which gives a zero topological number\(^{27} \). Since the bulk and vacuum belong to different topological sectors, the boundary defines a domain wall between the two phases, and there should exists gapless (chiral) Majorana edge states in the \( p_x + ip_y \) state following the analysis of Read and Green\(^{27} \). In this sense, the \( p_x + ip_y \)-state describes a time-reversal symmetry breaking topological spin liquid.

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FIG. 4: (Color online) The spinon dispersion the f-wave pairing state with constraint \( \langle N_i \rangle = \frac{1}{2} \). The red dot 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.
```

Next we consider the specific heat and spin susceptibility for the \( f \)- and \( p_x + ip_y \) pairing 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 behavior\(^{22} \) 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 \( E = 3 \sum_k \frac{E_k}{E_k} \) in mean field theory. At low temperature, the low energy 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 re-scaling of momentum and will not affect the result qualitatively). The magnetic specific heat
consistent with the experimental result. Several plausible ground states have been proposed for this system, including an antiferromagnetic (AFM) state 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)\textsuperscript{25}. For example, we show in Ref.\textsuperscript{22} 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 anti-ferro nematic order may exist when the bi-quadratic ($K(S_i \cdot S_j)^2$) 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.\textsuperscript{29}

Another very important issue is whether the spin liquid states we find are stable against gauge fluctuations. In 1-D, the gauge fluctuations can be removed by a time-dependent Read-Newns gauge transformation and thus have no effect to the low energy properties.\textsuperscript{26} 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\textsuperscript{20} and gapless $U(1)$ Dirac fermionic spin liquids is stable at 2D in the large-\textit{N} limit.\textsuperscript{24} 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 consequence 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 wavefunctions 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 $\psi$ 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 $(c_m, (-1)^{S-m}c_m) = (-1)^{S-m}(c_m, (-1)^{S-m}c_m)\sigma_x$, 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

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

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

Eq. (A1a) and Eq. (A1b) impose the condition

\[ \sigma_x W^* \sigma_x = (\sigma_z)^{2S} W (\sigma_z)^{2S} . \] (A2)

For integer spin, Eq. (A2) becomes $W^* = \sigma_x W \sigma_x$, which results in $W = e^{i\theta} \sigma_x$ or $W = e^{i\theta} \sigma_x$, i.e. $W \in U(1) \otimes Z_2$, where $U(1) = \{ e^{i\theta} \}$ is the usual gauge symmetry group and $Z_2 = \{ 1, 2 \}$ 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 $U(1) \otimes Z_2 = \{ e^{i\sigma_x \theta}, \sigma_x e^{i\sigma_x \theta} = e^{-i\sigma_x \theta} \sigma_x ; \theta \in R \}$. For half-odd-integer spin, Eq. (A2) implies $W^* = \sigma_y W \sigma_y$, which is equivalent to $\det W = 1$ since $W^* W = 1$. This indicates 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:

\[ B = \begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix} . \] (B1)

The matrix is the CG coefficients combining two spin-$S$ to a spin-singlet state, i.e. $\langle 0,0 | B_{mn} | S,m_1 \rangle = C_n^m (\text{vac})$. Thus $C$ can be expressed as $\tilde{C} = BC^* = (c_S^c, c_{S-1}^c, \ldots, c_{-S}^c)^T$. 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 $\tilde{R}$ is an rotation operation, and $D(R)$ is its $(2S+1) \times (2S+1)$ dimensional matrix representation, then we have $\tilde{R}C = D(R)C$ and

\[ \tilde{R}C = D(R)C = D(R)BC^* . \]

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

\[ \tilde{R}C = \tilde{R}BC^* = B\tilde{R}C^* = BD(R)^* C^* . \]

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

\[ B^{-1} D(R) B = D(R)^* . \] (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 $D(R) = e^{iR}$, where $R$ are the $SU(2)$ group parameters (real numbers) for the operator $R$, and consequently $D(R)^* = e^{-iR}$. From Eq. (B2) we have

\[ B^{-1} D(R) B = B^{-1} e^{iR} B = e^{-iB^{-1} R} = D(R)^* = e^{-iR} . \]

So we have

\[ B^{-1} B = I^* = I^T . \]

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

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

\[ \psi_1 \psi_j = \begin{pmatrix} C_1^j C_j & C_1^j \bar{C}_j \\ \bar{C}_1^j C_j & \bar{C}_1^j \bar{C}_j \end{pmatrix} , \] (B3)

\[ \psi_1^\dagger I \psi_j = \begin{pmatrix} C_1^j I C_j & C_1^j \bar{C}_j \\ \bar{C}_1^j I C_j & \bar{C}_1^j \bar{C}_j \end{pmatrix} . \] (B4)

We define $\chi_{ij} = C_1^j C_j$, $\Lambda_{ij} = \bar{C}_1^j C_j$ and $u_{ij} = C_1^j I C_j$, $v_{ij} = C_1^j \bar{C}_j$. The following discussions distinguish integer- and half-odd-integer-spins and prove the results in section III.C.
integer spins \((B^\dagger = B^T = B^{-1} = B)\)  

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

\[
C_i^\dagger C_j = C_i^\dagger BC_j^* = -(C_i^\dagger BC_j^*)^T = -C_j^\dagger BC_i^* = -C_j^\dagger \bar{C}_i = -\Delta_{ij}^\dagger 
\]

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, \(\Delta_{ij}^\dagger = (\bar{C}_j^\dagger C_i)^\dagger = C_i^\dagger \bar{C}_j\), so \(\Delta_{ji} = -\Delta_{ij}\).

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

\[
\bar{C}_i^\dagger \bar{C}_j = C_i^\dagger BBC_j^* = -(C_i^\dagger C_j^*)^T = -C_i^\dagger C_j = -\chi_{ij}^\dagger 
\]

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

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

\[
C_i^\dagger I \bar{C}_j = C_i^\dagger IBC_j^* = -(C_i^\dagger IT C_j^*)^T = -(C_i^\dagger IT C_j^*) = -C_i^\dagger IC_j = -\chi_{ij}^\dagger 
\]

On the other hand, above operator can be written into another form, \(C_i^\dagger IC_j = (\bar{C}_j^\dagger I C_i)^\dagger = u_{ij}^\dagger\). Comparing with Eq. (B3) we get \(u_{ij} = u_{ji}\).

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

\[
\bar{C}_i^\dagger I \bar{C}_j = C_j^\dagger IT C_i^* = (C_j^\dagger IT C_i^*)^T = C_j^\dagger IC_i = v_{ij}^\dagger 
\]

And the relation \(v_{ji}^\dagger = v_{ij}\) manifests itself.

half-odd-integer spins \((B^\dagger = B^T = B^{-1} = -B)\)

Repeating the above procedures, it is straightforward to show that 

\[
C_i^\dagger C_j = \Delta_{ij}, C_i^\dagger \bar{C}_j = -\chi_{ij}, 
\]

\[
C_i^\dagger \bar{C}_j = -u_{ij}^\dagger, \bar{C}_i^\dagger C_j = v_{ij}^\dagger, 
\]

with \(\chi_{ij} = \chi_{ji}^\dagger, \Delta_{ji} = \Delta_{ij}, u_{ij} = -u_{ji}, v_{ji} = v_{ij}^\dagger\).

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. Majorana fermion edge states also exist in our mean field theory under open boundary condition. Our discussion will follow the argument of Ref. 27 for 2D pairing fermions. Firstly, 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 \(\chi_k\) and \(\Delta_k\)). 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 \((u^*, v^*)|\sigma(u, v)|^T = (0, \sin \theta_k, \cos \theta_k)^T = (0, \Delta_{ik}, \chi_{ik})^T\) where we have used Eq. (205). 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 \(S^1\) (spinor space) to \(S^1\) (spinor space). The mapping degree is characterized by the first homotopy group \(\pi_1(S^1) = Z\). When \(-2J_X < \lambda < 2J_X\) (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 \(|\lambda| > 2J_X\), the mapping is topologically trivial since \(\chi_k\) 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 \(|\lambda| = 2J_X\). 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 wavefunction 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 \(|\lambda| > 2J_X\) 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 \(\mu(x) = 2J_X - \lambda(x)\) such that \(\mu\) is positive in the bulk, becomes zero near the edge and turns negative outside the edge. Expanding \(\chi_k\) and \(\Delta_k\) 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. (205), which can be written in position space as 

\[
\begin{align*}
\frac{\partial u}{\partial t} &= -\mu u - 2J\Delta \frac{\partial v}{\partial x}, \\
\frac{\partial v}{\partial t} &= \mu v + 2J\Delta \frac{\partial u}{\partial x},
\end{align*}
\]

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 normalizeable zero energy solution for the above equations. Putting \(u = v\), then 

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

and the solution is 

\[
u(x) = \nu(x) = \infty e^{-\frac{i}{\hbar} \int \mu(x)dx}.
\]
Notice that the BdG equation Eq. (31)
\[ Eu = -\mu u - 2J \Delta \frac{\partial v}{\partial x} \]
\[ Ev = \mu v + 2J \Delta \frac{\partial u}{\partial x} \]

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,
\[ E^2(u \pm v) = [\mu^2 - (2J\Delta)^2 \frac{\partial^2}{\partial x^2} + (2J\Delta) \frac{\partial \mu}{\partial x}](u \pm v), \]
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 Eq. (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 chains \( S^1 \) 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
\[
\chi_z(k, i\omega) = \frac{2}{V} \int d\tau e^{i\omega \tau} \sum_q \left[ \left[ C_q^2 G_A(q, -\tau) - S_q^2 G_B(-q, \tau) \right] \left[ -C_{q+k}^2 G_A(q + k, \tau) + S_{q+k}^2 G_B(-q - k, -\tau) \right] - C_q S_q [G_A(q, -\tau) + G_B(-q, \tau)] \times C_{q+k} S_{q+k} [G_A(q + k, \tau) + G_B(-q - k, -\tau)] \right]
\]
\[
= \frac{2}{\beta V} \sum_{q, \Omega} \left[ \left[ C_q^2 G_A(q, i\Omega) - S_q^2 G_B(-q, -i\Omega) \right] \left[ -C_{q+k}^2 G_A(q + k, i\Omega + i\omega) + S_{q+k}^2 G_B(-q - k, -i\Omega - i\omega) \right] - C_q S_q C_{q+k} S_{q+k} [G_A(q, i\Omega) + G_B(-q, -i\Omega)] \left[ G_A(q + k, i\Omega + i\omega) + G_B(-q - k, -i\Omega - i\omega) \right] \right]
\]

with the notations \( C_q = \cos \frac{q}{2} \) and \( S_q = \sin \frac{q}{2} \). Using the results \( G_A(k, i\omega) = G_B(k, i\omega) = G(k, i\omega) \) and \( G(-k, i\omega) = G(k, -i\omega) = G(k, -i\omega) = \frac{1}{i\omega + \Delta} \), we get the static susceptibility
\[
\chi_z = \lim_{k \to 0} \chi_z(k, 0)
= \lim_{k \to 0} \frac{2}{\beta V} \sum_{q, \Omega} \left[ -(C_q C_{q+k} + S_q S_{q+k})^2 G(q, i\Omega) G(q + k, i\Omega) + (C_q S_{q+k} - S_q C_{q+k})^2 G(q, i\Omega) G(q + k, -i\Omega) \right]
\]
\[
= \lim_{k \to 0} \frac{2}{\beta V} \sum_{q} \left[ -(C_q C_{q+k} + S_q S_{q+k})^2 \frac{n_f(\varepsilon_{q+k}) - n_f(\varepsilon_q)}{\varepsilon_{q+k} - \varepsilon_q} \right]
\]
\[
\chi_z = -2 \int d^2q \frac{\partial n_f(\varepsilon_q)}{\partial \varepsilon_q} \frac{\partial n_f(\varepsilon_q)}{\partial q} dq
= 4\pi \int_0^\infty n_f(\varepsilon_q) dq \frac{T}{v_F} \quad \text{(D1)}
\]

which is the Pauli susceptibility for free fermions. At low temperature, the excitation spectrum can be approximated by Dirac cones, so we have
\[
\chi_z \approx -2 \int_0^\infty 2\pi q \frac{\partial n_f(\varepsilon_q)}{\partial q} dq
= \frac{4\pi}{v_F} \int_0^\infty n_f(\varepsilon_q) dq \propto \frac{T}{v_F} \quad \text{(D2)}
\]
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Actually, a similar expression like Eq. (10) also holds for $S = 1/2$, $\hat{S}_i \cdot \hat{S}_j = -\frac{2}{3} \left[ -\text{Tr}(\psi_i^\dagger I \psi_j \cdot \psi_j^\dagger I \psi_i) + S^2 \text{Tr}(\psi_i^\dagger \psi_j \psi_j^\dagger \psi_i) \right]$. Notice that the first term in the square bracket has different sign comparing to the expression for $S = 1$ and 3/2. The two terms in the square bracket are also identical.

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We note that another method to deal with disordered spin states is modified spin-wave theory where zero magnetization is enforced by a magnon number constraint. Minoru Takahashi [Prog. Theor. Phys. Suppl. 87, 233 (1986); Phys. Rev. B 40, 2494 (1989)] applied this method to study 1D ferromagnets and 2D antiferromagnets on square lattice. The results agree well with that of Bethe Ansatz and Schwinger boson mean field theory, 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-1/2 spinons. However, for 1D half-odd-integer antiferromagnetic spin chains, elementary excitations are spin-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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We note that another method to deal with disordered spin states is modified spin-wave theory where zero magnetization is enforced by a magnon number constraint. Minoru Takahashi [Prog. Theor. Phys. Suppl. 87, 233 (1986); Phys. Rev. B 40, 2494 (1989)] applied this method to study 1D ferromagnets and 2D antiferromagnets on square lattice. The results agree well with that of Bethe Ansatz and Schwinger boson mean field theory, 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-1/2 spinons. However, for 1D half-odd-integer antiferromagnetic spin chains, elementary excitations are spin-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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