Schwinger-Boson mean-field study of spin-1/2 $J_1$-$J_2$-$J_x$ model in honeycomb lattice: thermal Hall signature

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We theoretically investigate, within the Schwinger-Boson mean-field theory, the transition from a gapped $Z_2$ quantum spin-liquid, in a $J_1$-$J_2$ Heisenberg spin-1/2 system in a honeycomb lattice, to a chiral $Z_2$ spin liquid phase under the presence of time-reversal symmetry breaking scalar chiral interaction (with amplitude $J_x$). We numerically obtain a phase diagram of such $J_1$-$J_2$-$J_x$ system, where different ground-states are distinguished based on the gap and the nature of excitation spectrum, topological invariant of the excitations, the nature of spin-spin correlation and the symmetries of the mean-field parameters. The chiral $Z_2$ state is characterized by non-trivial Chern number of the excitation bands and lack of long-range magnetic order, which leads to large thermal Hall coefficient.

I. INTRODUCTION

Quantum spin liquid (QSL) is an exotic state of matter where a spin system does not develop magnetic order nor break any lattice symmetry even at the absolute zero temperature. Instead, the system develops a topological order with fractionalized excitations [1–3]. QSLs cannot be described by the traditional Landau’s paradigm where different phases are characterized by local order parameters and broken symmetry. Historically QSL was originally proposed by Anderson as a quantum ground state for a geometrically frustrated triangular lattice antiferromagnet [4] and since then, the search for QSL in quantum magnets has primarily focused on the frustrated triangular, Kagome, pyrochlore lattice systems. Among possible candidates, the Kitaev model for spin-1/2 on Honeycomb lattice is a promising candidate to support QSL states, where strong quantum fluctuations arising from bond-dependent interaction destroys the magnetic orders [3, 5, 6]. This led to experimental search of Kitaev materials and signature of QSL state [7, 8]. In addition to the Kitaev’s honeycomb model and the search for Kitaev materials, the anti-ferromagnetic Heisenberg $J_1$-$J_2$ model has been studied extensively for possible QSL state [9, 10]. The conventional ground state of nearest neighbor Heisenberg model (without the $J_2$ coupling), say on the honeycomb lattice, is a Néel ordered state, but when the second nearest interaction is turned on and increased, the long-range order can get destroyed and the system can enter into a quantum disordered state for intermediate coupling regime. Various numerical studies have been conducted that suggests there is QSL phase for intermediate ratio of $J_2/J_1$ although the parameter range of it has been somewhat debated [11–18]. Apart from the novel physics associated with the QSLs, they also hold potentials for applications, especially in the field of quantum information processing [19], using properties of the long range entangled spins. Such as, the Kitaev QSL can support fractional excitations represented by Majorana fermions [8], which can be made to act as anyons obeying non-abelian statistics in the presence of a magnetic field. Braiding these anyons could be an important step toward topological quantum computation [2].

In recent years, there have also been numerous studies to identify chiral spin liquids (CSL) with realistic spin models having various geometries, such as, the Kagome [20–24], triangular [25–28], square [29], and honeycomb lattices [30]. CSL is a non-magnetic phase, characterized by scalar chiral order (i.e, $\langle \hat{S}_i \cdot (\hat{S}_j \times \hat{S}_k) \rangle \neq 0$, where $\hat{S}_i$ is the spin-operator at the $i^{th}$ site) and finite spin gap. The presence of such time-reversal symmetry breaking chiral order can give rise to non-zero chern numbers of the excitations, which can result in enhanced thermal hall conductivity. In particular, a recent work [8] on the Kitaev honeycomb model predicted that there are two topologically inequivalent phases, within the intermediate disordered regime, one of which is a CSL phase. In that case, the $J_2$ interaction in the CSL phase may itself play the same role as a flux term in the Haldane model [31], and the $J_2$ term acts as a spin-orbital coupling for the spinons in similarity with the Kane-Mele model [32]. Very Recently authors in the Ref 33 have investigated the topological phase transition and nontrivial thermal Hall signatures in honeycomb lattice magnets in presence of Zeeman coupling using the Abrikosov-fermion...
mean-field theory, which reports similar findings of unusual thermal Hall effect for pseudogap phase of copper-based superconductors [34].

In the present work, we consider the $J_1$-$J_2$ spin $S = 1/2$ Heisenberg model along with a scalar chiral three-spin term. Without the scalar chiral term, in the classical limit, $S \to \infty$, the system is Néel ordered for $J_2/J_1 < 1/6$ and magnetically ordered in a spiral manner for $J_2/J_1 > 1/6$ [35–37]. For the quantum-case, the nature of the ground-state has been extensively studied (without the scalar chiral term), using spin-wave theory [36–39], non-linear $\sigma$ model [40], exact diagonalization [41, 42], variational Monte-Carlo [18, 43] and other methods [44]. The general understanding is that, for $J_2/J_1 \lesssim 0.21$, it orders magnetically as a Néel phase; between 0.37 $\lesssim J_2/J_1 \lesssim 0.37$ there is a gapped spin-liquid (GSL) phase; between 0.4 $\lesssim J_2/J_1 \lesssim 0.37$ there is a $C_3$ rotational symmetry broken disordered valence-bond crystal (VBC) state and for $J_2/J_1 \gtrsim 0.4$, the system orders magnetically in a spiral manner. In the present work, based on the Schwinger-Boson mean-field theory (SBMFT), we investigate the effect of the scalar spin-chiral term on the disordered (gapped) phases and we theoretically observe a transition to a chiral $Z_2$ (CZSL) state, where the Chern numbers of the excitation bands change. We also theoretically study its signature in the thermal Hall measurement.

The paper is organized as following. In Sec. II we briefly review the formalism of SBMFT and various technicalities involved in solving for the ground-state properties. We provide details of the numerical simulation and further discussion of how we identify various phases from numerical data in Sec. III and we present the numerical results in Sec. IV. We discuss the results further and summarize our findings in Sec. V.

II. FORMALISM

In this work, we study the effect of the scalar three-spin chiral term, with coefficient $J_\chi$, in the $J_1$-$J_2$ Heisenberg spin-1/2 Hamiltonian:

$$H = \sum_{nn} J_1 \vec{S}_i \cdot \vec{S}_j + \sum_{nnn} J_2 \vec{S}_i \cdot \vec{S}_j + \sum_{\Delta} J_\chi \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k)$$  \hspace{1cm} (1)

where $\vec{S}_i$ is the spin operator at site $i$, $J_1$ and $J_2$ are the coupling amplitude for nearest and next nearest neighbors, whereas $J_\chi$ is the amplitude of the scalar spin-chiral term, as outlined in the Fig. 1. In the third term, the sum involves the triangular plaquettes $\Delta$ formed by the nearest-neighbors, as shown in the same figure.

As a passing comment, strong coupling expansion of Hubbard model yields $J_1 = 4t_1^2/U$ and $J_2 = 4t_2^2/U$, where $t_1$ and $t_2$ are the nearest and next-nearest neighbor hopping amplitudes of electrons, respectively, and $U$ being the onsite repulsion. On the other hand, scalar spin chirality is proportional to $-24t_1^2t_2/U^2 \sin \Phi$, where $\Phi$ is the magnetic flux through the triangular plaquette [45]. Starting from the Haldane-Hubbard model, one may also naturally lead to $J_\chi$ term without any further application of magnetic field [21, 30, 45–48].

We study this spin-model, Eq. (1), using the Schwinger-Boson mean-field theory (SBMFT), where we represent the spin-operators in terms of Bosons. The nature of the bosonic excitations on top of the mean-field ground-state predicts order-disorder transition and other physical properties of the system, as we discuss later. Before we discuss our numerical findings, we present a short review of the SBMFT below.

A. Schwinger-boson mean-field theory

The principle idea behind SBMFT is to express the spin operators in terms of bosonic operators that carry spin. In the SU(2) representation where two bosonic flavors are introduced to describe the spin operators, we write [46]

$$\vec{S}_i = \frac{1}{2} b_{i,\sigma}^\dagger \vec{\sigma}_{\sigma\sigma} b_{i,\sigma}$$  \hspace{1cm} (2)

where $\tau^i$ are the Pauli matrices, and $b_{i,\sigma}^\dagger$ are the bosonic creation operator of spin $\sigma$ on site $i$. In order to preserve the SU(2) commutation rule, the following local constraint has to be fulfilled on every site:

$$\sum_{\sigma} b_{i,\sigma}^\dagger b_{i,\sigma} = 2S.$$  \hspace{1cm} (3)

Where $S$ is the value of spin under consideration, which we take to be 1/2 for the present work. However it is typically difficult to impose this constraint exactly [50]; thus we impose it on the average over the mean-field ground-state.

As we do not impose any symmetry to be broken in the ground-state, only possible bilinears that preserves the spin rotation symmetry are the following:

$$\hat{A}_{ij} = \frac{1}{2} [b_{i\uparrow} b_{j\downarrow} - b_{i\downarrow} b_{j\uparrow}]$$  \hspace{1cm} (4)

$$\hat{B}_{ij} = \frac{1}{2} [b_{i\uparrow}^\dagger b_{j\uparrow} - b_{i\downarrow}^\dagger b_{j\downarrow}]$$  \hspace{1cm} (5)

It is clear that $A_{ij}$’s measure singlet type correlations while the $B_{ij}$’s measure triplet correlations [51]. In a gapped phase, the first one is favored, whereas the triplet correlation allows the spinons to hop between sites giving rise to long range orders.

It can be easily verified that,

$$\vec{S}_i \cdot \vec{S}_j = : \hat{B}_{ij}^\dagger \hat{B}_{ij} : - \hat{A}_{ij}^\dagger \hat{A}_{ij},$$  \hspace{1cm} (6)

where : $\hat{O}$ : refers to the normal ordering. Now, we perform the mean-field decoupling of $\hat{A}$, $\hat{B}$ operators as

$$\hat{A}_{ij}^\dagger \hat{A}_{ij} \rightarrow A_{ij}^\dagger A_{ij} + \hat{A}_{ij}^\dagger A_{ij} - A_{ij}^\dagger A_{ij},$$  \hspace{1cm} (7)

$$\hat{B}_{ij}^\dagger \hat{B}_{ij} \rightarrow B_{ij}^\dagger B_{ij} + \hat{B}_{ij}^\dagger B_{ij} - B_{ij}^\dagger B_{ij},$$  \hspace{1cm} (8)
with \( A, B \) are the mean-field order parameters that are computed, self-consistently, from the average over the mean-field ground-state, \(|gs\rangle\),

\[
A_{ij} = \langle gs| \hat{A}_{ij} |gs\rangle, \quad B_{ij} = \langle gs| \hat{B}_{ij} |gs\rangle. \tag{9}
\]

These expectation values, collectively define the parameters of the mean-field ansatz. The expectation values are calculated in the new basis that diagonalizes the Hamiltonian and using,

\[
\gamma_{q,\lambda} |gs\rangle = 0, \tag{10}
\]

where, \(|gs\rangle\) is the vacuum state for the resulting bosonic excitation, \(\gamma_{q,\lambda}\), details of these procedure we shall discuss in the sub-section II.C. Once the decomposition Eq. (8) is done, the effective mean-field Hamiltonian is now completely expressed in terms of bosonic bilinears. In the same way we can do the SBMFT decoupling of the scalar chirality term where we use the following identity,

\[
\hat{S}_i (\hat{S}_j \times \hat{S}_k) = 2i(\hat{B}_{ki} \hat{B}_{jk} \hat{B}_{lj} + \hat{B}_{lj} \hat{B}_{kj} \hat{B}_{ki}), \tag{11}
\]

Which we write, using the mean-field decomposition as,

\[
\hat{B}_{ij} \hat{B}_{jk} \hat{B}_{ki} \approx \hat{B}_{ij} \langle \hat{B}_{jk} \hat{B}_{ki} \rangle + \langle \hat{B}_{ij} \rangle \hat{B}_{jk} \langle \hat{B}_{ki} \rangle + \langle \hat{B}_{ij} \rangle \langle \hat{B}_{jk} \rangle \hat{B}_{ki} - 2 \langle \hat{B}_{ij} \rangle \langle \hat{B}_{jk} \rangle \langle \hat{B}_{ki} \rangle. \tag{12}
\]

In our original Hamiltonian we have the Heisenberg interactions up to second nearest neighbor. Now, if we want to preserve the translational symmetry but break all the point group symmetries, we can get at most 18 inequivalent mean-field ansatz (bond parameters), 9 for each \( A_{ij} \) and \( B_{ij} \). These are schematically shown in the Fig. 2. For nearest neighbor interactions, the bonds are between one \( u \) to one \( v \) sublattices, denoted by \( O_{1d} \) where \( d \) are the three possible orientations (subscript 1 denotes nearest neighbor). For the next nearest interactions, the bonds are connections between two \( u \) or \( v \) sublattices. We denote them with \( O_{2w} \), where the superscript represents sublattice index and \( d \) is the three possible orientations as before. Each \( O \) can be chosen as \( A \) or \( B \) type of order parameters, totaling 18 of them.

The final mean-field Hamiltonian can be expressed as,

\[
H_{mf} = \sum_{ij} J_{ij} (\gamma_{ij}^0 \hat{A}_{ij} + B_{ij}^{\dagger} \hat{B}_{ij} + h.c.)
- \sum_i \mu_i \left( \sum_{\sigma} \hat{b}_{i\sigma}^{\dagger} \hat{b}_{i\sigma} - 2S \right) + 2i \sum_{\Delta} J_\chi (B_{ki} B_{jk} B_{ij} + B_{ij} B_{jk} B_{ki} - h.c.) + K \tag{13}
\]

with,

\[
K = \sum_{ij} J_{ij} (|A_{ij}|^2 - |B_{ij}|^2) + 8 \sum_{\Delta} J_\chi 3 (B_{ij} B_{jk} B_{ki}). \tag{14}
\]

The final term in the Hamiltonian is the consequence of the constraint Eq. (3). For simplicity, we assume the chemical potential to be either \( \mu_u \) or \( \mu_v \), depending on the sublattices. Schwarz inequality restricts the upper bounds on the moduli \(|A| \leq S + 1/2, |B| \leq S \), which must be obeyed for any self-consistent ansatz in SBMFT [50].

**B. Diagonalization of bosonic quadratic Hamiltonian**

The mean-field Hamiltonian, Eq. (13), can be diagonalized using the Bogoliubov-Valentin canonical transformation [52, 53]. The procedure is following for a generic quadratic bosonic Hamiltonian,

\[
H = \frac{1}{2} \Psi \Gamma \Psi \dagger; \quad \Psi = (b_1^\dagger, ..., b_N^\dagger, b_1, ..., b_N). \tag{15}
\]

\( N \) is the degree of freedom and \( M \) is an \( 2N \times 2N \) matrix. \( b_n^\dagger \) (\( b_n \)) are the creation (annihilation) operators in moment, spin or any other degrees of freedom. In order to find the eigenvectors corresponding to the matrix \( M \), we introduce creation (annihilation) operators \( \gamma_m^\dagger \) (\( \gamma_m \)) such that,

\[
\Psi = TT; \quad \Gamma = (\gamma_1^\dagger, ..., \gamma_N^\dagger, \gamma_1, ..., \gamma_N), \tag{16}
\]

where \( T \) is the basis-transformation matrix. We choose our \( T \) such that Hamiltonian in Eq. (15) can be written in a diagonal form as:

\[
H = \frac{1}{2} \Gamma \Gamma \dagger MM T T, \tag{17}
\]

with, \( T \Gamma T \dagger = \begin{pmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_{2N} \end{pmatrix} \).
FIG. 3. Dispersion of the lowest spinon-band with $J_{\chi} = 0$ and $J_1 = 1$. (a), (b), (c) and (d) are the dispersions of the spin bands, when the system is in the Néel phase ($J_2 = 0.197$), GSL phase ($J_2 = 0.35$), VBC phase ($J_2 = 0.38$) and spiral anti-ferromagnetic phase ($J_2 = 0.43$), respectively.

In order to preserve the bosonic commutation rules, the $\Psi$ and $\Gamma$ matrices should obey the following matrix equation,

$$[\Psi_i, \Psi_j^\dagger] = [\Gamma_i, \Gamma_j^\dagger] = (\rho_3)_{ij},$$

where

$$\rho_3 \equiv \begin{pmatrix} I_{N \times N} & 0 \\ 0 & -I_{N \times N} \end{pmatrix}.$$  \hspace{1cm} (18)

Here $I_{N \times N}$ is the identity matrix of dimension $N$. This implies that the transformation matrix must satisfy,

$$T \rho_3 T^\dagger = \rho_3,$$  \hspace{1cm} (19)

In a more formal language, $T$ is a paraunitary $\text{SU}(N,N)$ matrix. The elements of the transformation matrix can be found from the eigenvectors of the dynamic matrix, defined as

$$K = \rho_3 M,$$  \hspace{1cm} (20)

which satisfies the Heisneberg equation of motion for $\Psi$ \cite{34}. All the eigenvalues of the dynamic matrix (when it is diagonalizable) appears in pairs of opposite sign, and are real. $T$ is also referred as the derivative matrix, consisting of all the eigenvectors of $K$ sorted in the form,

$$T = [V(\omega_1), ..., V(\omega_N), V(-\omega_1), ..., V(-\omega_N)],$$  \hspace{1cm} (21)

with the eigenvectors normalized as,

$$V^\dagger(\omega_i) \rho_3 V(\omega_i) = 1, \hspace{0.5cm} V^\dagger(-\omega_i) \rho_3 V(-\omega_i) = -1,$$  \hspace{1cm} (22)

for all the sets of $(V(\omega_i), V(-\omega_i))$. After the diagonalization we have,

$$T^{-1} K T = \text{diag} (\omega_1, ..., \omega_N, -\omega_1, ..., -\omega_N),$$  \hspace{1cm} (23)

and

$$T^\dagger M T = \text{diag} (\omega_1, ..., \omega_N, \omega_1, ..., \omega_N).$$  \hspace{1cm} (24)

Both $M$ and $K$ are simultaneously diagonalized. We call the the positive (negative) bands with indices $n = 1, ..., N$ ($n = N + 1, ..., 2N$) as the particle (hole) bands.

C. Mean-field dispersion

We use the method of the preceding section for diagonalization of the mean-field Hamiltonian Eq. (13), in the momentum space. We write the Bosonic annihilation operator in the Fourier space as,

$$b_{\vec{r},w,\sigma} = \frac{1}{\sqrt{n_c}} \sum_{\vec{q}} e^{i\vec{q}.\vec{r}} b_{\vec{q},w,\sigma},$$  \hspace{1cm} (25)

where $n_c$ is the total number of unit cells in the real-space lattice (each containing two sub-lattices); $\vec{r}$ are the positions of the unite cells and $w = u, v$ are sub-lattice indices. The combination ($\vec{r}, w$) defines position of a particular site and $\sigma = \uparrow / \downarrow$ are the flavors of the Schwinger-Bosons. Then the mean-field Hamiltonian is...
in the momentum space is written as:

\[ H_{mf} = \frac{1}{2} \sum_q \Psi_q^\dagger M_q \Psi_q - (2S + 1)n_c \sum_w \mu_w + K, \]  

(26)

with,

\[ \Psi_q^\dagger = (b_{\bar{q},u,1}^\dagger, b_{\bar{q},u,1}^\dagger, b_{\bar{q},u,\downarrow}, b_{\bar{q},u,\downarrow}). \]  

(27)

where the co-efficient matrix \( M_q \) is given by,

\[ M_q^{(1)} = \begin{pmatrix} \sum_j 2J_2(B_{2d}^u \phi_{2d}^j + B_{2d}^u \phi_{2d}^j) + 2\mu_u & J_1 B_{1d} \phi_{1d}^j & J_2 A_{2d}^u (\phi_{2d}^j - \phi_{2d}^j) + 2\mu_v & J_2 A_{2d}^u (\phi_{2d}^j - \phi_{2d}^j) \\ J_1 B_{1d} \phi_{1d}^j & \sum_j J_2 B_{2d}^u \phi_{2d}^j + B_{2d}^u \phi_{2d}^j + 2\mu_u & J_1 A_{1d} \phi_{1d}^j & J_2 A_{2d}^u (\phi_{2d}^j - \phi_{2d}^j) \\ -J_1 A_{1d} \phi_{1d}^j & J_2 A_{2d}^u (\phi_{2d}^j - \phi_{2d}^j) & \sum_j J_1 B_{1d} \phi_{1d}^j & J_2 B_{2d}^u \phi_{2d}^j + B_{2d}^u \phi_{2d}^j + 2\mu_u \\ & & & \sum_j J_2 B_{2d}^u \phi_{2d}^j + B_{2d}^u \phi_{2d}^j + 2\mu_v \end{pmatrix}, \]

(28)

Now the mean-field Hamiltonian takes the form, in this new basis:

\[ H_{mf} = \frac{1}{2} \sum_q \Gamma_q^\dagger \Gamma_q - (2S + 1)n_c \sum_w \mu_w + K \]  

(30)

the matrix \( T_q \) satisfies the following conditions,

\[ T_q^\dagger \rho_3 T_q = \rho_3, \]  

(31)

\[ T_q^\dagger M_q T_q = \omega_q, \]  

(32)

where

\[ \omega_q = I_2 \otimes \begin{pmatrix} \epsilon_{\bar{q},u} & \epsilon_{\bar{q},v} \end{pmatrix}. \]  

(33)

Now that we have found the mean-field spinon dispersion, one can find the fixed point in the mean-field parameter space by minimizing the free energy,

\[ F_{mf} = \sum_{\bar{q},w} \epsilon_{\bar{q},w} - (2S + 1)n_c \sum_w \mu_w + K \]  

(34)

with respect to the mean-field parameters and the chemical potentials:

\[ \frac{\partial F_{mf}}{\partial \mu_w} = 0, \quad \frac{\partial F_{mf}}{\partial \mu_w} = 0. \]  

(35)

These equations can be solved numerically. In a second procedure, which we employ in the present work, we solve for the mean-field order parameters by self-consistently solving Eq. (9).

\[ \text{D. spin structure factor} \]

Although we work in a finite size lattice system, how the static spin-structure factor \( \langle \hat{S}_{\bar{q}}^\dagger \hat{S}_{\bar{q}} \rangle \) behaves as a function of \( R_c \) reveals the nature of the underlying ground-state. In such finite size system the spin-rotation symmetry is never broken in the ground-state, which allows
us to write
\[
\langle \tilde{S}_0 \cdot \tilde{S}_i \rangle = 3\langle \tilde{S}_0^z \tilde{S}_i^z \rangle \\
= \frac{3}{4} \left( \langle \hat{b}^{\dagger}_i \hat{b}_{i\uparrow} - \hat{b}^{\dagger}_i \hat{b}_{i\downarrow} \rangle \langle \hat{b}^{\dagger}_i \hat{b}_{i\uparrow} - \hat{b}^{\dagger}_i \hat{b}_{i\downarrow} \rangle \right). \tag{36}
\]
In the Fourier-space, we have
\[
\langle \tilde{S}_0^z \tilde{S}_i^z \rangle = \frac{1}{4N^2} \sum_{\vec{k}, \vec{q}, \vec{r}} e^{i(\vec{k} - \vec{r}) \cdot \vec{q}} \left[ \hat{b}^{\dagger}_i \hat{b}_{i\uparrow} \hat{b}^{\dagger}_i \hat{b}_{i\downarrow} - \hat{b}^{\dagger}_i \hat{b}_{i\downarrow} \hat{b}^{\dagger}_i \hat{b}_{i\uparrow} \right] \\
+ \hat{b}^{\dagger}_i \hat{b}_{i\uparrow} \hat{b}^{\dagger}_i \hat{b}_{i\downarrow} - \hat{b}^{\dagger}_i \hat{b}_{i\downarrow} \hat{b}^{\dagger}_i \hat{b}_{i\uparrow}, \tag{37}
\]
where we have suppressed the sublattice index for brevity. The expectation values of these operators can be calculated in the diagonal basis of the Hamiltonian and using Eq. (40) [54].

E. Berry Curvature and Thermal Hall effect

Once we diagonalize the bosonic Hamiltonian, we have the Hamiltonian of the excitation
\[
H^D = \sum_{\vec{q}} \sum_{n=1}^{N_{\text{band}}} \epsilon_{\vec{q},n} \left( \hat{b}^{\dagger}_{\vec{q},n} \gamma_{\vec{q},n} \hat{b}_{\vec{q},n} + \frac{1}{2} \right), \tag{38}
\]
where \(N_{\text{band}}\) is the number of bosonic particle bands (with \(\epsilon_{\vec{q},n} > 0\)), which is two in our case. The thermal hall co-efficient is then defined as [55],
\[
\kappa_{xy} = -\frac{k_B T}{hV} \sum_{\vec{q}} \sum_{n=1}^{N_{\text{band}}} \left[ c_2(n_B(\epsilon_{\vec{q},n})) - \frac{\pi^2}{3} \right] \Omega_{n\vec{q}}, \tag{39}
\]
where \(n_B(\omega)\) is the Bose distribution function and,
\[
\Omega_{n\vec{q}} = \int_0^x dt \left( \ln \frac{1+t}{t} \right)^2. \tag{40}
\]
\(\Omega_{n\vec{q}}\) is the Berry curvature in momentum space, for the \(n\)th band, defined as,
\[
\Omega_{n\vec{q}} = i\epsilon_{\mu\nu} \left[ \rho_3 \frac{\partial T^\dagger_{\vec{q},\mu}}{\partial k_\mu} \rho_3 \frac{\partial T_{\vec{q},\nu}}{\partial k_\nu} \right]_{nn}, \tag{41}
\]
which can also be recasted in the following form,
\[
\Omega_{n\vec{q}} = i\epsilon_{\mu\nu} \langle \partial_\mu \psi_n(q) \rangle \langle \partial_\nu \psi_n(q) \rangle, \tag{42}
\]
where \(\psi_n(k)\) is the \(n\)th column of the \(T_q\) matrix. The numerical evaluation of the Berry curvature follows the U(1)-link variable method, outlined in the Appendix. The Chern number is then evaluated as
\[
C_n = \frac{1}{2\pi} \int_{BZ} \Omega_{n\vec{q}} \, d\vec{q}, \tag{43}
\]
which is always an integer and also it obeys the following constraints
\[
\sum_{n=1}^{N_{\text{band}}} C_n = \sum_{n=N_{\text{band}}+1}^{2N} C_n = 0, \tag{44}
\]
that is the sum of Chern numbers over particle and hole bands are individually zero [55].

III. DETAILS OF THE NUMERICAL SIMULATION

We solve for self-consistent values of the mean-field parameters in a finite lattice of \(n_c = N \times N\) unit-cells,
The original idea of projective symmetry groups (PSG) classification for spin-liquids was introduced by Wen and collaborator [56–58], in the context of Schwinger-Fermion approach. PSG analysis in Schwinger-Boson approach was extended by Wang et all [50]. Study of PSG provides the allowed symmetries and sign structures of the mean field ansatz. In disordered phase we want our mean-field state to obey the underlying microscopic symmetries of the spin model. For honeycomb lattice this symmetry transformations are lattice translations, point group symmetries (ie $C_3$ rotation and reflections), spin rotation symmetry and time reversal symmetry. Additionally, for the case of Schwinger-bosons, under the local U(1) transformation

$$b_{\vec{r}\sigma} \rightarrow e^{i\phi(\vec{r})}b_{\vec{r}\sigma},$$

(45)

under which the mean-field ansatz transform as:

$$A_{ij} \rightarrow e^{-i\phi(i)-i\phi(j)}A_{ij}, \quad B_{ij} \rightarrow e^{+i\phi(i)-i\phi(j)}B_{ij}.$$  

(46)

all the physical observables should remain invariant. But a subset of this U(1) transformation keeps the ansatz itself invariant. The set of all transformations that keep the ansatz invariant form the PSG. The set of the elements of PSG that are of kind Eq. (45), form a group called Invariant Gauge Group (IGG) [56]. For Honeycomb lattice with both nonzero $A_{ij}$ and $B_{ij}$, this IGG is simply $Z_2$ [59]. For the honeycomb lattice, such PSG classification found to give two distinct spin liquid states classified as 0 and $\pi$ flux states [59]. The spin liquid states
we found from numerical simulations, starting from completely unrestricted ansatz, matches with the 0 flux states mentioned above.

The symmetries of the ansatz that identifies the nature of the ground-state are following [51, 59]

- In Spin Liquid State and Neel state:
  \[ A_{11} = A_{12} = A_{13} = A \]
  \[ A^u_{21} = A^u_{22} = A^u_{23} = A^v_{21} = A^v_{22} = A^v_{23} = 0 \]
  \[ B_{11} = B_{12} = B_{13} = 0 \]
  \[ B^u_{21} = B^u_{22} = B^u_{23} = B^v_{21} = B^v_{22} = B^v_{23} = B. \] (47)

- In VBC State:
  \[ A_{11} \neq A_{12} = A_{13} = A \]
  \[ A^u_{21} \neq A^u_{22} = A^v_{21} \neq A^v_{22} = -A^u_{23} \]
  \[ B_{11} \neq B_{12} = B_{13} \]
  \[ B^u_{21} \neq B^u_{22} = B^v_{21} \neq B^v_{22} = B^u_{23}. \] (48)

- In Spiral State:
  \[ A_{11} = A_{12} \neq A_{13} \]
  \[ A^u_{21} \neq A^u_{22} = -A^u_{23} \]
  \[ B_{11} = B_{12} \neq B_{13}, B^u_{21} \neq B^u_{22} = B^u_{23} \]
  \[ B^v_{21} \neq B^v_{22} = B^v_{23}. \] (49)

The broken time-reversal symmetry of state give rise to non-vanishing imaginary part of the mean-field parameters we obtain [50, 60], in the chiral state. As the A and B, in Eq. (47), are both non-zero in numerical finding, we identify the GSL state as a $Z_2$ quantum spin-liquid [50].

**C₃-symmetry breaking order parameter**

In the intermediate spin disordered region, in the VBC state, the spin rotational symmetry SU(2) and translational symmetries are intact, but it may break the C₃ rotational symmetry of the lattice. Following Okumura et al., [61] we define a C₃ rotational symmetry breaking order parameter,

\[ \psi_3 = p_1 \bar{a}_1 + p_2 \bar{a}_2 + p_3 \bar{a}_3, \quad (50) \]

with, \( p_i = J_i(B^i_{11} - A^i_{11}) \).

\( p_i \) \((\alpha = 1, 2, 3)\) are nothing but the bond energies corresponding to nearest-neighbor bonds \( \bar{a}_\alpha \) \((\alpha = 1, 2, 3)\). This order parameter is zero as long as the bond energies remain same along three different direction.

**IV. NUMERICAL RESULTS**

Without application of the scalar chiral term (i.e., \( J_x = 0 \)), numerically we find, for \( J_2 \leq 0.22 \), the ground-state is gapless (defined as a gap less than \( 1/N \)), with Néel order and spiral magnetic order is also found for larger value of \( J_2 > 0.4 \). A gapped phase is found in the intermediate range \( 0.22 < J_2 < 0.4 \) between the Néel and the spiral order. Within a range of \( 0.37 \leq J_2 < 0.4 \) we find the staggered valence bond crystal (VBC) phase, with non-zero C₃ symmetry breaking order parameter, Eq. (50). We call the rest of the gapped region GSL state. These findings match with previous studies [51, 62].

In Fig. 3, we show the lower spinon (particle) bands, without the application of \( J_x \) in all the four different phases. The Brillouin-zone is from \( -\pi \) to \( \pi \) in both momentum, measured along the directions along the reciprocal translation vectors. The dispersion in the Néel ordered phase shows the characteristic minima (with gap
\(< 1/N\) at the (0, 0) momentum, which shifts away from this point in the case of the spiral ordered state. The spectrum for the GSL and the VBC states are gapped with different positions of minima in the band. The gap in the spectrum for different phase is shown in the Fig. 4, where we also show, in the inset of the same figure, the sudden rise in the \(\chi_3\) order-parameter in the VBC state.

Within the GSL state, as the the \(J_\chi\) is increased, we find, beyond a certain value of \(J_\chi\), either the state becomes gapless with Néel ordering, or the bands acquire non-zero Chern number, which we identify as a CZSL state. It is important to note that, in CZSL state, spinon bands remain gapped but with increasing perturbation (\(J_\chi\)), the particle bands themselves come closer leading to topological phase transition for a critical \(J_\chi\). If we start instead from a VBC state, for a critical perturbation we also observe a topological transition in the spinon bands (the ground-state still remains gapped). Interestingly, we observe that, if we start in GSL state, we end up with a Chern number \(C = 1\), whereas, if we start from a VBC state, we obtain a Chern number \(C = 2\), after the topological transition.

In the Fig. 5 (a), we show the full phase-diagram including the \(J_\chi\) perturbation which leads to possible CZSL state, characterized by non-zero Chern number. We also show the static spin-spin correlation, defined in the Sec. II D in Fig. 5 (b) and (c) for the phases without \(J_\chi\) and with \(J_\chi\), respectively. From these logarithmic-scaled plots, it is evident that the spin-spin correlation, \(\langle \hat{S}_0 \cdot \hat{S}_R \rangle\), decays at a much faster rate, as a function of the distance \(R\), in the GSL, CZSL and VBC state in comparison to magnetically ordered states, which is expected.

With increasing \(J_\chi\), at a critical \(J_\chi\), there is a topological transition to a non-zero Chern number (C) state, which can also be seen from the Berry curvatures of the spinon bands. When \(C \neq 0\), the symmetry the Berry curvature is lost, i.e, \(\Omega(\bar{q}) \neq \Omega(-\bar{q})\). The plot of Berry curvature is shown in Fig. 6, before and after such a topological transition.

Finally, in Fig. 7, we show the thermal Hall coefficients in the states with \(C \neq 0\), which peaks to an appreciable value at a temperature equal to the gap in the lower spinon band. Due to the preserved symmetry of the Berry curvature, the Hall coefficients is vanishingly small in the case of the state with \(C = 0\).

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Appendix A: Berry curvature and U(1)-link variable

Here we briefly summarize the method of Berry-curvature computation, especially for the Bosonic case, following Ref. 71 and Ref. 72. We first consider a two
We discretize the Brillouin zone as following:

\[ \partial \]

where \( H \) is the Hamiltonian. The corresponding field-strength \( F_{12}(q) \) for the \( n^{th} \) band, are given by

\[ A_n^\mu(q) = \langle n(q) | \partial_\mu | n(q) \rangle, \quad (S1) \]

\[ F_{12}^n(q) = \partial_1 A_2^\mu(q) - \partial_2 A_1^\mu(q), \quad (S2) \]

where \( | n(q) \rangle \) is a normalized wave function of the \( n^{th} \) Bloch band. The field-strength is then numerically approximated by

\[ F_{12}^n(q) \delta q_1 \delta q_2 \approx \log_e U_1^n(q) U_2^n(q + \vec{\delta} q) U_1^n(q + \vec{\delta} q) U_2^n(q) \quad (S8) \]

with,

\[ -\pi < \frac{1}{4} F_{12}^n(q) \delta q_1 \delta q_2 \leq \pi. \quad (S9) \]

Finally, the Chern number on the lattice corresponding to the \( n^{th} \) band is defined as,

\[ C_n \equiv \frac{1}{2\pi i} \sum_{\vec{q}} F_{12}^n(q) \delta q_1 \delta q_2. \quad (S11) \]

For Bosonic case

To accommodate the commutation relations among the bosonic operators, the generalized eigenvalue equation in case of a bosonic Hamiltonian \( M \) is written as,

\[ M(q) | n(q) \rangle = E(q) \rho_3 | n(q) \rangle, \quad (S12) \]

as a consequence the inner product in U(1)-link variable has the form [72],

\[ U_\vec{q}(\vec{q}) \equiv \langle n(\vec{q}) | \rho_3 | n(\vec{q} + \vec{\mu}) \rangle / N_\vec{q}(\vec{q}) \quad (S13) \]

where,

\[ N_\vec{q}(\vec{q}) \equiv | \langle n(\vec{q}) | \rho_3 | n(\vec{q} + \vec{\mu}) \rangle |. \quad (S14) \]

\( E(q) \) has eigenvalues of the form,

\[ (\epsilon_{\vec{q},+}, \epsilon_{\vec{q},+}, -\epsilon_{\vec{q},+}, -\epsilon_{\vec{q},+}) \quad (S15) \]

For particle/ hole bands the eigenvector \( | n(\vec{q}) \rangle \) is normalized as follows,

\[ \langle n^{\text{particle}}(\vec{q}) | \rho_3 | n^{\text{particle}}(\vec{q}) \rangle = 1, \quad (S16) \]

\[ \langle n^{\text{hole}}(\vec{q}) | \rho_3 | n^{\text{hole}}(\vec{q}) \rangle = -1. \quad (S17) \]