Supplemental Material

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TRANSFORMATION FROM THE SPIN TO THE BOSONIC LANGUAGE

The spin-1/2 Heisenberg model is defined on the bcc and fcc lattices, shown in Fig. 1. By using the Matsubara-Matsuda transformation introduced in the main text, the Hamiltonian is transformed into the bosonic language, up to a constant term:

\[
\hat{H} = \frac{J_1}{2} \sum_{ij} (b_i^+ b_j + b_j^+ b_i) + \frac{J_2}{2} \sum_{\langle ij \rangle} (b_i^+ b_j + b_j^+ b_i) + U \sum_i n_i(n_i - 1) + J_3 \sum_{\langle\langle ij \rangle\rangle} n_in_j + \left(\frac{z_1 J_1 + z_2 J_2 + z_3 J_3}{2} - H\right) \sum_i n_i
\]

where \(U\) is the on-site hard-core repulsion, which is sent to infinity in the calculation, and \(z_1, z_2, z_3\) are the coordination numbers of the 1st, 2nd and 3rd nearest neighbors.

FIG. 1. The Heisenberg interactions \(J_1, J_2, J_3\) are defined on the 1st, 2nd and 3rd nearest neighbors. (a) bcc lattice. (b) fcc lattice.

By Fourier transformation \(b_i^n = \frac{1}{N} \sum_k e^{-i k \cdot r_i} b_k^n\), the Hamiltonian is written down in \(k\)-space:

\[
\hat{H} = \sum_k [\epsilon(k) - \epsilon(0) + H] b_k^+ b_k + \sum_{k,k',q} (U + V_q) b_{k+q}^+ b_{k'}^+ b_{k'} b_k
\]

where

\[
\epsilon(k) = \frac{J_1}{2} \sum_{\eta_1} e^{i k \cdot r_{\eta_1}} + \frac{J_2}{2} \sum_{\eta_2} e^{i k \cdot r_{\eta_2}} + \frac{J_3}{2} \sum_{\eta_3} e^{i k \cdot r_{\eta_3}}
\]

and \(r_{\eta}\) denote the positions of the neighboring sites. And

\[V_q = 2\epsilon(q)\]

To be explicit, for bcc lattice:

\[
\epsilon(k) = 4J_1 \cos k_x \cos k_y \cos k_z + 2J_2 \left(\cos k_x + \cos k_y + \cos k_z\right) + 2J_3 \left(\cos k_x \cos k_y + \cos k_y \cos k_z + \cos k_z \cos k_x\right)
\]

For fcc lattice:

\[
\epsilon(k) = 2J_1 \left(\cos k_x \cos k_y \cos k_z + \cos k_y \cos k_z \cos k_x + \cos k_z \cos k_x \cos k_y\right) + 4J_3 \left(\cos k_x \cos k_y \cos k_z + \cos k_y \cos k_z \cos k_x\right)
\]

We define the minimum value of \(\epsilon(k)\) to be \(\epsilon_{\text{min}}\), in this way \(\omega_k \equiv \epsilon(k) - \epsilon_{\text{min}}\) has minimum value equals to zero. The Hamiltonian is rewritten as:

\[
\hat{H} = \sum_k (\omega_k - \mu) b_k^+ b_k + \frac{1}{2N} \sum_{k,k',q} (U + V_q) b_{k+q}^+ b_{k'}^+ b_{k'} b_k
\]
where the chemical potential:

\[ \mu = [\epsilon(0) - \epsilon_{\text{min}}] - H \equiv H_\text{sat} - H \]  

Because of the frustration, the single magnon dispersion \( \omega_k \) can have multiple degenerate minima at different \( \mathbf{Q} \)-vectors. In Fig. 2, we compute the number of minima in \( \omega_k \), for both bcc and fcc lattices.

For concreteness, we focus on the regions with 6 degenerate minima, whose positions are denoted by \( \pm \mathbf{Q}_n = \pm \mathbf{Q} \mathbf{e}_n \), where \( n = 1, 2, 3 \). The value of \( \mathbf{Q} \) is given by \( \cos \frac{\mathbf{Q}}{2} = -J_1/(J_2 + 4J_3) \) for the bcc lattice and \( \cos \frac{\mathbf{Q}}{2} = -(J_1 + 2J_2)/(J_2 + 4J_3) \) for the fcc lattice. Correspondingly, the saturation field values are:

\[ H_\text{sat}^{\text{bcc}} = \frac{2J_1^2}{J_2 + 4J_3} + 4J_1 + 2J_2 + 8J_3 \]  
\[ H_\text{sat}^{\text{fcc}} = \frac{2(J_1 + 2J_2)^2}{J_2 + 4J_3} + 4J_1 + 2J_2 + 16J_3 \]

CALCULATION OF EFFECTIVE INTERACTIONS

The effective interactions in the dilute limit for hard-core bosons are calculated by the Bethe-Salpeter equation, which is equivalent to summing over all the ladder diagrams (Fig. 3).

\[ \Gamma_q(k, k') = U + V_q - \int d^3q' \frac{\Gamma_q(k, k')(U + V_{q-q'})}{V_{\text{BZ}}} \]  

where \( V_{\text{BZ}} \) is the volume of the 1st BZ.

When the magnetic field \( H \) is close to the saturation value \( H_\text{sat} \), the system is unstable towards BEC at the dispersion minima. In this case we can take the long wave length limit \( k \rightarrow \pm \mathbf{Q}_i \), and calculate the corresponding vertex functions (schematically shown in Fig. 4):

\[ \Gamma_1 = \Gamma_0(\mathbf{Q}_n, \mathbf{Q}_n) \]  
\[ \Gamma_2 = \Gamma_0(\mathbf{Q}_m, -\mathbf{Q}_n) + \Gamma_2(\mathbf{Q}_n, -\mathbf{Q}_n) \]  
\[ \Gamma_3 = \Gamma_0(\mathbf{Q}_m, \mathbf{Q}_m) + \Gamma_3(\mathbf{Q}_m, \mathbf{Q}_m) \]  
\[ \Gamma_4 = \Gamma_0(\mathbf{Q}_n, -\mathbf{Q}_n) + \Gamma_4(\mathbf{Q}_n, -\mathbf{Q}_n) \]

To solve the Bethe-Salpeter equation, we start from the following ansatz:

\[ \Gamma_q = \langle \Gamma \rangle + \sum_\eta A_\eta V(r_\eta) e^{i \mathbf{q} \cdot r_\eta} \]  

where \( r_\eta \) denotes the positions of the 1st, 2nd, and 3rd neighboring sites. The \( k, k' \) index in \( \Gamma_q(k, k') \) are omitted for simplicity, and \( \langle \Gamma \rangle = \int d^3q V(q) = 0 \)

By substituting the ansatz into the Bethe-Salpeter equation and taking the hard-core limit, we get the following form of linear equations:

\[ \sum_\eta V(r_\eta)(\tau_\eta^T)^* \eta \eta + \tau_0(\Gamma) = 1 \]  
\[ \sum_\nu (\tau_\nu^T V(r_\nu) + \delta_\nu) \eta \eta + \tau_0(\Gamma) = 1 \]

where the integrals are defined as:

\[ \tau_0 = \int d^3q \frac{1}{V_{\text{BZ}}} \]  
\[ \tau_1 = \int d^3q \frac{e^{-i \mathbf{q} \cdot \mathbf{r}_\eta}}{V_{\text{BZ}}} \]  
\[ \tau_2 = \int d^3q \frac{e^{-i \mathbf{q} \cdot \mathbf{r}_\eta}}{V_{\text{BZ}}} \]

Denote:

\[ B_\eta = \tau_2^{\eta^*} V(r_\eta) + \delta_\eta \]  
\[ C_\eta = V(r_\eta)(\tau_1^T)^* \]

The above equations are now organized into a matrix form:

\[ \begin{pmatrix} B_{11} & \cdots & B_{1z} & \tau_1^1 \\ \vdots & \ddots & \vdots \\ C_{11} & \cdots & C_{1z} & \tau_0 \end{pmatrix} \begin{pmatrix} A_1 \\ \vdots \\ A_z \end{pmatrix} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \]

By solving the linear equations Eq. (17), we obtain all the unknown coefficients in the ansatz Eq. (12). Then we can substitute the values of \( \Gamma_1, \ldots, \Gamma_4 \) into the expression of effective energy, and determine which multi-\( \mathbf{Q} \) state will be stabilized.
EFFECT OF SYMMETRIC EXCHANGE ANISOTROPY

We consider short-range symmetric exchange anisotropy (cutoff at 2nd nearest neighbor):

\[ \hat{H}_A \propto \sum_{\langle ij \rangle} -3(\mathbf{S}_i \cdot \mathbf{r}_{ij})(\mathbf{S}_j \cdot \mathbf{r}_{ij}) \] (18)

such terms can arise directly from dipole-dipole interactions, or perturbatively from spin-orbit coupling[1].

Similar to the treatment of the Heisenberg exchange interactions, we choose the quantization axis along [111] direction, and represent the spin-\( \frac{1}{2} \) operators with hard-core bosons. In the long-wavelength limit, for both bcc and fcc lattices:

\[ \hat{H}_A \propto \left[ \left( \frac{\sqrt{3}}{2} + i \frac{1}{2} \right) b_{Q_1}^\dagger b_{Q_1}^\dagger - \left( -\frac{\sqrt{3}}{2} + i \frac{1}{2} \right) b_{Q_2}^\dagger b_{Q_2}^\dagger \right] + h.c \] (19)

Then we condense the bosons by \( \langle b_{\sigma Q_n} \rangle / \sqrt{N} = \sqrt{\rho_{Q_n}} \exp\left( i \phi_{Q_n} \right) \), which gives the energy correction of symmetric exchange anisotropy:

\[ E_A \propto J_A \sum_n \sqrt{\rho_{Q_n} \rho_{-Q_n}} \cos(\Phi_n + 2n\pi/3 - \pi/2). \] (20)

where \( \Phi_n = \phi_{Q_n} + \phi_{-Q_n} \).