Ground state properties of quantum Kagomé ice hardcore bosons

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Abstract

We study the quantum Kagomé ice hardcore bosons, which correspond to the $XY$ limit of the quantum spin ice Hamiltonian. We estimate the values of their zero-temperature thermodynamic quantities using the large-$S$ expansion. We show that our semiclassical analysis is consistent with the finite temperature quantum Monte Carlo estimates.

Keywords: hardcore bosons, condensate fraction, dynamical structure factors

(Some figures may appear in colour only in the online journal)

1. Introduction

The recent search for a putative quantum spin liquid (QSL) state in three-dimensional (3D) pyrochlore lattice quantum spin ice (QSI) has led to a new proposal for a quantum spin Hamiltonian devoid of the debilitating quantum Monte Carlo (QMC) sign problem for a wide range of the parameter regime [1–3]. Recently, Carrasquilla et al [3] studied the projected 3D QSI Hamiltonian of Huang, Chen, and Hermele [1] on a 2D frustrated Kagomé lattice with a [111] crystallographic field. They explored this model with explicit finite temperature QMC simulations and identified the interactions that promote a QSL state. In a recent study, we complemented the QMC analysis using linear spin wave theory [4]. In this study, we found that quantum fluctuations are suppressed in the quantum Kagomé ice model; hence, the semiclassical analysis captures the broad trend of the quantum phase diagram and ground state properties uncovered by QMC [3].

However, the possibility of an $XY$ limit remains for the quantum Kagomé ice (QKI) model. The $XY$ model essentially controls the dynamics of the fully frustrated system, [1, 3] and forms the basis of the ultra-cold atoms trapped in quantum optical lattices [5–7]. The
quantum XY model is also known to describe quantum magnetic insulators and quantum Hall bilayer systems [8]. Thus, it is crucial to understand the nature of the XY limit of this model. We consider the hardcore boson model

\[ \mathcal{H} = -t \sum_{\langle lm \rangle} (b_l^\dagger b_m + b_m^\dagger b_l) - t' \sum_{\langle lm \rangle} (b_l^\dagger b_m^\dagger + b_m b_l) - \mu \sum_{l} n_l, \]  

where \( t \) and \( t' \) are the hopping amplitudes between neighboring sites, \( \mu \) is a chemical potential, \( b_l^\dagger (b_l) \) are the bosonic creation (annihilation) operators at site \( l \), and \( n_l = b_l^\dagger b_l \) is the occupation number. This Hamiltonian maps to the XY model via the Matsubara–Matsuda transformation [9],

\[ \mathcal{H} = - \sum_{\langle lm \rangle} \mathcal{J}_{\pm} (S_l^x S_m^x + S_l^y S_m^y) + \mathcal{J}_{\pm} (S_l^x S_m^y + S_l^y S_m^x) - H \sum_{l} S_l^z, \]

where \( S^x = S^\dagger \pm iS^\dagger \) are operators that flip the spins at site \( l \), \( t \rightarrow \mathcal{J}_{\pm}, t' \rightarrow \mathcal{J}_{\pm}, \) and \( \mu \rightarrow H \). The Hamiltonian [2] corresponds to theXY limit of the QSI model [1, 3]. A crucial observation in this model is that the \( \mathcal{J}_{\pm} \) sign is irrelevant. It can be changed by a \( \pi/2 \)-rotation about the \( z \)-axis: \( S_{l,m}^z \rightarrow \pm i S_{l,m}^z \), leaving the other terms invariant. Hence, the ground state of equation (2) is independent of the sign of \( \mathcal{J}_{\pm} \) but depends on the sign of \( \mathcal{J}_{\pm} \) for non-bipartite lattices. We consider \( \mathcal{J}_{\pm} > 0 \). The usual hardcore bosons are recovered when \( \mathcal{J}_{\pm} = 0 \) [10–18]. The effects of a dominant \( \mathcal{J}_{\pm} \) are only well pronounced on non-bipartite lattices, and they have not been reported in the existing literature for the Kagomé lattice.

The goal of this paper is to provide the estimated values of the thermodynamic quantities for the quantum Kagomé ice hardcore bosons in the dominant \( t' \) limit. For this purpose we study the nature of equation (2), focusing mainly on the large \( \mathcal{J}_{\pm} \) limit. Henceforth, we take \( \mathcal{J}_{\pm} \) as the energy unit and consider the Hamiltonian

\[ \mathcal{H} = - \frac{1}{2} \sum_{\langle lm \rangle} \{ (S_l^x S_m^x + S_l^y S_m^y) + \Delta (S_l^x S_m^y + S_l^y S_m^x) \} - H_z \sum_{l} S_l^z - H_x \sum_{l} S_l^x, \]

where \( 0 \leq \Delta = \mathcal{J}_x / \mathcal{J}_{\pm} \leq 1 \). The external magnetic fields are introduced to enable the calculation of magnetizations and susceptibilities. The Hamiltonian [3], retains \( Z_2 \)-invariance in the \( xy \) plane when \( H_x = 0 \), which is a \( \pi \)-rotation about the \( z \)-axis in spin space: \( S_{l,m}^z \rightarrow S_{l,m}^z \), \( S_{l,m}^x \rightarrow -S_{l,m}^x \). At \( H_z = 0 \), the limits \( \Delta = 0 \) and \( \Delta = 1 \) correspond to the isotropic \( Z_2 \)-invariant XY model and the fully polarized \( S_x \) (Ising) ferromagnet respectively. We present an analysis based on the semiclassical large-\( S \) expansion and we show that the estimated values of our analysis are in good agreement with the finite temperature QMC simulation by Carrasquilla [1] on the Kagomé lattice.

2. Linear spin wave theory

2.1. Mean-field theory

In the mean-field analysis or large-\( S \) limit, the spin operators in equation (3) are replaced with classical vectors: \( \mathbf{S}_l = S_l \mathbf{n}_l \), where \( \mathbf{n}_l = (\sin \theta_l \cos \phi_l, \sin \theta_l \sin \phi_l, \cos \theta_l) \) is a unit vector. For this model, there is only one possible phase at zero magnetic fields—an easy-axis ferromagnet

\[ \text{The QMC results were provided by J Carrasquilla from his analysis of the fully frustrated system in [3].} \]
resulting from the spontaneously broken \(Z_2\) symmetry along the \(x\)-direction. This phase becomes a canted ferromagnet (CFM) for small \(H_z\). For large \(H_z\), there is a fully polarized (FP) ferromagnet, with the spins aligned along the \(z\)-axis. Both ferromagnets are described with \(q = l\) and \(f = 0\), hence the classical energy is given by

\[
e_c = -\zeta (1 + \Delta) \sin^2 \theta - h_z \sin \theta - h_z \cos \theta,
\]

where \(e_c = \mathcal{E}/N S^2\), \(N\) is the total number of sites, and \(\zeta = 2, 3\) on the Kagomé and the triangular lattices respectively, and \(h_{x,z} = H_{x,z}/S\). Minimizing the classical energy with respect to \(\theta\) yields

\[
h_z = \tan \theta [h_z - 2\zeta (1 + \Delta) \cos \theta],
\]

hence

\[
e_c (\theta) = \zeta (1 + \Delta) \sin^2 \theta - h_z \sec \theta,
\]

where \(\theta\) is a function of \(h_z\). At \(h_z = 0\), we get \(h_z = h_z^c \cos \bar{\theta}\) and the corresponding energy is \(e_c (\bar{\theta} = \bar{\theta}) = -\zeta (1 + \Delta)(1 + \cos^2 \bar{\theta})\), where \(h_z^c = 2\zeta (1 + \Delta)\) is the critical field between the CFM and the FP. For \(h_z \ll 1\), the energy is obtained perturbatively in \(h_z\):

\[
e_c = e_c (h_z = 0) + h_z \frac{\partial e_c (\bar{\theta})}{\partial h_z} \bigg|_{h_z = 0} + \cdots,
\]

where \(e_c (h_z = 0) = e_c (\bar{\theta} = \bar{\theta})\).

### 2.2. Holstein–Primakoff transformation

We perform linear spin wave theory (LSWT) by rotating the coordinate about the \(y\)-axis so that the \(z\)-axis coincides with the local direction of the classical polarization. The corresponding rotation matrix is

\[
\mathcal{R}_y (\theta) = \begin{pmatrix}
\cos \theta & 0 & \sin \theta \\
0 & 1 & 0 \\
-\sin \theta & 0 & \cos \theta
\end{pmatrix}
\]

Next, we employ a three-sublattice Holstein–Primakoff transformation [19] with the bosonic creation and annihilation operators, \(a_{\alpha}^\dagger\) and \(a_{\alpha}\) [20] respectively, where \(\alpha = A, B, C\) labels...
the three sublattices on the Kagomé lattice, as depicted in figure 1(a). After the Fourier transform, the linearized momentum space Hamiltonian is given by

\[ \mathcal{H} = S \sum_{\mathbf{k},\mathbf{\alpha},\mathbf{\beta}} (\mathcal{M}_0^{\alpha\beta} \delta_{\alpha\beta} + \mathcal{M}_0^{\alpha}) (a^+_{\mathbf{k}\alpha} a_{\mathbf{k}\beta} + a^+_{-\mathbf{k}\alpha} a_{-\mathbf{k}\beta}) + \mathcal{M}_0^{\alpha} (a^+_{\mathbf{k}\alpha} a^+_{-\mathbf{k}\beta} + a_{-\mathbf{k}\alpha} a_{\mathbf{k}\beta}), \]

where \( \alpha, \beta = A, B, C \) and the coefficients are given by \( \mathcal{M}_0^{\alpha} = \xi \text{ diag}(1, 1, 1) \), with \( \xi = (h_1 \cos \theta + h_x \sin \theta)/2 + \zeta (1 + \Delta) \sin^2 \theta \), and the matrices \( \mathcal{M}^{\alpha} \) differ only by a pre-factor:

\[ \mathcal{M}^{\pm} = -\frac{\chi \pm (1 - \Delta)}{2} \Omega, \]

where \( \chi = (1 + \Delta) \cos^2 \theta \) and \( \Omega \) is given by

\[ \Omega = \begin{pmatrix} 0 & \cos k_1 & \cos k_2 \\ \cos k_1 & 0 & \cos k_3 \\ \cos k_2 & \cos k_3 & 0 \end{pmatrix}, \]

with \( k_j = \mathbf{k} \cdot \mathbf{e}_j \); \( \mathbf{e}_1 = -(1/2, \sqrt{3}/2) \); \( \mathbf{e}_2 = (1, 0) \); \( \mathbf{e}_3 = (-1/2, \sqrt{3}/2) \). The eigenvalues of \( \Omega \) are given by

\[ \omega_1 = -1; \quad \omega_{2,3} = \frac{1}{2} (1 \pm \sqrt{1 + 8g_k}); \]

where \( g_k = \cos k_1 \cos k_2 \cos k_3 \). The Hamiltonian (9) is diagonalized in two steps [20]. Firstly, we make a linear transformation

\[ a_{\mathbf{k}\alpha} = \sum_{\mu} U_{\alpha\mu}(\mathbf{k}) d_{\mu}, \]

where \( U_{\alpha\mu}(\mathbf{k}) \) is a unitary matrix constructed from the eigenvectors of \( \Omega \) associated with the eigenvalues \( \omega_\mu \). Secondly, we apply the Bogoliubov transformation

\[ d_{\mu} = u_{\mathbf{k}\alpha} \beta_{\mu} - v_{\mathbf{k}\alpha} \beta^*_{-\mu} ; \quad u_{\mathbf{k}\alpha}^2 - v_{\mathbf{k}\alpha}^2 = 1. \]

The resulting Hamiltonian is diagonalized with

\[ u_{\mathbf{k}\alpha}^2 = \frac{1}{2} \left( \frac{A_{\mathbf{k}\alpha}}{\epsilon_{\mathbf{k}\alpha}} + 1 \right) ; \quad v_{\mathbf{k}\alpha}^2 = \frac{1}{2} \left( \frac{A_{\mathbf{k}\alpha}}{\epsilon_{\mathbf{k}\alpha}} - 1 \right). \]

and

\[ A_{\mathbf{k}\alpha} = \xi + (1 - \Delta) \omega_{\mathbf{k}\alpha} + B_{\mathbf{k}\alpha} ; \quad B_{\mathbf{k}\alpha} = -\frac{\chi + (1 - \Delta)}{2} \omega_{\mathbf{k}\alpha}. \]

The energy is given by \( \epsilon_{\mathbf{k}\alpha} = \sqrt{A_{\mathbf{k}\alpha}^2 - B_{\mathbf{k}\alpha}^2} \). The diagonal Hamiltonian is given by

\[ \mathcal{H} = S \sum_{\mathbf{k},\alpha} (\gamma_{\mathbf{k}\alpha})^* \gamma_{\mathbf{k}\alpha} + \gamma_{-\mathbf{k}\alpha}^* \gamma_{-\mathbf{k}\alpha}. \]

For the triangular lattice, there is only one sublattice. We obtain

\[ A_{\mathbf{k}} = \xi + 3(1 - \Delta) g_{\mathbf{k}} + B_{\mathbf{k}} ; \quad B_{\mathbf{k}} = -\frac{\chi + 3(1 - \Delta)}{2} g_{\mathbf{k}}, \]

with \( \xi = (h_1 \cos \theta + h_x \sin \theta)/2 + 3(1 + \Delta) \sin^2 \theta, \chi = 3(1 + \Delta) \cos^2 \theta \), and \( g_{\mathbf{k}} = (\cos k_x + 2 \cos k_y/2 \cos \sqrt{3} k_x/2)/3 \). The corresponding Hamiltonian is diagonalized in a similar way but without the sublattice indices.
2.3. Excitation spectra

The features of the quantum Kagomé ice hardcore bosons can be understood by analyzing the momentum-dependent eigenfrequencies given by $\varepsilon_{k_0} = 2\varepsilon_{k_0}$. The energy bands for the Kagomé lattice are plotted in figure 2 along the Brillouin zone paths in figure 1(b) for $\Delta = h_{z,x} = 0$ (isotropic limit) and $\Delta = 0.25$; $h_x = 0; h_z = \pm 4.5$. We also show the energy band on the triangular lattice in figure 3. The excitation spectra of equation (2) are fully gapped on both lattices for all $\Delta$ between 0 and 1 for $h_{z,x} = 0$. The gap persists at all values of the magnetic field $h_z \leq h_x$ and $h_y = 0$. The absence of a zero (soft) mode in the quantum Kagomé ice hardcore bosons is a direct consequence of the discrete $Z_2$ symmetry of

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{The plots of the energy bands for the Kagomé lattice at $h_x = 0, \Delta = 0 = h_z$ (a); $\Delta = 0.25; h_z = \pm 4.5$ (b).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{The plot of the energy band on the triangular lattice at $h_x = 0$ and several values of $\Delta$ and $h_z$. There is only one band for each parameter.}
\end{figure}
equation (2). For the triangular lattice, a roton minimum occurs at the corners of the Brillouin zone for $\Delta = h_{t,z} = 0$, i.e., at $Q_K = (\pm 4\pi/3, 0)$ and the symmetry related points, whereas the dispersion has a maximum peak at $Q_F = (0, 0)$. This is in stark contrast with the pure $U(1)$-invariant $XY$ model.

2.4. Ground state energy

The spin wave correction to the mean field energy is given by

$$\Delta \mathcal{E} = \mathcal{E}_g - \mathcal{E}_c = S \sum_{k\alpha} [\epsilon_{k\alpha} - \xi].$$  \hspace{1cm} (19)

The correction to the ground state energy as a function of $h_z$ is plotted in figure 4 for the Kagomé lattice. The triangular lattice has a similar trend. We see that the trend of the quantum Kagomé ice hardcore bosons is different from that of the $U(1)$-invariant $XY$ model. In particular, the energy of the isotropic $Z_2$-invariant model at $\Delta = h_z = 0$ does not vanish at the saturated point $h_z = h_f$. The estimated ground state energy on the Kagomé lattice at the isotropic point $\Delta = h_{t,z} = 0$ is $\mathcal{E}_g = -0.5309$. The finite temperature QMC simulation (see footnote 1) for a relatively large cluster $V = 24 \times 24 \times 3$ spins at the inverse-temperature $\beta = 100$ gives $\mathcal{E}_g = -0.5359(2)$, in good agreement with the linear spin wave theory. For the triangular lattice, linear spin wave theory gives $\mathcal{E}_g = -0.7791$ \cite{21}; there is no QMC result in this case.

2.5. Particle and condensate densities

We now study the ground state properties of equation (3) by probing the sublattice magnetizations, which will quantify the strengths of the quantum fluctuations in this model. We first analyze the Kagomé lattice, and the triangular lattice follows a similar pattern. For the Kagomé lattice, the sublattice magnetizations are equivalent, and the total magnetizations per site are given by
Using equation (19) we obtain

\[ \langle S_z \rangle = -\frac{1}{SN} \frac{\partial E_{SW}(h_z, h_x = 0)}{\partial h_z}, \]

\[ \langle S_z \rangle = -\frac{1}{SN} \frac{\partial E_{SW}(h_z, h_x)}{\partial h_x} \bigg|_{h_y = 0}. \]

Using equation (19) we obtain

\[ \langle S_z \rangle = S \cos \vartheta \xi + \frac{1}{2 \xi} \frac{1}{N} \sum_{\mathbf{k}_z} (\hat{A}_{\mathbf{k}_z} - \hat{B}_{\mathbf{k}_z}) \frac{\omega_{\mathbf{k}_z}}{\xi_{\mathbf{k}_z}}. \]

For the linear order in \( h_z \), we find

\[ \langle S_z \rangle = S \sin \vartheta \xi - \frac{\cos^2 \vartheta \xi}{2 \xi} \frac{1}{N} \sum_{\mathbf{k}_z} (\hat{A}_{\mathbf{k}_z} - \hat{B}_{\mathbf{k}_z}) \frac{\omega_{\mathbf{k}_z}}{\xi_{\mathbf{k}_z}} \]

\[ - \frac{1}{2 \sin \vartheta \xi} \frac{1}{N} \sum_{\mathbf{k}_z} \left[ \frac{\hat{A}_{\mathbf{k}_z}}{\xi_{\mathbf{k}_z}} - 1 \right] \]

where \( \hat{A}_{\mathbf{k}_z} = A_{\mathbf{k}_z} (h_z = 0) \), etc. As seen in equations (22) and (23), the denominator in these expressions corresponds to the gapped energy spectrum. We define the particle density \( \rho \) and the ‘condensate density’ at \( \mathbf{k}_0 = 0 \) as \( \rho = S + \langle S_z \rangle \) and \( \rho_0 = \langle S_z \rangle^2 \) respectively. In LSWT we find

\[ \rho_0 = (S \sin \vartheta \xi)^2 - \frac{\cos^2 \vartheta \xi}{2 \xi} \frac{1}{N} \sum_{\mathbf{k}_z} (\hat{A}_{\mathbf{k}_z} - \hat{B}_{\mathbf{k}_z}) \frac{\omega_{\mathbf{k}_z}}{\xi_{\mathbf{k}_z}} \]

\[ - S \frac{1}{N} \sum_{\mathbf{k}_z} \left[ \frac{\hat{A}_{\mathbf{k}_z}}{\xi_{\mathbf{k}_z}} - 1 \right]. \]

The corresponding expressions for the triangular lattice are similar to the Kagomé lattice without the sublattice summation. Figure 5 shows the plot of the condensate against the particle density at \( \Delta = 0 \) (isotropic \( Z_2 \)-invariant XY model) for the Kagomé lattice. At half

\[ \text{Figure 5. The spin wave condensate density } \rho_0 \text{ against the particle density } \rho \text{ on the Kagomé lattice at } h_z = \Delta = 0 \text{ and } S = 1/2. \]
filling \((\rho = 0.5 \text{ or } h_{z,z} = \Delta = 0)\), the estimated values of the order parameter for the Kagomé lattice are \(\langle S_z \rangle = 0.4829\) and \(\rho_0 = \langle S_z \rangle^2\). The finite temperature QMC simulation (see footnote 1) for a relatively large cluster \(V = 24 \times 24 \times 3\) spins at the inverse-temperature \(\beta = 24\) gives \(\langle S_z \rangle = 0.4785(2)\). For the triangular lattice, linear spin wave theory gives \(\langle S_z \rangle = 0.4902\), which is closer to the mean-field value \(\langle S_z \rangle = 0.5000\), and there is no QMC result in this case. Clearly, the gapped energy spectrum of equation (23) enhances the thermodynamic quantities.

The out-of-plane magnetic susceptibility, \(\chi_{zz}\), is another important measurable quantity as it relates to the compressibility of the bosons. It is given by

\[
\chi_{zz} = \frac{1}{S} \frac{\partial \langle S_z \rangle}{\partial h_z} \bigg|_{h_z=0}.
\]

We find

\[
\chi_{zz} = \chi_{zz}^c + \frac{1}{4 \zeta^2 (1 + \Delta)^2 S N} \sum_{kz} (\bar{A}_{kz} - \bar{B}_{kz}) \frac{\omega_{kz}^2}{\epsilon_{kz}},
\]

where \(\chi_{zz}^c = [2\zeta (1 + \Delta)]^{-1}\) is the classical susceptibility and \(\bar{A}_{kz} = A_{kz} (h_{z,z} = 0)\), etc. The plots of \(\chi_{zz}^c\) and \(\chi_{zz}\) as a function of \(\Delta\) are shown in figure 6 for the Kagomé lattice. The triangular lattice has a similar trend. The classical and the quantum susceptibilities coincide as \(\Delta \to 1\), corresponding to the fully polarized \(S_z\)-ferromagnet. The estimated value of \(\chi_{zz}\) at the isotropic \(Z_2\)-invariant limit, \(\Delta = 0\) for the Kagomé is \(\chi_{zz} = 0.2807\). The finite temperature QMC simulation (see footnote 1) for a large cluster \(V = 24 \times 24 \times 3\) spins at the inverse-temperature \(\beta = 24\) gives \(\chi_{zz} = 0.2785(2)\). For the triangular lattice, linear spin wave theory gives \(\chi_{zz} = 0.1799\), and the mean-field value \(\chi_{zz} = 1/6\); again there is no QMC result in this case. In contrast to the \(U(1)\)-invariant model \([10-18]\), we see that the quantum fluctuation increases the classical susceptibility away from \(\Delta = 1\).

\[\text{Figure 6. The plot of the classical and the spin wave quantum susceptibilities as a function of } \Delta \text{ for the Kagomé lattice at } S = 1/2.\]
2.6. Dynamical structure factors

Furthermore, we explore the nature of the quantum Kagomé ice hardcore bosons by studying the dynamical structure factor, which is an important quantity in experiments for characterizing the ground state properties of a quantum system. The spin structure factor is given by the Fourier transform of the equal-time spin–spin correlation function

\[
S_{\mu \nu}(\mathbf{k}) = \frac{1}{N} \sum_{\mu \nu} e^{i \mathbf{k} \cdot (\mathbf{r}_\mu - \mathbf{r}_\nu)} \langle S^\mu_{\alpha \sigma} S_{m \rho}^\nu \rangle ,
\]

where \( \mu, \nu = (x, y, z) \) label the components of the spins, \( S^\mu_{\alpha \sigma} = \sum_{\alpha} S^\mu_{\alpha \sigma} \) on the Kagomé lattice, and \( \alpha \) labels the sublattices. We restrict the calculation of the structure factors to the case of half-filling (\( r = 0.5 \)) or zero magnetic fields (\( h_{x,z} = 0 \)).

The momentum distribution is related to the off-diagonal static structure factor \( S^{\pm}(\mathbf{k}) \). We have \( \langle S^x_{\alpha \sigma} S^y_{\alpha \sigma} \rangle = \langle S^y_{\alpha \sigma} S^x_{\alpha \sigma} \rangle + \langle S^z_{\alpha \sigma} S^z_{\alpha \sigma} \rangle \delta_{\alpha \sigma} \). At \( h_{x,z} = 0, \theta = \pi/2 \), hence rotation about the y-axis gives \( S^x \rightarrow S'^z \), \( S^y \rightarrow -S'^y \), and \( S^z \rightarrow S'^z \). The off-diagonal structure factor in the rotated coordinate up to order \( S \) is given by \( S^{\pm}(\mathbf{k}) = \langle S'^z_{\alpha \sigma} S'^z_{\alpha \sigma} \rangle + \langle S'^y_{\alpha \sigma} S'^y_{\alpha \sigma} \rangle \). At \( k_F = 0 \), \( S^{\pm}(\mathbf{k}) \) is related to the order parameter by \( \rho_0 = S^{-}(k_0)/N \) as \( N \rightarrow \infty \). For the Kagomé lattice we find that the off-diagonal structure factor for \( \mathbf{k} = k_F \) and the out-of-plane structure factor are given by

\[
S^{\pm}(\mathbf{k}) = \sum_{\mu} F^{\pm}_{\mu}(\mathbf{k}), \quad S^{zz}(\mathbf{k}) = \sum_{\mu} F^{zz}_{\mu}(\mathbf{k}),
\]

where \( F^{\pm}_{\mu}(\mathbf{k}) = S(u_\mu + v_\mu)/2 \sum_{\alpha \sigma \rho} U_{\alpha \rho \sigma}(\mathbf{k}) U_{\rho \sigma \mu}(\mathbf{k}) \) \( F^{zz}_{\mu}(\mathbf{k}) = S(u_\mu - v_\mu)/2 \sum_{\alpha \sigma \rho} U_{\alpha \rho \sigma}(\mathbf{k}) U_{\rho \sigma \mu}(\mathbf{k}) \). For the triangular lattice, the explicit expressions are

\[
S^{\pm}(\mathbf{k}) = \frac{S}{2} (u_\mu + v_\mu) = \frac{S}{2} \left( \frac{A_\mu + B_\mu}{\sqrt{A_\mu^2 - B_\mu^2}} \right), \quad (29)
\]

\[
S^{zz}(\mathbf{k}) = \frac{S}{2} (u_\mu - v_\mu) = \frac{S}{2} \left( \frac{A_\mu - B_\mu}{\sqrt{A_\mu^2 - B_\mu^2}} \right), \quad (30)
\]

Figure 7. The plot of the off-diagonal form factor \( F^{\pm}(\mathbf{k}) \) for the two dispersive bands on the Kagomé lattice at \( S = 1/2; \Delta = h_{x,z} = 0 \).
The denominator of equations (29) and (30) corresponds to the energy spectrum, which is gapped in the entire Brillouin zone. In figures 7 and 8 we have shown the off-diagonal form factor $\mathcal{F}^{\pm\pm}(\mathbf{k})$ and the out-of-plane form factor $\mathcal{F}^{zz}(\mathbf{k})$ for the two dispersive bands on the Kagomé lattice. Figure 9 shows the off-diagonal and the out-of-plane structure factors on the triangular lattice. The solid hexagons denote the respective Brillouin zones for the two lattices. For the Kagomé lattice, the momentum distribution shows noticeable non-divergent sharp peaks at the centre and corners of the Brillouin zones, whereas for the triangular lattice we observe non-divergent peaks at $\mathbf{Q}_K = (\pm 4\pi/3, 0)$ and the symmetry related points. This is due to the roton minima of the excitation spectrum at $\mathbf{Q}_K = (\pm 4\pi/3, 0)$ as opposed to the divergent peak at $\mathbf{k}_F = 0$ in the U(1)-invariant model [10–13]. On the other hand, the out-of-plane structure factor, $\mathcal{S}^{zz}(\mathbf{k})$, shows a non-divergent sharp peak at $\mathbf{k}_F = 0$. At $\mathbf{Q}_K = (\pm 4\pi/3, 0)$ and $\mathbf{Q}_\Gamma = (0, 0)$ we have

Figure 8. The plot of the out-of-plane form factor $\mathcal{F}^{zz}(\mathbf{k})$ for the two dispersive bands on the Kagomé lattice at $S = 1/2; \Delta = h_{xx} = 0$.

Figure 9. The plot of the off-diagonal structure factor $\mathcal{S}^{\pm\pm}(\mathbf{k})$ and out-of-plane structure factor $\mathcal{S}^{zz}(\mathbf{k})$ for the triangular lattice at $S = 1/2; \Delta = h_{xx} = 0$. 
We have shown that linear spin wave theory works remarkably well in the description of quantum Kagomé ice hardcore bosons. Due to the $Z_2$-invariance of the quantum Kagomé ice hardcore boson model, the excitation spectra are fully gapped at all momenta and the resulting occupation number is very small. The gapped nature of the excitation spectrum enhances the estimated values of the thermodynamic quantities. We have showed that these values are in very good agreement with finite temperature quantum Monte Carlo (QMC) simulations. We observed Bragg peaks in the structure factors at the centre and corners of the Brillouin zone for the Kagomé lattice. This is a special feature of the $Z_2$-invariance of the Hamiltonian. For the triangular lattice, we also observed Bragg peaks in the structure factors at the corners of the Brillouin zone. These are the consequences of the roton minimum in the energy spectrum. Although we have partially studied this model numerically, the results presented in this paper are sufficient for us to understand the nature of quantum Kagomé ice hardcore bosons. However, it would be interesting to explore the other properties of this model with an explicit zero-temperature QMC analysis.

$$S_{\pm}(Q_K) = S \sqrt{\frac{1 + \Delta}{(21 + 3\Delta)}}, \quad (31)$$

$$S_{\pm}(Q_T) = \frac{S}{(\sqrt{21 + \Delta})}. \quad (32)$$

Figure 10 shows the trend of $S_{\pm}(Q_K)$ and $S_{\pm}(Q_T)$ as a function of $\Delta$.
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References

[1] Huang Y-P, Chen G and Hermele M 2014 Phys. Rev. Lett. 112 167203
[2] Gingras M J P and McClarty P A 2014 Rep. Prog. Phys. 77 056501
[3] Carraquilla J, Hao Z and Melko R G 2015 Nat. Commun. 6 7421
[4] Owerre S A, Burkov A A and Melko R G 2016 Phys. Rev. B 93 144402
[5] Greiner M et al 2002 Nature 415 39
[6] Duan L-M, Demler E and Lukin M D 2003 Phys. Rev. Lett. 91 090402
[7] Struck J et al 2013 Nat. Phys. 9 738
[8] Kyriienko O et al 2015 EPL 109 57003
  Eisenstein J P and MacDonald A H 2004 Nature 432 691
  Burkov A A and MacDonald A H 2002 Phys. Rev. B 66 115320
[9] Matsubara T and Matsuda H 1956 Prog. Theor. Phys. 16 569
[10] Bernardet K et al 2002 Phys. Rev. B 65 104519
[11] Sandvik A W and Hamer C J 1999 Phys. Rev. B 60 6588
  Hen I and Rigol M 2009 Phys. Rev. B 80 134508
[12] Coletta T, Laflorence N and Mila F 2012 Phys. Rev. B 85 104421
[13] Gomez G and Joannopolos J D 1987 Phys. Rev. B 36 8707
[14] Sandvik A W and Melko R G 2006 Ann. Phys. 321 1651
[15] Fujiki S and Betts D D 1986 Can. J. Phys. 64 876
[16] Nishimori H and Nakamichi H 1988 J. Phys. Soc. Jpn. 57 626
[17] Weihtong Z, Oitmaa J and Hamer C J 1991 Phys. Rev. B 44 11869
  Oitmaa J, Hamer C J and Weihtong Z 1992 Phys. Rev. B 45 9834
[18] Hamer C J, Oitmaa J and Weihtong Z 1991 Phys. Rev. B 43 10789
[19] Holstein T and Primakoff H 1940 Phys. Rev. 58 1098
[20] Harris A B, Kallin C and Berlinsky A J 1992 Phys. Rev. B 45 2899
[21] Owerre S A 2016 Phys. Rev. B 93 094436