Effects of Dzyaloshinskii-Moriya interaction on Spin 1/2 XY Model with Ring Exchange on a Triangular Lattice

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We analyse the linear spin wave theory calculation of the superfluid phase of a hard-core boson model with nearest neighbour exchange interaction $J$, Dzyaloshinskii-Moriya (DM) exchange interaction $D$ and four-particle ring-exchange interaction $K$ at half filling on the triangular lattice, as well as the phase diagrams of the system at zero and finite temperatures. We find that the DM interaction can be removed from the Hamiltonian by redefining the spin operators but this leads to a change in the nearest neighbour exchange interaction. We also find that the pure $J$ model (XY model) which has a well known uniform superfluid phase with an ordered parameter $(S^x) \neq 0$ at zero temperature is quickly destroyed by the inclusion of a negative-$K$ ring-exchange interactions for $D \neq 0$, favouring a state with a $(\frac{\pi}{2}, 0)$ ordering wavevector. We further study the behaviour of the zero temperature superfluid density and finite-temperature Kosterlitz-Thouless phase transition ($T_{KT}$) in the uniform superfluid phase for some values of $\kappa = K/J, \eta = D/J$, by forcing the universal quantum jump condition on the finite-temperature spin wave superfluid density. At zero temperature, we find that the maximum values of the superfluid density as a function of $\kappa$ increases as $\eta$ increases which shows that the DM exchange interaction constant increases the zero temperature superfluid density.

I. INTRODUCTION

The effective studies of continuum field theories have resulted in detailed predictions for the low-energy physics of quantum spin systems in two dimensions. Spin wave theory can provide us with a rather accurate picture of the low-lying states of quantum spin systems. There are several versions of spin wave theory. The standard spin wave theory is based on Holstein-Primakoff representation\textsuperscript{[10]} which was first applied to the study of the Heisenberg model by Anderson\textsuperscript{[3]} and further extended to second order by Kubo\textsuperscript{[4]} and Oguchi\textsuperscript{[5]}. Spin wave theory was thought to be unsatisfactory in the case of XY model until Gomez-Santos and Joannopoulos\textsuperscript{[6]} showed that by a good choice of quantization axis, one can obtain a good theoretical result for XY model. Since then numerous applications of spin wave theory have been carried out on XY model with different lattice configurations and the results obtained so far are in a good agreement with quantum Monte Carlo simulations (QMC)\textsuperscript{[11,12]}. Magnetic spin models can be supplemented with antisymmetric spin exchange interaction called Dzyaloshinskii-Moriya (DM) interaction which arises from spin-orbit coupling. This interaction was first proposed by Dzyaloshinskii\textsuperscript{[23]} and later derived by Moriya\textsuperscript{[24]}. We shall see later that such additional interaction does not change the form of the original Hamiltonian, it only leads to changes in the exchange interaction constants.

Another interesting area is the multiple (ring) spin-exchange models. This model was first introduced to describe the magnetic properties of solid $^3$He\textsuperscript{[15]}. It incorporates ring-exchange interactions over plaquettes such as spin 1/2 four-spin XY ring exchange of the form:

$$H_K = -K \sum_{ijkl} (S^+_i S^-_j S^+_k S^-_l + S^-_i S^+_j S^-_k S^+_l), \quad (1)$$

where the summation runs over plaquettes with the indices running counter-clockwise, $i$ and $j$ are nearest neighbours lying opposite to $k$ and $l$.

The ring exchange interaction is important in Wigner crystal near the melting density.\textsuperscript{[13]} This model, alone or in competition with pure XY model with nearest neighbour exchange has attracted considerable attention over the years and has been studied extensively on a square lattice using a stochastic series expansion (SSE) quantum Monte Carlo method\textsuperscript{[3]}, also a comprehensive theoretical study (spin wave theory) has been done on a square lattice.\textsuperscript{[3]} It has been suggested in recent works that models of this form may harbour exotic ground state properties, including de-confined quantum critical points or quantum spin liquid phases.

In this paper, we shall calculate the exact (numerical) value of the Kosterlitz-Thouless temperature, superfluid density and other low temperature thermodynamical properties of spin 1/2 XY model with ring exchange and DM interactions on a triangular lattice using linear spin wave theory without the inclusion of the repulsive interaction between bosons.

The format of the paper is as follows: In Sec.II, we present the model Hamiltonian. In Sec.III, we apply linear wave theory by choosing our quantization axis along the $z$-direction and use it to diagonalize the Hamiltonian and obtain its energy. In Sec.IV, we analyze the dispersion and plot it for some values of $\kappa$ and $\eta$. In Sec.V, we explore the zero temperature superfluid density using the diagonalized Hamiltonian and plot it as a function of $\kappa$ for some values of $\eta$. In Sec.VI, we calculate the finite
temperature superfluid density for some values of $\kappa$ and $\eta$ and the values of the Kosterlitz-Thouless temperature for this model and in Sec. VII, we make some concluding remarks.

II. MODEL

In this section, we shall present the model Hamiltonian and the mean field theory argument of the J-K model on a triangular lattice, similar work was done on a square lattice\cite{12} for $\vec{D} = 0$. Our model Hamiltonian is given by

$$H = -2 \sum_{(ij)} \left( J \vec{S}_i \cdot \vec{S}_j + \vec{D} \cdot (\vec{S}_i \times \vec{S}_j) \right)$$

$$-K \sum_{(ijkl)} \left( S^+_{i} S^-_{j} S^+_{k} S^-_{l} + S^+_{i} S^-_{j} S^-_{k} S^+_{l} \right). \quad (2)$$

where $\vec{S}_i = (S^x_{i}, S^y_{i})$ and $S^\pm_{i} = S^{x}_{i} \pm i S^{y}_{i}$.

The first summation is over nearest neighbour pairs on a triangular lattice and the second summation runs over the three possible plaquette orientations on a triangular lattice as shown in Fig. 1. It has been shown that this Hamiltonian undergoes a Kosterlitz-Thouless phase transition for $\vec{D}, K = 0$ at $T_{KT} \approx 0.69$ for 2D model and a superfluid phase for temperatures less than $T_{KT}$\cite{12}. For $\vec{D} = 0, K < 0$, there is a sign problem which prevents (QMC) simulation\cite{12} though it is not possible to capture this sign problem in the linear spin wave theory. QMC simulation on a square lattice has been performed for $\vec{D} = 0, K > 0$ in which there is no sign problem\cite{12}. For simplicity, let’s assume that $\vec{D} = D e_x$, that is $\vec{D}$ points in the z-direction. Then $\vec{D}$ takes the form

$$H = -\sum_{(ij)} [(J + iD)S^+_{i} S^-_{j} + (J - iD)S^+_{i} S^+_{j}]$$

$$-K \sum_{(ijkl)} \left( S^+_{i} S^-_{j} S^+_{k} S^-_{l} + S^+_{i} S^+_{j} S^-_{k} S^-_{l} \right). \quad (3)$$

Rotating globally about the z-axis\cite{22} by an angle $\pm \alpha/2$ we have

$$S^+_{i} \rightarrow S^+_{i} e^{i\alpha/2}, S^-_{j} \rightarrow S^-_{j} e^{-i\alpha/2},$$

$$S^+_{k} \rightarrow S^+_{k} e^{-i\alpha/2}, S^+_{l} \rightarrow S^+_{l} e^{i\alpha/2}. \quad (4)$$

where $\alpha = \arctan(D/J)$. Plugging $\begin{pmatrix} 1 \end{pmatrix}$ into $\begin{pmatrix} 3 \end{pmatrix}$, the Hamiltonian transforms into

$$H = -J_D \sum_{(ij)} \left( S^+_{i} S^-_{j} + S^-_{i} S^+_{j} \right)$$

$$-K \sum_{(ijkl)} \left( S^+_{i} S^-_{j} S^+_{k} S^-_{l} + S^-_{i} S^+_{j} S^-_{k} S^+_{l} \right). \quad (5)$$

where $J_D = \sqrt{J^2 + D^2} = J \sqrt{1 + D^2}, \quad \eta = D/J$.

Therefore we see that the redefinition of the spin operators removes the DM interaction and rescales the nearest neighbour interaction but has no effect on the ring exchange term.

Let’s define the spins as classical vectors by making the transformation $S^\pm_{i} = \rho e^{i\phi_i}$. The model Hamiltonian becomes

$$H = -2J_D \sum_{(ij)} \rho^2 \cos(\phi_i - \phi_k)$$

$$-2K \sum_{(ijkl)} \rho^4 \cos(\phi_i - \phi_j + \phi_k - \phi_l). \quad (6)$$

Now lets consider the case $J_D, K > 0$, in this case, minimizing the energy we have $\phi_i = \phi_j$ for the $J_D$ term and $\phi_i = \phi_j, \phi_k = \phi_l$ for the $K$ term which leads to a ferromagnetic ordering of spins. Consider the case $J_D, K < 0$, in this case, minimizing the energy we have $\phi_i - \phi_j = \pi$ or $\phi_i = \phi_j - \phi_k - \phi_l = 0$ or $\phi_i = \phi_j = \phi_k = 0, \phi_i = \pi$ for the $K$ term which leads to ud (up-down) state for the $J_D$ term and und state on the plaquettes, basically we have two configurations of spins on the lattice.

This model has also been considered by L. Balents and A. Paramakant with the inclusion of the repulsive interaction $U$ term between bosons without the DM term $D = 0$, that is $J_D = J$ and also in the regime where $J << K$. They showed that when $J = 0$, the four-spin exchange leads to a manifold of ground states with gap less excitations and critical power-law correlations and when $J \neq 0$, fluctuations select a four-fold ferromagnetically ordered ground state with a small spin (superfluid) stiffness which breaks the global $U(1)$ and translational symmetry but they did not obtain any exact (numerical) value of the Kosterlitz-Thouless temperature and the superfluid density.

From their Hamiltonian they argued that with $J = 0$, the ground state is independent of the sign of $K$ and for non-zero $J$, the sign of $K$ is vital, for $J < 0$ with $K < 0$, there is a ferromagnetic phase while $J > 0$ leads to a $\sqrt{3} \times \sqrt{3}$ Neel order which are also the ground states for large $|J/K|$. They finally concluded that there are no phase transitions at any non-zero $J$ other than the well known phases.

III. LINEAR SPIN WAVE THEORY

The basic assumption of spin wave theory lies on selecting a classical ground state and determining the fluctuation around it. In other words, one considers quantum fluctuations very close to an ordered ground state configuration of the system under study. By the usual mapping between spins $S = 1/2$ and the hard-core bosons, we can view $\begin{pmatrix} 2 \end{pmatrix}$ as a hard-core boson model. For $J >> D, K$ or $D, K = 0$, the $T = 0$ ground state (in-plane ferromagnet) has an ordered parameter $M_x = \langle S_x^\uparrow \rangle \neq 0$ which breaks the $U(1)$ global rotational symmetry or a superfluid phase in the hard-core boson version\cite{15,20}. One can therefore perform a spin wave expansion around this ordered state configuration by introducing the boson operators $a_i^\dagger$ and $a_i^\dagger$ which represent the low-energy spin wave
excitations out of \( \langle S_i^x \rangle \) and treat other terms in \([5]\) as perturbations.

We shall proceed by analysing the dispersion of this model in the limit \( D, K = 0 \) as expected. This diagonalized Hamiltonian \([8]\) will be used to analyse some properties such as dispersion, ground state, internal energy, superfluid density etc., all as a function of \( \kappa \) and \( \eta \).

### IV. SPIN WAVE ENERGY DISPERSION

We shall now proceed by analysing the dispersion of this model for some values of \( \kappa \) and \( \eta \). We shall set \( J = 1/2 \) which corresponds to the parameter value of pure XY model for which \( D, K = 0 \). From the diagonalized form of the Hamiltonian, the dispersion for \( \kappa = -4/3 \) is given by

\[
\epsilon (\mathbf{k}) = 2\omega_k = 2\sqrt{A_k^2 - B_k^2} = \sqrt{1 - \gamma_k}.
\]  

(18)

The graph of \([18]\) is shown in Fig.\(2\) for \( \eta = 0 \). It shows a zero mode at the corners and the center of the Brillouin zone of a triangular lattice. The dispersion along the \( k_x \) direction for \( k_y = 0 \) is \( 2\pi/\sqrt{3} \) and \( \kappa = -4/3 \) is also shown in Fig.\(2\) for several values of \( \eta \). There are three zero modes at \( \mathbf{k} = \mathbf{Q} = (0,0), \mathbf{k} = \pm \mathbf{Q} = (\pm 2\pi/3, 0) \) for \( \eta = 0, k_y = 0 \), away from this value of \( \eta \), there is only one zero mode which is at the center of the Brillouin zone \( \mathbf{k} = \mathbf{Q} = (0,0) \).

For \( \eta = 0, k_y = 2\pi/\sqrt{3}, \) there is only one zero mode at \( \mathbf{k} = \pm \mathbf{Q} = (\pm 2\pi/3, 0) \). If one chooses ferromagnetic ordering along the \( k_y \) axis then the corresponding ordering wave
vector is \( \mathbf{k} = \pm \mathbf{Q} = (\pm \frac{2\pi}{3}, 0) \) which is the soft modes of the dispersion for \( \kappa = -4/3, \eta = 0 \). The linear spin wave instability of the excitation spectrum at the corner of the Brillouin zone \( \mathbf{k} = \pm \mathbf{Q} = (\pm \frac{2\pi}{3}, 0) \) occurs for \( \eta = 0, \kappa = -4/3 \). For the pure \( XY \) model \( \eta = 0, K/J = 0 \), there is a gapless excitation at \( \mathbf{Q} = (0,0) \) (Goldstone mode of the superfluid phase), but there is no minima at the ordering wave vector. Near the zero modes for \( \eta = 0, \kappa = -4/3 \) we have

\[
\epsilon(\mathbf{k}) = \frac{\sqrt{3}}{2} (k_x^2 + k_y^2)^{1/2} = \sqrt{3} J k.
\]  

(19)

V. SUPERFLUID DENSITY AT \( T = 0 \)

In this section we shall explore the superfluid density of this model on a triangular lattice. This is done by making a phase twist \( \theta \) on the lattice sites. The relevant transformations have been worked out for a similar model on the square lattice, with this transformations it was found that the ring exchange term is independent of the phase angle. Using this transformation, the twisted Hamiltonian becomes

\[
H(\theta) = -2J_D \sum_{\langle ij \rangle} \left\{ (S^x_i S^x_j + S^y_i S^y_j) \cos \theta + (S^x_i S^y_j - S^y_i S^x_j) \sin \theta \right\} - K \sum_{\langle ijkl \rangle} (S^+_i S^-_j S^+_k S^-_l + S^-_i S^+_j S^-_k S^+_l).
\]  

(20)

Comparing (5) and (21), we see that the effect of the twist is to rescale the nearest-neighbour exchange interaction in (2) as \( J_D \to J_D \cos \theta \). Therefore, the diagonalized form of (21) is exactly of the form (8) with \( J_D \) replaced by \( J_D \cos \theta \). That is

\[
H(\theta) = H_{MF}(\theta) + \sum_{\mathbf{k}} (\omega_{\mathbf{k}}(\theta) - A_{\mathbf{k}}(\theta)) \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \sum_{\mathbf{k}} \omega_{\mathbf{k}}(\theta) \left( \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}^\dagger \right),
\]  

(22)

where the twisted mean-field energy and the coefficients are given by

\[
H_{MF}(\theta) = -3 \left( \frac{1}{2} J_D N \cos \theta + \frac{1}{8} KN \right),
\]  

(23)

\[
\omega_{\mathbf{k}}(\theta) = \sqrt{A_{\mathbf{k}}(\theta)^2 - B_{\mathbf{k}}(\theta)^2},
\]  

(24)

\[
A_{\mathbf{k}}(\theta) = J_D Q_{\mathbf{k}} \cos \theta + K R_{\mathbf{k}},
\]  

(25)

\[
B_{\mathbf{k}}(\theta) = J_D S_{\mathbf{k}} \cos \theta + K T_{\mathbf{k}}.
\]

The free energy is given by

\[
F(\theta) = -\frac{1}{\beta} \ln Z(\theta) = E_0(\theta) + \frac{1}{\beta} \ln \left( 1 - e^{-\beta \epsilon(\theta)} \right),
\]  

(26)

where the ground state energy \( E_0(\theta) \) is given by

\[
E_0(\theta) = H_{MF}(\theta) + \sum_{\mathbf{k}} (\omega_{\mathbf{k}}(\theta) - A_{\mathbf{k}}(\theta)).
\]  

(27)
At zero temperature, the free energy is simply the ground state energy. Taylor expanding the ground state energy we have

$$ E_0(\theta) = E_0(\theta = 0) + \frac{1}{2} \rho_s \theta^2 + O(\theta^4), $$

(28)

$$ \rho_s(T = 0) = \frac{1}{N} \frac{\partial^2 E_0(\theta)}{\partial \theta^2} \bigg|_{\theta = 0}. $$

(29)

The expression for $\rho_s$ can be obtained from (27) by expanding the $\cos \theta$ to order $\theta^2$ and differentiating. This gives

$$ \rho_s(T = 0) = \frac{3J_D}{4} + \frac{J_D}{2N} \sum_k \left[ Q_k - \frac{1}{\omega_k} \right] \left( J_D \left( Q_k^2 - S_k^2 \right) + K \left( Q_k R_k - S_k T_k \right) \right), $$

(30)

where we have divided by 2 to account for the dimensionality of the lattice.

The plot of $\rho_s(T = 0)$ is shown in Fig. 3 for a range of $\kappa$ and several values of $\eta$. The superfluid density curve shows a maximum at $\kappa = 0$, with a value of $\rho_s = 0.4140$ for $\eta = 0$, $\rho_s = 0.4140$ for $\eta = 0.2$, $\rho_s = 0.4372$ for $\eta = 0.4$, $\rho_s = 0.4734$ for $\eta = 0.6$. We see that the maximum of the superfluid density increases as $\eta$ increases, therefore the effect of the DM interaction is to increase the superfluid density. We also notice that the curves decrease monotonically with increasing $|K|$ as one moves away from these maxima, in other words the ring exchange term decreases the value of $\rho_s(T = 0)$ from the pure XY result. On the positive-$K$ side, $\rho_s$ decreases relatively gradually, only becomes zero for extremely large values. This is consistent with the result obtained in the dispersion, which indicates that no soft modes develop for moderate values of positive $K$. Similar result was observed on a square lattice for $\eta = 0$, which is consistent with quantum Monte Carlo simulation. On the negative-$K$ side, the value of $\rho_s$ decreases rapidly as it approaches $\kappa = -4/3$.

**VI. SUPERFLUID DENSITY AND KOSTERLITZ-THOULESS TRANSITION AT FINITE TEMPERATURE**

In this section we shall discuss the uniform superfluid phase of our model at finite temperatures. In order to calculate the finite temperature superfluid density, we replace the twisted ground state energy in (29) with the twisted free energy, that is

$$ \rho_s(T \neq 0) = \frac{1}{N} \frac{\partial^2 F(\theta)}{\partial \theta^2} \bigg|_{\theta = 0}. $$

(31)

Using (26) we obtain

$$ \rho_s(T \neq 0) = \frac{3J_D}{4} + \frac{J_D}{2N} \sum_k \left[ Q_k - \frac{1}{\omega_k} \right] \left( J_D \left( Q_k^2 - S_k^2 \right) + K \left( Q_k R_k - S_k T_k \right) \right) \left( 1 + 2 \frac{e^{\epsilon_k/T}}{1 - e^{\epsilon_k/T}} \right). $$

(32)

This expression for $\rho_s(T)$ is plotted as a function of $T/J$ in Fig. 4 for some values of $\kappa$ and $\eta$.

![Graph showing the superfluid density as a function of $T/J$ for different values of $\kappa$ and $\eta$.](image)

**FIG. 4:** (Color online) The superfluid density as a function of $T/J$ for $\kappa = 0$ (top), lines are labelled by the parameter value $\eta$ and for $\kappa \neq 0$ (bottom), lines are labelled by the parameter value $\eta$ and $\kappa$. The dashed line is the universal jump condition.

The graph shown in Fig. 4 is similar to the one obtained on a square lattice for $\eta = 0$ which shows slowly...
decaying superfluid density. We see that the superfluid phase for $\kappa = 0, \eta = 0$ is being destroyed for $\kappa < 0$ regardless of the value of $\eta$. The dash line is the so-called universal jump condition

$$\frac{\rho_s(T_{KT})}{T_{KT}} = \frac{2}{\pi},$$

(33)

which accounts for the discontinuity in $\rho_s(T)$. The estimate of $T_{KT}$ can be found by solving $\rho_s(T)/T = 2/\pi$, using $\rho_s(T)$ from our spin wave theory. Using this procedure we found the $KT$ transition temperature at $T_{KT} = 0.9295J$ for $\kappa = 0, \eta = 0$ and $J = 1/2$, the parameter values for the pure XY model. This is shown in Fig. 1, where the dashed line crosses the curve for $\kappa = 0, \eta = 0$. We can as well read off the values of $T_{KT}$ for $\kappa \neq 0, \eta \neq 0$. The full analysis of this model for $\eta = 0$ has been worked out previously by the same author of this article.\(^{23}\)

VII. CONCLUSION

We have analysed the study of linear spin wave theory of hard-core bosons (zero field XY model) with DM and ring exchange interactions at half filling on the triangular lattice. We studied through linear spin wave theory the destruction of uniform superfluid phase by the bosonic ring exchange model on a triangular lattice at half filling. The dispersion of this model was calculated by applying the traditional Holstein-Primakoff representation and summing over the three plaquettes orientations on a triangular lattice. This calculation showed a spin wave instability and a development of three minima at $k = \pm\mathbf{Q} = (\pm \frac{2\pi}{a}, 0)$, and $k = \mathbf{Q} = (0, 0)$ for $\kappa = -4/3, \eta = 0$. One should expect a phase transition from a superfluid phase to another phase at this wave vector $k = \mathbf{Q} = (\frac{2\pi}{3a}, 0)$ for $\kappa = -4/3, \eta = 0$. We hope that quantum Monte Carlo data should provide further insight into this issue.

The mean field superfluid density and ground state (zero temperature) spin wave superfluid density obtained in this model for $\kappa = -4/3, \eta = 0$ is bigger than that of a square lattice.\(^{3}\) despite the fact that both are 2D systems. This might be due to a larger number of nearest neighbours and plaquettes on a triangular lattice. We calculated the finite temperature uniform superfluid density and use it to estimate the Kosterlitz-Thouless transition temperature by forcing it to obey the universal quantum jump condition. We also analyse the effect of DM interaction on the superfluid density by plotting it for several values of $\eta$ as a function of $\kappa$. It was found that the DM interaction increases the maximum of superfluid density at zero temperature. It has been shown with the model Hamiltonian \((5)\) on a square lattice using QMC simulations for $\eta = 0$ that for small $K > 0$ away from the XY point, the zero-temperature spin stiffness value of the XY model is decreased.\(^{3}\) Our results above seem to agree with this trend found in QMC simulations.

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