THE PHYSICS OF SPIN-1/2 XY MODEL WITH FOUR-SITE EXCHANGE INTERACTION ON THE KAGOME LATTICE

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ABSTRACT

The quantum spin liquid (QSL) state, proposed more than three decades ago by Fazekas and Anderson remains surprisingly elusive. Although recent experiments provide a strong evidence of their existence in the frustrated spin systems, the microscopic model for this state is still rare. The extensive theoretical framework, developed over decades, continues to extend further motivated by these and other discoveries from large-scale computer simulations of a relatively small number of models. In this work, we discuss the physics of the ground-state phase diagram of a two-dimensional Kagome lattice spin-1/2 XY model with a four-site ring-exchange interaction using quantum Monte Carlo simulation. We found the second order phase transition from superfluid state to a Z_2 quantum spin liquid phase driven by the four-site ring exchange interaction. We have characterized the QSL by its vanishing order parameters such as the spin-spin structure factor, the plaquette-plaquette structure factor. Moreover, we have found the large anomalous exponent $\eta_{XY^*} \approx 1.325$ which belongs to a different universality class other than 3D XY universality class. There is no signal of supersolid phase intervening between the superfluid state and QSL state.

Keywords: Quantum Spin Liquid, Kagome Lattice, Quantum Monte Carlo, Ring Exchange Model, critical exponents.

1. INTRODUCTION

Although Fazekas and Anderson [1] proposed an idea of quantum spin liquid (QSL) state three decades ago, recent neutron scattering experiments on the spin-1/2 Kagome lattice $ZnCu_3(OH)_6Cl_2$ (Herbertsmithite) [2] and prochlore compounds mapping to Kagome ices, particularily $Tb_2Ti_2O_7$, $Yb_2Ti_2O_7$, $Pr_2Zr_2O_7$, and $Pr_2Sn_2O_7$, provide the significant evidences of its existence [3,4,5]. The extensive study of QSL is expected to have a large impact on the future computing technology like a topological quantum computing [6,7]. It is believed that the geometric frustration is a main ingredient for a microscopic model of QSL state. The theoretical framework has developed for three decades, and still needs to explore further due to the complexity of QSL phase structure [8,9]. The significant motivation came from the power of large-scale computer simulation after Yan et al. has recently applied density matrix renormalization group to explain the existence of QSL in the ground state of the Kagome-lattice

Heisenberg antiferromagnet [10]. However, the study of a gapped QSL using Quantum Monte Carlo simulation of the honeycomb lattice Hubbard model at half filling predicted some contradiction [11]. The difficulty in finding models for Quantum Monte Carlo is the fact that the frustration typically leads to the infamous sign problem. Fortunately, Balents et al. proposed a sign-problem free Hamiltonian of spins on Kagome lattice exhibited the QSL state which can be attacked by Quantum Monte Carlo simulation [12]. Recently Dang et al. has also utilized the large-scalable Quantum Monte Carlo to extract the signals of QSL in Kagome lattice [13]. The interesting transition to QSL state characterized by an exotic XY* universality class, namely XY* universality class, caused by the condensation of bosonic spinons, which has unfortunately not been addressed yet. Although the neutron scattering experiments in Cs_2CuCl_4 suggested the large anomalous dimension η_{XY*} in the range of 0.7-1.0 [14,15].

More interestingly, Bloch et al. [16] has proposed a unique experiment setting for quantum simulation of the artificial structure in optical lattice with the high degree of controlability. And, Buchler et al. [17] have also provided an experimental design of a ring exchange interaction for ultracold atoms in 2D optical lattice. These settings make the ring exchange model more realiable and controllable.

In this paper, we carry out a study of Z_2 QSL phase using a model with competition between two purely kinetic terms, namely spin-1/2 model with four-site ring exchange interaction in the Kagome lattice. A large scale finite temperature Quantum Monte Carlo (QMC) simulation is applied to characterize the different quantum phases as well as their transition. We find that there is a second order quantum phase transition between the superfluid and quantum spin liquid state driven by the ring exchange interaction. A significant large anomalous critical exponent $\eta_{XY*} \approx 1.325$ is qualitatively consistent with the classical Monte Carlo simulation [18] as well as the broad line shapes seen in experiment of Cs_2CuCl_4 [14,15].

Moreover, the geometrical frustration does not typically induce the supersolid state [19]. In this study, we have also supported to this claim, i.e. there is no signature of supersolid state intervening between the superfluid state and QSL state.

2. QUANTUM MONTE CARLO SIMULATION

The well-known model of spin-1/2 XY model with four-site exchange interaction Hamiltonian reads:

$$H = -J\sum_{<ij>} B_{ij} - K\sum_{<ijkl>} P_{ijkl} \qquad (1)$$

Where $<i,j>$ denotes a pair of nearest neighbor sites and $<ijkl>$ denotes the sites on the corners of a bow-tie plaquette on 2D Kagome lattice, J factor is the nearest neighbor coupling strength and K factor is the foursite ring exchange strength; the bond operator $B_{ij} = (S_i^+ S_j^- + S_i^- S_j^+)$ describes the nearest neighbor XY exchange interaction; and the plaquette operator $B_{ij} = (S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+)$ (the labelling rule is defined in Figure 1 a) describes the four-site ring exchange interaction (Figure 1b). Hamiltonian (1), in short J-K model, can be mapped into the Bose-Hubbard model using the Holstein-Primakoff transformation. In the bosonic language, the bond operator represents the hopping energy between two nearest neighbor interaction whereas the plaquette operator represents the ring hopping around the 4 sites on Kagome lattice (Figure 1 c). Interestingly, two terms J and K are all purely kinetic energy which is different from the regular model in which the exotic phase driven by the competition between the kinetic and potential energy. For simplicity, J = 1 has been chosen for energy scale. The same version of Hamiltonian (1) , except for the square lattice XY ring exchange model, has shown the deconfined quantum critical point between a superfluid and valence-bond-solid (VBS). VBS has shown a non-magnetic order but its plaquette correlation displays a long range feature, meaningly, there is no QSL state in the square lattice model.

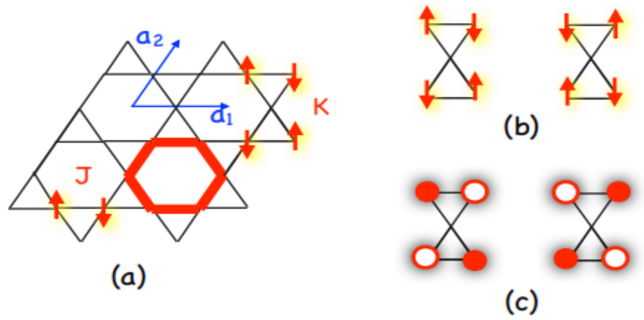

Figure 1÷. (a) Kagome lattice and a labeling convention for the indices of the bond operator B_{ij} and plaquette operator P_{ijkl}. Two primitive vectors $\vec{a}_1, \vec{a}_2$ are shown. (b) Two spin plaquette configuration describes the four-site spin ring exchange. (c) Particle-hole configuration represents the plaquette configuration in the bosonic language.

We investigate the J-K model (1) using QMC technique namely the stochastic series expansion (SSE) algorithm [20,21] which does not suffer from sign problem. The system size are defined as $\vec{L}_1 = n_1\vec{a}_1$ and $\vec{L}_2 = n_2\vec{a}_2$ with two primative vectors $\vec{a}_1 = \vec{a}_2 = 1$(shown in Figure 1.a). Moreover, the total number of sites in the simulation cell is defined as $N_s = n_1 \times n_2 \times 3$. In principle, we can make $n_1 \neq n_2$ to investigate the structure as a ladder, we however take $n_1 = n_2 = L$ for simplicity.

The QMC simulations have been carried out at finite temperature but the ground state phase diagram can be extrapolated at very low temperature. In other words, the imaginary time β ≈ L has been fixed during the simulations. The finite temperature phase diagram could be addressed in the other MC studies. We characterize the various phases in this model by investigating the spin stiffness as well as the spin and plaquette structure factors. The spin stiffness is defined as:

$$\rho_s = \frac{1}{N_s}\frac{\partial^2 E(\phi)}{\partial \phi^2} \qquad (2)$$

Where ϕ is a twist in the periodic boundary of the lattice, hence the spin stiffness is the energy $E(\phi)$ response to the twist. In bosonic language, it is a superfluid density induced by the winding numbers in imaginary time space configuration. The spin structure factor can be calculated from the Fourier transformation of the z-component, $S^z_{k,l} = (1/2)\sigma^z_{k,l}$ with $\sigma^z_{k,l} = \pm 1$, of the spin-spin correlation function $\left\langle S_k^z S_l^z \right\rangle = \frac{1}{4}\left\langle \frac{1}{n}\sum_{p=1}^{n-1}\sigma_k^z(p)\sigma_l^z(p) \right\rangle$ with n is the number of non-identity operators in the Monte Carlo - SSE operator list at the wavevector $\boldsymbol{q}=(q_x, q_y)$: $S_s(q_x, q_y) = \frac{1}{N}\sum_{k,l} e^{i(r_k - r_l).q}\left(\left\langle S_k^z S_l^z \right\rangle - \left\langle S_k^z \right\rangle \left\langle S_l^z \right\rangle\right)$(3) Where, k and l are lattice sites and $r_i=(x_i, y_i)$ is the lattice corrdinate. Similarly, the plaquette structure factor reads:

$$B_p(q_x, q_y) = \frac{1}{N}\sum_{m,n} e^{i(r_m - r_n).q}\left(\left\langle P_m^z P_n^z \right\rangle - \left\langle P_m^z \right\rangle \left\langle P_n^z \right\rangle\right) \quad (4)$$

Where P_m, P_n are the plaquette operator

3. RESULTS AND DISCUSSION

Since QSL does not have a regular order parameter as the description in Landau theory of phase transition, the characteristic of the various phases in J-K model (1) must be investigated carefully. We first look at the finite size scaling behavior. In our simulation, we study the superfluid stiffness (2) using the general scaling form near the quantum critical transition point [22]:

$$\rho_S = L^{-z} F_{\rho_S}(tL^{1/\nu}, \beta / L^z) \quad (5)$$

where, F_{ρ_S} is a universal scaling function, and $t = K_c - K$, L is the linear system size, β is the inverse temperature or the imaginary time, z =1 is the dynamical critical exponent , and ν =0.43 is the correlation length exponent [19] which is slightly different from the typical 3D XY universality class. Our simulation shows the superfluid density vanishing with increasing the ring exchange interaction which suggests a second order phase transition. Now, we apply the scaling relation (5) and plot $\rho_S L^z$ as a function of $t = K_c - K$ to determine the critical point K_c= 21.8. Figure 2 shows that all the curves collapse into a single curve for the conventional 3D XY universality class. As the result, we have found the large anomalous exponent $\eta_{XY^*} \approx 1.325$ using the scaling relation [22]:

$$2\beta^* = \nu(d + z - 2 + \eta_{XY^*})$$

Where, β^*=0.5 is the critical exponent, $d = 2$ is the dimensionality for 2D system (taken from the well-known 3D XY universality class). It is worthy to note that an anomalous exponent belonging to the 3D XY universality class $\eta_{XY} \approx 0.04$ which is much smaller than our finding. This can be explained through the condensation of bosonic spinons at the transition. The transition from superfluid to insulating phase with the large anomalous critical exponent suggests that the insulating phase is Z_2 quantum spin liquid.

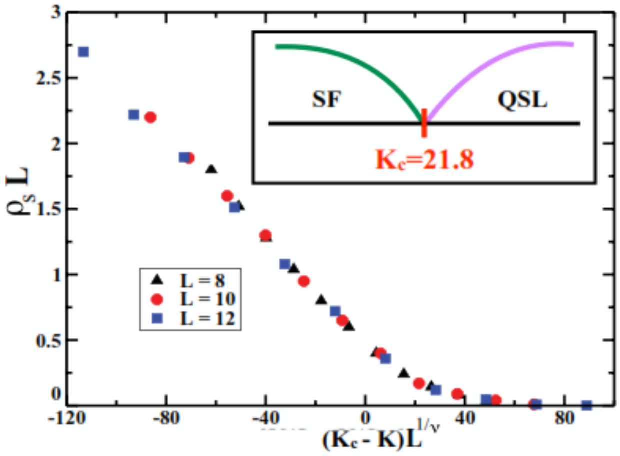

Figure 2÷. Collapse of the scaling function for superfluid density $\rho_s L^z$ at ground state as a function of four-site ring exchange. The critical value of the ring exchange K_c = 21.8 separates the quantum spin liquid with superfluid state. Inset: ground state diagram of Hamiltonian (1) with superfluid phase(SF) and quantum spin liquid (QSL) separated by the critical ring exchange interaction.

In order to rule out the other possibilities of the order phase such as the solid state or the valence bond state, we make a further investigation by examining the spin structure factor. Figure 3 shows the spin structure factor as a function of $1/L_s$ ($L_s = 3 \times L \times L$) of an insulating state with $K = 26$ at the wavevector $q_{max} = (0,\ 4\pi/\sqrt{3})$ corresponding to the Bragg peak required for the long range order such as solid order in crystal. The spin structure factor dies off with an increase of the system size and approaches zero in the thermodynamic limit. This feature signals a short range correlation and rule out the possibility of having solid order with a regular broken symmetry. It immediately rules out the possibility of supersolid phase in this system as well.

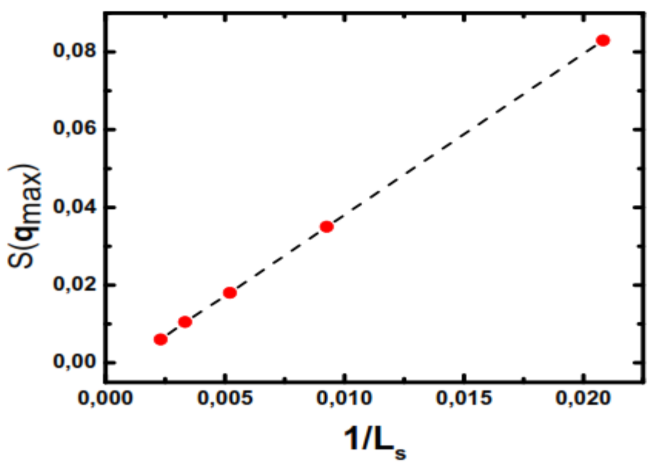

Figure 3÷. Spin structure $S(q_{max})$ at a certain wave vector $q_{max} = (0,\ 4\pi/\sqrt{3})$ as a function of $1/L_s$ $L_s = 3 \times L \times L$) for an insulating state with K =26.

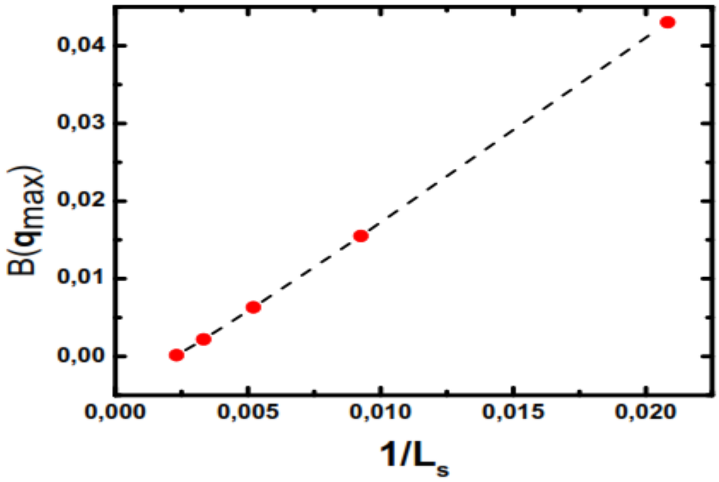

Figure 4÷. Plaquette structure factor $B(q_{max})$ at a certain wave vector $q_{max} = (0, 15\pi / 6\sqrt{3})$ as a function of $1/L_s$ ($L_s = 3 \times L \times L$) for an insulating state with K = 26.

In Figure 4, we illustrate the plaquette structure factor as a function of the inverse system size $1/L_s$. Similar to the spin structure factor, the plaquette structure factor at wavevector$q_{max} = (0, 15\pi / 6\sqrt{3})$ vanishes in the thermodynamic limit. This again shows no evidence of valence bond state for the insulating phase.

4. CONCLUSIONS

In conclusion, we have studied the ground state phase diagram of the Kagome lattice spin-1/2 XY model with a four-site ring exchange model using the modified SSE large-scale quantum Monte Carlo simulation. We have shown the second order transition from superfluid state to quantum spin liquid state belonging to the exotic 3D XY* universality class. The regular order structure such as the solid or spin wave order and valence bond order has not been observed in this system. We have also confirmed that the supersolid state does not exist in this frustrated system. This finding is consistent with the previous study [18]. Significantly, the quantum critical point has a dynamical exponent $z = 1$, the correlation length exponent $\nu = 0.44$ and large anomalous critical dimension $\eta_{XY*} \approx 1.325$. It is very interesting to point out that several system such as $CsCuCl_4$ even shows the spin liquid state at finite temperature instead of its appearance in the ground state phase diagram [14,15]. This suggests a further investigation of the finite temperature phase diagram which is also accessible with SSE simulation. Moreover, the interaction should be taken into account since this may give rise many interesting physics mechanism , i.e. a vison-condensation transition as well as the less computational resource to characterize the phase diagram with SSE simulation.

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