Journal of Physics: Conference Series

Chirality-spin separation in the Hubbard model on the kagome lattice

To cite this article: Masafumi Udagawa and Yukitoshi Motome 2010 *J. Phys.: Conf. Ser.* **200** 012214

Chirality-spin separation in the Hubbard model on the kagome lattice

Masafumi Udagawa and Yukitoshi Motome
Department of Applied Physics, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, Japan
E-mail: udagawa@ap.t.u-tokyo.ac.jp

Abstract. Effect of geometrical frustration in strongly-correlated metallic region is studied for the Hubbard model on the kagome lattice at half filling by a cluster extension of the dynamical mean-field theory combined with a continuous-time auxiliary-field quantum Monte Carlo method. We find that the electron correlation enhances the spin chirality in both vector and scalar channels. The chirality grows as decreasing temperature and exhibits a peak at a low temperature, indicating a new energy scale under strong correlation. The peak temperature is considerably lower than that for the local spin moment, namely, the characteristic temperatures for the chirality and the local moment are well separated. This is a signature of separation between spin and chiral degrees of freedom in the correlated metallic regime under geometrical frustration.

1. Introduction

For a long time, considerable attention has been focused on the role of geometrical frustration in localized spin systems. It has been discussed that large degeneracy due to geometrical frustration opens a way to realize non-trivial ground states, such as spin-liquid state [1, 2], by suppressing conventional long-range ordering. It has also been clarified that geometrical frustration can induce an exotic long-range order composed of some higher rank objects, such as spin chirality [3] and spin quadrupole [4].

On the other hand, much less is known about the effect of geometrical frustration in itinerant electron systems. Recently, several interesting phenomena have been found in itinerant systems and an importance of the geometrical frustration has been pointed out. A typical example is heavy-fermion behavior found in transition metal compounds such as LiV_2O_4 [5], Y(Sc)Mn_2 [6] and β-Mn [7]. In contrast to the heavy-fermion rare-earth compounds, these materials have no explicit localized moments, and therefore, it is difficult to explain their heavy-fermion behavior by the conventional Kondo mechanism based on the interaction between conduction electrons and localized spins. A candidate for the origin of the heavy-fermion behavior is a common feature among these transition metal compounds — geometrical frustration in the underlying lattice structure. In fact, in the related insulating materials, it has been reported that magnetic transition temperatures are strongly suppressed compared to the Curie-Weiss temperatures because of the frustration [8]. Furthermore, characteristic magnetic fluctuations under a suppression of long-range ordering are observed in these materials, and their relation to the heavy-fermion behavior has attracted much interests [9, 10, 11].

In general, in a weakly-correlated metal, the electronic state is well described by a Slater determinant of single-particle states which extend over the entire system. In this case, physical

properties of the system will be rather insensitive to the local lattice structure, i.e., whether or not the lattice is geometrically frustrated. The issue is how this picture is modified when the system enters into a strongly-correlated regime where the electrons tend to be localized due to strong electron interaction. In particular, in the vicinity of the Mott transition, spin moments grow with antiferromagnetic correlations between neighboring sites, and hence, it is expected that these moments suffer from the frustration and lead to some exotic behavior as seen in the localized spin systems. It is intriguing to examine how the geometrical frustration affects the electronic state through the interplay between spin and charge degrees of freedom.

Motivated by these considerations, in this paper, we investigate the effect of geometrical frustration in correlated metallic region for a simple model, the Hubbard model on the kagome lattice. In particular, we will focus on the behavior of spin chirality in comparison with that of the original spin degree of freedom.

2. Model and Methods

As a minimal model including both geometrical frustration and electron correlation, we consider the Hubbard model on the kagome lattice, whose Hamiltonian is given by

$$\mathcal{H} = -t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}\right) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}, \tag{1}$$

in the standard notations. We consider only the nearest-neighbor site hopping on the kagome lattice shown in the left panel of Fig. 1, and set $t = 1$ as an energy unit hereafter. The chemical potential μ is controlled so that the system is at half filling (one electron per site on average). The Mott transition and magnetic fluctuations near the transition have been recently studied for this model by several theoretical methods [12, 13, 14].

To investigate the correlated metallic region of the model (1), we use a cluster extension of the dynamical mean-field theory [15], which enables to describe the Mott transition with including spatial fluctuations within a finite-size cluster. In this method, the original lattice problem is mapped to a cluster impurity problem: In the present study, in order to take account of the effect of geometrical frustration, we consider a 3-site cluster (Fig. 1). We extended the cluster up to 12 sites and confirmed that the spin correlation hardly develops beyond the nearest-neighbors in the parameter range of the following calculations (not shown). To solve the impurity problem, we employ the continuous-time auxiliary-field quantum Monte Carlo method [16], which requires much smaller computational cost compared with the conventional Hirsch-Fye algorithm.

In the next section, we will show the results for the density of states, the spin chirality and the local spin moment. The density of states (DOS) $\rho(\omega)$ is calculated from the one-particle local Green's function, $G_{j\sigma}(\tau) = -\langle T_\tau c_{j\sigma}(\tau) c^\dagger_{j\sigma}(0)\rangle$, ($j = 1-3$ corresponds to the cluster sites in Fig. 1) by using $\rho(\omega) = -\frac{1}{\pi}\text{Im}G_{j\sigma}(\omega+i\delta)$. We use the maximum entropy method for the analytic continuation. Note that $\rho(\omega)$ does not depend on either j or σ within the paramagnetic solution assumed here. For the calculations of magnetic properties, we define the local spin at cluster site j as $\mathbf{s}^\nu_j \equiv \frac{1}{2}\sum_{s,s'} c^\dagger_{js}(\boldsymbol{\sigma}^\nu)_{ss'} c_{js'}$, with the ν-th component of Pauli matrix, $\boldsymbol{\sigma}^\nu$ ($\nu = x, y, z$). By using $\mathbf{s}_j$, we calculate the vector spin chirality, $\mathbf{K}_v \equiv \frac{2}{3\sqrt{3}}(\mathbf{s}_1 \times \mathbf{s}_2 + \mathbf{s}_2 \times \mathbf{s}_3 + \mathbf{s}_3 \times \mathbf{s}_1)$, and the scalar spin chirality, $\mathbf{K}_s \equiv (\mathbf{s}_1 \times \mathbf{s}_2) \cdot \mathbf{s}_3$. In the following, we present the squared moments of the vector chirality $K^2_v \equiv \langle \mathbf{K}^2_v\rangle$ and of the scalar chirality $K^2_s \equiv \langle \mathbf{K}^2_s\rangle$ as well as the local spin moment $s^2 \equiv \langle \mathbf{s}^2_j\rangle$ (s^2 is independent of j). Here, the bracket represents the statistical average taken in the grand-canonical ensemble at temperature T. s^2, K^2_v and K^2_s are two-, four- and six-body equal-time correlation functions, respectively, and obtained by applying the Wick's theorem for each Monte Carlo sampling.

3. Results

First, we present the result of DOS at $U = 6$ and $T = 0.05$ in Fig. 2. For comparison, we also show the non-interacting DOS at $U = 0$. At $U = 0$, $\rho(\omega)$ has peculiar structures, two van-Hove singularities ($\omega \simeq -0.47$ and -2.47) and a flat band ($\omega \simeq 1.53$). At $U = 6$, the system is still in the metallic region with finite DOS at the Fermi level $\omega = 0$, whereas $\rho(\omega)$ shows several characteristic features of strong correlation effect. One is the strong renormalization of the energy scales; the three peaks around $\omega = 0$ are considered as renormalized structures of the van-Hove singularities and the flat band. Another feature is the formation of the Hubbard bands which are observed as two broad humps at $\omega \sim \pm 3$. We note that the result is consistent with the previous one obtained by a similar method but with using the conventional Hirsch-Fye algorithm [14]. The previous study revealed that the critical value of U for the Mott transition is about 8.2. Below we show the results for the spin chirality degrees of freedom in this correlated metallic region at $U = 6$.

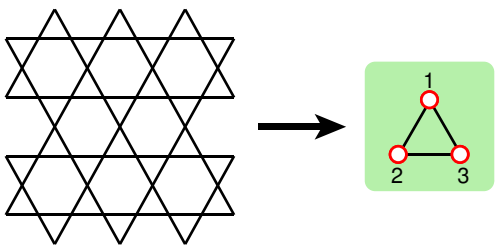

Figure 1. Schematic picture of the mapping of the Hubbard model on the kagome lattice to an effective cluster-impurity Anderson model.

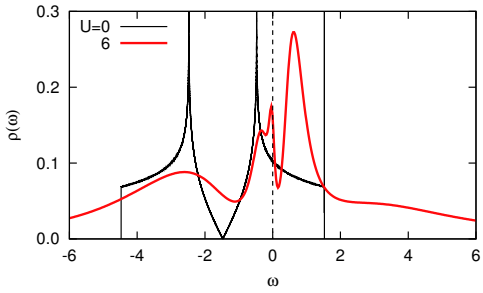

Figure 2. DOS at $U = 6$ and $T = 0.05$ (red) in comparison with the result at $U = 0$ (black). We set the chemical potential to be $\omega = 0$.

Figure 3 shows the temperature dependence of the spin chiralities K_v^2 and K_s^2. At $U = 0$, both K_v^2 and K_s^2 are small and featureless, in spite of the peculiar ω dependence of the DOS. The deviation from the high temperature limits $[K_v^2(T \to \infty) = 1/24$ and $K_s^2(T \to \infty) = 3/256]$ is within 0.03 % for the entire temperature range. In contrast, at $U = 6$, both K_v^2 and K_s^2 are largely enhanced compared with the non-interacting case. Furthermore, as decreasing T, they grow gradually and exhibit a peak at a low temperature $T_K^* \simeq 0.3$. This temperature T_K^* characterizes a new energy scale related with the spin chirality degrees of freedom.

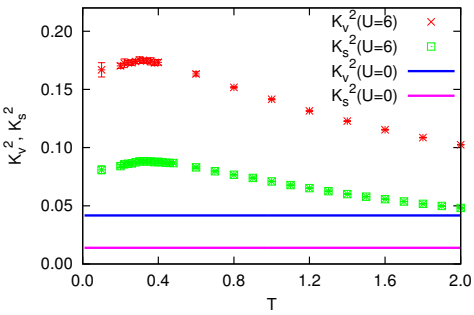

Figure 3. Temperature dependence of K_v^2 and K_s^2 at $U = 6$ and $U = 0$.

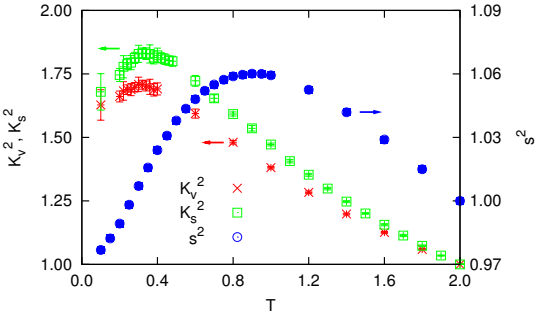

Figure 4. Temperature dependence of K_v^2, K_s^2 and s^2 at $U = 6$. All the data are normalized by the value at $T = 2.0$.

In Fig. 4, we compare this behavior of the chiralities with the local spin moment s^2. s^2 also shows a broad peak, but the peak temperature $T_s^* \simeq 0.9$ is considerably higher than T_K^*. In the intermediate temperature $T_K^* < T < T_s^*$, the chiralities are enhanced while the spin moment is suppressed as decreasing T. This contrastive behavior is surprising because of the following reasons. First of all, by definition, the spin chiralities are composed of the products of spin operators. In fact, their behavior is tightly related with that of the spin moment in most of the localized spin systems. Furthermore, in the present itinerant system, the decrease of s^2 is anticipated to reduce the spin chirality moments since it corresponds to the increase of doubly-occupied or empty sites: The spin chiralities have largest values when they operate on the 3-site triangle which includes no doubly-occupied or empty site. Therefore, the apparent separation between the spin and chirality found in Fig. 4 is highly non-trivial.

4. Summary and Concluding Remarks

We have studied the spin and chirality moments for the Hubbard model on the kagome lattice at half filling by applying the cluster dynamical mean-field theory combined with the continuous-time quantum Monte Carlo method. In metallic region under strong electron correlation, we obtained the following results. (1) The spin chirality is strongly enhanced in both vector and scalar channels, compared with the non-interacting case. It grows as decreasing T and exhibits a peak at a low temperature T_K^*, implying a new energy scale due to the electron correlation. (2) The local spin moment also shows a peak, but the peak temperature T_s^* is substantially higher than T_K^*. In the temperature range between T_K^* and T_s^*, the spin and chirality show opposite temperature dependences. These results suggest a separation of the spin and chirality degrees of freedom in the correlated metallic region in this strongly frustrated system.

The origin of the chirality-spin separation deserves further study. It is also interesting to clarify how the electronic state is affected by the appearance of the new energy scale T_K^* related with the chirality. Another issue is a possibility of some instabilities in the chiral sector by allowing symmetry breaking within the cluster dynamical mean-field framework. Systematic study in a wide region of U and T is now in progress.

We would like to thank S. Sakai for fruitful discussions. We also acknowledge S. Onoda and H. Tsunetsugu for helpful comments. This work was supported by Grant-in-Aid for Scientific Research on Priority Areas (Nos. 17071003, 19052008), Grant-in-Aid for Young Scientists(B) (No. 21740242), Global COE Program "the Physical Sciences Frontier" and by the Next Generation Super Computing Project, Nanoscience Program, MEXT, Japan.

References

[1] Anderson P W 1956 *Phys. Rev.* **102** 1008
[2] Fazekas P and Anderson P W 1974 *Phil. Mag.* **30** 423
[3] Miyashita S and Shiba H 1984 *J. Phys. Soc. Jpn.* **53** 1145
[4] Tsunetsugu H and Arikawa M, 2006 *J. Phys. Soc. Jpn.* **75** 083701
[5] Kondo S *et al.* 1997 *Phys. Rev. Lett.* **78** 3729
[6] Wada H, Nakamura H, Fukami E, Yoshimura K, Shiga M and Nakamura Y 1987 *J. Magn. Magn. Mater.* **70** 17
[7] Shinkoda T, Kumagai K and Asayama K 1979 *J. Phys. Soc. Jpn.* **46** 1754
[8] Ueda Y, Fujiwara N and Yasuoka H 1997 *J. Phys. Soc. Jpn* **66**, 778
[9] Lee S-H, Qiu Y, Broholm C, Ueda Y and Rush J J 2001 *Phys. Rev. Lett.* **86** 5554
[10] Ballou R, Lelievre-Berna E and Fak B 1996 *Phys. Rev. Lett.* **76** 2125
[11] Nakamura H, Yoshimoto K, Shiga M, Nishi M and Kakurai K 1997 *J. Phys.: Condens. Matter* **9** 4701
[12] Imai Y, Kawakami N and Tsunetsugu H 2003 *Phys. Rev.* B **68** 195103
[13] Bulut N, Koshibae W and Maekawa S 2005 *Phys. Rev. Lett.* **95** 037001
[14] Ohashi T, Kawakami N and Tsunetsugu H 2006 *Phys. Rev. Lett.* **97** 066401
[15] Kotliar G, Savrasov S Y, Palsson G and Biroli G 2001 *Phys. Rev. Lett.* **87** 186401
[16] Gull E, Werner P, Parcollet O and Troyer M 2008 *Europhys. Lett.* **82** 57003