Spin and Mass Excitations in the Doped Multiple Spin Exchange Model on a Triangular Lattice: $^3$He on Graphite

K Seki$^1$, T Shirakawa$^{1,2}$ and Y Ohta$^1$

$^1$Department of Physics, Chiba University, Chiba 263-8522, Japan
$^2$Institut für Theoretische Physik, Leibniz Universität Hannover, D-30167 Hannover, Germany

Abstract. Using an exact-diagonalization technique on small clusters, we calculate the spin and density excitation spectra as well as the temperature dependence of the specific heat for the triangular-lattice $t$-$J$ model with the multiple-spin exchange interactions, whereby we consider the low-energy excitations of the two-dimensional liquid $^3$He adsorbed on graphite. We find that, for a relevant set of the parameter values, the spectral weight for the spin excitations is concentrated on a very low-energy region, while that of the density excitations extends over a wide energy range, indicating the clear separation of their energy scales. The double-peak structure in the temperature dependence of the specific heat is also obtained.

1. Introduction

$^3$He atoms adsorbed on a graphite surface is known to be an ideal two-dimensional correlated fermion system. A variety of phenomena have been found to appear depending on the density of $^3$He atoms in the second layer, including a correlated fermi-liquid phase and a solidified commensurate phase at a $4/7$ density of the underlying first layer [1, 2]. The latter $4/7$ phase has been studied by using the triangular-lattice Heisenberg model with the multiple-spin exchange interactions [3, 4], where the opening of the spin gap has been suggested [5]. However, experiments on the magnetic susceptibility [4, 6] and specific heat [7, 8] indicate that the system has the gapless nature of the quantum spin liquid. A double-peak structure in the temperature dependence of the specific heat has also been reported in the doped-Mott region of monolayer $^3$He [9].

Recently, Watanabe and Imada [10] pointed out that the density fluctuations between the second and third layers of $^3$He atoms are essential for understanding the gapless spin-liquid nature. Then, Fuseya and Ogata [11] proposed the doped triangular-lattice $t$-$J$ model with multiple-spin exchange interactions as an effective model for the doped-Mott region of this system and obtained the ground-state phase diagram of the model. The low-energy excitations of the model were also discussed. They thereby argued that there is an anomalous quantum-liquid phase, characteristic of the spin-charge separation, which may be relevant with the anomalous features observed in the $^3$He system.

Motivated by such developments in the field, we study in this paper the triangular-lattice $t$-$J$ model with the multiple-spin exchange interactions further. In particular, we directly calculate the spin and density excitation spectra and single-particle spectra as well as the temperature dependence of the specific heat and uniform magnetic susceptibility by using the
exact-diagonalization technique on small clusters. We thus discuss the peculiar nature of the low-energy physics of the system.

2. Model and method

The triangular-lattice $t$-$J$ model with the multiple-spin exchange interactions is defined by the Hamiltonian

$$
\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} \left[ (1 - n_{i,-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} (1 - n_{j,-\sigma}) + \text{H.c.} \right] + J \sum_{\langle ij \rangle} \left( S_i \cdot S_j - \frac{n_i n_j}{4} \right)
$$

$$
+ K \sum_{\langle ijkl \rangle} (P_4 + P_4^{-1}) + S \sum_{\langleijklmn \rangle} (P_6 + P_6^{-1})
$$

(1)

where $c_{i\sigma}$ is the annihilation operator of a fermion ($^3$He atom) at site $i$ and spin $\sigma (= \uparrow, \downarrow)$, $S_i$ is the spin-1/2 operator, and $n_i (= n_{i\uparrow} + n_{i\downarrow})$ is the number operator. $P_4$ and $P_6$ are the four-spin and six-spin operators, respectively. The nearest-neighbor hopping parameter $t$ and two-spin and four-spin exchange interaction parameters $J$ and $K$ are estimated as follows $^{11}$: $t = 50 - 100 \text{ mK}$, $-J = 1 - 10 \text{ mK}$, and $K/J \sim 0.2$. $S$ is small and is neglected in this paper. Throughout the paper, we use $t = 1$ as the unit of energy and we set $\hbar = k_B = 1$.

We use the Lanczos exact-diagonalization technique on small clusters to calculate the ground state and excitation spectra of the model. In particular, we study the dynamical spin ($\alpha = s$) and density ($\alpha = d$) correlation functions defined as

$$
C_{\alpha}(q, \omega) = \frac{1}{\pi} \Im \langle \Psi_0 | O_{\alpha}^\dagger (q, \omega) O_{\alpha}(q, \omega) | \Psi_0 \rangle
$$

(2)

where $\Psi_0$ and $E_0$ are the ground-state wave function and energy, respectively, and $O_{\alpha}$ is the Fourier transform of either the spin ($\frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$) or density ($n_{i\uparrow} + n_{i\downarrow}$) operator. We define $S(q, \omega) (= C_s(q, \omega))$ and $N(q, \omega) (= C_d(q, \omega))$. We also calculate the single-particle spectral function $A(k, \omega)$ to see the dynamics of a doped hole and possible quasiparticle dispersion and fermi-surface topology. We use a cluster of 20 sites with periodic boundary condition for these calculations. To calculate the temperature dependence of the specific heat $C(T)$ and uniform magnetic susceptibility $\chi(T)$, the Hamiltonian for a smaller-size cluster of 12 sites is fully diagonalized.

3. Results of calculation

Before discussing our results, let us first briefly review the ground-state phase diagram obtained by Fuseya and Ogata $^{11}$. Phases obtained are as follows: the region of phase separation (phase-I), the region of fermi liquid with strong spin fluctuations (phase-II), the region of new-type quantum liquid (phase-III), and the region of ferromagnetism (phase-IV). They put special emphasis on the phase-III, which is argued to be the region of spin-charge separation and may be relevant with the anomalous features of the $^3$He system. In the following, we in particular examine the region of phase-III using the parameter values $J = -0.3$ and $K = 0.06$, which we compare with the results of other regions, i.e., the phases II ($J = -0.3$ and $K = 0.15 - 0.2$) and IV ($J = -0.3$ and $K = 0$).

Now let us discuss our results. First, we discuss the spin and density excitation spectra calculated for the region of phase-III. The results are shown in Fig. 1. We find the following: The spectral weight for the spin excitations is concentrated on a very low-energy region of about $\omega < 0.8t$. This reflects the presence of a large number of nearly degenerate low-energy states coming from the frustrated nature of the spin degrees of freedom. The low-energy spectral weight is extended over the entire Brillouin zone, reflecting the spatially localized nature of spin...
fluctuations. The spectral weight for the density excitations, on the other hand, extends over the wide energy range of about $0 < \omega < 9t$ (entire band width), which is more or less resembles the spectrum of the noninteracting system. From these results, we may say that the spin and density excitations are clearly separated in their energy scales. With increasing $K$, we find the upward shift of the low-energy spectral weight of the spin excitations; e.g., at $K = 0.2$, we find the peaks at a higher-energy region of about $0 < \omega < 2t$, where the momentum dependence of the positions of the peaks becomes significant as well. Thus, the separation between the energy scales of the spin and density excitations becomes weaker.

Figure 2. Calculated temperature dependence of the specific heat of the $t$-$J$-$K$ model at $J = -0.3$. We use a cluster of 12 sites with two holes.

Temperature dependence of the specific heat $C(T)$ calculated for the 12-site clusters with two
holes is shown in Fig. 2. We find that there appears the double-peak structure in \( C(T) \) when we use the parameter set corresponding to the anomalous quantum-liquid phase (phase-III); i.e., a sharp peak at low temperature that comes from the spin excitations and a broad peak extending over high temperatures that comes from the density excitations. In fact, the temperature ranges correspond well to the energies of the spectral weight of the spin and density excitations (see Fig. 1). The obtained two-peak structure is consistent with experiment [8, 9]. We also find that the uniform magnetic susceptibility calculated shows unique temperature variations, depending on the value of \( K \).

We also calculate the single-particle spectral function \( A(k, \omega) \) both at half filling to examine the propagation of a single hole and at a two-hole doping level to examine the possible quasiparticle dispersion and fermi-surface topology. The results will be presented elsewhere [12] but we find the following: The sharp quasiparticle-like peaks with a characteristic dispersion appear at the lowest energies in the spectra at half filling, just as in the square-lattice \( t-J \) model; this is in particular the case at \( K = 0.2 \) but remains significant even at \( K = 0.06 \). Further analyses are required to clarify the nature of the hole dynamics, quasiparticle dispersion and fermi-surface topology in this system, which will be presented elsewhere [12].

4. Summary
To consider the low-energy excitations of the two-dimensional liquid \(^3\)He adsorbed on graphite, we have calculate the spin and density excitation spectra as well as the temperature dependence of the specific heat for the triangular-lattice \( t-J \) model with the multiple-spin exchange interactions by an exact-diagonalization technique on small clusters. We have shown for a relevant set of the parameter values that the spectral weight for the spin excitations is concentrated on a very low-energy region, while that of the density excitations extends over a wide energy range. We have also shown that the double-peak structure appears in the temperature dependence of the specific heat, with the identification that the low-temperature peak corresponds to the spin excitations and the high-temperature broad peak corresponds to the density excitations. We have thus demonstrated that the spin and density excitations are clearly separated in their energy scales. Further details will be published elsewhere [12].

Acknowledgments
This work was supported in part by Grants-in-Aid for Scientific Research (Nos. 18028008, 18043006, 18540338, and 19014004) from the Ministry of Education, Culture, Sports, Science and Technology of Japan. TS acknowledges financial support from JSPS Research Fellowship for Young Scientists. A part of computations was carried out at the Research Center for Computational Science, Okazaki Research Facilities, and the Institute for Solid State Physics, University of Tokyo.

References
[1] Elser V 1989 \textit{Phys. Rev. Lett.} \textbf{62} 2405
[2] Greywall D S 1990 \textit{Phys. Rev. B} \textbf{41} 1842
[3] Roger M, Bäuerle C, Munkov Y M, Chen A S and Godfrin H 1998 \textit{Phys. Rev. Lett.} \textbf{80} 1308
[4] Ikemai H, Masutomi R, Obara K and Ishimoto H 2000 \textit{Phys. Rev. Lett.} \textbf{85} 5146
[5] Misguich G, Bernu B, Lhuillier C and Waldmann C 1998 \textit{Phys. Rev. Lett.} \textbf{81} 1098
[6] Masutomi R, Karaki Y and Ishimoto H 2004 \textit{Phys. Rev. Lett.} \textbf{92} 025301
[7] Ishida K, Morishita M, Yawata K and Fukuyama H 1997 \textit{Phys. Rev. Lett.} \textbf{81} 1098
[8] Matsumoto Y, Tsuji D, Murakawa S, Akiwato H, Kambara H and Fukuyama H 2005 \textit{J. Low Temp. Phys.} \textbf{138} 271
[9] Matsutomo Y, Tsuji D, Murakawa S, Bäuerle C, Kambara H and Fukuyama H 2007 unpublished
[10] Watanabe S and Imada M 2007 \textit{J. Phys. Soc. Jpn.} \textbf{76} 113603
[11] Fuseya Y and Ogata M 2008 \textit{J. Phys. Soc. Jpn.} preprint cond-mat/0804.4329
[12] Seki K, Shirakawa T and Ohta Y 2008 in preparation.