Journal of Physics: Conference Series **391** (2012) 012155 doi:10.1088/1742-6596/391/1/012155

Mott Insulator in Two-Channel Kondo Lattice

S Hoshino[1,†], J Otsuki[1,2] and Y Kuramoto[1]

[1]Department of Physics, Tohoku University, Sendai 980-8578, Japan
[2]Theoretical Physics III, Center for Electronic Correlation and Magnetism, Institute of Physics, University of Augsburg, Augsburg 86135, Germany

E-mail: [†]hoshino@cmpt.phys.tohoku.ac.jp

Abstract. The Mott insulator is found in the two-channel Kondo lattice by using the dynamical mean-field theory combined with continuous-time quantum Monte Carlo method. At quarter filling of two conduction bands, the paramagnetic state shows metal-insulator crossover with increasing the coupling constant at low temperatures. The insulating state is explained by the strong coupling limit, where the system is effectively interpreted as the half-filled Hubbard model. It is shown that the present Mott insulating state is well described by the Hubbard I approximation.

1. Introduction

In Pr- and U-based systems with even number of f electrons per site, the ground state can be a non-Kramers doublet [1]. When this doublet strongly couples with conduction electrons, exotic behaviors are expected as in URu_2Si_2 [2, 3] and $PrAg_2In$ [4, 5]. Recently non-Kramers doublet systems attract renewed attention due to the discovery of Γ_3 doublet compounds such as $PrIr_2Zn_{20}$ [6, 7] and PrV_2Al_{20} [8]. Theoretically, the simplest description of the non-Kramers doublets coupled with conduction electrons is given by the two-channel Kondo lattice (2ch KL) [9]. It is desirable to reveal basic properties of this fundamental model, since it is not restricted to a particular compound.

The 2ch KL is described by the following Hamiltonian:

$$\mathcal{H} = \sum_{\boldsymbol{k}\alpha\sigma} (\varepsilon_{\boldsymbol{k}} - \mu) c^{\dagger}_{\boldsymbol{k}\alpha\sigma} c_{\boldsymbol{k}\alpha\sigma} + J \sum_{i\alpha} \boldsymbol{S}_i \cdot \boldsymbol{s}_{ci\alpha}, \tag{1}$$

where $c_{\boldsymbol{k}\alpha\sigma}$ is the annihilation operator of conduction electrons with channel α and spin σ. The operators $\boldsymbol{S}_i$ and $\boldsymbol{s}_{ci\alpha} = \frac{1}{2}\sum_{\sigma\sigma'} c^{\dagger}_{i\alpha\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} c_{i\alpha\sigma'}$ are the localized and conduction spins at site i, where $\boldsymbol{\sigma}$ is a spin-1/2 Pauli matrix. The 2ch KL forms ordered states in the wide parameter region. At half filling, which corresponds to the case with two conduction electrons per site, antiferromagnetic order is found [10]. The channel symmetry breaking is also reported if suppression of staggered ordering is assumed [11]. At quarter filling, an instability toward the antiferro-channel order is pointed out [1, 12]. The antiferro-channel order actually realizes in infinite dimensions [13]. On the other hand, the paramagnetic state of the 2ch KL has been identified as an incoherent metal [9]. In this paper, we show that the paramagnetic state at quarter filling becomes the Mott insulator [14] in strong coupling region. The Mott insulating state is well described by the Hubbard I approximation [15] as will be demonstrated in the following.

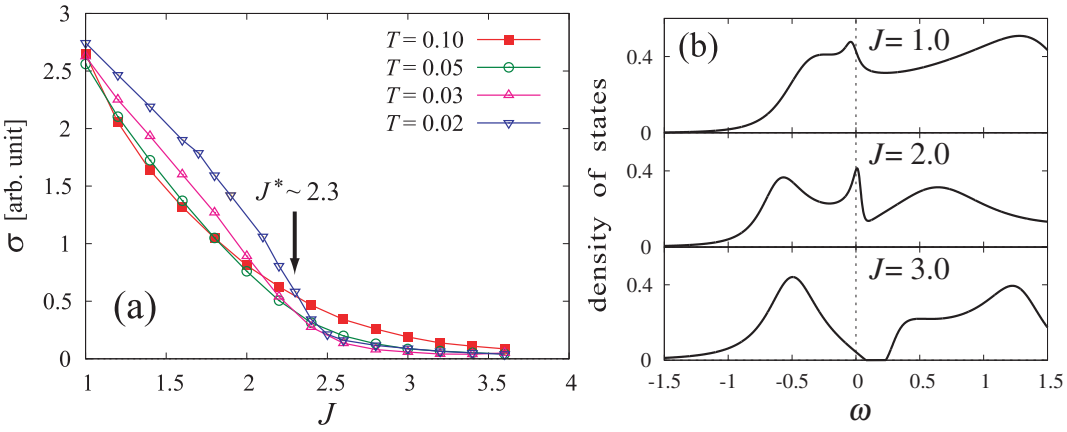

Figure 1. J dependence of the (a) electrical conductivity at quarter filling, and (b) density of states at $T = 0.02$ with several values of J.

We analyze the 2ch KL by using the dynamical mean-field theory (DMFT) [16] combined with the continuous-time quantum Monte Carlo method (CT-QMC) [17, 18]. We take the semi-circular density of states given by $\rho_0(\omega) = N^{-1}\sum_{\boldsymbol{k}} \delta(\omega - \varepsilon_{\boldsymbol{k}}) = (2/\pi D)\sqrt{1-(\omega/D)^2}$ where N is the number of sites, and D is a half of the band width with $D = 1$ as a unit of energy. For analytic continuation from imaginary axis onto real one, we have employed the Pade approximation [19]. In this paper, we concentrate mainly on the paramagnetic state at quarter filling, and do not allow for the staggered ordering. The suppression of the staggered order is expected in realistic situations because of *e.g.* substantial nearest neighbor hopping or geometrical frustration. Note that the present discussion is valid only at finite temperatures, since the paramagnetic state cannot be the ground state because of the residual entropy.

2. Metal-Insulator Crossover

In this section, we discuss the metal-insulator crossover in the 2ch KL at quarter filling. Figure 1(a) shows the J dependence of the electrical conductivity calculated from the current-current correlation function [16]. At $T = 0.10$, the conductivity smoothly decreases with increasing J. On the other hand, the result at $T = 0.02$ shows the characteristic behavior near $J^* \sim 2.3$. The conductivity steeply decreases around this point, and the system tends to become an insulator when $J > J^*$. Although we could not go to further low temperatures because of the increasing computing time, the change in conductivity seems to become steeper at J^*.

The change in the electronic states is clearly seen in the density of states as shown in Fig. 1(b). In the cases with $J = 1.0, 2.0 (< J^*)$, the value at $\omega = 0$ is finite and the system is metallic. However, the density of states with $J = 3.0 (> J^*)$ forms the gap structure near the Fermi level. Thus, the the electronic state changes from metal to insulator near the crossover point $J \sim J^*$. On the other hand, it is also characteristic that the sharp peak develops at the Fermi level when $J \lesssim J^*$. These behaviors are very similar to that of the Mott transition in the half-filled Hubbard model [14].

The origin of the insulating state can be understood in terms of the strong coupling limit. Figure 2(a) shows the schematic illustration of the quarter-filled 2ch KL in $J \to \infty$. In this limit, the electron at each site does not have spin degrees of freedom owing to the formation of the Kondo singlet with the localized spin, and has only the channel degrees of freedom. If we regard the channel $\alpha = 1$ as the spin 'up' state and $\alpha = 2$ as 'down' state, the system is mapped onto the half-filled Hubbard model which shows the Mott physics. Such situation is schematically drawn in Fig. 2(b). In the 2ch KL, the repulsive interaction between conduction electrons is

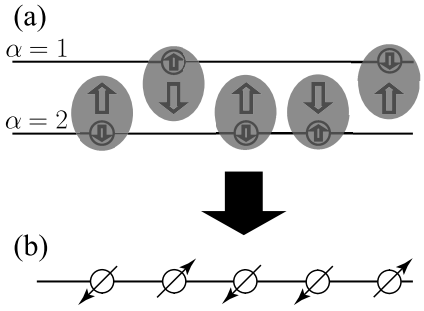

Figure 2. Schematic illustrations of (a) quarter-filled 2ch KL in the strong coupling limit and (b) half-filled Hubbard model.

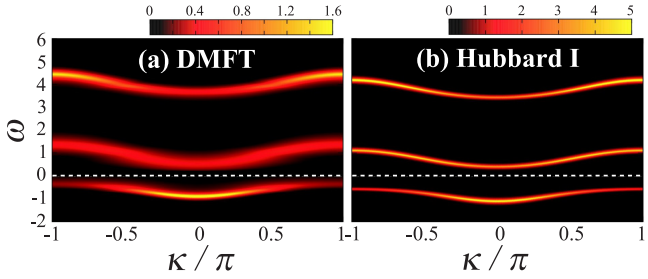

Figure 3. Single-particle spectrum for the quarter-filled 2ch KL with $J = 3.0$ and $T = 0.02$ obtained by the (a) DMFT and (b) Hubbard I Approximation.

caused by the Kondo exchange J instead of the Coulomb interaction. Although the present mapping is valid only in $J \to \infty$, the system at low temperatures can show the properties in this limit in wide parameter region, since the effective exchange interaction is scaled to strong coupling by the Kondo effect.

We note that the Mott insulator realizes also in the half-filled 2ch KL in the strong coupling region. This is understood in a manner similar to the quarter-filled case by considering the limit $J \to \infty$. The difference is that the electrons in the strong coupling limit have only the spin degrees of freedom instead of channel.

3. Single-Particle Spectrum and Hubbard I Approximation

Let us consider the single-particle spectrum in the Mott insulating state. The spectrum is derived from the Green function as

$$A(\boldsymbol{k}, \omega) = -\mathrm{Im}\, G(\boldsymbol{k}, \omega + \mathrm{i}\delta)/\pi, \tag{2}$$

where δ is a positive infinitesimal. In the present condition, the spectrum does not depend on the spin and channel. Since the self energy is local in the DMFT, the wave-vector dependence of the spectrum enters only through $\varepsilon_{\boldsymbol{k}}$. We introduce the parameter κ defined by $\varepsilon_{\boldsymbol{k}} = -D\cos\kappa$, and draw the spectrum as if the system were in one dimension.

Figure 3(a) shows the single-particle spectrum of the 2ch KL with $J = 3.0$ and $T = 0.02$ obtained by the DMFT. We can see the formation of the gap at the Fermi level, which is consistent with Fig. 1(b). The bands below and above the Fermi level are due to the emergence of lower and upper Hubbard bands. On the other hand, we observe another band in the high-energy region near $\omega \sim 4$, which does not appear in the Hubbard model.

Now we show that the spectrum in the Mott insulating states are well explained by the Hubbard I approximation [15]. Let us consider the model in atomic limit:

$$\mathcal{H}_{\mathrm{atom}} = -\mu \sum_{\alpha\sigma} c^{\dagger}_{\alpha\sigma} c_{\alpha\sigma} + J \sum_{\alpha} \boldsymbol{S} \cdot \boldsymbol{s}_{\mathrm{c}\alpha} \tag{3}$$

Here only the local operators appear. We define the Green function in the atomic limit by

$$G_{\mathrm{atom}}(\tau) = -\langle T_\tau c_{\alpha\sigma}(\tau) c^{\dagger}_{\alpha\sigma} \rangle. \tag{4}$$

In the Hubbard I approximation, the Green function in the original Hamiltonian (1) is approximated as

$$G(\boldsymbol{k}, \mathrm{i}\varepsilon_n)^{-1} = G_{\mathrm{atom}}(\mathrm{i}\varepsilon_n)^{-1} - \varepsilon_{\boldsymbol{k}}, \tag{5}$$

where $\varepsilon_n = (2n+1)\pi T$ is the fermionic Matsubara frequency. Thus we obtain the single-particle properties in the 2ch KL. We note that the Hubbard I approximation is reasonable only in the strong coupling regime. At $T = 0$, the quarter-filled situation is realized by the condition $\mu = -3J/4$. When we plot the spectrum, the infinitesimal constant δ is replaced by $0.05D$.

The single-particle spectrum obtained by the Hubbard I approximation is shown in Fig. 3(b). The bands below and above the Fermi level originate from removal and addition processes of local electrons, respectively. Since there are two final states in the electron-addition process in the atomic limit of the quarter filled 2ch KL, we observe two bands above the Fermi level. Compared with Fig. 3(a), the Hubbard I approximation well reproduces the spectrum obtained by the DMFT not only qualitatively but quantitatively. However, we should mention that the Hubbard I approximation fails in metallic states away from integer filling, since the correct Fermi volume is not reproduced. This approximation can describe only the Mott insulator at integer filling.

4. Summary

We have analyzed the paramagnetic phase of the 2ch KL at quarter filling by using the DMFT+CT-QMC method. The system shows the metal-insulator crossover by tuning strength of the Kondo coupling. The resultant insulating state is regarded as the Mott insulator, which is understood in the strong coupling limit. The electronic structure of the Mott insulating state is well described by the Hubbard I approximation.

One of the author (SH) is supported by Research Fellowships of the Japan Society for the Promotion of Science for Young Scientists. This work is partly supported by a Grant-in-Aid for Scientific Research on Innovative Areas “Heavy Electrons” (No 20102008) of MEXT, Japan.

References

[1] D. L. Cox and A. Zawadowski: Adv. Phys. **47** (1998) 599.
[2] Y. Kuramoto, H. Kusunose and A. Kiss: J. Phys. Soc. Jpn. **78** (2009) 072001.
[3] J. A. Mydosh and P. M. Oppeneer: arXiv:1107.0258.
[4] A. Yatskar, W. P. Beyermann, R. Movshovich, P. C. Canfield, A. Panchula and S. L. Bud'ko: Physica B **230-232** (1997) 46.
[5] O. Suzuki, H. S. Suzuki, H. Kitazawa, G. Kido, T. Ueno, T. Yamaguchi, Y. Nemoto and T. Goto: J. Phys. Soc. Jpn. **75** (2006) 013704.
[6] T. Onimaru, K. T. Matsumoto, Y. F. Inoue, K. Umeo, Y. Saiga, Y. Matsushita, R. Tamura, K. Nishimoto, I. Ishii, T. Suzuki and T. Takabatake: J. Phys. Soc. Jpn **79** (2010) 033704.
[7] T. Onimaru, K. T. Matsumoto, Y. F. Inoue, K. Umeo, T. Sakakibara, Y. Karaki, M. Kubota and T. Takabatake: Phys. Rev. Lett. **1061** (2011) 177001.
[8] A. Sakai and S. Nakatsuji: J. Phys. Soc. Jpn. **80** (2011) 063701.
[9] M. Jarrell, H.-B. Pang, D. L. Cox and K.-H. Luk: Phys. Rev. Lett. **77** (1996) 1612.
[10] M. Jarrell, H. Pang and D. L. Cox: Phys. Rev. Lett. **78** (1997) 1996.
[11] R. Nourafkan and N. Nafari: J. Phys. Condens. Matter **20** (2008) 255231.
[12] T. Schauerte, D. L. Cox, R. M. Noack, P. G. J. van Dongen and C. D. Batista: Phys. Rev. Lett. **94** (2005) 147201.
[13] S. Hoshino, J. Otsuki and Y. Kuramoto: J. Phys. Soc. Jpn. Suppl. A **80** (2011) SA135.
[14] M. Imada, A. Fujimori and Y. Tokura: Rev. Mod. Phys. **70** (1998) 1039.
[15] J. Hubbard: Proc. Roy. Soc. A **276** (1963) 238.
[16] A. Georges, G. Kotliar, W. Krauth and M. J. Rozenberg: Rev. Mod. Phys. **68** (1996) 13.
[17] J. Otsuki, H. Kusunose, P. Werner and Y. Kuramoto: J. Phys. Soc. Jpn **76** (2007) 114707.
[18] E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer and P. Werner: Rev. Mod. Phys. **83** (2011) 349.
[19] H. J. Vidberg and J. W. Serene: J. Low Temp. Phys. **29** (1977) 179.