Variational Monte Carlo analysis of the Mott transition in multi band electron systems

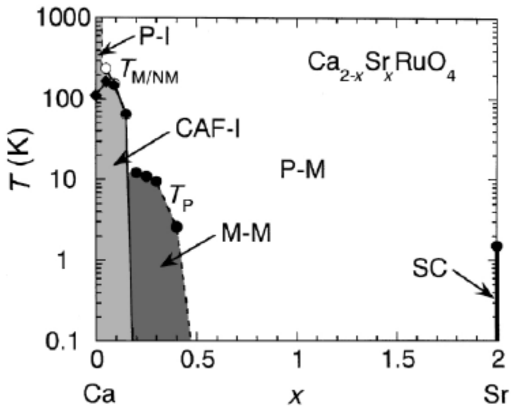
Yuto Takenaka and Norio Kawakami

Department of Physics, Kyoto University

Introduction

Mott transitions in multi-orbital systems have been investigated

(ex) Orbital-selective Mott transitions in ruthenium alloy



・Phase diagram of Sr2RuO4

[S. Nakatsuji & Y. Maeno, Phys. Rev. Lett. 84,2666 (2000)]

Hund's coupling and inter- (,intra-)orbital Coulomb interactions are important

Previous studies ⇒ mainly performed by DMFT

Low dimensionality?
Spatial fluctuation?

We focus on a two-dimensional two-orbital Hubbard model
and study the Mott transition by using the variational Monte Carlo method

Model and Method

- Two-dimensional two-orbital Hubbard model

$$H = -t \sum_{<i,j>\alpha\sigma} c^{\dagger}_{i\alpha\sigma} c_{j\alpha\sigma} + U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow}$$
$$+ (U' - J) \sum_{i\sigma} n_{i1\sigma} n_{i2\sigma} + U' \sum_{i\sigma} n_{i1\sigma} n_{i2\bar{\sigma}}$$

We study this model on a square lattice at half filling

- Method

Variational Monte Carlo method (VMC)

Optimization method

Stochastic reconfiguration method
[S. Sorella Phys. Rev. B **64**, 024512 (2001) ; S. Sorella Phys. Rev. B **71**, 241103 (2005)]

Trial function

$$|\Psi> = P_Q P_G |\Phi_F>$$

$|\Phi_F>$: Fermi Sea

No.	$\|\Gamma\rangle$	α_Γ	N_e	S^z
1	$\|0,0\rangle$		0	0
2	$\|\uparrow,0\rangle$		1	1/2
3	$\|0,\uparrow\rangle$		1	1/2
4	$\|\downarrow,0\rangle$		1	−1/2
5	$\|0,\downarrow\rangle$		1	−1/2
6	$\|\uparrow,\downarrow\rangle$	α_1	2	0
7	$\|\downarrow,\uparrow\rangle$		2	0
8	$\|\uparrow,\uparrow\rangle$	α_2	2	1
9	$\|\downarrow,\downarrow\rangle$		2	−1
10	$\|\uparrow\downarrow,0\rangle$	α_3	2	0
11	$\|0,\uparrow\downarrow\rangle$		2	0
12	$\|\uparrow,\uparrow\downarrow\rangle$	α_4	3	1/2
13	$\|\uparrow\downarrow,\uparrow\rangle$		3	1/2
14	$\|\downarrow,\uparrow\downarrow\rangle$	α_5	3	−1/2
15	$\|\uparrow\downarrow,\downarrow\rangle$		3	−1/2
16	$\|\uparrow\downarrow,\uparrow\downarrow\rangle$	α_6	4	0

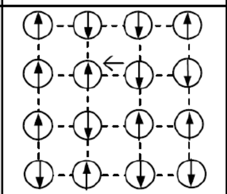
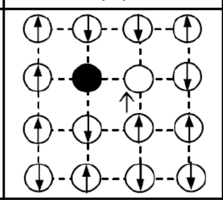
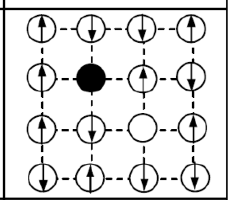
P_G: Gutzwiller factor

P_G gives different weights to the wave function depending on the configurations (number of double occupancy) of electrons

P_Q: Doublon Holon factor

Attractive correlation between doublon and holon sites

In order to describe the Mott transition, this factor plays an important role

		(a)	(b)	(c)
configuration				
factor	$P_Q P_G$	1	α	$\alpha \cdot \alpha'$
	P_G	1	α	α

In our poster ,

(1) Equivalent bandwidths case

・We clarify the nature of
the Mott transition in this model

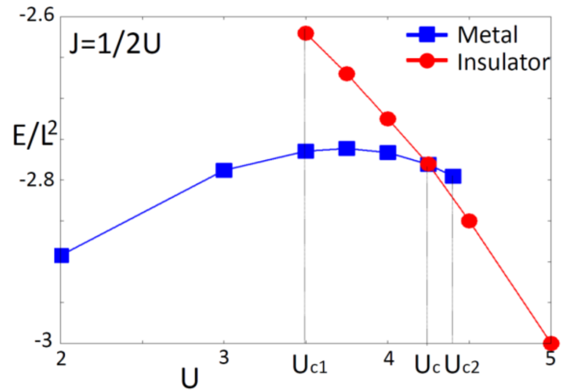
(Coexistence region of
metallic and Mott insulating states
Hysteresis)

・We discuss how Hund's coupling
affects the Mott transition

(2) Inequivalent bandwidths case

・Orbital Selective Mott transition
does not occur
・Non-fermi liquid behavior
appears in narrow band

・Optimized energy



・U-U' phase diagram