Report
Research stay of Dr. Fabien Trousselet in Cracow

This document describes results of the research stay of F. Trousselet (from Max-Planck Institute for Solid State Research in Stuttgart — MPI FKF) at Institute of Physics of the Jagiellonian University in Cracow, in the frame of a collaboration with Andrzej M. Oleś (professor at this institute) which was started during their common stay at MPI FKF in Stuttgart.

We first report of the work and progress being made in the understanding of low-temperature properties of some strongly correlated materials, more precisely of some systems with degenerate and active t_{2g} orbitals. In these systems a model of Kugel-Khomskii type [1] is well adapted to the description of spin and orbital degrees of freedom in a limit of strong on-site Coulomb repulsion with respect to both direct- and superexchange hopping amplitudes. In the case of $NaTiO_2$, a previous work [2] has shown the variety of possible phases to be considered within this model, depending on the importance of Hund's coupling, and on the ratio of direct- over superexchange processes ; in most regions of the corresponding phase diagram, a tendency to dimerization within planes with a triangular lattice geometry was found — a dimer being there either constituted of a spin singlet/ orbital triplet or of an orbital singlet/ spin triplet depending on the situation. As the manifold of candidate dimer patterns has a macroscopic degeneracy at the classical level, it remains to investigate whether ordered phases (of Valence Bond Crystal type) are favored by quantum fluctuations with an Order by Disorder mechanism, or whether some disordered phase (spin- and/or orbital- liquid) are stabilized in some regions of the phase diagram.

To that purpose, a derivation of a Quantum Dimer Model (QDM) in the spirit of the work of Rokhsar and Kivelson [4,5] is of importance and constitutes the first step of the present project. We focused mainly on the limit of large Hund's coupling, favoring spin-ordered phases polarized ferromagnetically, and first determined the manifold of nearest neighbor dimer (i.e. orbital singlet) coverings that would be as many degenerate ground states in a limit of zero overlap between distinct coverings. The derivation of an effective QDM model acting within this subspace took into account, on the one side, couplings of the original spin-orbital model on interdimer bonds ; and on the other side, non-orthogonality of different dimer coverings. The resulting model contains various local dimer resonance terms (2-dimer and 3-dimer flips). A second part of the project, consisting on the implementation of an exact diagonalization code to treat numerically this effective model, has been initiated and is currently under progress ; we also intend to compare the phase diagram found in this model with the one corresponding to the (spin-polarized) original orbital model, also to be treated numerically (with smaller accessible system size), and eventually with previously studied [2] features of the full spin-orbital model at large Hund's coupling. This should allow to determine whether and under which conditions an orbitally-disordered phase (orbital liquid) can be formed, as whether it might be expected from the properties of Quantum Dimer Models on the triangular lattice [3,5]. We intend to publish the results of this ongoing work within a few months, in one of the leading journals in the field with high impact factor.

A possible extension of the project is the consideration of smaller Hund's couplings, where spin singlets / orbital triplets are also to be considered in the low-energy manifold and which could be a route to the stabilization of a spin-orbital liquid phase.

Independently from this project, we also continued our earlier research project started in Stuttgart a few months before by F. Trousselet, A.M. Oleś, and P. Horsch (from MPI FKF), on a model called Compass-Heisenberg model — motivated by the physics of strongly correlated materials with orbital degeneracy. The model, studied by purely numerical and various complementary (e.g. perturbative) methods on a square lattice, is characterized by the strongly frustrated interactions which lead to a rich phase diagram, and interesting properties concerning low-energy excitations in phases stabilized by weak Heisenberg interactions. Thanks to these properties a system with such interactions could be a good candidate for quantum computing device. During the stay of F. Trousselet in Cracow, discussions between him and A.M. Oleś enabled numerous improvements to this work and eventually led to the final form of an article submitted for publication a few days later [6] — consequently, the HFM Network was acknowledged in this article.

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