Charge degrees of freedom on a pyrochlore lattice

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Final report from the visit of Karlo Penc in Budapest (17/2/07 – 22/2/07).

The study of charge degrees of freedom on a checkerboard (planar pyrochlore) lattice has revealed interesting effects. It has been shown that excitations which carry fractional charges in a model of strongly correlated spinless fermions on the checkerboard lattice are linearly confined. Even though the checkerboard lattice and pyrochlore lattice show many similarities, there exist certain differences between them, e.g., due to the higher spatial dimensionality. Particular differences of the two lattices arise in the U(1) lattice gauge theory, which describes the low energy excitations of the considered systems. It allows for a deconfined phase in 3+1 dimensions in contrast to 2+1 dimensions where such a phase cannot form.

In our ongoing project, we perform numerical studies of an effective Hamiltonian for the 3D pyrochlore lattice. Numerical exact diagonalization has been shown to be a powerful tool to study such models. Systematic studies provide a deeper insight and show explicitly the differences between the 3D pyrochlore lattice and the 2D projection. In particular, we hope to provide a proof for the existence of a deconfined phase in the 3D pyrochlore lattice.

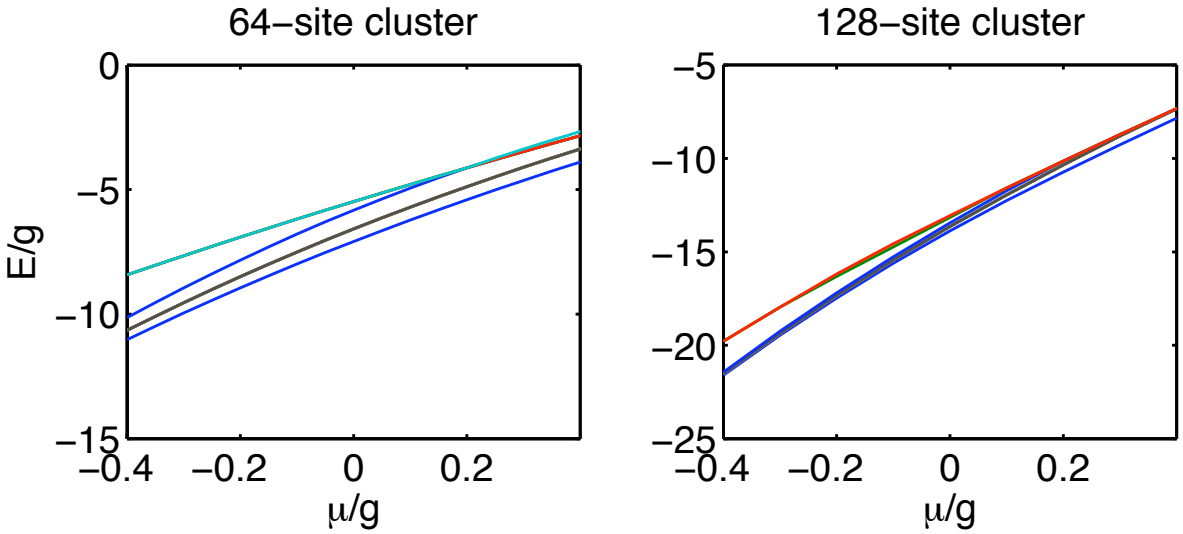

Figure 1: *Energies of the ground states and first excited states are shown for the 64–site and 128–site cluster. Only the sector containing the maximal flippable configurations of the quarter filled pyrochlore lattice is considered.*

During the visit, we improved the implementation of the exact diagonalization code for an effective Hamiltonian and discussed first results. For a deeper understanding of the nature of the ground state, we study a Hamiltonian which includes an extra term that counts the number of flippable hexagons, motivated by Rokshar–Kivelson. In other words, flippable hexagons gain kinetic energy –g and are punished by a diagonal term μ. The number of flippable hexagons is an essential parameter to understand the effect of the ring–exchange term. By using an efficient algorithm for the generation of 'allowed' configurations which describe the low–energy physics, we can now diagonalize an effective Hamiltonian

on systems with up to 128 sites. For the diagonalization we use clusters with periodic boundary conditions which have the full symmetry of the pyrochlore lattice. Calculations of ground states and first excited states for different parameters give a first view on a possible phase diagram. Level crossings might here be interpreted as indication for phase transitions (see Figure 1). Furthermore, we compared the energies which were obtained by exact diagonalization with a series expansion starting from the maximal flippable configuration.

For definite statements about the occurrence of phase transitions and a numerical proof for the existence of a U(1) liquid phase we have to perform careful finite size scaling. This involves further diagonalizations as well as the application of Green's Function Monte Carlo techniques (which are currently implemented in an ongoing project together with Olga Sikora). In addition, we are considering different expansions in order to understand the low–lying excitations of the model.

Upon successful completion of our project we plan to publish our results in a refereed journal.