Hierarchical Mean Field

In collaborations with L. Isaev, G. Ortiz and S. Rombouts

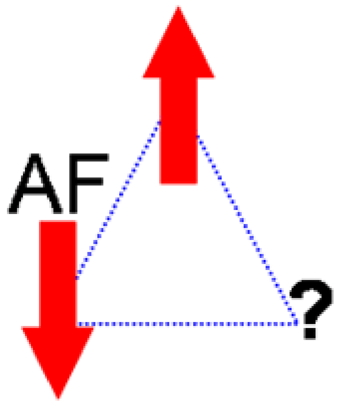
- Hierarchical mean-field approach to the J_1-J_2 Heisenberg model on a square lattice.

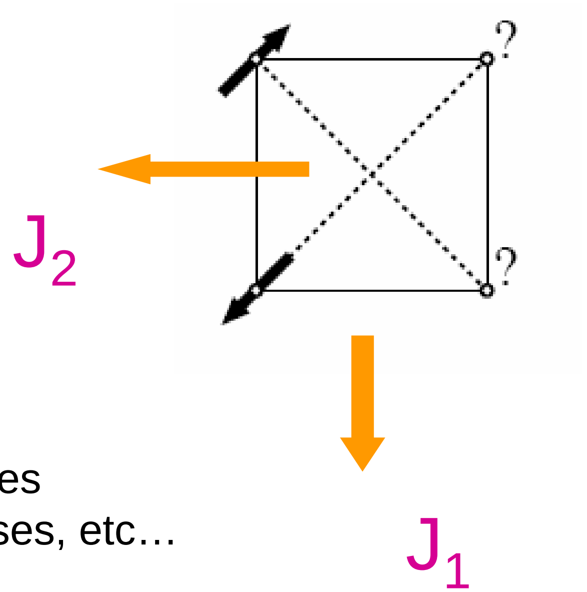
Phys. Rev. B 79, 024409 (2009).

- Phase diagram of the Heisenberg antiferromagnet with four-spin interactions. arXiv:0903.1630.
- Local physics of magnetization plateaux in the Shastry-Sutherland model. arXiv:0906.4991.
- Work in progress for Hubbard systems. (Preliminary results)

Frustrated Magnets

Frustration is a phenomenon in condensed matter physics in which the geometrical properties of the crystal lattice or the presence of conflicting atomic forces forbid simultaneous minimization of the interaction energies acting at a given site.



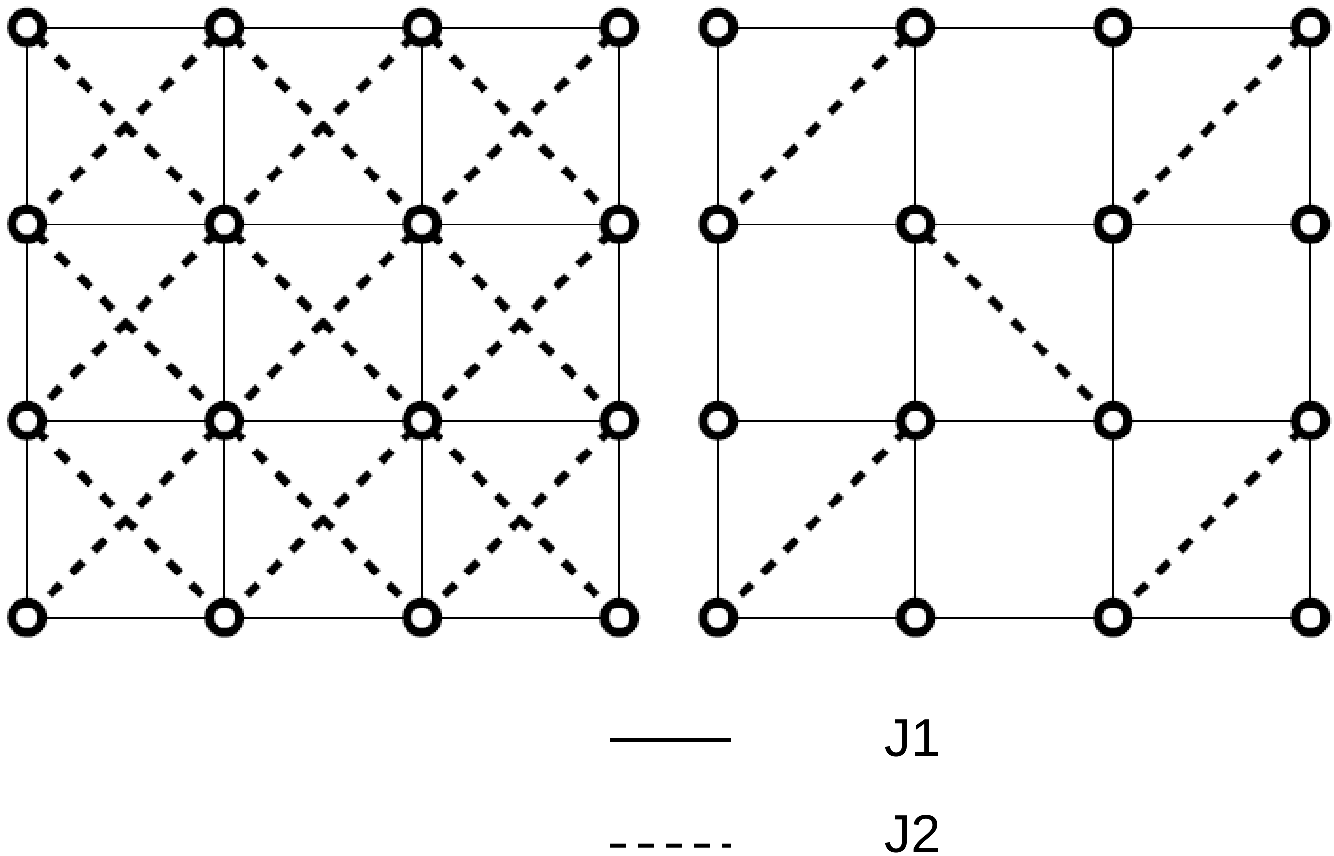


Frustration gives rise o a variety of spin phases
(valence bond cristals, spin liquids, spin glasses, etc…

Li_2VOSiO_4

$VOMo_2O_4$

$SrCu_2(BO_3)_2$



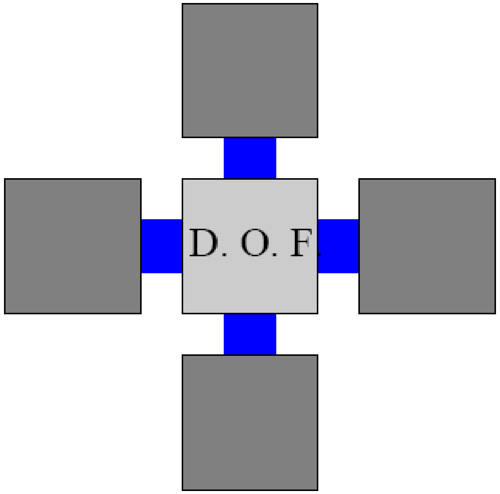
Hierarchical Mean Field (HMF)

Basic assumption: the physics of the problem is “local”.

Fist problem: identify the minimal “cluster” that contains the relevant degrees of freedom (DOF).

Coarse grain the lattice into a new lattice of clusters.

Each cluster does not contain all the physics of the problem.



HMF takes into account cluster interaction at the mean field level

Schwinger Represention

For a given cluster of N_s ½ spins the dimension is 2^{N_s}. The eigenstates and eigenvalues of the cluster are $|\alpha>$ and ε_α .
We associate each degree of freedom with a Schwinger boson.

$$\left|\beta\right\rangle_i \Rightarrow b_{i\alpha}^{+}\left|0\right\rangle, \left|0\right\rangle_i \Rightarrow b_{i0}^{+}\left|0\right\rangle$$

With the local physical constraint $\sum_{\beta} b_{i\beta}^{+} b_{i\beta} = 1$

A spin Hamiltonian with up two cluster interactions is mapped into:

$$H = \sum_{i\beta} \varepsilon_\beta b_{i\beta}^{+} b_{i\beta} + \sum_{\langle ij\rangle\sigma\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}^{\sigma} b_{i\alpha}^{+} b_{j\beta}^{+} b_{j\gamma} b_{i\delta}$$

Cluster Hartree-Fock: The Ground State

We treat the Schwinger Hamiltonian in the simplest HF approximation by performing a canonical transformation on the composite bosons.

$$\Gamma^{+}_{in} = \sum_{\beta} R^{n}_{\beta} b^{+}_{i\beta}, \quad \sum_{\beta} R^{n}_{\beta} R^{n'}_{\beta} = \delta_{nn'}, \quad \sum_{n} R^{n}_{\beta} R^{n}_{\beta'} = \delta_{\beta\beta'}$$

The GS state ansatz is:

$$\left|\Psi\right\rangle = \prod_{i} \Gamma^{+}_{i0} \left|0\right\rangle$$

We made no further assumption about the symmetries present in the GS. The formalism allows the treatment of competing phases present in the cluster on equal footing.

HF equations and observables

The energy is

$$E = \sum_{\beta} \varepsilon_{\beta} \left(R_{\beta}^{0} \right)^{2} + \sum_{\sigma} z_{\sigma} V_{\alpha\beta\gamma\delta}^{\sigma} R_{\alpha}^{0} R_{\beta}^{0} R_{\gamma}^{0} R_{\delta}^{0}$$

Minimizing the energy we obtain the HF equations

$$\sum_{\beta} \left\{ \varepsilon_{\alpha} + 2 \sum_{\sigma\gamma\delta} z_{\sigma} V_{\alpha\varphi\delta\beta}^{\sigma} R_{\gamma}^{0} R_{\delta}^{0} \right\} R_{\beta}^{n} = e_{n} R_{\alpha}^{n}$$

Expectation values inside a cluster can be easily calculated for example the spin polarization in site **m** of cluster **l**.

$$\langle \Psi | S_{im}^{z} | \Psi \rangle = \sum_{\beta\beta'} \left(S_{m}^{z} \right)_{\beta\beta'} R_{\beta}^{0} R_{\beta'}^{0}$$

The J1-J2 Model

$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j$$

The 2x2 plaquette

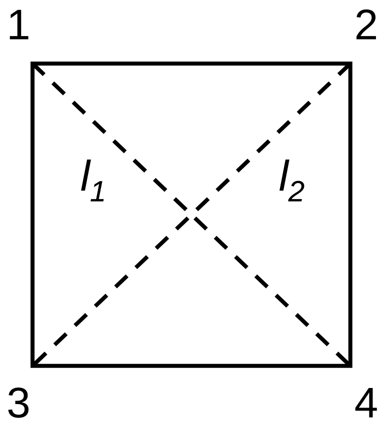
$$H = J_1 (S_1 + S_4) \cdot (S_2 + S_3) + J_2 [S_1 \cdot S_4 + S_2 \cdot S_3]$$

$$E_{l_1 l_2 L} = \frac{J_1}{2} [L(L+1) - l_1(l_1+1) - l_2(l_2+1)] + \frac{J_2}{2} [l_1(l_1+1) + l_2(l_2+1) - 3]$$

l_1	l_2	L	E
0	0	0	$-3x/2$
0	1	1	$-x/2$
1	0	1	$-x/2$
1	1	0	$-2 + x/2$
1	1	1	$-1 + x/2$
1	1	2	$1 + x/2$

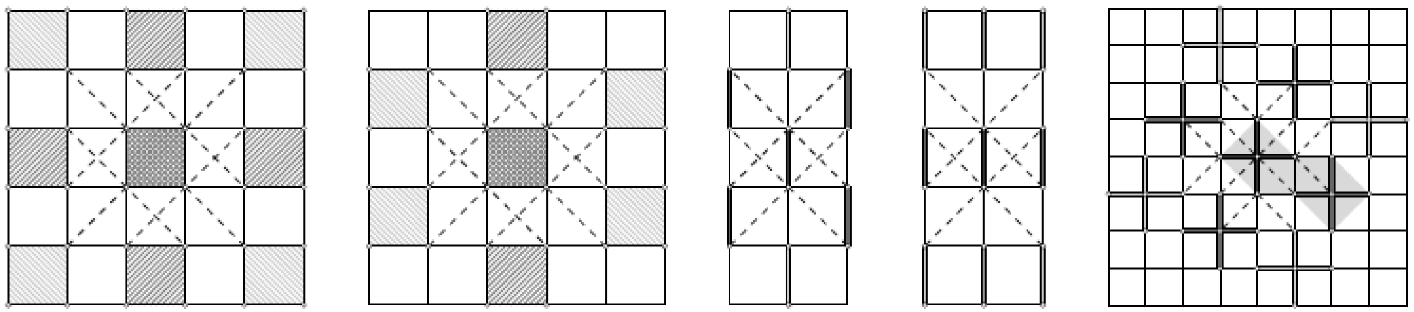
$$\Gamma_{in}^{+} = \sum_{l_1 l_2 J} R_{l_1 l_2 J}^{n} b_{i l_1 l_2 J 0}^{+}$$

X=J1/J2



Selection of the cluster

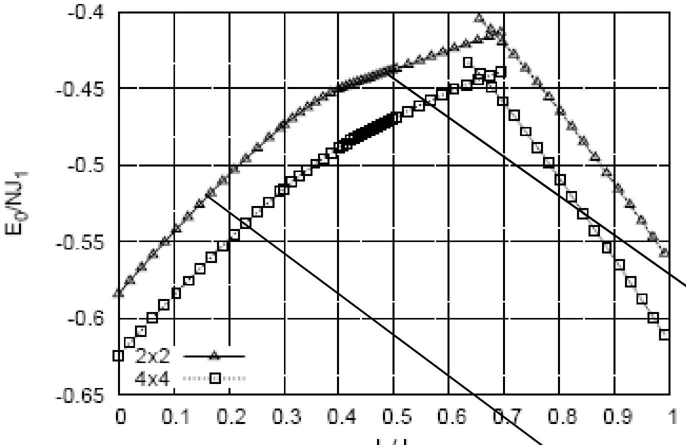
Several ways of covering the lattice



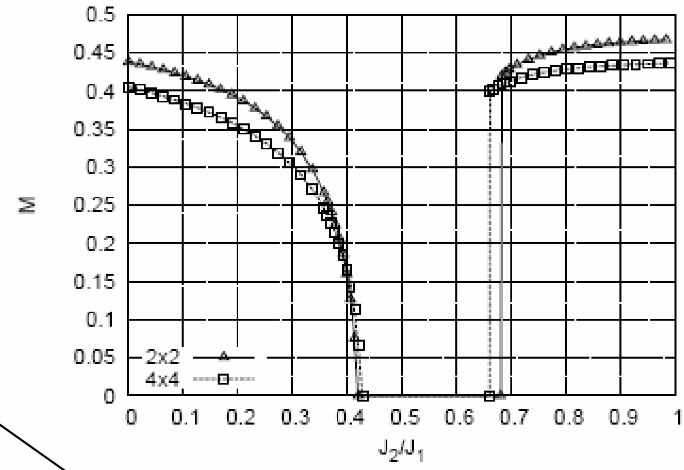
plaquettes dimers crosses

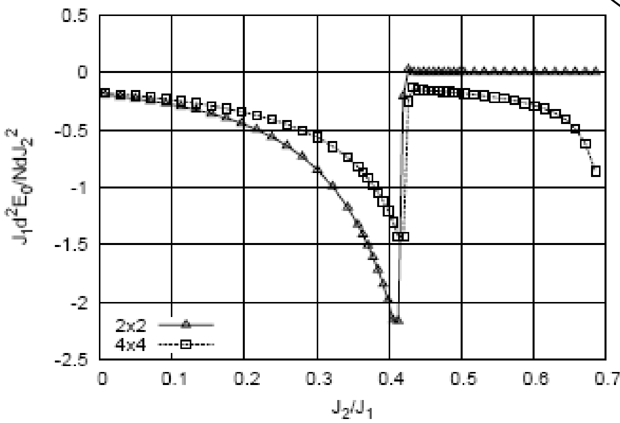
Only the symmetric 2x2 plaquette covering and extensions and extensions 4x4 capture all the phases of the system.

Phase Diagram



$R^0_{11J} \neq 0$

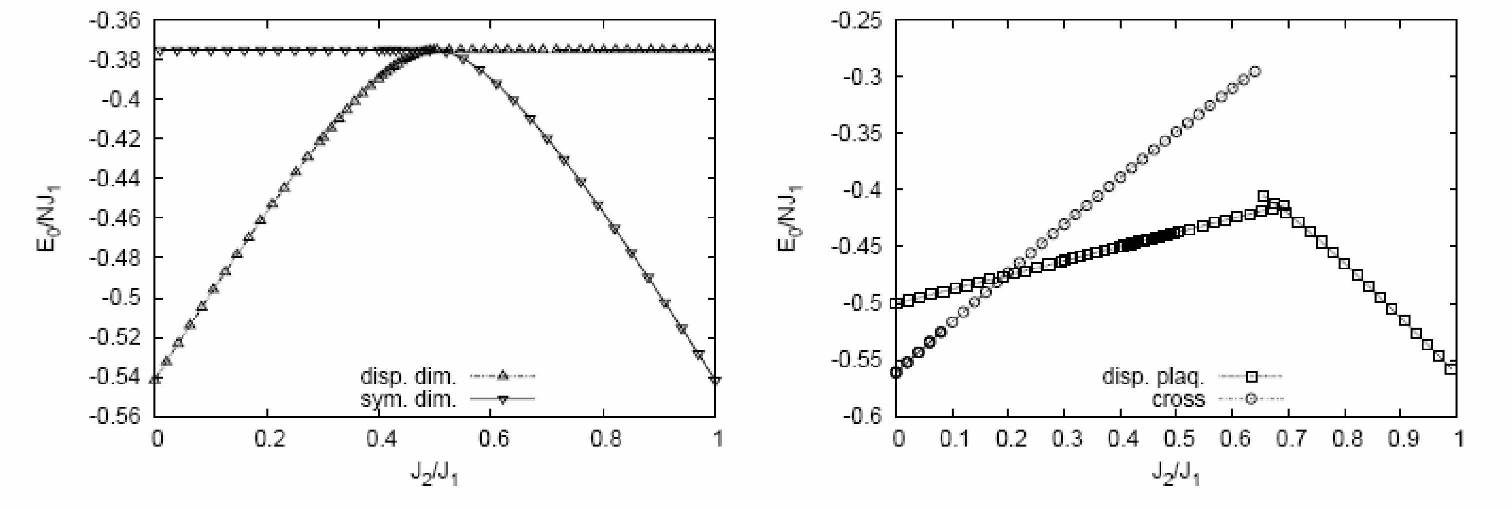


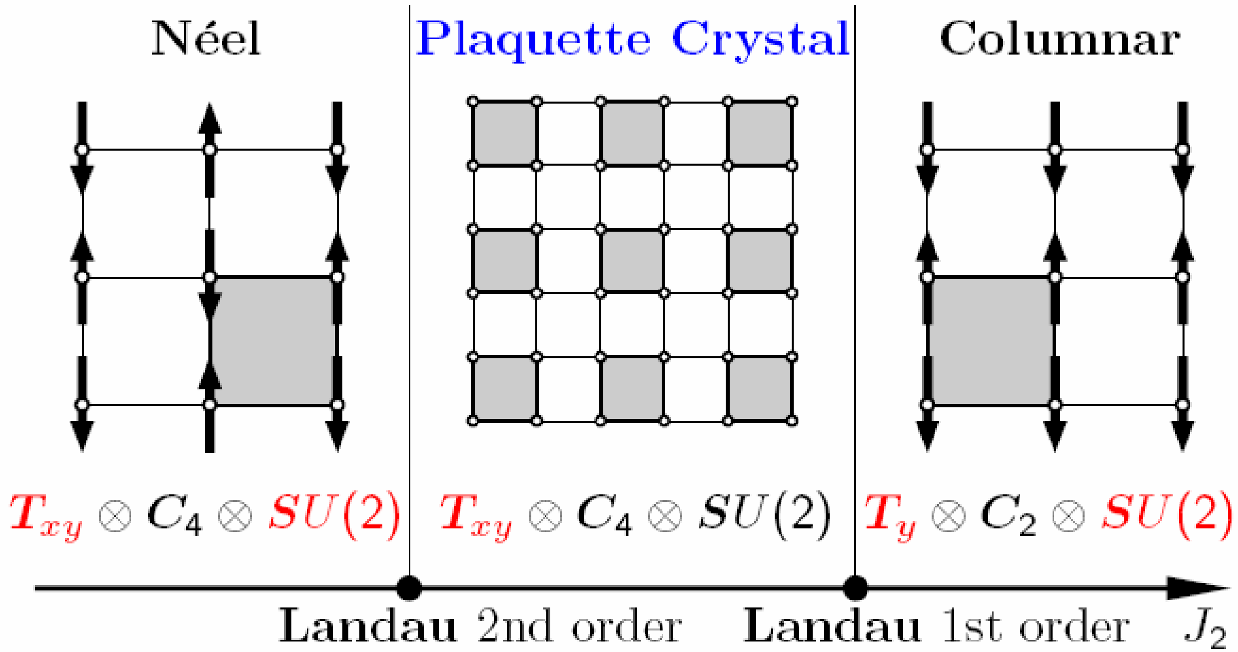


O

$$R_{11J} \neq 0 \qquad R_{110} = 1$$

Other coarse graining scenarios fail to describe all phases




Néel
Plaquette Crystal
Columnar
$T_{xy} \otimes C_4 \otimes SU(2)$
$T_{xy} \otimes C_4 \otimes SU(2)$
$T_y \otimes C_2 \otimes SU(2)$
Landau 2nd order
Landau 1st order
J_2

HMF for fermions

Within each cluster there are configuration with even number of fermions that behaves like composite bosons and configurations with odd number of fermions that behave like composite fermions.

$$\left|\beta s\right\rangle_i^{even} \Rightarrow b_{i\beta s}^{+}\left|0\right\rangle, \left|0\right\rangle_i \Rightarrow b_{i00}^{+}\left|0\right\rangle \qquad \left|\alpha s\right\rangle_i^{odd} \Rightarrow a_{i\alpha s}^{+}\left|0\right\rangle$$

Physical constraint and number of fermions:

$$\sum_{\alpha s} a_{i\alpha s}^{+} a_{i\alpha s} + \sum_{\beta s} b_{i\beta s}^{+} b_{i\beta s} = 1, \quad \sum_{i\alpha s} n_{i\alpha s}^{a} a_{i\alpha s}^{+} a_{i\alpha s} + \sum_{i\beta s} n_{i\beta s}^{b} b_{i\beta s}^{+} b_{i\beta s} = N$$

Mapping of the fermion creation operator:

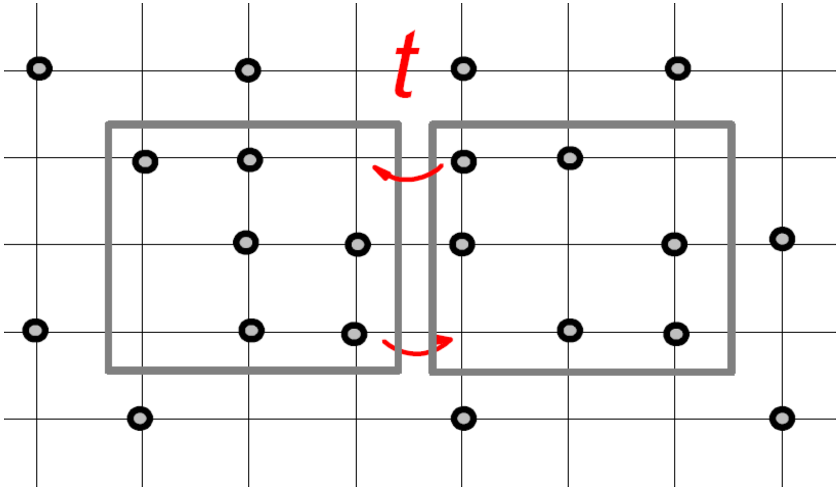
$$c_{ls}^{+} = \sum_{\alpha\beta s'} \left\langle \beta, s'+s \right| c_{ls}^{+} \left| \alpha, s' \right\rangle b_{i\beta s'+s}^{+} a_{i\alpha s'} + \left\langle \alpha, s'+s \right| c_{ls}^{+} \left| \beta, s' \right\rangle a_{i\alpha s'+s}^{+} b_{i\beta s'}$$

Cluster Hamiltonian

Though we can proceed with a general Hamiltonian in an arbitrary single particle basis, for the ease of the presentation I will concentrate in the Hubbard Hamiltonian:

$$H = -t\sum_{l\delta s} c_{ls}^{+} c_{l+\delta s} + U\sum_{l} c_{l\uparrow}^{+} c_{l\uparrow} c_{l\downarrow}^{+} c_{l\downarrow}$$

Within the cluster picture the cluster interaction is mediated by hopping



The more general fermion two-body Hamiltonian gives rise to eight body terms. However, they at most quartic in bosons and fermions.

Assuming cluster translational invariance, the cluster Hamiltonian in terms of composite bosons and fermions is:

$$H = \sum_{i\beta s} \omega_{\beta s} b^{+}_{i\beta s} b_{i\beta s} + \sum_{i\alpha s} \varepsilon_{\alpha s} a^{+}_{i\alpha s} a_{i\alpha s} +$$

$$\frac{1}{2} \sum_{i\delta\alpha\alpha'\beta\beta' s_1 s_2 s_3 s_4} V_{\delta\alpha\alpha'\beta\beta' s_1 s_2 s_3 s_4} \left(b^{+}_{i\beta s_1} b_{i+\delta\beta' s_2} a^{+}_{i+\delta\alpha' s_3} a_{i\alpha s_4} + h.c. \right) +$$

$$\frac{1}{2} \sum_{i\delta\alpha\alpha'\beta\beta' s_1 s_2 s_3 s_4} W_{\delta\alpha\alpha'\beta\beta' s_1 s_2 s_3 s_4} \left(b^{+}_{i\beta s_1} b^{+}_{i+\delta\beta' s_2} a_{i+\delta\alpha' s_3} a_{i\alpha s_4} + h.c. \right)$$

Mean Field Decoupling

Decoupling at the mean-field level bosons and fermions we arrive to a problem of coupled one-body fermion and boson Hamiltonians with constraints

$$H_F = \sum_{i\alpha s}(\varepsilon_{\alpha s} - \lambda - \mu n_{\alpha s})a^+_{i\alpha s}a_{i\alpha s} + \frac{1}{2}\sum_{i\delta\alpha\alpha'\beta\beta'ss'} V_{\delta\alpha\alpha'\beta\beta'sss's'}\left(\left\langle b^+_{i\beta s'}b_{i+\delta\beta's'}\right\rangle a^+_{i+\delta\alpha's}a_{i\alpha s} + h.c.\right) +$$
$$\frac{1}{2}\sum_{i\delta\alpha\alpha'\beta\beta'ss'} W_{\delta\alpha\alpha'\beta\beta'-sss'-s'}\left(b^+_{i\beta s'}b^+_{i+\delta\beta'-s'}a_{i+\delta\alpha'-s}a_{i\alpha s} + h.c.\right)$$

$$H_B = \sum_{i\beta s}(\omega_{\beta s} - \lambda - \mu n_{\beta s})b^+_{i\beta s}b_{i\beta s} + \frac{1}{2}\sum_{i\delta\alpha\alpha'\beta\beta'ss'} V_{\delta\alpha\alpha'\beta\beta's's'ss}\left(b^+_{i\beta s}b_{i+\delta\beta's}\left\langle a^+_{i+\delta\alpha's'}a_{i\alpha s'}\right\rangle + h.c.\right) +$$
$$\frac{1}{2}\sum_{i\delta\alpha\alpha'\beta\beta'ss'} W_{\delta\alpha\alpha'\beta\beta'-s's's-s}\left(b^+_{i\beta s}b^+_{i+\delta\beta'-s}\left\langle a_{i+\delta\alpha'-s'}a_{i\alpha s'}\right\rangle + h.c.\right)$$

Constraints

$$\sum_{i\beta s} n_{\beta s}b^+_{i\beta s}b_{i\beta s} + \sum_{i\alpha s} n_{\alpha s}a^+_{i\alpha s}a_{i\alpha s} = N, \quad \sum_{i\beta s} b^+_{i\beta s}b_{i\beta s} + \sum_{i\alpha s} a^+_{i\alpha s}a_{i\alpha s} = M$$

Comparison with DMFT in the 1d Hubbard

Few words on cellular or cluster DMFT.

Basic idea: model the effect on the cluster of the remaining system by a bath of uncorrelated orbitals that exchange fermions with the cluster, whose interaction parameters are determined selfconsistently.

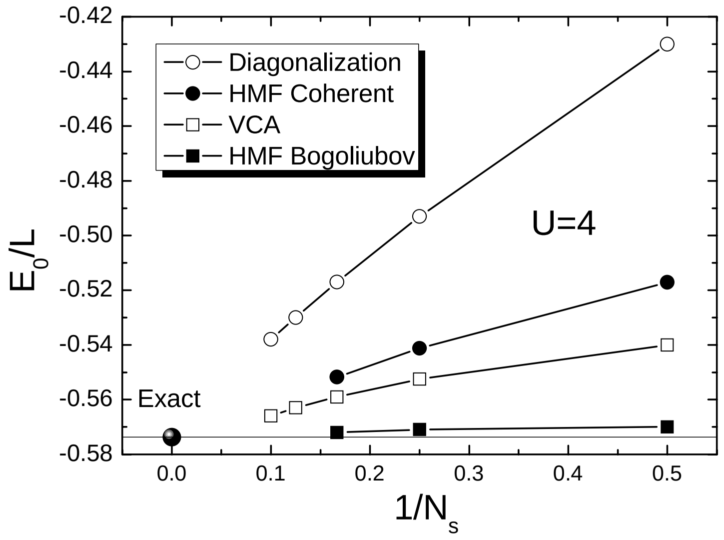
$$H_{DMFT} = \sum_{lms} E_{lm} c_{ls}^{+} c_{ms} + U \sum_{l} n_{l\uparrow} n_{l\downarrow} + \sum_{ks} e_k f_{ks}^{+} f_{ks} + \sum_{kls} \left(V_{kl} f_{ks}^{+} c_{ls} + h.c. \right)$$

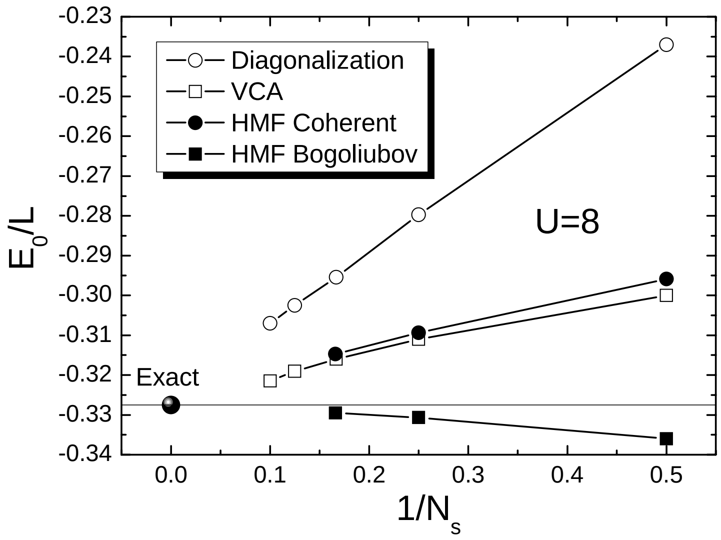
Solve iteratively the impurity model in the superlattice and in the cluster lattice varying the cluster-bath parameters till selfconsistency in the corresponding selfenergies.

In practice, on has to diagonalize the impurity Hamiltonian. Calculations are restricted to ~4sites in the cluster and ~8 sites in the bath.

Preliminary results

(VCA are taken from M. Balzer, W. Werner and M. Potthof, Phys. Rev. B 77, 045133.





SUMMARY

- We propose a simple and “symmetry” preserving mean-field approach for quantum spin systems and strongly correlated fermions.

- We were able to derive the correct phase diagrams of quantum spin systems (J1-J2, J-Q, Shastry-Sutherland) with minimal effort.

- The results seems to be very competitive with other well established approaches. In particular, the fermion HMF looks very promising.

- HMF is a zero order approximation. It can be used as a reference state for CCM or Jastrow-type extensions.

- We are now working on an adaptive DMRG procedure based on the ideas of HMF.