Computation of the Susceptibility

for the Anderson Impurity Model

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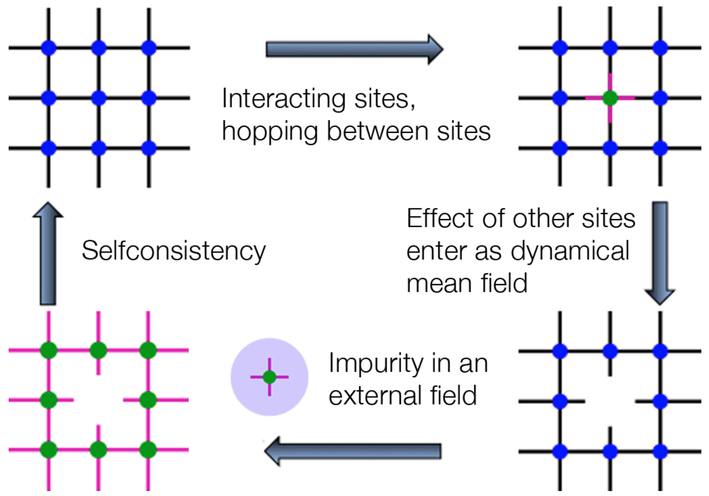
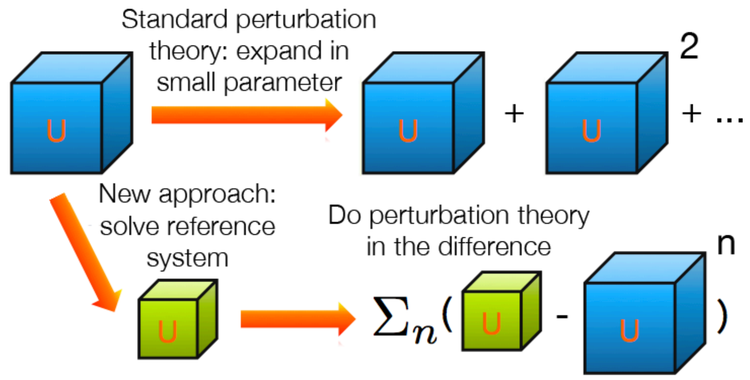
The Anderson Impurity Model (AIM) describes a magnetic impurity embedded into a bath of non-interacting electrons. Solving the AIM is important to show the properties of quantum lattice models within the Dynamical Mean-Field Theory (DMFT). Current solvers of the AIM provides controlled results for spectral and thermodynamic properties but are computationally expensive and non-scalable for multiorbital problems. We consider the AIM utilizing the superperturbation solver, a new method that has been proposed recently [1].

Dynamical Mean-Field Theory

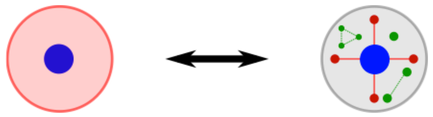


An interacting lattice (upper left) is replaced by a single site that exchanges particles with an electronic bath (upper right). The bath is given by the cavity, i.e. the lattice with one site missing (lower right). The problem is then reduced to the solution of the AIM with a self-consistency condition.

Superperturbation

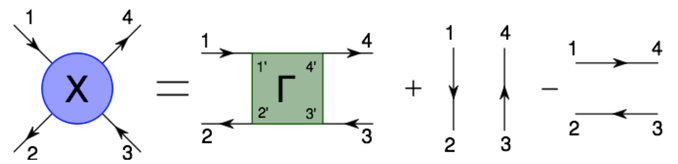


Instead of expanding a large interacting problem in a small parameter, a reference system is constructed with most of the essential physics. The reference system is treated with Exact Diagonalization (ED), which solves the Hamiltonian precisely. To decrease the computational time, the bath is approximated with a small number of bath orbitals.



The idea is based on the transformation to a set of new fermionic variables (green dots) and reformulation of the perturbation theory in the difference between the systems.

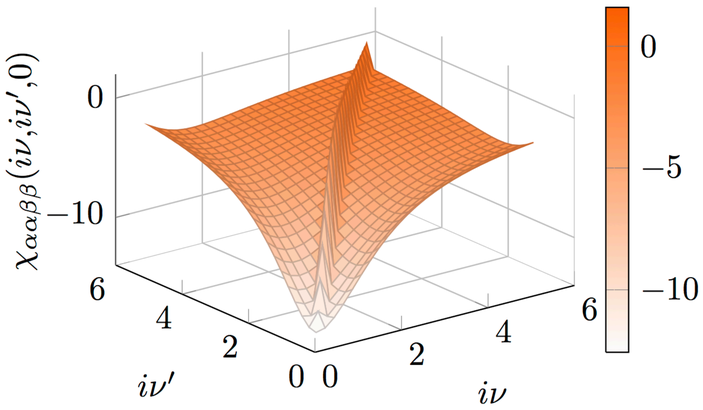
The susceptibility shows the response of a material to a perturbation, for example a magnetic field. It grows exponentially with the size of the problem and is computationally expensive. The two-particle Green function, and thereby the susceptibility, is a major building block in developing the superperturbation theory.



In the composition of the two-particle Green function, the susceptibility is the fully irreducible vertex part.

RSPt is an Open Source project for band structure calculations using DMFT and ED. It is written in Fortran 90. By extending and employing parts of the RSPt code the susceptibility can be computed efficiently.

The result is a Fortran 90 module that extends the RSPt code and computes the susceptibility for a multiorbital model. It is verified with analytical results for the one-band model using Matlab.



Future research is to finalize the implementation of the superperturbation routine for the multi-orbital models, which will be able to treat the AIM for a large range of hybridization and coupling strengths at a reasonable computational cost.

[1] H. Haffermann, *et. al.*, EPL **85**, 27007 (2009).

Images by C. Jung