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M2 Internship subject: Rotationally-invariant Slave-Spin dynamical mean field.

<u>Description and expected results</u>: Slave-variable techniques are very successful semi-analytic methods to treat the quantum many-body problem. They have been applied to solving models relevant for strongly-correlated materials, cold atomic quantum simulators, quantum dots and out-of-equilibrium quantum systems.

In these methods the original model is rewritten in an enlarged Hilbert space including auxiliary degrees of freedom (still, constrained to some extent to follow the dynamics of the original ones), where approximations result less harsh compared to applying them on the original problem. Notably, a Hartree-Fock-type of mean-field on the auxiliary variables results in a dynamical mean-field on the original problem. Still simplified but numerically much cheaper than the more accurate Dynamical Mean-Field Theory (DMFT), these are ideally complementary techniques.

In particular the Slave-Spin method¹ (in which quantum spins are the auxiliary variables "slaves" to the original fermions of the model) is particularly versatile in approaching multi-orbital Hubbard models, which are essential in interpreting and describing the electronic properties of several strongly-correlated materials, like e.g. the Fe-based high-Tc superconductors², which have polarized the attention of the quantum materials international community in the last decade or so. Still, the method has to be generalized to "rotationally invariance", which implies the possibility of treating off-diagonal interactions and spin-orbit coupling, for instance, and off-diagonal symmetry breaking orders like superconductivity.

This generalization, which was already performed for some similar methods³, is the main subject of this internship.

Success in this generalization will lead to a powerful and versatile technique which will have a vast number of applications both in and out of equilibrium. First problems to be tackled will be the effect of spin-orbit coupling on the correlations of Hund metals (see below) and multi-orbital photo-doped Mott insulators.

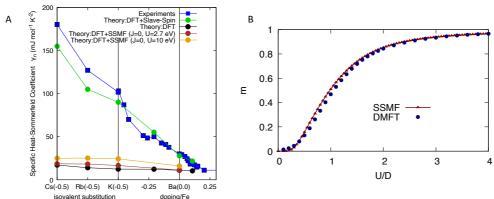


Figure 1 A. Slave-spin mean-field (SSMF) study of the normal state of a family of Fe-based superconductors (Ref. 2). Experimental values of the Sommerfeld coefficient (low-temperature slope of the electronic specific heat) are reported in blue and calculated withing band-theory (DFT) in black. This mismatch shows the need of including strong correlations with a dynamical mean-field like SSMF or DMFT (results in green). These materials are now portrayed as "Hund metals" since turning off the atomic "Hund coupling" exchange J, even preserving strong electronic interactions (U) is enough to make the modeling fall back basically to the band-theory results. B. Staggered magnetization in a one-band antiferromagnet as a function of interaction strength: SSMFT vs DMFT. The SSMF is one million times faster.

¹ Crispino et al. "Slave-spin mean field for broken-symmetry states: Néel antiferromagnetism and its phase separation in multiorbital Hubbard models", PRB 107 155149 (2023)

² L. de' Medici "<u>Hund's Metal Physics in the Iron-Based Superconductors</u>", Eva Pavarini, Erik Koch, Alexander Lichtenstein, and Dieter Vollhardt (eds.), <u>Understanding Correlated Materials with DMFT Modeling and Simulation</u>, Vol. 15, Verlag des Forschungszentrum Jülich, 2025, ISBN 978-3-95806-813-1, doi:<u>10.34734/FZJ-2025-03722</u>

³ Lechermann et al. "Rotationally invariant slave-boson formalism and momentum dependence of the quasiparticle weight", PRB 76, 155102 (2007)