Rotationally Invariant Slave-Boson Method and application in combination with Density Functional Theory

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The density functional theory (DFT) [1, 2] proved to be a good starting point for deriving model Hamiltonians [3, 4], that can be studied with more elaborated methods able to treat correlations. While early approaches to solve the realistic many-body problem in solids focused on perturbative treatments of the interactions [5], over the last two decades several non-perturbative methodologies have emerged. Dynamical mean field theory (DMFT) was combined with realistic electronic structure methods, for example in the LDA+DMFT approach [6, 7]. This methodology can be thought as a spectral density functional [8], and is nowadays widely used to study 3d, 4d, 5d, 4f and 5f systems, see, e.g., Refs. [9-13]. LDA+DMFT has been implemented in different basis sets, such as linearized augmented planewave (LAPW) [14, 15] plane wave pseudopotentials, [16] projector augmented wave method [17] and linearized muffin-tin orbitals [18]. Another important approach — which is not as accurate as DMFT, but has the advantage to be less computationally demanding — is the GA [19], which was first implemented to study real solids in Ref. [20]. The GA approximation has been thereafter extensively developed [21-27], and it has been formulated and implemented in combination with realistic electronic structure calculations such as the LDA+GA approach [23, 28], which has been applied successfully to many systems [29-36]. A third important many-body technique is the slave boson approach (SB) [37, 38], which is, in principle, an exact reformulation of the quantum many-body problem for model Hamiltonians, and reproduces the results of the GA at the saddle-point level [24, 39]. This technique was recently extended to treat full rotationally invariant [38, 40, 41]. This approach, which is commonly named Rotationally Invariant Slave Boson (RISB) mean field theory has also been combined with LDA for the study of real materials [8, 42, 43]. The three above-mentioned methods are closely connected, and largely complementary of each other.

In this lecture we introduce the RISB theory [37, 38, 40], and we show that the mean field approximation can be derived from an *exact* operatorial reformulation of the many-body problem, see Ref. [41], which reproduces the Gutzwiller approximation [19] at the mean-field level [24, 39]. Furthermore, we present several mathematical ideas that result into substantial algorithmic advancements, which enable us, e.g., to study interesting low-symmetry phases of matter and to derive accurate equations of state for materials currently far beyond the reach of LDA+DMFT. In particular, we display a connection between the SB amplitudes and the coefficients of the Schmidt decomposition [44] and show that, based on this connection, it is possible to formulate an algorithm which consists in calculating recursively the ground state of a series of Anderson impurity Hamiltonians, whose baths have the same dimension as the corresponding impurities.

The following hands-on session will focus on the practical applications of the RISB mean field approximation in combination with DFT. For this purpose, the participants will employ the numerical implementation of the RISB equations formulated in Refs. [41, 46], where the LAPW interface with the DFT WIEN2K [45] code is implemented as following Ref. [14]. In this session, the participants will learn how to perform in practice elementary LDA+RISB simulations based on a few simple examples of strongly correlated materials and to extract several key physical quantities from the calculation.

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