Density reconstruction via entropy optimization: Applications to disordered solids

The maximum entropy approach to local electronic structure rests on two important observations. The moment theorem of Cyrot-Lackmann (1968) connects the local density of states to the topology of the local environment of an atom. The moments of the (local) density of states can be expressed as a sum of irreversible paths that start and end at the same atomic site. This makes it possible to map the problem onto the Hausdorff moment problem, which can be solved by maximizing the Shannon information entropy associated with the density, subject to the moment constraints. The approach is based on the maximum entropy principle (MEP), proposed by Jaynes', which states that in the absence of sufficient information, the solution that maximizes the entropy is the most unbiased solution among others. The reconstruction of a density from its moments is an archetypal example of an inverse problem, which quickly becomes ill-conditioned as the number of moments grows beyond 10-12 power moments.

The present activity of the group is primarily focused on two aspects of entropy optimization problems. First, it is essential to develop a robust algorithm that can deal with reasonable noise that might be present in numerically obtained moments for a physical problem. The presence of noise can affect the necessary conditions for solving an MEP problem and make the problem intractable even though an MEP solution may exist for a set of noise-free moments. A suitable perturbation of the moments or a regularization of the problem might be necessary in order to obtain an MEP solution in such cases. Second, from the point of view electronic-structure calculations, this problem is also related with the calculation of electronic forces upon perturbation of moments via atomic displacements. While the problem is nontrivial for disordered systems, it is particularly difficult for crystalline solids, owing to the presence of van Hove's singularities. The latter require information from higher-order moments, which are increasingly difficult to obtain and include in the MEP solution via conventional optimization algorithms. The reconstruction of the electronic density of states for ordered Hamiltonians with fine structure in the spectral distribution is a difficult inverse problem in electronic structure theory. Current efforts to address these problems are largely based on the use of orthogonal polynomials. Biswas and his collaborators proposed an efficient scheme for entropy optimization, based on Chebyshev polynomials, which is proved to be particularly useful and robust in dealing with a large number of moments of up to 200 for reconstructing highly nontrivial density distributions with fine structure.