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Accelerating the convergence of the SCF Iteration through charge mixing and preconditioning

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Kohn-Sham density functional theory (KSDFT) is the most widely used electronic structure theory for condensed matter systems. Although KSDFT is often stated as a nonlinear eigenvalue problem, an alternative formulation of the problem, which is more convenient for understanding the convergence of numerical algorithms for solving this type of problem, is based on a nonlinear map known as the Kohn-Sham map. The solution to the KSDFT problem is a fixed point of this nonlinear map. The simplest way to solve the KSDFT problem is to apply a fixed point iteration to the nonlinear equation defined by the Kohn-Sham map. This is commonly known as the self-consistent field (SCF) iteration in the condensed matter physics and chemistry communities. However, this simple approach often fails to converge. The difficulty of reaching convergence can be seen from the analysis of the Jacobian matrix of the Kohn-Sham map, which we will present in this talk. The Jacobian matrix is directly related to the dielectric matrix or the linear response operator in the condense matter community. We will show the different behaviors of insulating and metallic systems in terms of the spectral property of the Jacobian matrix. We discuss how to use these properties to approximate the Jacobian matrix and to develop effective preconditioners to accelerate the convergence of the SCF iteration. Approximations to the Jacobian can also be constructed directly using the Broyden-like technique. In computational condense matter physics, this is often known as the charge mixing scheme. We will present and compare different mixing schemes and point out some open questions regarding the effects of mixing and preconditioning on the convergence of the SCF iteration.