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Linear Scaling Solvers for Density Functional Theory Calculations

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The theory of matrix functions is a well developed framework with a wide range of applications including differential equations, graph theory, and electronic structure calculations. One particularly important application area is diagonalization free methods in density functional theory calculations. When the input and output of the matrix function are sparse, methods based on polynomial expansions can be used to compute matrix functions in linear time. In this talk, we present a library based on these methods that can compute a variety of matrix functions. We will describe the algorithms at the heart of this library, and show how can be integrated into a variety of programs to enable large scale calculations.

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