Simplified pseudopotential problems for the classroom

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Abstract. In the computational quantum mechanical study of condensed matter systems *ab initio* methods have been used for many decades to accurately predict properties of crystalline solids such as equilibrium lattice constants, band structure, optical properties, elastic constants, etc. In the early 80's and 90's many research groups developed their own programs to perform *ab initio* calculations. In doing so, generations of research students and postdoctoral fellows acquired useful, transferable skills. Over time however, collaborations between various research groups within academia and in industry have resulted in the creation of more than 50 open-source and commercial software packages. These software packages are widely used today for condensed matter research by students who, unfortunately, often have have very little understanding of the theoretical framework, and algorithmic and programming details of these codes. To address this shortcoming, our research group has embarked on a programme to devise a range of simplified computational problems appropriate for the classroom, which can be used to teach undergraduate students about particular theoretical and numerical aspects of the electronic structure method. These problems are easily programmable. In this presentation, we will focus on the pseudopotential method, which is an important ingredient in modern *ab initio* methods. Whereas the full implementation of this concept in a real electronic structure code requires complicated numerical methods, e.g. accelerated convergence to selfconsistency including the interactions between all the electrons in the system, we show that the essential principles of the pseudopotential can, nevertheless, be presented in a simpler class of problems, which can readily be coded by students.