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Quantum Mechanics and Density Functional Theory of the Rosen-Morse Potential ERIC HINOJOSA, ANTONIO CANCIO, Ball State University — Density Functional Theory (DFT) is an electronic structure method widely used to calculate the electronic, optical and magnetic properties of materials in terms of atoms and the electrons that glue them together. One way to test and improve DFT theories is to apply them to simple, one-dimensional potentials. Such potentials allow easy testing of new theories, as calculations can be made quickly and analytic answers are sometimes known. We study the Rosen-Morse potential, a quantum potential used to model vibrations and predict energy spectra of molecules. It is also used in nanoscience to model an electron trapped in a thin layer between two materials. We adapt previously written code to study this potential, using Python along with the numpy and matplotlib library. We calculate eigen-orbitals and bound state energies and then study "pseudo-atom" systems consisting of RM potentials with all bound states completely occupied, simulating the electronic shell structure of the atom. We use these systems to test the predictions of density functionals of the kinetic energy, including the Thomas-Fermi, Von Weizsacker, and local gradient-expansion. Our data indicates that kinetic energy models that are typically poor in three-dimensions are nearly exact for this model.

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