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Band Gap Studies in Density Functional Theory[1] THOMAS E. BAKER, Department of Physics & Astronomy, University of California, Irvine, California 92697 USA, LUCAS WAGNER, Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling,FEW, Vrije Universiteit, De Boelelaan 1083, 1081HV Amsterdam, The, MILES STOUDENMIRE, Perimeter Institute for Theoretical Physics, Waterloo, Ontario, N2L 2Y5 Canada, KIERON BURKE, Department of Chemistry and of Physics, University of California, Irvine, California 92697 USA, STEVEN WHITE, Department of Physics & Astronomy, University of California, Irvine, California 92697 USA — We examine the exact properties of Density Functional Theory (DFT) in one dimension and compare it with the numerically exact answer provided by Density Matrix Renormalization Group. Using the exact answers, we can compare exact Density Functional Theory quantities against commonly used approximations. Approximations tend to underestimate the band gap of the material. We compare the exact DFT quantities with the approximations to explore the band gap problem and provide numerical proofs of principle.

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