Remarks on Local Energy and Perturbations

M. G. Marmorino

Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Warinchamrap, Ubon Ratchathani, 34190. Thailand

Reprint requests to Dr. M. G. M.; E-mail: mgm@sci.ubu.ac.th

Z. Naturforsch. **55a.** 912–914 (2000); received March 3, 2000

The local energy is first reviewed and compared with the expected energy. We then present the perturbative local energy method which uses an exactly soluble base problem and a perturbing potential to greatly simplify the expression of the local energy. This is demonstrated with two-electron atoms for which the method gives upper bounds with errors from 18% for He to 4% for Ne⁸⁺. Finally a call to develop a local energy method for large systems is issued.

Key words: Local Energy; Variation Theorem; Perturbations.