

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

A problem with the stress theorem commonly used in DFT codes¹

DONALD NICHOLSON, Department of Physics, University of North Carolina Asheville — The change in energy when an affine transformation (strain) is applied to a lattice of ions can be obtained by evaluating the algebraic derivative of the DFT energy (in practice a local or other approximation) of an electron density that has been similarly strained [1]. Because the DFT energy is stationary in the density, it is only required that the strained density reduces to the exact density at zero strain; it does. The algebraic derivatives of the Hartree and exchange energies are straightforward. The derivative with respect to strain of the non-interacting kinetic energy depends on two assumptions: 1) the modulus squared of the strained orbitals equals the strained electron density, and 2) the strained orbitals minimize the non-interacting kinetic energy. The first assumption is correct. I find that the second assumption applies only in special cases. The limitations and possible modifications of the stress theorem are discussed.

[1] Nielsen, O. H. & Martin, R. M. 1983 First-Principles Calculation of Stress. *Physical Review Letters* 50, 697.

[2] D. M. Nicholson, Madhusudan Ojha, and T. Egami, *Journal of Physics Condensed Matter* 10/2013; 25(43):435505.

¹Work at the University of North Carolina Asheville and Oak Ridge National Laboratory was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division.

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Date submitted: 13 Nov 2014

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