Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Density Functional Theory Revisited: The Mathematical and Physical Conditions for the Physical Content of the Eigenvalues DIOLA BAGAYOKO, LASHOUNDA FRANKLIN, YURIY MALOZOVSKY, BETHUEL KHAMALA, Southern University and A&M College in Baton Rouge (SUBR), Louisiana, USA, CHINEDU EKUMA, Department of Physics and Astronomy, Louisiana State University (LSU), Baton Rouge, Louisiana, USA, YACOUBA DIAKITE, Deparment of Studies and Research (DSR) in Physics, University of Science (USTTB), Bamako, Mali, AZIZJON SALIEV, Binghamton University, Binghamton, New York, USA — We briefly recall the derivation of density functional theory (DFT) and of its local density approximation (LDA). From this derivation, we show that eigenvalues resulting from self consistent DFT calculations utilizing a single input basis set do not necessarily have much physical content. We subsequently present *the necessary conditions for obtaining eigenvalues with a physical content, for the ground state and low energy excited states.* These conditions include the verifiable attainment of the minima of the occupied energies, on the one hand, and the avoidance of a mathematical artifact stemming from the Rayleigh theorem, on the other. We show a few new results, obtained with DFT potentials, that agree very well with corresponding experimental ones. These results include band gaps, effective masses, and structural properties of selected semiconductors. Our calculations utilized the Bagayoko, Zhao, and Williams (BZW) method as enhanced by Ekuma and Franklin (BZW-EF). The distinctive feature of the method includes its strict adherence to the necessary conditions described noted above.

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Date submitted: 15 Nov 2013 Electronic form version 1.4