J Material Sci Eng 2015, 4:3
http://dx.doi.org/10.4172/2169-0022.C1.032

OMICS International
conferenceseries.com

International Conference and Exhibition on
Mesoscopic & Condensed Matter Physics
June 22-24, 2015 Boston, USA

On N-representability problem in density functional theory

Eugene S Kryachko
Bogolyubov Institute for Theoretical Physics, Ukraine

In Table, we report the ground-state energies of some representative atoms, obtained within the Kohn-Sham density functional theory (DFT), and compare them with the corresponding exact energies. Table demonstrates that for these atoms there holds the inequalities EoDFT < Eoexact that break the variational principle. These inequalities remind the known situation with the N-representability problem for second-order reduced density matrix (2-RDM) which arose as follows: Since an electronic Hamiltonian H of N electrons, no matter describing a given molecule or solid, contains at most two-particle operators, the corresponding energy functional / can be written in terms of so-called second-order reduced density matrix (2-RDM). Omitting the Pauli conditions for 2-RDM which are in fact the necessary ones only to satisfy that a given 2-RDM is derivable from N-electronic wave function, Bopp obtained the ground-state energies for the He-isoelectronic series below the exact ones. Altogether, this implies that the xc-density functional potentials GGA, TH1, Bx88/Bc95, and many others are non-N-representable.

System	DFT methods	E_{o} DFT	E_{o} exact
H	GGA	-0.502	-0.500
	TH1	-0.502	
He	GGA	-2.909	-2.904
Li	GGA	-7.486	-7.478
	Bx88/BC95	-7.482	
Be			
O	*GGA*	*-75.069*	*-75.067*
	TH1		
F	*GGA*	*-99.737*	*-99.734*

Table: The ground-state energies, Kohn-Sham DFT and exact, (in Hartrees), of representative atoms.

Biography

Eugene S Kryachko has completed his PhD from Bogolyubov Institute for Theoretical Physics of the National Academy of Science of Ukraine. For about 20 years he worked abroad after receiving the Alexander v. Humboldt Fellowship in 1988 in LMU (Munich). He is the leading research scientist in the Department of Computational Methods in Theoretical Physics in Kiev. He has published more than 250 papers in reputed journals and serving as an Editorial Board Member of some of them.

eugene.kryachko@ulg.ac.be