Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Landscape of the exact energy functional for a simplified universe
PAULA MORI-SANCHEZ, Universidad Autonoma de Madrid, ARON COHEN, University of Cambridge — One of the great challenges of electronic structure theory is the quest for the exact functional of density functional theory (DFT). Its existence is proven, but it is a complicated multivariable functional that is almost impossible to conceptualize. In this talk we study the asymmetric two-site Hubbard model because it has only a two-dimensional universe of density matrices, hence the exact functional becomes a simple function of two variables whose three dimensional energy landscape can be visualized and explored. A walk on this unique landscape, tilted to an angle defined by the one-electron Hamiltonian, gives a valley whose minimum is the exact total energy. This is contrasted with the landscape of some approximate functionals, explaining their failure for electron transfer in the strongly correlated limit. We show concrete examples of pure-state density matrices that are not v-representable due to the underlying non-convex nature of the energy landscape. The exact functional is calculated for all numbers of electrons, including fractional, allowing the derivative discontinuity to be visualized and understood. The fundamental gap for all possible systems is obtained solely from the derivatives of the exact functional.

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Date submitted: 06 Nov 2015 Electronic form version 1.4