

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

On the Edge of Koopmans' Theorem PAUL GRABOWSKI, KIERON BURKE, University of California, Irvine — It is well known that the density of an atom falls off exponentially with increasing distance to the nucleus, with a falloff length inversely proportional to the square root of the ionization energy. It is less well known what happens when the ionization energy goes to zero, which is the case if the nuclear charge is artificially reduced to the critical value. At this critical value, there is a normalizable state at the bottom of the continuum, but the density only falls off as an exponential of the square root of the radius. We calculate this state for the two-electron atom using the pseudospectral method finding the critical value of the nuclear charge to 12 digits. This is a single-center system with strong correlation, and so is a difficult test case for DFT methods.

Paul Grabowski
University of California, Irvine

Date submitted: 15 Nov 2013

Electronic form version 1.4