Relativistic Effects on Atoms In Molecules: Theory and Properties for 1- and 2-Component Hamiltonians

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The quantum theory of atoms in molecules (QTAIM) as originally formulated is a successful method for computing atomic properties within a nonrelativistic quantum mechanical framework. Prof. R.F.W. Bader and coworkers showed that AIM satisfies the Schwinger principle of stationary action and as such justifying its utility for computing atomic properties in a nonrelativistic setting. Relativity must be accounted for when computing properties of chemical systems that include nuclei with atomic number larger than 37. I will demonstrate how to formulate QTAIM to include relativistic effects in defining a proper quantum subsystem that satisfies Schwinger's principle of stationary action for one- and two-component Hamiltonians. This will be carried out in an analogous way to the nonrelativistic treatment of QTAIM using the same assumptions. I will concentrate on some popular two-component Hamiltonians including the popular scalar-relativistic zeroth-order regular approximation (SR-ZORA). I will show how relativistic effects can alter the molecular graph and atomic properties.