Symmetry Based Determination of Relativistic Wave Equations

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The determination of increasingly accurate density functionals is one of the most active fields in quantum chemistry. Many of the wave-equations for elementary particles were derived in the 1930's and 40's using the symmetry group of flat space-time, and it seems worthwhile to try and adapt these techniques to provide information about the corresponding density functionals.

This talk will highlight some of the accomplishments and limitations of the symmetry approach to wave-equations. It is the author's opinion that the symmetry of flat space-time is not always sufficient to determine the wave-equation for an elementary particle. In particular it does not seem to be sufficient for a relativistic electron, and this finding casts doubt on whether the symmetry group contains useful information about the density functional. One way out of the impasse is to use a larger symmetry group. A promising candidate is obtained by requiring the wave-equation to be an invariant of both flat and slightly curved space time. The enhanced symmetry constraints do give rise to the Dirac equation, and the enhanced symmetry group emerges as a promising candidate for application to density functional theory.