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An Extended Electron Approach to the General Many-Body Problem

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Extended electrons, a new model in fundamental physics recently introduced, fully recovers many of the experimental results of quantum mechanics while avoiding its notorious pit falls and paradoxes [1-3]. The formulation for many-body electronic structure calculations in this context resembles the Kohn-Sham formulation of standard density functional theory, but rather than basing the density on a large set of single electron orbitals, the model is based only mass density and field components, potentially leading to a massive increase in computational efficiency. To date, the Hohenberg-Kohn theorems have yet to be proved for a model of this type. Here, we address this problem and show that the theorems do in fact hold. Following on from this result, we present a density functional method derived from the extended electron model. As a simple illustration of the new procedure we show how the model works in practice for a hydrogen molecule.

Keywords: DFT, many-body, condensed matter

Biography:

Professor Werner Hofer holds a master degree in Engineering Physics and a PhD in Condensed Matter Theory. He is internationally known for his work on the nanoscience of surfaces and interfaces, and has worked for more than fifteen years in this field with international collaborators, based at University College London, the University of Liverpool, and Newcastle University. In 2010 he became Founding Director of the Stephenson Institute for Renewable Energy in Liverpool, which he led until 2014. His current role as Dean involves coordinating and supervising all research activities within the Faculty of Science, Agriculture, and Engineering at Newcastle University.