Introducing Relativistic Reduced Density Matrix Functional Theory

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The applicability of reduced density matrix functional theory (RDMFT) is increasing among the chemists and physicist communities. Recent studies using the Hubbard model have proven that some RDMFT functional approximations are suitable for studying systems where strong electron correlation effects are dominant[1,2]. Moreover, as another example, RDMFT has been recently adapted as an alternative methodology to study superconductivity[3].

To further extend RDMFT applicability, we introduce in this work its relativistic version. Relativistic RDMFT[4] is presented using the Dirac 4-component Hamiltonian and including the effects of creation and annihilation of electron-positron pairs. To this end, we have properly adapted the recent work of Toulouse[5], where relativistic density functional theory including effective quantum electron dynamics was established. Then, considering the so-called no-pair approximation[6] we also present the relativistic version of some of the most accurate RDMFT functional approximations[7,8]. Finally, we analyze some properties of these functional approximations.

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