University of Crete
Department of Physics

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Approximating electronic correlations with functionals of the one-body reduced density matrix

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ABSTRACT

The quest for accurate and at the same time numerically efficient approximations of the many-electron problem holds a central position in the theoretical material science. Multiconfigurational methods are quite accurate but computationally demanding. On the other hand, theoretical frameworks that are based on functionals compromise sufficiently between accuracy and efficiency. Two such frameworks are density functional theory (DFT) and the reduced density matrix functional theory (RDMFT). In DFT, the fundamental variable is the electron density and certain terms of the total energy are expressed as functionals of it. Similarly, in RDMFT the fundamental variable of the one-body reduced density matrix and the total energy is expressed in terms of this quantity. DFT is computationally efficient and is the workhorse of electronic structure theory. However, there are classes of problems that DFT results deviate from experiment and for them, RDMFT is a promising alternative. In this presentation, we overview the fundamentals of RDMFT in a comparative perspective to DFT, review its main approximate functionals and assess the performance when applied to molecular and infinite systems. Finally, we present extensions for open-shell systems and the problem of N-representability in view of the so-called generalized Pauli conditions that were recently derived systematically.

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