Geometric Aspects of Functional Theories

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We provide a fresh and more concise perspective on fundamental aspects of functional theories with an emphasis on one-particle reduced density matrix functional theory (1RDMFT). First, in a general context, we introduce the so-called *scope* of a functional theory [1]. This novel concept identifies in a direct manner the natural variables, reveals the existence of a universal functional and explains how symmetries can be incorporated in functional theories.

Then, we discuss the significance of the one-body N-representability problem for 1RDMFT. We first recall the Levy [2] and Valone [3] approach to 1RDMFT. Exploiting basic tools from convex analysis then allows us to derive a striking relation between both universal functionals [4]. This result demonstrates that the complexity of the generalized Pauli constraints cannot be circumvented [4] in 1RDMFT. By utilizing recent results in quantum information theory [5,6], we finally demonstrate in a more general context how such one-body N-representability constraints shape the universal functional. In particular, we reveal the existence of an *exchange force* in fermionic systems [7] and a *Bose-Einstein force* in bosonic systems [8,9] with remarkable implications for our understanding of many-particle quantum systems.

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