Abstract Submitted
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Continuum mechanics for quantum many-body systems[1] GIOVANNI VIGNALE, University of Missouri-Columbia, JIANMIN TAO, Los Alamos National Laboratory, XIANLONG GAO, Zhejiang Normal University, ILYA TOKATLY, Universidad del Pais Vasco — Continuum mechanics is a theory of the dynamics of classical liquids and solids in which the state of the body is described by a small set of collective, such as density and current. A similar description is possible for quantum many-body systems, and indeed its existence is guaranteed by the basic theorems of time-dependent current density functional theory. In this paper we show how the exact Heisenberg equation of motion for the current density of a many-body system can be closed by expressing the quantum stress tensor as a functional of the current density. Several approximation schemes for this functional are discussed. The simplest scheme allows us to bypass the solution of the time-dependent Schrödinger equation, resulting in an equation of motion for the current that requires only ground-state properties as an input. We illustrate the formalism by applying it to the calculation of excitation energies in simple one- and two-electron systems.

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