Abstract Submitted
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Density-Functional Theory of Thermoelectric Phenomena[1] FLORIAN G. EICH, GIOVANNI VIGNALE, Department of Physics, University of Missouri-Columbia, Columbia, Missouri 65211, MASSIMILIANO DI VENTRA, University of California - San Diego, La Jolla, CA 92093 — Thermoelectric phenomena play an important role in the development of sustainable energy sources. We have introduced a non-equilibrium density-functional theory of local temperature and associated energy density that is particularly suited for the study of thermoelectric phenomena from first principles [1]. This theory rests on a local temperature field coupled to the energy-density operator. We identify the excess energy density, in addition to the charge density, as fundamental variable. These densities are obtained from an effective non-interacting Kohn-Sham system. We show that the Schrödinger equation for the Kohn-Sham system features a spatially varying mass representing the effect of local temperature variations. Furthermore we discuss strategies to approximate the Kohn-Sham potential and the spatially varying mass emerging in the Kohn-Sham equation.

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