Density-Functional Theory of Thermal Transport[1] F.G. EICH, A. PRINCIPI, University of Missouri - Columbia, M. DI VENTRA, University of California - San Diego, G. VIGNALE, University of Missouri - Columbia — We have recently introduced a non-equilibrium density-functional theory of local temperature and associated energy density that is suitable for the study of thermoelectric phenomena from first principles [1]. This theory rests on a local temperature field coupled to the energy-density operator. Here we apply the theory to a simple two-terminal setup, in which the terminals are held at different temperatures. We show that our treatment becomes equivalent to the standard Landauer-Büttiker formulation of thermal transport in the non-interacting limit.

[1] arXiv:1308.2311

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