

Abstract Submitted
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Thermal connection formula and linear response time-dependent density functional theory for thermal ensembles AURORA PRIBRAM-JONES, Lawrence Livermore National Lab and Department of Chemistry, University of California, Berkeley, PAUL GRABOWSKI, Department of Chemistry, University of California, Irvine, KIERON BURKE, Departments of Physics and Chemistry, University of California, Irvine — The finite-temperature adiabatic connection formula is cast as an integral over the temperature and used to write new relations between correlation components in terms of temperature and the coupling constant. Next, the van Leeuwen proof of time-dependent density functional theory is generalized to thermal ensembles, along with the Gross-Kohn relation and the fluctuation-dissipation theorem. These results are combined with the thermal connection formula to produce a method for generating new exchange-correlation approximations.

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