

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Time-dependent V-representability on lattice systems¹ YONGHUI LI, CARSTEN A. ULLRICH, Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211 — We study the mapping between time-dependent densities and potentials on small lattices. As discovered recently by Baer (arXiv:0704.1787), there exist well-behaved time-dependent density functions on lattices which cannot be constructed from any real potential. However, one finds that such densities can always be reproduced by complex potentials. We analyze the breakdown of time-dependent V-representability on lattices and show that it is related to problems with the continuity equation which ultimately arise from discretization of the momentum operator. This imposes fundamental restrictions on practical numerical applications of TDDFT. In the continuum limit, time-dependent V-representability is restored.

¹Supported by Research Corporation and NSF DMR-0553485.

Carsten Ullrich
Department of Physics and Astronomy,
University of Missouri, Columbia, MO 65211

Date submitted: 26 Nov 2007

Electronic form version 1.4