

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

A new approach to the treatment of uniform electric fields¹

ROBERTO D'AGOSTA, GIOVANNI VIGNALE, University of Missouri - Columbia

— It has been known for a long time that the treatment of an external uniform electric field in a periodic system presents conceptual and practical difficulties. At the heart of these difficulties lies the fact that, when a uniform electric field is present, the ground state does not exist: thus one is faced with the dilemma of either breaking the periodicity by a scalar potential or making the problem time-dependent by a vector potential. Within the context of density functional theory this seems to imply that the conventional description of many-body effects in terms of the time-dependent density should be abandoned in favor of a description in terms of the current density.¹ However, we will show that it is possible to describe the uniform electric field without leaving the framework of ordinary time-dependent DFT, by passing to a non-inertial reference frame. By leaving the distances invariant, this transformation preserves the periodicity of the lattice, and at the same time the appearance of an “inertial force” compensates for the vector potential. Thus, we end up with a system subjected to a periodic time-dependent external potential – a perfectly legitimate candidate for the application of TDDFT.

1. N.T. Maitra, I. Souza, and K. Burke, Phys. Rev. B. **68**, 045019, (2003).

¹Work supported by NSF Grant No. DMR-0313681

Roberto D'Agosta
University of Missouri - Columbia

Date submitted: 30 Nov 2004

Electronic form version 1.4