

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Gaussian-type orbitals in *ab-initio* calculations for periodic systems: Solving the so-called “linear-dependence” problem with efficient dual space summation** CRISTIAN DIACONU, JOACHIM PAIER, GUSTAVO SCUSERIA, Rice University — Expanding single-particle wave functions in a local basis set using Gaussian-type orbitals (GTO) is well established. All-electron GTO basis sets of so-called multi- $\zeta$  quality are available for a large number of elements. However, the application of GTOs in *ab-initio* calculations for periodic systems is not straightforward. Diffuse *i.e.* low-exponent basis functions are necessary for an accurate treatment of metals and small-gap semiconductors, but their use leads to the well documented problem of so-called “linear dependence.” However, we found out that the problem is not due to linear dependence, but rather to the vanishingly small norms of some of the Bloch functions. The present work introduces Poisson summation for alleviating this problem. Moreover, this approach will lead to a much more efficient calculation of Hamiltonian matrix elements. Exploiting the dual properties of real and momentum space, computations involving tight, *i.e.* high-exponent basis functions, are carried out in real space, whereas calculations using diffuse basis functions are carried out in Fourier space. This is what we mean with “dual space summation”. Roughly speaking, exploiting “the best of both worlds”, *i.e.* real as well as momentum space, can solve the technical problems incurred by the so-called “linear-dependence” of crystal orbitals.

Cristian Diaconu  
Rice University

Date submitted: 20 Nov 2009

Electronic form version 1.4