Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Analytical minimization of total spread of generalized Wannier functions in one-dimensional crystals[1] DENIS R. NACBAR, ALEXYS BRUNO-ALFONSO, Universidade Estadual Paulista, Brazil — Since their introduction in 1937, Wannier functions have become key theoretical and computational tools in Solid State Physics. In this work, generalized Wannier functions of several bands in a one-dimensional crystal are investigated. For the case of two bands, necessary condition for minimum of total variance leads to a non-linear set of four second-order differential equations having a simple analytical solution. This is a new alternative to current iterative numerical procedures. Results are displayed for diatomic crystals with inversion symmetry. The relation between generalized Wannier functions and orthogonalized atomic orbitals is discussed. It is shown that such functions may present increased exponential localization when compared with Wannier functions of separate bands. Our findings should be relevant in studies of layered semiconductor and photonic structures and linear atomic chains. Hopefully, it will speed progress both in understanding and applications of Wannier functions.

[1]We thank Brazilian Agencies CNPq and FAPESP for financial support.

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Date submitted: 11 Nov 2011 Electronic form version 1.4