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NEW POTENTIALITIES OF THE RECURSION METHOD FOR PERIODIC LATTICES

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Abstract : The recursion method has been generally applied without fully exploiting the translational symmetry or the other point group symmetries of the system. This has as consequence a practical limitation in the dimension of the clusters generated by the method, due to computer storage capabilities. Only very recently it has been shown how to exploit the point group symmetry and the special **k**-point technique in the recursion method. We present here for the case of Si an unprecedent number of recursions for the representation of the corresponding Green's functions. This opens the road to an interesting number of perspectives also for non perfect crystals.

The implementation of the recursion method for periodic structures have first been proposed by Anlaghe el al. [1] exploiting the point group symmetry of the perfect crystal with the use of the special **k**- point technique. In the same framework Cordelli et al. [2] have devised a peculiar procedure to fully exploit the translational symmetry and obtained more than 300

recursions in the case of the simple cubic crystal with s-orbitals. We have now undertaken a similar approach for realistic IV and III-V semiconductors . The more than hundreed coefficients obtained for the continued fractions representing the density of states, allow a very accurate description of the Green's function of the perfect crystals. The starting point is the microscopic description of the crystal in terms of localized orbitals. The recursion method is applied to different subzones of the Brillouin zone of the crystal, giving rise to a set of independent linear chains. A final application of the recursion method to these chains allows to sum them and to arrive to the final result. As an example we present in figure 1 the density of states of Silicon projected on the s- states, obtained with 150 continued fraction coefficints.

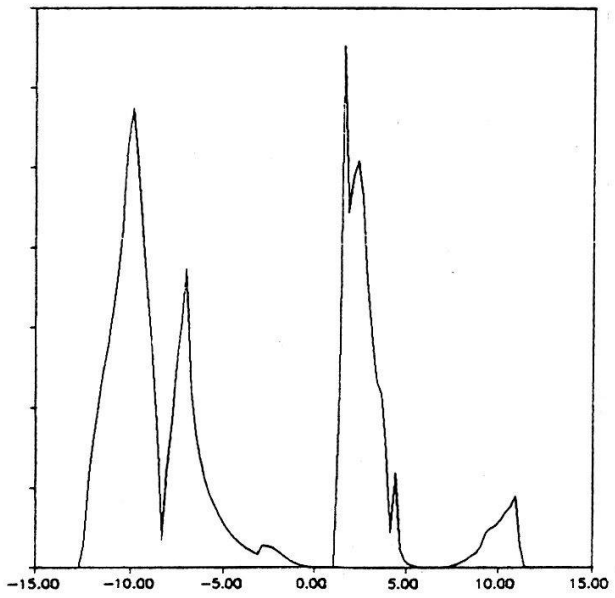

Fig.1 : s-projected density of states for Si

[1] S.M.Anlaghe and D.L.Smith, Phys.Rev. B34, 2336(1986)

[2] A.Cordelli,G.Grosso and G.Pastori Parravicini,Phys.Rev.B38, 2154(1988)