Title

MOMENTS AND AVERAGES OF THE ELECTRONIC DENSITY OF STATES OF AMORPHOUS AND CRYSTALLINE HOMOPOLAR SOLIDS

Authors

Joannopoulos, J.D.
Yndurain, F.

Publication Date

1974-10-01

Submitted to Physics Letters

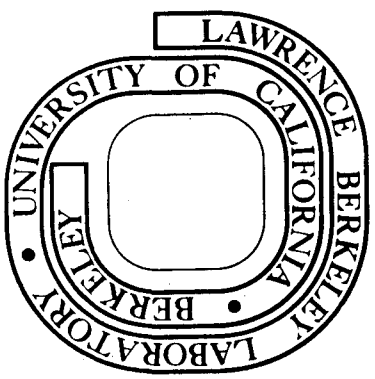
LBL-3567
Preprint c.

MOMENTS AND AVERAGES OF THE ELECTRONIC DENSITY OF STATES OF AMORPHOUS AND CRYSTALLINE HOMOPOLAR SOLIDS

J. D. Joannopoulos and F. Yndurain

October, 1974

Prepared for the U. S. Atomic Energy Commission
under Contract W-7405-ENG-48



DISCLAIMER

MOMENTS AND AVERAGES OF THE ELECTRONIC DENSITY OF STATES OF AMORPHOUS AND CRYSTALLINE HOMOPOLAR SOLIDS

J.D. Joannopoulos† and F. Yndurain‡

Department of Physics
University of California

and

Inorganic Materials Research Division
Lawrence Radiation Laboratory, Berkeley, California
94720
U.S.A.

† Supported in part by the National Science Foundation through Grant GH 35688. Present Address: Department of Physics, MIT, Cambridge, Massachusetts.

‡ Fulbright fellow under the auspices of the "Program of Cultural Cooperation between the U.S.A. and Spain." Work supported in part by the National Science Foundation through Grant GH 34438.

ABSTRACT

We have calculated the first fifteen moments of the density of states of the BC-8 and ST-12 structures and of the Polk random network model. Using these moments we calculate exact averages of the density of states of these structures.

* * *

In the last few years a great effort has been devoted to the study of the density of states (DOS) of crystalline and non-crystalline systems in terms of the moments of the local DOS (LDOS) [1]. The moments, $\mu_{0,k}$, of the LDOS, n_0, are defined as

$$\mu_{0,k} \equiv \int_{-\infty}^{\infty} n_0(E)E^k dE \quad , \qquad (1)$$

where E stands for the energy.

It can be easily seen that the kth moments of the LDOS, $\mu_{0,k}$, is directly related to the number of paths, $\Lambda_{0,k}$, that, starting at one orbital in one atom, return to the same orbital after k steps. In consequence, the first few moments

of the LDOS are related to the local configuration if no long-range interactions are present in the hamiltonian describing the system. We have calculated by a counting path method, the moments of the LDOS for the BC-8 and ST-12 structures [2] and for the Polk random network model as well [3]. We assume that there is only one s-orbital per atom and there is only a nearest-neighbour interaction V which is constant throughout the system. In consequence, $\mu_{0,k} = V^k \Lambda_{0,k}$. Our results up to Λ_{14} along with the results for the perfect diamond lattice [4] are listed in Table I. For the Polk model we have averaged over the central atom and its sixteen neighbours, and for the ST-12 structure* we have averaged over the two different atoms in the unit cell.

In order to get information about the LDOS, we have calculated exact averages of the LDOS at isolated energies. The averages are given by:

$$\langle n_o(E^{(i)}) \rangle = \int_{-\infty}^{+\infty} \sum_{\ell=o}^{N} P_\ell^{(i)} E^\ell n_o(E) dE = \sum_{\ell=o}^{N} P_\ell^{(i)} \mu_{o,\ell} \qquad (2)$$

* In the ST-12 structure, we get the same first eleven moments previously calculated by Wang and Dy (Dy private communication).

where $\sum_{\ell} P_{\ell}^{(i)} E^{\ell}$ are the Bernstein polynomials (see Reference [5], and references therein).

The advantage of these averages is that they are mathematically exact, and do not depend at all on higher order moments. In consequence, the information provided by them is reliable.

In Table II, we have listed the averages of the LDOS for the diamond, ST-12 and BC-8 structures and for the Polk model taking as input the first fifteen ($\mu_0, \mu_1, \ldots, \mu_{14}$) moments (see Table I).

We realize at once that the averages are symmetric for both diamond and BC-8 structures. This is due to the fact that, for these structures, the odd moments are zero, in other words, there are no odd-numbered rings of bonds.

The dip that appears at the middle of the band in the diamond and BC-8 structures is filled up in the ST-12 structure. This is due to the presence of five-fold and seven-fold rings of bonds in the ST-12 structure as the values of the fifth and seventh moments indicate (see Table I). In the Polk model, the dip moves to the negative energies (see Table II) and, although experiments in amorphous Si and Ge presently indicate [6] a filling-up of the dip, in the Polk model we do not find a complete filling-up. To

get that filling-up, the fifth and seventh moments should be larger as in the ST-12 structure (see Table I).

Although our results are for an oversimplified hamiltonian, its corresponding DOS is related by an analytical transformation to a more realistic hamiltonian which itself gives a good description of the s-part of the valence band of these structures [7-9].

It should be worthwhile to notice that our above-reported results are in accordance with previous calculations by the authors using the cluster-Bethe method [8,9].

This work was done in part under the auspices of the U. S. Atomic Energy Commission.

TABLE CAPTIONS

Table I: Returning paths up to 14 steps for the perfect diamond, BC-8 and ST-12 lattices and for the Polk model.

Table II: Averages of the one-band DOS of a perfect diamond, BC-8 and ST-12 lattices and of the Polk model. The energy is in units of 4V.

Table I

	Diamond	BC-8	ST-12	Polk
Λ_o	1	1	1	1
Λ_1	0	0	0	0
Λ_2	4	4	4	4
Λ_3	0	0	0	0
Λ_4	28	28	28	28
Λ_5	0	0	6.666	4.118
Λ_6	256	250	235.999	245.411
Λ_7	0	0	149.333	88.235
Λ_8	2716	2596	2241.333	2418.
Λ_9	0	0	2496.	1582.706
Λ_{10}	31504	29704	23257.333	26013.529
Λ_{11}	0	0	37693.333	25500.706
Λ_{12}	387136	362170	259099.999	297021.706
Λ_{13}	0	0	545237.333	385129.647
Λ_{14}	4951552	4611394	3060964.	3548138.412

Table II

E	Diamond	BC-8	ST-12	Polk
-.88	.209	.203	.131	.173
-.76	.359	.365	.409	.396
-.65	.500	.513	.588	.543
-.53	.606	.608	.622	.605
-.41	.646	.629	.574	.616
-.29	.618	.598	.525	.584
-.18	.555	.555	.516	.528
-.06	.506	.528	.544	.495
.06	.506	.528	.581	.545
.18	.555	.555	.608	.610
.29	.618	.598	.620	.634
.41	.646	.629	.611	.614
.53	.606	.608	.571	.578
.65	.500	.513	.490	.495
.76	.359	.365	.369	.367
.88	.209	.203	.219	.215

REFERENCES

[1] J.P. Gaspard and F. Cyrot-Lackmann, J. Phys. C: Solid State Phys. 6 (1973) 3077.

[2] J.D. Joannopoulos and M.L. Cohen, Phys. Rev. B7 (1973) 2644.

[3] D. Polk, J. Non-crystal. Solids 5 (1971) 365.

[4] M.F. Thorpe, D. Weaire and R. Alben, Phys. Rev. B7 (1973) 3777.

[5] C. Lopez, F. Yndurain and F.J. Yndurain, J. Phys. C: Solid State Phys. 7 (1974) 61.

[6] L. Ley, S. Kowalczyk, R. Pollak and D.A. Shirley, Phys. Rev. Lett. 29 (1972) 1088.

[7] M.F. Thorpe and D. Weaire, Phys. Rev. B4 (1971) 3518.

[8] F. Yndurain, J.D. Joannopoulos, M.L. Cohen and L.M. Falicov, Solid State Commun. (at press).

[9] J.D. Joannopoulos and F. Yndurain, Phys. Rev. B (to be published).

TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720