An average cluster Bethe lattice method for electronic structure calculation

1992 J. Phys.: Condens. Matter 4 6751

(http://iopscience.iop.org/0953-8984/4/32/010)

J. Phys.: Condens. Matter 4 (1992) 6751–6754. Printed in the UK

An average cluster Bethe lattice method for electronic structure calculation

S Q Wang and H Q Ye

Laboratory of Atomic Imaging of Solids, Institute of Metal Research, Academia Sinica, Wenhua Road 72, Shenyang 110015, People's Republic of China

Received 3 February 1992, in final form 14 April 1992

Abstract. An average cluster Bethe lattice method is developed for the calculation of the electronic density of states of an infinite system of atoms. The correctness and efficiency of the method are tested by two examples of calculating the electronic structure for square and honeycomb lattices.

1. Introduction

The investigation of the electronic structure of solids is a very important topic in solid state physics research. One effective way to do this is to calculate the local density of states (LDOS) of the system. Several ways have been developed to achieve the LDOS calculation. Among them, some typical methods are the self-consistent method [1], the method of moments [2, 3], the recursion method [1, 4] and the cluster Bethe lattice (CBL) method [5, 6].

In dealing with an infinite system, the first three methods are used to calculate the LDOS for a finite cluster with some kind of boundary condition to imitate the infinite system. In order to approach the situation in which the boundary condition does not affect the result seriously, a very large cluster must be used. So it may need strenuous calculations. On the other hand, the CBL method chooses a finite part of the system as a cluster and replaces the infinite environment by a Bethe lattice; the LDOS of the system is then calculated by considering the interaction of the cluster and the Bethe lattice.

The CBL method is a very useful tool for studying the electronic structure of non-periodic systems but, when used for periodic systems, the convergence is usually very slow. Then arduous calculation is needed. Hence an improvement to the method is essential. In this paper, an average cluster Bethe lattice (ACBL) method will be presented. The correctness of our method is tested by calculating the LDOSs of two periodic lattices.

2. The improved cluster Bethe lattice method

To improve the CBL method, an ACBL method is proposed and a simplification of the cluster's selection is suggested. Firstly a finite cluster with the symmetry of the reference site is chosen in order that the reference site is located at the symmetry

0953-8984/92/326751+04$04.50

centre of the cluster. Then an irreducible section of the cluster is selected. Suppose that the number of sites in it is N; the reference lattice site is labelled as the first site. Then the LDOS of the reference site can be given as

$$n_1(E,N) = (1/\pi)\,\mathrm{Im}\langle 1|G|1\rangle. \tag{1}$$

$\langle 1|G|1\rangle$ can be obtained by solving the following Dyson equation of the cluster:

$$E\langle i|G|1\rangle = \delta_{i1} + \sum_k \langle i|H|k\rangle\langle k|G|1\rangle \qquad i = 1,2,\ldots,N \tag{2}$$

and

$$H = \sum_i U_i|i\rangle\langle i| + \sum_{(i,j)} V_{ij}|i\rangle\langle j| \tag{3}$$

with nearest neighbours i, j.

By calculating $n_1(E,N)$ with a series of different sizes of clusters from those only consisting of the basic ring topology where the number of sites is m_L to a fairly complex topological structure where the number of sites is m_H in the irreducible section, then we define

$$n_1(E) = \left(\sum_m n_1(E,m)\right) \Big/ (m_H - m_L) \tag{4}$$

i.e. the average LDOS of the CBL method. This is the ACBL method.

3. The electronic structure calculation of periodic lattices by the ACBL method

This part of the paper gives examples using the ACBL method to test its correctness and precision. The lattice parameters U_i and V_{ij} are taken as 0.0 and 1.0, respectively, in the calculations.

Each site is equivalent in the square lattice. The exact LDOS calculation can be carried out by other methods [7, 8]. The LDOS of the square lattice calculated by the ACBL method for 297 sites, by the CBL method for 1385 sites and by exact calculation are shown in figure 1 by short-dashed, long-dashed and full curves, respectively. From the figure, one can see that the existence of a large number of oscillatory peaks makes it unsuitable for the CBL method to deal with a periodic system. On the other hand, the ACBL method possesses a great advantage when dealing with this problem. Even for a very small cluster, one can obtain a fairly good result.

The honeycomb lattice is the same kind of two-dimensional periodic lattice as the square lattice. The exact LDOS result has been evaluated [7, 8]. The results obtained by the ACBL method for 223 sites, by the CBL method for 1039 sites and by exact calculation are shown in figure 2 by short-dashed, long-dashed and full curves, respectively. Once more, the efficiency of the ACBL method in dealing with the periodic system is demonstrated.

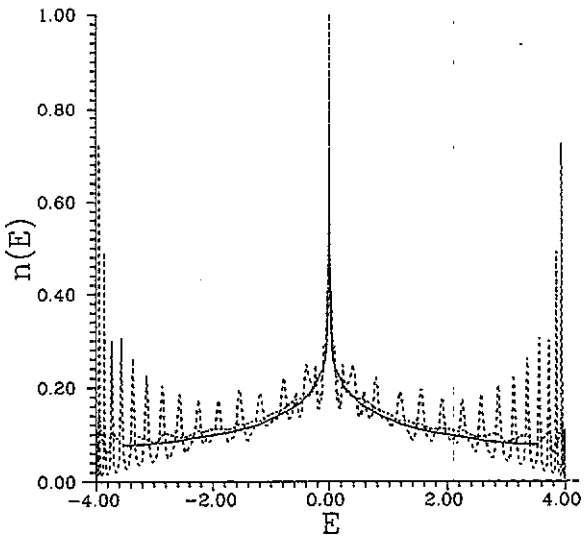

Figure 1. LDOSs of the square lattice: ----, result obtained by the ACBL method; – – –, result obtained by the CBL method; ——, exact result.

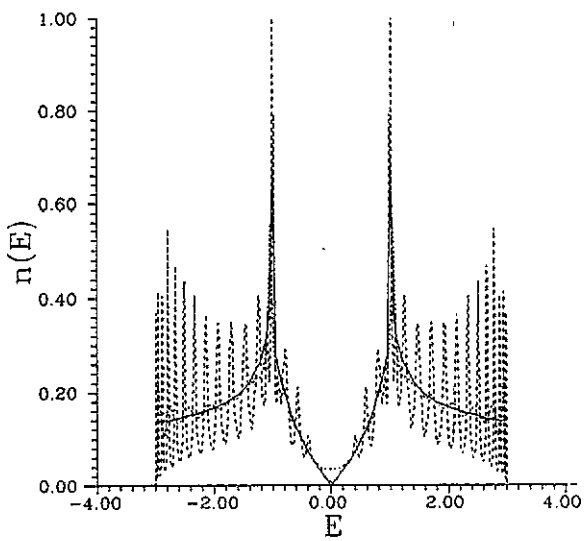

Figure 2. LDOSs of the honeycomb lattice: ----, result obtained by the ACBL method; – – –, result obtained by the CBL method; ——, exact result.

4. Conclusion

An improved CBL method, namely the ACBL method, for calculating the LDOS of an infinite system is presented. The validity and accuracy of the method are tested by the electronic structure calculation of the square and honeycomb lattices. It is shown that the ACBL method is appropriate for the LDOS calculation of periodic systems.

Acknowledgments

We are grateful to Professor Y K Wu for a beneficial discussion and to Professor D X Li and Mr T S Xie for technical help. This work was partly supported by the National Science Foundation of China.

References

[1] Haydock R, Heine V and Kelly M J 1972 *J. Phys. C: Solid State Phys.* **5** 2845
[2] Gaspard J P and Cyrot-Lackmann F 1973 *J. Phys. C: Solid State Phys.* **6** 3077
[3] Ducastelle F and Cyrot-Lackmann F 1970 *J. Phys. Chem. Solids* **31** 1295
[4] Haydock R, Kelly M S and Heine V 1980 *Solid State Physics* vol 35 (New York: Academic)
[5] Joannopoulos J D and Yndurain F 1974 *Phys. Rev.* B **10** 5164
[6] Yndurain F, Joannopoulos J D, Cahen M L and Falicov L M 1974 *Solid State Commun.* **15** 617
[7] Montroll E W 1986 *Proc. 3rd Berkeley Symp. on Mathematical Statistics and Probability* ed J Neyman (Berkeley, CA: University of California Press)
[8] Horiguchi T 1972 *J. Math. Phys.* **13** 1411