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A convolution technique for the calculation of local densities of states

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Abstract. A convolution technique is proposed for the calculation of local densities of states (LDOS) within the tight-binding (TB) model. It relies on the separability of the variables in the Hamiltonian. This technique allows one to carry out calculations for the two- and three-dimensional lattices if the one-dimensional LDOS is known. The approach avoids K-space integration as well as the processing of large clusters. The results are checked against known results produced by the straight TB model, and some new cases, such as that of the LDOS for a two-dimensional lattice in the presence of an external electric field, are also considered.

1. Introduction

The local density of states (LDOS) is one of the most characteristic features of any quantum system [1, 2]. Usually the calculation of the LDOS for one-dimensional model crystals poses no problems, but for two or three dimensions the calculations may become cumbersome [1, 2]. The tight-binding approximation which accounts for an interaction restricted to the first neighbours allows an analytical solution for a chain of atoms with one orbital each (the one-band one-dimensional model) [3] to be obtained. For two or three dimensions, even for simple cubic structures the TB model has to be evaluated numerically [4–6] and various fast computational schemes have been considered for the purpose [7]. The case with imperfect periodicity in some direction has to be considered in many instances [5, 6], e.g. when a constant electric field is applied to a solid, producing the well known Wannier–Stark effect. For the simplest case of this effect, an infinite one-dimensional chain, the analytical solution for the LDOS was obtained recently [3]. A generalization of this result in two and three dimensions for one- or two-band TB models would be an interesting step. There are various approaches to computing the LDOS for crystals in the TB approximation, but two of them are especially popular. The first one relies on periodicity and uses integration over the Brillouin zone. Such an integration is usually carried out numerically and depends on choosing some selected points or subdividing the zone in an appropriate manner [4, 6]. The other commonly used alternative for obtaining the LDOS is the so-called cluster approximation [4, 6]. The matrix of the Hamiltonian for a sufficiently large one-, two- or three-dimensional cluster is diagonalized and a histogram of its eigenvalues is used to approximate the LDOS [4, 6]. The size of the matrix increases

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with the number of atoms and, even with a good algorithm for the eigenvalues, this method is time consuming. However, the cluster approach does not need periodicity in all of the spatial directions [5, 6].

Here we propose a new approach to LDOS calculations in two or three dimensions for the TB model of simple cubic crystals. The idea is to utilize the separability of the Hamiltonian, which allows one to perform a convolution of the one-dimensional result with the LDOS for one or two dimensions so as to obtain the result for the case with a higher dimensionality. This way of proceeding avoids both the huge matrices of the cluster approximation and the awkward integration over the Brillouin zone. As was pointed out, obtaining the LDOS in the TB model for one dimension is not a problem: for the one-dimensional one-band case the analytic solution is known [3] and for two bands the numerical calculation is fairly easy [8]. Our approach has been implemented for two- and three-dimensional one- or two-band crystals in order to compare its merits with those of the already known methods. The investigation has been extended to the calculation of the LDOS in two dimensions in the presence of an external electric field. The results concerning the Wannier–Stark effect in two-dimensional crystals are a further generalization of the analytical results obtained recently [3] for the one-dimensional one-band case.

2. Model and method

We consider within the TB model a simple cubic crystal with a dimensionality D and first neighbours. For a one-band case the Hamiltonian of a one-electron system can be written as a sum of commutating operators $H = H_{x_i}$, $i = 1, \ldots, D$. In this case the spectrum of eigenvalues is a sum of the eigenvalues of each H_{x_i}, and their overall distribution is a 'convolution' or a 'composition' [9]. This formulation suggests that the one-dimensional LDOS of a chain can be used as an operator that increases the dimensionality of the solution:

$$\rho^{(D)}(E) = \int_{-\infty}^{\infty} \rho^{(D-1)}(\epsilon)\rho^{(1)}(E-\epsilon)\,\mathrm{d}\epsilon.$$

The trivial case in which $D - 1 = 0$ is indeed $\rho^{(0)}(\epsilon) = \delta(\epsilon)$. For $D = 2$ and identical variables, the one-dimensional LDOS has to be convolved with itself:

$$\rho^{(2)}(E) = \int_{-\infty}^{\infty} \rho^{(1)}(\epsilon)\rho^{(1)}(E-\epsilon)\,\mathrm{d}\epsilon.$$

For $D = 3$ the autoconvolution of ρ has to be performed twice. The idea of our approach is summarized in a graphical form in figure 1. The top row presents the convolution of the one-dimensional LDOS with itself, producing the corresponding two-dimensional LDOS; as can be seen, the width of the band is doubled, as its centre remains fixed; the singularities at the two ends of the one-dimensional curve cancel one another and, combined, produce the logarithmic singularity in the middle. In the same figure, shown below is the convolution of the two-dimensional LDOS with the one-dimensional LDOS producing the three-dimensional result; the width is three times the original. An alternative way to perform convolutions is to multiply the Fourier transforms and then to take the inverse Fourier transform of the result. The transform of the LDOS for a simple chain is a zeroth-order Bessel function J_0, so one can write $\rho^{(D)} = \mathrm{FT}(J_0^D)$ and thus the curves shown in figure 1 are readily produced. The calculations outlined are rather simple and can be done with almost any mathematical software such as the Matlab package [10], which we used.

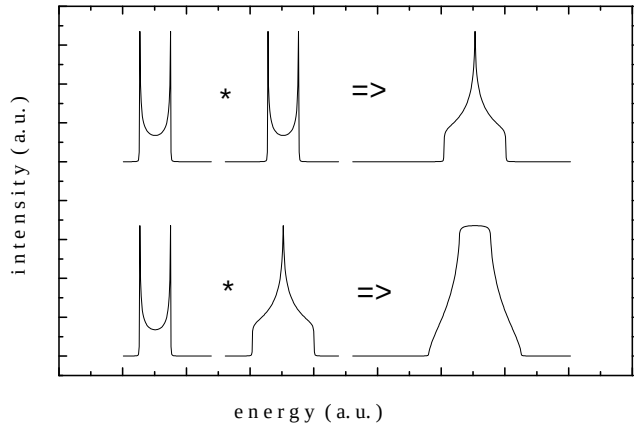

Figure 1. Top row: a convolution of two one-dimensional LDOS producing a two-dimensional LDOS; bottom row: a convolution of a two-dimensional and a one-dimensional LDOS producing a three-dimensional LDOS.

3. Results and discussion

Whenever this way of proceeding is applicable, its output is in perfect agreement with results produced by other known methods, the main difference being of course in the cost of the computational power. In order to compare results, we used the cluster approximation relying on the well known formula $\rho = (-1/\pi)\,\mathrm{Im}\,G(E + 0\mathrm{i})$ where G is the Green function for the orbitals of the central atom and it is calculated as the inverse of $H - E$, H being the Hamiltonian. The one-electron Hamiltonians with semi-empirical parameters were taken as in [8]. The resonance integral was taken to be zero while the value for the exchange integral was typically -1 eV. The size of the system is chosen such as to allow a precision of 1 meV for the eigenvalues. The checking has been done for the TB model of two- and three-dimensional one- or two-band simple cubic crystals with first neighbours. An excellent agreement of the curves produced by direct TB calculations and by convolution is shown in figure 2 for a case with $N = 51$. The saving in computational effort is considerable: the matrix for a two-dimensional structure of $N \times N$ atoms is N times larger than the matrix for the one-dimensional chain and, as the usual calculations involve inversions, the number of operations is about N^3 larger. Typically, the time needed here would be reduced by 2–3 orders of magnitude. For instance on a PC586/100 MHz it took several hours to obtain the upper curve in figure 2, while the lower one was produced in just about a minute.

Since the one-dimensional LDOS in the presence of an external electric field is known [3], there was no problem in constructing the curve for the two-dimensional case. For the two cases (with a field or without) the analytical expressions are available and here it is possible to simplify the calculation further. When a field γ is applied, $\rho = \rho(\epsilon; \gamma)$, but if it is along the x-axis, the movement would be free for the other directions, so

$$\rho^{(1)}(\epsilon; 0) = (1/\pi)/\sqrt{1 - \epsilon^2}$$

and in this particular case there is an ingenious formula for the convolution:

$$\rho^{(2)}(E; \gamma) = (1/n) \sum_{i=1}^{n} \rho^{(1)}(E - \epsilon_i; \gamma)$$

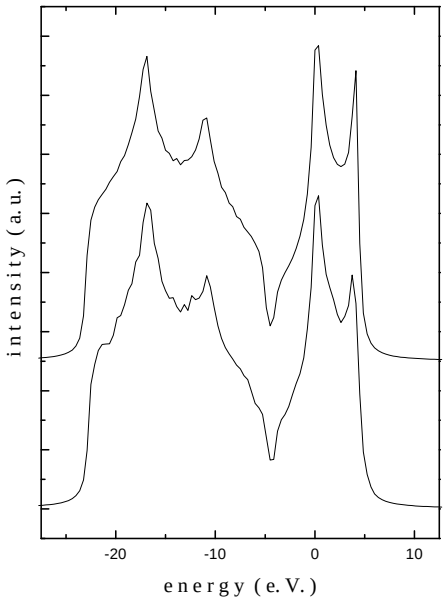

Figure 2. A model two-dimensional two-band LDOS obtained by standard TB calculations (above) and by convolution (below).

where $\epsilon_i = \cos((2i-1)\pi/(2n)); i = 1, 2, \ldots, n$ [11], $\rho^{(1)}(E;\gamma)$ being the solution for a chain in the presence of an electric field [3]. In figure 3 the two one-dimensional curves are plotted on the left and the two-dimensional result calculated by direct convolution and by using the simplified formula is on the right. One can note that the singularity is reproduced better with the second variant. A further investigation of this way of proceeding is likely to be fruitful; we hope to pursue this in future work.

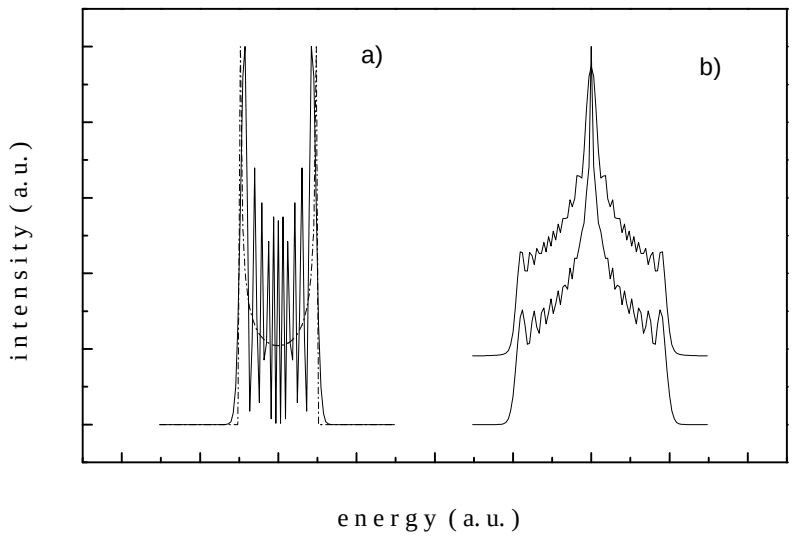

Figure 3. (a) A plot of the one-dimensional LDOS in the presence of a field and without a field (dash–dot curve); (b) a plot of the corresponding two-dimensional LDOS calculated using a numerical convolution (above) and the simplified formula (below).

4. Conclusions

The present work proposes a convolution technique for fast calculation of the LDOS in some two- and three-dimensional cases. This method produces exact results, while most of the previous accelerated computational schemes rely on converging iterations. It is applicable only when the Hamiltonians are separable, which is of course a severe limitation. A more detailed consideration of transforms which might produce their full or partial separation would allow one to delineate more clearly the scope of its possible utilization. Developing further the result of Davison *et al* [3] has provided an example of its usefulness.

Acknowledgments

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