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The convolution method for calculations of local densities of states

A Losev

Bulgarian Academy of Sciences, Institute of General and Inorganic Chemistry,
11 G Bonchev street, Sofia BU-1113, Bulgaria

E-mail: banchem@argo.bas.bg

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Abstract

The convolution method for the calculation of local densities of states is presented more thoroughly along with its expression in terms of Green functions. This constructive approach allows us to produce results for a higher dimensionality from lower-dimensional parts. Its applications and different aspects are discussed for some simple cases.

1. Introduction

Recently we proposed and demonstrated a new convolution technique for the calculation of the local density of states (LDOS) [1, 2]. The idea of this novel approach is intuitively accessible, so its mathematical description has not been revealed yet. The analytic formulation offers the advantage of a more comprehensive view of the interplay of parameters in the models utilized, which could be beneficial as regards further developments. Exact analytic results being rather scarce in this area [3–7], the calculations of the LDOS and other characteristics rely on numerical schemes, but usually they become onerous tasks even for some of the simplest systems. In consequence, a wealth of alternatives have been produced and among them the ones exploiting tight-binding (TB) models appear particularly useful [8–10]. In this context Green functions (GFs) have proved to be a most versatile tool with applications that are constantly expanded [11, 12]. The approach considered here proposes to utilize in a constructive manner the already known LDOSs in analytic or numeric form, no matter how they have been arrived at, and shows also that the GF can be obtained in the same way.

2. Model and method

We consider a particular class of Hamiltonians, such that in some representation they can be written as $H = \sum_i H_i(k_i)$. This is a severe restriction, of course, but at least an important case is included in that class, as will be demonstrated in the next section. The meaning of the

LDOS is that $dk \sim \rho(E) dE$ or $\rho \sim dk/dE$, while the dependence of the wavenumber k on the energy E is given in the Hamiltonian equation; in one dimension this leads eventually to

$$\rho^{(1)}(E) = a[H_1^{-1}(E)]',$$

assuming that this derivative exists and its integral can be scaled to a unit by some coefficient a .

In two dimensions we suppose first a constant k_2 and we consider the partial LDOS

$$\rho^{(1)}(E; k_2) = a[H_1^{-1}(E - H_2(k_2))'].$$

Then the whole two-dimensional LDOS is obtained by integrating over k_2 :

$$\rho^{(2)} = a \int [H_1^{-1}(E - H_2(k_2))'] dk_2.$$

Here the substitution $\eta = H_2(k_2)$ produces the integral

$$\rho^{(2)} = a \int [H_1^{-1}(E - \eta)]'[H_2^{-1}(\eta)]' d\eta$$

which is indeed a convolution. This result can be rewritten more concisely using the commonly adopted sign $*$ to denote the convolution operation and ρ_i for $[H_i^{-1}]'$:

$$\rho^{(2)} = \rho_1 * \rho_2.$$

In three dimensions the same reasoning leads to

$$\rho^{(3)} = \rho_1 * \rho_2 * \rho_3.$$

As the convolution is equivalent in Fourier space to a simple multiplication of the transforms, it has the properties of this operation, namely being associative and commutative, and the result can be presented more generally as

$$\rho^{(D)} = \rho^{(D-1)} * \rho^{(1)},$$

where $D = 1, 2, 3$ is the dimensionality of the system and $\rho^{(0)}$ is the delta function $\delta(E)$. This is the defining equation of the method: it reveals an important property of the LDOS which can be utilized independently of the way in which the LDOS itself has been obtained.

The same result was reached straightforwardly [1] by adopting a statistical viewpoint: the distribution of the values generated by a form such as H is a 'composition' or 'convolution' [13] of the distributions of its additive parts which correspond to the independent variables. Thus the energy in the Hamiltonian equation is to be seen as a variable produced as a sum of independent variables. So, the density of its distribution is the convolution of the densities of the summed variables. This observation implies also that the eigenvalues of the system are indeed obtained by additive combinations of eigenvalues corresponding to its components. Within the framework of renormalization, Oliveira *et al* [14] have arrived at a rather similar idea.

In terms of the GF the LDOS is expressed as

$$\rho(E) = -\frac{1}{\pi} \text{Im } g(E + i0)$$

where $i0$ is a vanishingly small imaginary quantity. In the two-dimensional case, the formula now reads

$$\text{Im } g^{(2)} = -\frac{1}{\pi} \text{Im } g_1 * \text{Im } g_2.$$

Keeping in mind that $\text{Re } g$ and $\text{Im } g$ are a Hilbert transform (HT) pair, i.e.

$$\text{HT}(\text{Im } g) = \text{Re } g,$$

and that the transform is performed as a convolution with the reciprocal of the variable [15], the two-dimensional result can be written as

$$\text{Im } g^{(2)} = -\frac{1}{\pi} \text{Re } g_1 * \frac{1}{E} * \text{Re } g_2 * \frac{1}{E}.$$

Using the properties of the convolution and noting that the effect of two HTs is simply a sign inversion, one arrives at

$$\text{Im } g^{(2)} = \frac{1}{\pi} \text{Re } g_1 * \text{Re } g_2.$$

But as

$$\text{Re } g^{(2)} = \text{HT}(\text{Im } g^{(2)})$$

we also have

$$\text{Re } g^{(2)} = -\frac{1}{\pi} \text{Im } g_1 * \text{Re } g_2$$

and

$$\text{Re } g^{(2)} = -\frac{1}{\pi} \text{Im } g_2 * \text{Re } g_1.$$

These equations for the real and imaginary parts of $g^{(2)}$ are in fact contained in the formula

$$g^{(2)} = -\frac{1}{2\pi i} g_2 * g_1$$

and by the same reasoning they can be extended to the next dimension.

3. Results and discussion

We shall consider briefly some applications to a few typical cases concerning finite or infinite structures involving eventually some degree of disorder. They offer a rather new point of view on examples which for the most part are known.

3.1. A simple crystal

Within the TB model the Hamiltonian of a simple D -dimensional crystal is written in a plane-wave representation as $H = \alpha + 2 \sum_i \beta_i \cos(k_i d_i)$, $i = 1, \dots, D$. Assuming the spacing to be $d_i = 1$ and the energy ϵ to be expressed through the dimensionless variable $E = (\epsilon - \alpha)/2\beta$, we would have $k_1 = \arccos(E)$ and thus

$$\rho^{(1)} = \frac{1}{\pi \sqrt{(1 - E^2)}},$$

the coefficient $-1/\pi$ being included in order to scale the overall density to a unit, considering it equal to zero outside the energy interval $(-1, 1)$. In two and three dimensions,

$$\rho^{(2)} = \frac{1}{\pi^2} \int_{-1}^1 \frac{1}{\sqrt{1 - (E - \eta)^2} \sqrt{1 - \eta^2}} d\eta$$

and

$$\rho^{(3)} = \frac{1}{\pi^3} \int_{-1}^1 \int_{-1}^1 \frac{1}{\sqrt{(1 - ((E - \eta) - \xi))^2} \sqrt{1 - \eta^2} \sqrt{1 - \xi^2}} d\eta d\xi.$$

The curves representing the LDOS obtained for this case are shown in figure 1 where they have been scaled to the same maximum height, instead of keeping the same (unit) area, in order to

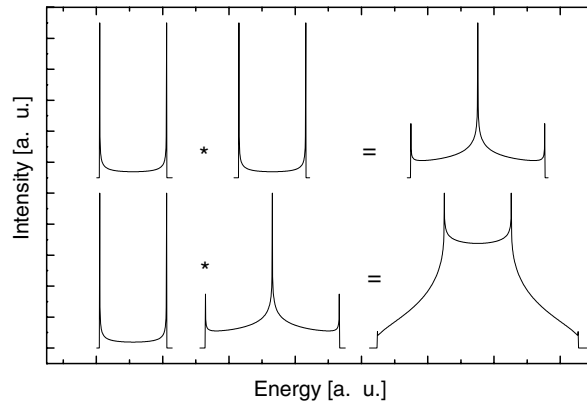


Figure 1. The LDOS of a 3D simple cubic crystal obtained by self-convolution. Upper panel: the convolution of two 1D LDOSs produces a 2D LDOS; lower panel: the convolution of the 2D LDOS and 1D LDOS produces the 3D LDOS.

offer a better view. If the singularities of the one-dimensional curve are well pronounced, they are reproduced in subsequent calculations, as can be seen in this figure. It was not evident that these well resolved features could be obtained at such low computational costs. In numerical form the convolutions are reduced to sums of the type $s_k = \sum_i u_{k-i} v_i$. In Fourier space they are multiplications of the transforms and here we would have $\rho^{(D)} = FT(|J_0^D|)$, J_0 being the zeroth-order Bessel function. The attempts to obtain the same curves from the GF are unlikely to succeed for computational reasons but, reformulated in terms of GF, the method can be linked to various other approaches. The analytical formulae suggest that the two- or three-dimensional LDOS can be expressed through elliptic integrals; the convolutional form has a rather intuitive meaning, which is perhaps more intelligible.

3.2. A semi-infinite slab

The model of a slab is a structure which might be taken to be a little more realistic than the infinite 3D crystal. Now two of the axes are infinite on both sides, while the third is restricted to one direction only. In this case the LDOS corresponding to an infinite plane should be convoluted with the LDOSs for atoms in a semi-infinite chain, which differ according to their distance from the origin [16]. This has been illustrated in figure 2 which in fact reproduces results presented by Haydock and Kelly, who in their turn were assessing the possibilities of their own approach by repeating a plotting originally performed by Kalkstein [17]. The last curve in the plot is essentially a replication of the lower row of curves in figure 1, as for atoms far from the beginning of the chain the LDOS is the same as in an infinite structure. However, one might presume that here we have gained some insight into the constitution of these well known results.

3.3. A percolating cluster

Percolation phenomena are usually instances where finite and infinite structures interplay. A well known result states that for a simple cubic crystal the critical concentration of bonds for which a percolating cluster appears is close to 0.25 [18]. A reasonably good approximation for the LDOS of such a structure can be easily produced now. A bond concentration less than a unit means that a ‘chain’ of length N does indeed consist of isolated shorter fragments

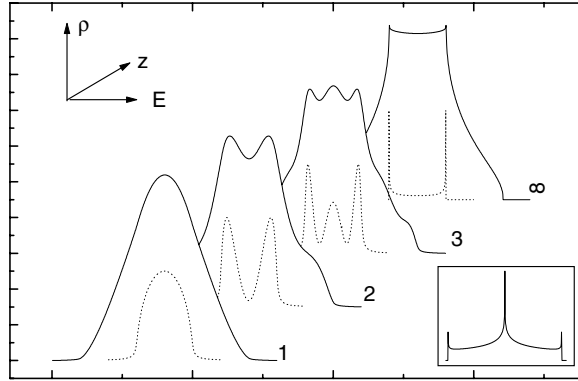


Figure 2. The LDOS in a semi-infinite slab for the first three atomic layers and bulk ($z = 0, 1, 2, \dots, \infty$). The dotted curves present on a smaller scale the LDOS in a semi-infinite chain, while the inset shows the 2D LDOS in a plane used to produce the curves.

and its LDOS is just a weighted sum of the LDOSs of its elements, while the LDOS of the whole crystal is the convolution of the results for three such broken chains. Statistics for the length of the fragments are the only supplementary data needed. A crude numerical experiment shows that for a chain of 201 sites, the available bonds (0.25) are distributed in dimers, trimers and tetramers with frequencies of 0.187, 0.046 and 0.015 respectively; longer fragments occur in less than 0.002 of the cases while the remainder (0.75) are isolated atoms. For these data the result is shown in figure 3 but it could have been obtained fully *ab initio* as the distribution of fragments according to their length follows some power law [18]. The present result and its computational costs might be compared with the example presented by Lambin and Gaspard [19] for their generalized-moments method.

3.4. A Fibonacci quasicrystal

Another related case would be a Fibonacci (quasi)crystal which is constructed from chains built in correspondence with the law for this sequence. In one dimension a Fibonacci chain is obtained when using bonds with two different strengths t_w and t_s alternating in accordance with the Fibonacci generating rule. The two-dimensional lattice has been investigated by Yang and Xing [20] but here the third dimension will be added. In the limit when the weak and the strong bonds tend to the same value ($t_w/t_s \rightarrow 1$) a plain cubic crystal is obtained. For $t_s > t_w > 0$ the LDOS is rather similar to that of the percolating cluster (in figure 3). If t_w decreases down to 0, a Fibonacci chain breaks down into non-interacting fragments, but here they are just atoms, dimers or trimers, so the LDOS for any dimension consists of a fixed number of discrete levels. As it is expressed as a sum of delta functions, its convolutions produce again sums of delta functions whose poles are obtained by simple addition. Thus, assuming that $t_w = 0$ and $t_s = 1$, one can write for the eigenvalues

$$e_k^{(D)} = e_i^{(D-1)} + e_j^{(1)} \quad \text{where } i = 1 \dots n; j = 1 \dots m; k = ij; \quad \text{and } e^{(0)} = 0.$$

The sets of different levels are easily enumerated:

$$\begin{aligned} e^{(1)} &= \{0, \pm 1, \pm \sqrt{2}\}, \\ e^{(2)} &= \{e^{(1)}, \pm 2, \pm 2\sqrt{2}, \pm 1 \pm \sqrt{2}\}, \\ e^{(3)} &= \{e^{(2)}, \pm 3, \pm 3\sqrt{2}, \pm 2 \pm \sqrt{2}, \pm 1 \pm 2\sqrt{2}\}. \end{aligned}$$

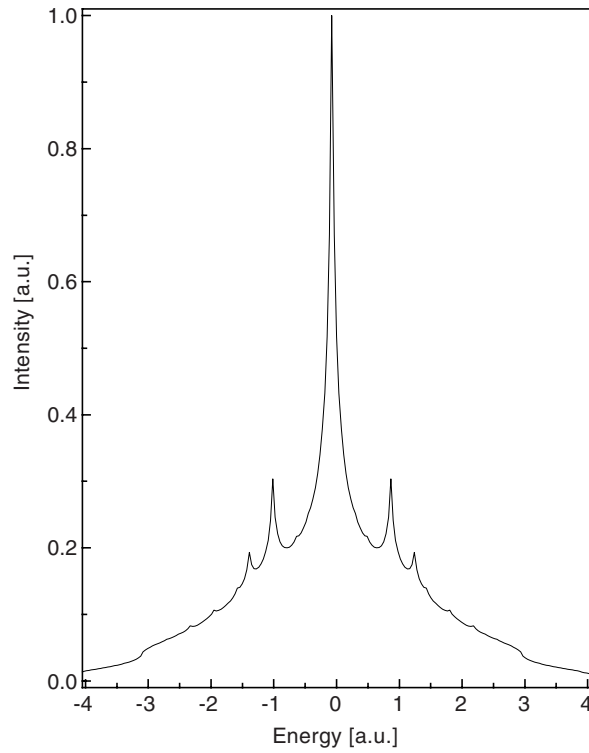


Figure 3. The LDOS for a percolating cluster in a cubic crystal.

A non-zero t_w produces the interaction between finite fragments and the degeneracy is lifted, so the eigenvalues are smeared into bands, which remain separated by gaps as long as t_w is sufficiently small. Figure 4 presents the eigenspectrum of a crystal with $N = 56$, for $t_s = 1$ and $t_w = 0.01$, when all the 25 bands of $e^{(3)}$ are visible. (It should be noted that here the ‘width’ of a trimer is $2\sqrt{2}$, i.e. larger than 2, and accordingly the full width of the spectrum, which is $6\sqrt{2}$, is greater than 6.) This approach allows one to treat also variants of the Fibonacci or similar sequences and their combinations into exotic (quasi)crystals.

3.5. The effect of a constant electric field

The two preceding examples involve a weakening or cancelling of some particular bonds in a structure. When all the bonds along one dimension disappear, the dimensionality D of the system is reduced to $D - 1$ and in fact this could be interpreted as representing the effect produced on the LDOS by a constant electric field with sufficient strength. For the simple crystal considered above (section 3.1), the Fourier transform of the LDOS with dimensionality D being J_0^D , this form makes it easier to account for the electrical effect. The result for an infinite chain obtained by Davison *et al* [5] when a field with strength F is applied along some axis becomes in Fourier space $J_0(|2 \sin(\omega)/F|)$ [21]. Now the transform of the LDOS, being represented by a product of such factors each corresponding to an axis, for higher field strength along any one of them turns into a constant ($J_0(0) = 1$), so its original form is a delta function and the dimensionality of the system is lowered. We have already considered the physical aspect of this phenomenon in previous work [22].

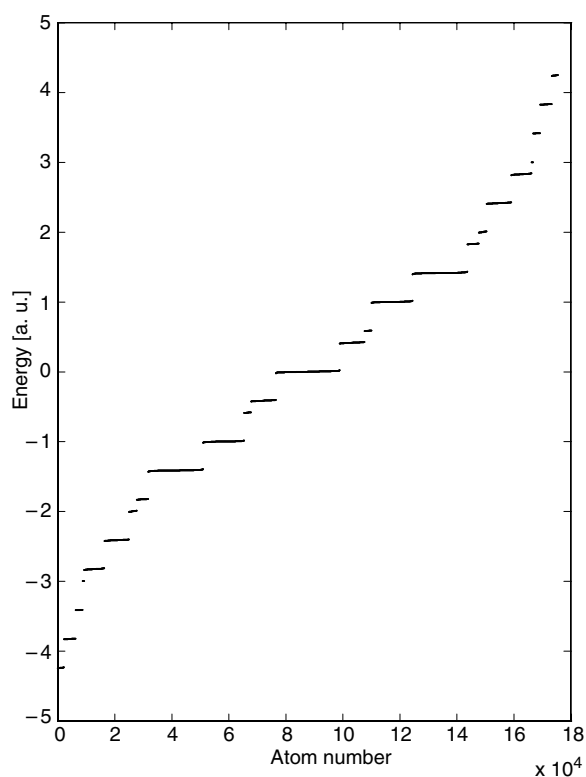


Figure 4. The eigenspectrum of a Fibonacci quasicrystal.

The limitations for this way of proceeding are fairly evident as it relies on the additivity of the Hamiltonians. However, some insight into the production of the LDOS has been gained. For instance, a $\rho^{(2)}$ -curve now can be seen as (the way to the limit for) a weighted sum of ‘U’ shapes centred at different energies. If second neighbours are to be included in a TB Hamiltonian with dimensionality greater than one, it ceases to be additively separable but it can still be factorized, now as a product, and then the summation would include not just weighted and displaced one-dimensional ‘U’ shapes but also ones with a different spread.

In one dimension there is no problem in considering neighbours further than first ones and obtaining the LDOS for such chains as a derivative of the inverted Hamiltonian, a result that has also been obtained by Oliveira *et al* [14]. Yuan *et al* [23] have investigated the so-called labyrinth tiling, which is constructed from two diagonally oriented ‘octonacci’ chains and so the sites appear as if they were ‘pure’ second neighbours. In this case the eigenvalues for the TB Hamiltonian defined on the tiling are simply the products of the eigenvalues from the two chains. These remarks could be used to suggest some perspectives for future developments of the method discussed here.

4. Conclusions

The proposed method allows one to utilize effectively results already obtained and to extend them further. It is able to generate new ones and, in many instances, results that are otherwise difficult to obtain become easily accessible. However, the method relies on the

separability of the Hamiltonian, which severely limits its scope. The analytic formulation of the method suggests a novel view even if the complexity of the calculations mostly prevents their completion. Some discrete and/or finite cases however turn out to be trivial.

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