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Local densities of states for some embedded structures

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Abstract

The convolution method for calculations of the local densities of states is applied to some simple embedded model structures and quasiperiodic sequences of two types of layers are briefly considered. Some analytic results are derived along with a discussion about the limitations of this approach.

1. Introduction

Recently we proposed and demonstrated a convolution method for the calculation of the local density of states (LDOS) [1, 2]. It has been shown to be applicable to relatively simple structures including some quasicrystals and other cases of disorder. Our efforts overlap with earlier work by Schwalm and Schwalm [3] even if we proceed along different lines. Here we investigate the case of embedded structures which are a particular case of heterogeneity. Over the years there has been a sustained interest about such objects and particularly the effect of localization observed in them, which is reflected in a wealth of papers and ideas [4–10]. There are indeed six simple embedded structures which we will consider: a pointlike impurity in a chain, a lattice or a solid (a crystal); a chain embedded in a lattice or a solid and a lattice embedded in a solid. The last three cases will be referred to as 'extended' impurities while the first three are naturally called 'pointlike'. They have been drawn schematically in figure 1. It will be shown that the characteristics of the former derive from the latter and also that some more complicated structures can be seen as variations of these simple cases. We construct the LDOS for the six basic cases starting with a one-dimensional solution. The convolution method provides analytic results even if they might be rather awkward to write explicitly. Implemented as a computational scheme it has the advantages of simplicity and speed, which stand out when compared with other numerical approaches. However, the method is shown to have some severe limitations. Nevertheless it offers some new insight into the constitution of already known results.

2. Model and method

The convolution method is applicable for Hamiltonians that can be written in some representation as $H = \sum_i H_i(k_i)$. It was shown [1–3] that in such cases the LDOS, $\rho(E)$, can

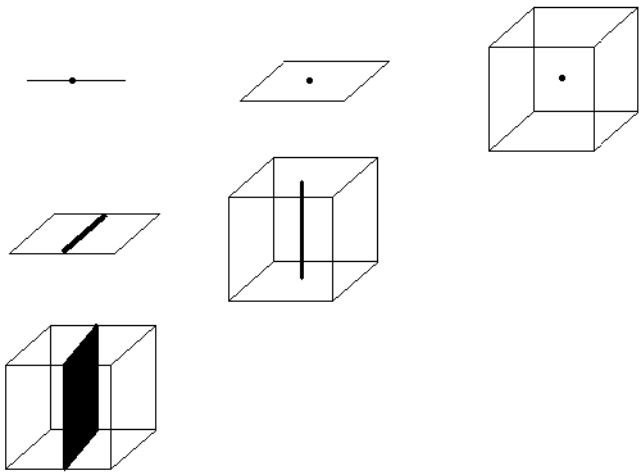

Figure 1. The six cases of simple embedded structures. Top row: pointlike impurities; middle row: a chain embedded in a lattice and in a solid; bottom: a lattice embedded in a solid.

be obtained through the recurrence

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

where $D = 1, 2, 3$ is the dimensionality of the system and $\rho^{(0)}$ is the delta function $\delta(E)$. This result can be reached directly, relying only on the form (i.e. the separability) of the Hamiltonian but also in a roundabout way using Green functions (GF). The LDOS is obtained from the GF solution of the Hamiltonian as $\rho(E) = \frac{-1}{\pi} \operatorname{Im} g(E + \mathrm{i}o)$, where o is a vanishingly small quantity, and conversely the GF can be reconstructed from the LDOS, relying on the fact that its real and imaginary parts are a Hilbert transform pair. A convolution formula is also valid for the GF:

$$g^{(D)} = -\frac{1}{2\pi \mathrm{i}} g^{(D-1)} * g^{(1)},$$

where $D = 2$ or 3.

If the solution for a 'perfect' unperturbed structure is known, the case of a pointlike impurity has a solution given generally by

$$g^{(D)}(u) = \left(u + \frac{1}{g^{(D)}(0)} \right)^{-1} \tag{2}$$

which is indeed the appropriately modified Dyson's formula. The LDOS and GF are, of course, functions of the energy E and they depend on the parameter u, but for brevity we omit the argument E. We denote by u the potential introduced by any heterogeneous structure. Writing an index 0, 1, 2 to it, we mean a single point impurity, a whole chain or a plane. Thus, for instance, we write $\rho^{(3)}(u_1)$ for the LDOS of a chain embedded in a crystal or $\rho^{(2)}(0)$ for a perfect lattice. In matrix notation u has to be interpreted with respect to the dimensionality of the perturbing heterogeneous potential.

Of the six simple embedded structures enumerated in the introduction the pointlike cases are solved by utilizing the GF formula (2) above, while the extended ones are covered by the convolution formula for the LDOS (1). Of course the convolution is just an integral operation but we may offer a spatial description corresponding to it. As a start we have a chain strung along the x axis with an embedded impurity which is located at the origin. Next we consider

a whole set of parallel noninteracting chains, equidistant in the xy plane. The convolution 'creates', i.e. takes into account, bonds between the atoms from adjacent chains and so a lattice is produced, containing an embedded chain of impurities along the line $x = 0$. Further, we consider a stack of such lattices: the convolution produces the interaction along the z axis and a solid is formed, containing now the embedded plane of impurities $x = 0$. This is illustrated by the first column of drawings in figure 1. In the same way a stack of lattices with an impurity in the middle will be transformed into a solid, containing an embedded chain along the z axis, which can be seen in the second column of figure 1.

In brief, starting with just one element, either the GF or the LDOS of a simple chain of particles, all the rest can be derived.

3. Results and discussion

We consider a tight-binding Hamiltonian with first neighbours only and just one band. More than one band could have been used but then the results lose some of their clarity; using further neighbours is apparently impossible as the Hamiltonian loses its additive separability.

3.1. Pointlike impurities

The case of a pointlike impurity is solved by the following sequence:

$$\rho^{(D)}(0) = \rho^{(D-1)}(0) * \rho^{(1)}(0)$$
$$g^{(D)}(0) = \pi(\mathrm{HT}(\rho^{(D)}(0)) - \mathrm{i}\pi\rho^{(D)}(0))$$
$$g^{(D)}(u_0) = \left(u + \frac{1}{g^{(D)}(0)}\right)^{-1}$$
$$\rho^{(D)}(u_0) = \frac{-1}{\pi}\,\mathrm{Im}\, g^{(D)}(u_0).$$

This equation sequence produces the analytic results for a pointlike impurity in a chain, a lattice and a volume when $D = 1, 2, 3$. As a preliminary step, the well known formula (see, e.g., [11]) for $g^{(1)}(0)$ is used to obtain $\rho^{(1)}(0)$. Convoluting it with itself $D - 1$ times, the LDOS for the dimension D is obtained. The GF corresponding to it is constructed using a Hilbert transform (HT), which is commonly performed as a fast Hilbert transform. Next the modified Dyson's formula gives the GF of a pointlike impurity and finally the LDOS is retrieved from its imaginary part.

The LDOS for the heterogeneous central atom of a chain ($D = 1$) is plotted for different values of u in the left panel of figure 2. We assume the hopping parameter to be $b = 1$, which gives a scale for u. Increased values of u lead to trapping of electrons at that point.

3.2. Extended impurities

For the one-dimensional case the third formula of the sequence may be rewritten as

$$g^{(1)}(u_0) = g^{(1)}(0) - \frac{g^{(1)}(0)ug^{(1)}(0)}{ug^{(1)}(0) + 1}$$

from where the LDOS is crudely approximated as

$$\rho^{(1)}(u_0) \approx \rho^{(1)}(0) + |u|\delta_u.$$

The result of its convolution with $\rho^{(D)}(0)$ would be then

$$\rho^{(D+1)}(u_D) \approx \rho^{(D+1)}(0) + |u|\rho^{(D)}(0),$$

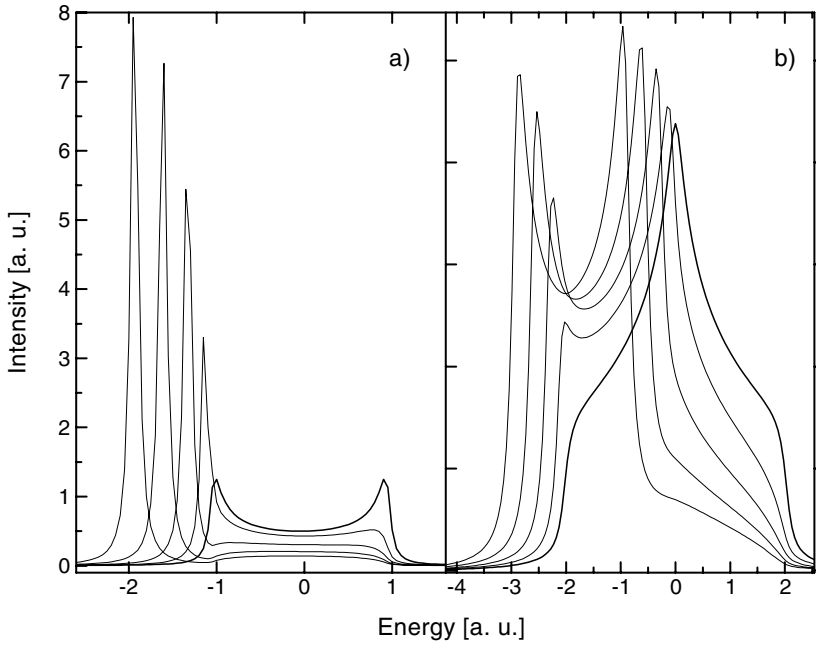

Figure 2. The LDOS of (a) a chain with an impurity for $u = 0, 0.8, 1.6, 2.4, 3.2$ and (b) a chain embedded in a lattice, the result being obtained by a convolution from the previous (see the text).

where $D = 1$ or 2 and this suggests how the results would look: the usual curve with a displaced lower-dimensional one added. In the two-dimensional case

$$\rho^{(2)}(u_1) = \rho^{(1)}(u_0) * \rho^{(1)}(0),$$

the result corresponds to a chain embedded in a lattice. Its plot in figure 2(b) has been obtained by convoluting the LDOS of a chain with an impurity (figure 2(a)) with an unperturbed LDOS.

In three dimensions

$$\rho^{(3)}(u_1) = \rho^{(2)}(u_0) * \rho^{(1)}(0)$$

is the LDOS of a chain embedded in a volume. The results are presented in figure 3(a). Apparently the one-dimensional density does not grow straight out of the three-dimensional one. For values of u higher than 0.25 the curves tend to replicate the ones in figure 1(b). One may suppose that the localization occurs first in the planes containing the embedded chain. (There are just two such planes in a cubic crystal with first neighbours; perhaps the argument is more cogent if one takes the curves from left to right, i.e. considering decreasing values of u.) For higher values of u the behaviour is the same as in the 2D case. It is not clear if this is an artefact of the too simplistic model or reflects some real effect.

The last possible combination here is a lattice embedded in a volume. Its LDOS is obtained either from

$$\rho^{(3)}(u_2) = \rho^{(2)}(u_1) * \rho^{(1)}(0)$$

or, as the convolution is associative, from

$$\rho^{(3)}(u_2) = \rho^{(1)}(u_0) * \rho^{(2)}(0).$$

The result is presented in figure 3(b). The first of these two equivalent formulae would correspond to the last step of construction shown in figure 1 while the second suggests another

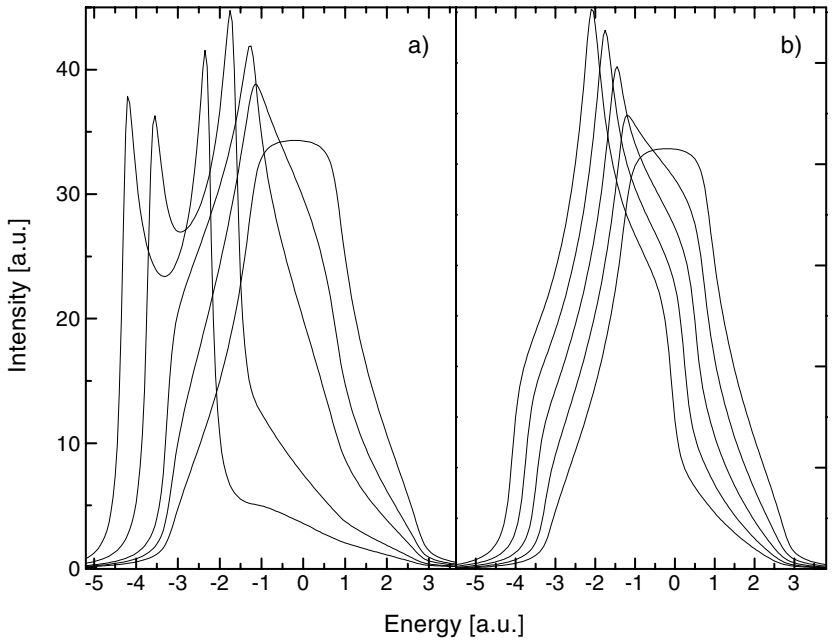

Figure 3. The LDOS of (a) a chain embedded in a solid for $u = 0, 0.2, 0.4, 0.8, 1.2$ and (b) a lattice embedded in a solid for $u = 0, 0.8, 1.6, 2.4, 3.2$, the result being obtained by a convolution from the curves in figure 2 (see the text).

interpretation: following the chain along the x axis, the solid is built by replacing each atom with a whole lattice. Thus at the origin there appears one heterogeneous plane. If the chain has more impurities, a corresponding number of such planes would appear in the solid and this idea will be put to use in the next subsection.

The analytic derivation of the last three plotted results (figures 2(b) and 3) is not as immediate as in the pointlike cases even if it follows from general principles [3]. However the plotted curves have been checked repeatedly against results obtained from other direct calculations and the coincidence has always been unambiguous. The three cases are summarized in the formula

$$\rho^{(D+1)}(u_{k+1}) = \rho^{(D)}(u_k) * \rho^{(1)}(0),$$

where $D = 1$ or 2 and $k = 0$ or 1, being strictly smaller than D. A similar formula is possible for the GFs. In reciprocal space the convolutions are just multiplications, so the result for the GFs shows that they can be obtained as a product. Recently Burioni, Cassi *et al* [11, 12] have proposed a somewhat similar technique to deal with impurities and topological peculiarities which embodies the same constructive approach. Investigating the so-called 'bundled structures' they have found a separation of the LDOS into distinct bands, which has not been observed here. In all the presented cases our results support the same trivial interpretation: increasing the parameter u increases the localization on the embedded structure.

3.3. A quasiperiodic crystal

A possible step towards more complicated structures would be to consider quasicrystals. An impressive amount of work has been published on their electronic properties [3, 13–15] but here we will just show that now it is easy to obtain by convolution the LDOS for a volume

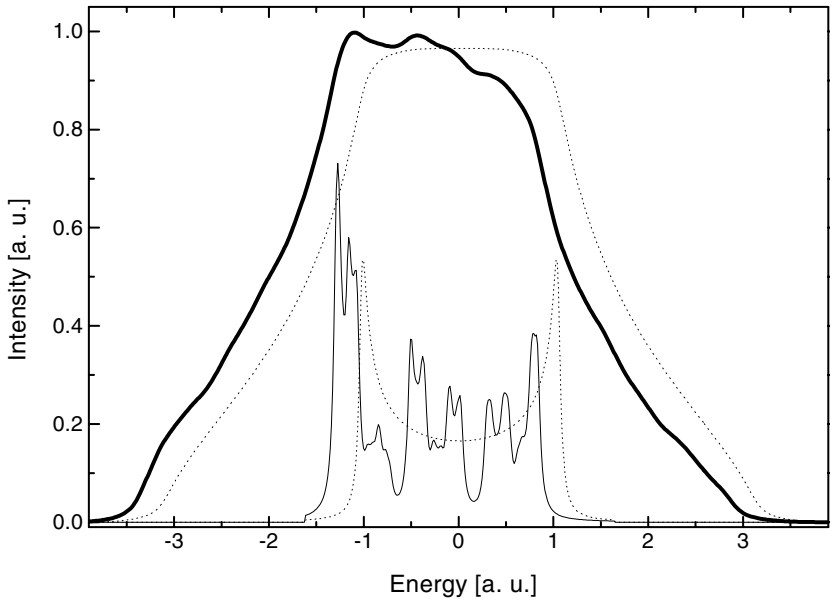

Figure 4. The LDOS of a Fibonacci sequence of 987 planes (thick curve). Plotted by dots is shown the LDOS of the corresponding simple crystal. Below, on a smaller scale, are the LDOS of the Fibonacci chain (full curve) and the pure chain (dots) which have been used for the convolutions.

constructed out of a quasiperiodic sequence of layers. Starting with a chain of atoms where the impurities appear according to the generating rule, its LDOS, convoluted with the function for the (homogeneous) 2D case, produces the LDOS of a volume built from two types of layers alternating according to the rule. The result for a sequence of 987 layers arranged in a Fibonacci sequence is presented in figure 4. The fine features of the 1D LDOS are smeared over after the convolution and a rather smooth curve is produced. This is inevitable as $\rho^{(2)}$ has a width that is two times larger than the whole $\rho^{(1)}$. The result has been obtained numerically but it may be obtained also in analytic form. Using, for instance, Newman's result for the GF of a generalized one-dimensional quasicrystal [15], its corresponding LDOS has to be convoluted twice with $1/\sqrt{(}1 - E^2)$, which is the LDOS of a simple chain or with the elliptic integral [3, 5] which gives the LDOS of a lattice.

The main concern of this paper is the method and its constructive effectiveness. It has been shown how some results for more computationally demanding cases are produced from simpler ones.

The case of neighbours further than the first, however, is an obstacle for the convolution method. The LDOS of a chain with second neighbours can be obtained analytically by inverting its Hamiltonian or by some other method [2, 16]. Then the embedding of an impurity can be done as above (section 3.1). But it is no longer possible to obtain the LDOS of a lattice by a convolution. Considering the numbering of neighbours already gives a hint: second neighbours in 1D are counted as third neighbours in 2D. If we follow the reasoning that allowed us to establish the convolution method [2] it will appear, as we will demonstrate briefly, that here it leads to an altogether different result. In a plane waves representation the tight-binding Hamiltonian of a square lattice with first and second neighbours is written as $H = \alpha + 2\beta_1(\cos(k_x) + \cos(k_y)) + 4\beta_2 \cos(k_x)\cos(k_y)$. If $\beta_2 > 0$ the Hamiltonian is not additively separable into independent parts and the convolution formula cannot be utilized, but

now it can be written as a product:

$$H = \alpha - \frac{\beta_1^2}{\beta_2} + 4\beta_2(\beta + \cos(k_x))(\beta + \cos(k_y)),$$

where $\beta = \frac{\beta_1}{2\beta_2}$, or more generally as $H = H_1 H_2$. Adopting a statistical point of view one might see the LDOS as a distribution of eigenvalues. Now the eigenvalues of H are products of the eigenvalues of H_1 and H_2 and if their distributions are ρ_1 and ρ_2, correspondingly, then the overall distribution [17] or LDOS for the two-dimensional Hamiltonian will be

$$\rho^{(2)}(E) = a \int_L \rho_1\left(\frac{E}{\eta}\right)\frac{1}{\eta}\rho_2(\eta)\,\mathrm{d}\eta.$$

The extension to $D = 3$ being unproblematic, we note that now we have a method for the LDOS of Hamiltonians which are factorizable as products. Establishing the set of limits L can be a tiresome task, especially when both positive and negative values of the variables are possible, but need not be considered here. It appears clearly that the result is no longer expressed by a convolution integral.

4. Conclusion

The convolution method allows us to treat effectively some model cases of embedded structures. It might be seen as a means to obtain results for higher dimensionality results out of one-dimensional ones; already known results, either in numerical or analytical form, may be extended further and, in many instances, otherwise difficult to reach results became easily accessible. However, the method relies on the separability of the Hamiltonian, which severely limits its scope. Establishing this has led to an observation which has its own interest. The analytic formulation provided by the method suggests a novel view even if the complexity of the mathematical expressions most often defies their explicit completion.

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