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## Decomposition of the density of states via the recursion method

Š Varga

Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta,  
842 36 Bratislava, Czechoslovakia

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**Abstract.** A scheme for a fast decomposition of the total density of states evaluated by the recursion method is presented. It is suggested that all the projected densities can be obtained in a single recursion calculation instead of applying the complete recursion procedure to each projection separately. The proposed scheme appears to be exact for the correct choice of the initial vector of the recursion transformation. It is shown that when the random initial vector approach to the total density of states is implemented, good results can be obtained in particular for calculating the partial densities of states.

The applicability and efficiency of the proposed method is demonstrated on two model systems. A simple criterion of reliability is formulated. Possible ways to eliminate spurious effects caused by the random initial vector approach are discussed.

### 1. Introduction

The recursion method (Haydock *et al* 1972, 1975) has become a well established and powerful tool for the effective diagonalization of large Hamiltonians in the last decade. (For an exhaustive review of the topic see Heine *et al* (1980); the generalization to non-orthogonal basis sets was done by Ballentine and Kolář (1986).) Besides its natural application in the density of states (DOS) calculations the method has proved its efficiency also in less straightforward cases, such as the electronic transport properties (Stein and Krey 1980, Bose *et al* 1983) and it turned out to be also a suitable framework for determining effective interatomic interaction (Stankey and Allen 1986, Esterling *et al* 1987).

The DOS calculations within the recursion method scheme are usually performed by summing up over an adequate set of respective local density of states (LDOS) contributions. Of course, for periodic systems comprising only a small number of non-equivalent sites this is the most efficient and exact way (within the exactness of the method itself) as well, while for a cluster simulating an amorphous system, typically consisting of  $10^3$ – $10^5$  orbitals, an alternative conception of the random initial vector may turn out to be more efficient for evaluating the total density of states (TDOS) (e.g. Ishii and Fujiwara 1980, Krajčí 1987) and the partial densities of states (PDOS) (Varga and Krempaský 1989). In some cases use of the selected random initial vector appears to be advantageous (Varga and Krempaský 1989). However, if self-consistency in the electronic structure determination is desired a need for more effective LDOS or PDOS calculations arises.

Evidently, to employ the recursion method framework for recent challenging first-principles computer simulations of solids (Hafner and Jaswal 1988), even faster schemes are required to enable local electronic structure and electronic interaction evaluation to be repeated many times over all the orbitals of the cluster. Various termination techniques can be used to lower the computational effort by lowering the number of exactly evaluated recursion levels. Esterling *et al* (1987) even suggested speeding up the electronic force computational scheme by terminating the recursion drastically after the first exactly evaluated level.

We propose a completely different way to make electronic structure calculations more effective. Instead of attempting lowering the effort for each particular calculation we suggest performing the recursion transformation only once for the whole system and then somehow extracting all the local quantities of interest from it. In §2 the philosophy of the scheme, as well as the computational aspects of the method, are described. The results of test runs on model systems are presented in §3. A simple criterion of reliability is also formulated here. In §4 the applicability and consequences of implementing the random initial vector approach are discussed. Finally, §5 contains the conclusions.

## 2. Method

### 2.1. Background

Let us summarize the basic equations we will need for the description of our method first. Let the Hamiltonian of the electronic system have a simple tight-binding form:

$$\mathbf{H} = \sum_{\alpha} \varepsilon_{\alpha} |\alpha\rangle\langle\alpha| + \sum_{\alpha} \sum_{\beta \neq \alpha} t_{\alpha\beta} |\alpha\rangle\langle\beta| \quad (1)$$

in the basis set of atomic orbitals. Once the set of eigenvalues  $E_n$  and eigenvectors  $|\Phi_n\rangle$  of  $\mathbf{H}$  is known, the density of states can be expressed as

$$g(E) = \frac{1}{N} \sum_n \delta(E - E_n). \quad (2)$$

Similarly, the LDOS on the state  $|\alpha\rangle$  is a projection of the DOS onto this state:

$$g^{\alpha}(E) = \frac{1}{N} \sum_n |\langle\alpha|\Phi_n\rangle|^2 \delta(E - E_n). \quad (3)$$

By means of the recursion transformation (for the explicit form see e.g. Haydock *et al* (1975)) the Hamiltonian is transformed into a symmetric chain form:

$$\mathbf{h} = \sum_{i=0}^{L-1} [a_i |u_i\rangle\langle u_i| + b_{i+1} (|u_i\rangle\langle u_{i+1}| + |u_{i+1}\rangle\langle u_i|)] \quad (4)$$

where the orthogonal  $u$ -basis set and  $h$ -matrix elements  $a_n, b_n$  are generated successively in the process of the transformation. In practice,  $L \ll N$  is sufficient for reasonable results. The choice of the initial vector of the transformation  $|u_0\rangle$  is discussed below.

The truncated Hamiltonian  $\mathbf{h}$  can easily be diagonalized in the  $u$ -basis set

$$\mathbf{e} = \mathbf{p}^\dagger \mathbf{h} \mathbf{p} \quad (5)$$

where  $\mathbf{e}$  and  $\mathbf{p}$  are the matrices of eigenvalues  $e_n$  and eigenvectors  $|\varphi_n\rangle$ , respectively.† For the matrix elements of the latter we adopted the notation

$$p_k^n = \langle u_k | \varphi_n \rangle. \quad (6)$$

The eigenvectors  $|\varphi_n\rangle$  are commonly understood to be normalized to unity, e. g.

$$\sum_k |\langle u_k | \varphi_n \rangle|^2 = 1. \quad (7)$$

Now the projected density of states onto the initial vector  $|u_0\rangle$  can be expressed as

$$g^{(0)}(E) = \sum_n^L w_n^{(0)} \delta(E - e_n) \quad (8)$$

where the weight is

$$w_n^{(0)} = |\langle u_0 | \varphi_n \rangle|^2 \quad (9)$$

such that

$$\sum_n^L w_n^{(0)} = 1 \quad (10)$$

As a consequence of the truncation, all the quantities are now dependent on the initial vector, which is indicated by the superscript in equations (8)–(10). (Precisely, the eigenvalues and eigenvectors should be denoted in the same way, however, we will mostly omit this for simplicity of notation.)

By the local orbital choice of the vector  $|u_0\rangle$  each LDOS can easily be evaluated. All the component densities as well as the TDOS itself can be summed up from these local projections; of course, the whole recursion transformation has to be repeated for each projection separately. Our goal would rather be the opposite, namely to perform the expensive recursion procedure only once for a projection representing the TDOS and then to decompose all the required local weights from this single projection. Such a scheme is proposed in the following subsection.

## 2.2. Decomposition scheme

Let us emphasize first that, as a consequence of the truncation, all the weights (9) are strongly dependent on  $n$  even if they represent the TDOS which is, of course, not the case for the full Hamiltonian  $\mathbf{H}$  where (see (2))  $w_n = 1/N$  regardless of  $n$ .

† Instead of stressing the  $L$ -dependence of eigenvalues and eigenfunctions of  $\mathbf{h}$  explicitly, we adopted the use of small letters and capitals to distinguish between the quantities referring to the truncated and full Hamiltonians, respectively.

Let us assume now that the projection vector  $|u_0\rangle$  is chosen in such a way that (8) represents the TDOS. In this case it might seem obvious to consider the quantities  $|\langle\alpha|\varphi_n\rangle|^2$  which follow from the expansion†

$$\langle\alpha|\varphi_n\rangle = \sum_k^L \langle\alpha|u_k\rangle\langle u_k|\varphi_n\rangle \quad (11)$$

to be (in analogy with (3)) directly the required LDOS weights,  $w_n^\alpha$ . As can be easily verified (see (7)), regardless of  $n$ :

$$\sum_\alpha |\langle\alpha|\varphi_n\rangle|^2 = 1. \quad (12)$$

(Notice in this context that contrary to the full Hamiltonian, the sum  $\sum_n |\langle\alpha|\varphi_n\rangle|^2 \neq 1$  for  $L < N$ .‡) However, as has already been pointed out above, a strongly  $n$ -dependent weight  $w_n^{(0)}$  (9) is expected to be a result of (12) for  $L \ll N$ . The straightforward way to cope with this shortcoming is to suggest a ‘renormalized’ form for the LDOS weights:

$$w_n^\alpha = |\langle\alpha|\varphi_n\rangle|^2 \times w_n^{(0)} \quad (13)$$

provided that  $w_n^{(0)}$  corresponds to the TDOS of the system. The form (13) requires that the eigenfunctions be normalized to  $w_n^{(0)}$  instead of unity. We will refer to such normalization by an asterisk, e.g.

$$|\langle\varphi_n^*|\varphi_n^*\rangle|^2 = \sum_k |\langle u_k|\varphi_n^*\rangle|^2 = w_n^{(0)}. \quad (14)$$

In this notation, (13) reads

$$w_n^\alpha = |\langle\alpha|\varphi_n^*\rangle|^2. \quad (15)$$

Now,  $w_n^\alpha$  obviously has the correct behaviour with regard to the sum over  $\alpha$  for both  $L \ll N$  and  $L \rightarrow N$  cases. Thus we have good reasons to consider the quantity (15) to be the true LDOS weight required for our decomposition scheme.

In the following subsection we will concentrate on the technical problems of employing the scheme.

### 2.3. Technical details

The crucial problem in implementing the scheme proposed in §2.2 is that we do not know any exact form for the initial vector  $|u_0\rangle$ , projection onto which would return the TDOS directly. (We refer to such a hypothetical vector by a superscript e.g.  $|u_0^{(t)}\rangle$ ,  $w_n^{(t)}$  etc.)

Because of the lack of any true  $|u_0^{(t)}\rangle$ , we used the well known approach of random initial vectors of the form

$$|u_0^{(t)}\rangle = N^{-1/2} \sum_\alpha^N \xi_\alpha |\alpha\rangle. \quad (16)$$

where  $\xi_\alpha$  are random numbers,  $\xi_\alpha = \pm 1$ . In an attempt to get rid of the randomness in

† Though the  $u$ -subspace  $\Gamma_L$  of dimension  $L \ll N$  is, in general, insufficient for the correct expansion of a vector from the  $\alpha$ -space  $\Gamma_N$ , the expansion is exact for the scalar product  $\langle\alpha|\varphi_n\rangle$  as  $|\varphi_n\rangle \in \Gamma_L$  does not have any non-zero projection out of  $\Gamma_L$ .

‡ Though  $\mathbf{U}^t\mathbf{U} = \mathbf{I}$ ,  $\mathbf{U}\mathbf{U}^t \neq \mathbf{I}$  for the truncated recursion transformation matrix  $\mathbf{U}$  ( $\mathbf{I}$  and  $\mathbf{I}$  being the respective unit matrices).

(16), averages of the evaluated quantities over several, say  $n_i$ , different choices of (16) are taken usually.

Starting now from the random state (16) the recursion procedure is performed. The products  $\langle \alpha | \varphi_n \rangle$  for the evaluation of local weights (13) follow from the expansion (11). (To evaluate (11) effectively, the set of successively generated  $u$ -vectors should be stored in a backing storage in the process of the recursion transformation (4).) The desired weights  $w_n^A$  are easily summed up from the local weights  $w_n^\alpha$  (13) over all the  $A$ -states of our interest. The set of  $\{e_n, w_n^A\}$  now fully defines† the corresponding DOS,  $g^A(E)$  (see (3)). For  $L \ll N$ , however, the set of weighted  $\delta$ -functions is too small to produce even a quasi-smooth function. The  $\varepsilon$ -broadening of the  $\delta$ -functions is a straightforward remedy; however, it suffers from the arbitrariness of  $\varepsilon$ . Fortunately, a one-to-one correspondence exists between the set  $\{e_n, w_n\}$  and the  $\mathbf{h}$ -matrix elements (the recursion coefficients)  $\{a_n, b_n\}$  (see appendix). Thus the standard routines for evaluation of the DOS from the recursion coefficients (Nex 1978, Haydock and Nex 1985) can be used without change also in our case.

In addition, one important point deserves to be mentioned in this context. It follows from the physical sense of the sum

$$n_A = \sum_n w_n^A = \sum_n \sum_{\alpha \in A} w_n^\alpha \quad (17)$$

that  $n_A$  should be equal to the relative number of  $A$ -states in the system  $n_A^0$ . Because of the approach (16) this condition is never fulfilled exactly, as will be demonstrated in § 3. However, if the difference between the sum (17) and its expected value,  $n_A^0$ ,

$$\delta_A = n_A - n_A^0 \quad (18)$$

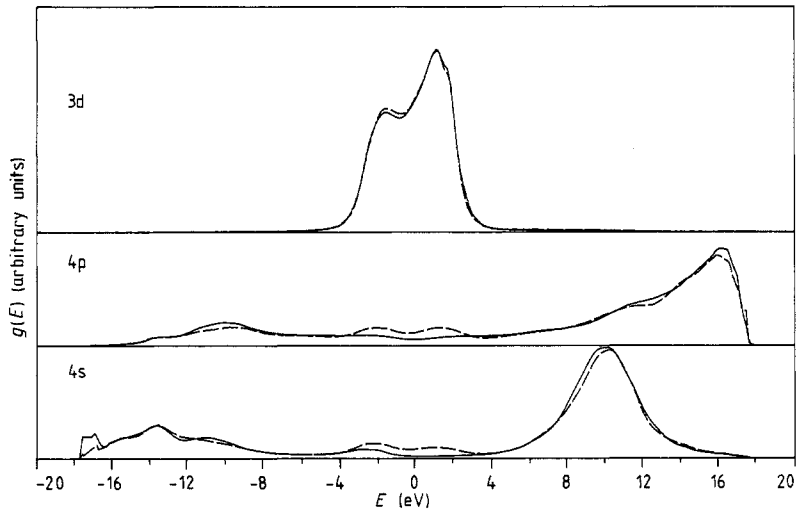
is not too large, the discrepancy does not notably influence the resulting DOS. (Anyhow, the weights  $w_n^A$  entering the  $g(E)$  calculation are correctly normalized first.) Moreover, as will be demonstrated below, the deviation (18) may be considered as a simple criterion of the reliability of application.

### 3. Test calculations

To verify the applicability of our scheme the method was tested on two different systems, which we believe to be quite representative and for which reference DOS curves can be easily found.

As a first test system a realistic model of amorphous Fe (a-Fe) was chosen. This system has already been intensively studied by many authors (see Varga and Krempaský (1989) and references therein). The structural model and the Hamiltonian parameters were taken from our earlier work (Varga and Krempaský 1989). Random partial initial vector choice was used for the evaluation of reference PDOS curves. Their comparison

† The question may arise, whether the set of eigenvalues  $\{e_n^{(i)}\}$  can be used also in connection with  $w_n^A$ . For  $L = N$ , of course, both eigenvalue sets are equivalent. Though this is not exactly true for the truncated Hamiltonian, the differences between eigenvalue-sets we have found to be only very slightly sensitive to the choice of  $|u_0\rangle$ .



**Figure 1.** Comparison of the reference (full curve) and decomposed (broken) PDOS for the a-Fe system. (The scales for different orbital types are not the same.)

**Table 1.** An illustration of the dependence of sum (17) on the level of the truncation  $L$  for the a-Fe system. The expected value ( $L \rightarrow \infty$ ) is also indicated.

$L$	s	p	d
15	0.122	0.364	0.514
30	0.116	0.351	0.539
50	0.115	0.343	0.542
100	0.115	0.337	0.548
$\infty$	0.111	0.333	0.556

with the decomposition-calculated PDOS curves is shown in figure 1. (Averages over  $n_i = 5$  sets were used for reference curve evaluation; this number was found to be sufficient for the decomposition scheme as well.) The dependence of the sum (17) on the level of the Hamiltonian truncation  $L$  was also studied for this case. The results are summarized in table 1.

In figure 2 an attempt to decompose the TDOS of the model above into the local density of d states on a single specified site in the central part of the cluster is presented. The reference curves were evaluated as the sums over the respective local initial orbital contributions here. Though the decomposed densities reproduce the general shape of the reference curve fairly well, the agreement is not as excellent as for the d-PDOS in figure 1. We attempted to improve the result by the use of selected random initial vectors (Varga and Krempaský 1989), however, this had no significant effect on improving the agreement (see figure 2). Averages over  $n_i = 30$  sets were used here. Increasing  $n_i$  over this value produced almost no improvement of the decomposed curves. The agreement of sums (17) with their expected values was found to be typically of an order worse than for the PDOS case.

An artificial FCC cluster containing two different types of sites, both sites occupied by  $d$  orbitals only, was our second test system. It was chosen to verify whether our decomposition scheme is able to cope with a many-peaked curve. Considering the highly oscillatory shape of the curves the decomposed densities turned out to be in surprisingly good agreement with the reference case. Again,  $n_i = 5$  was found to be sufficient. The sum (17) agreed with the expected value within 0.005 for each calculation. In figure 3 the site-type decomposed DOS curves for two different cluster sizes are presented.

Concluding this section, we remark that we have found the last few pairs of reconstructed recurrence coefficients  $(a_n, b_n)$  to be unreliable in some cases. Hence the  $u$ -basis dimension  $L$  should be chosen to be such a size that the last few pairs  $(a_n, b_n)$  might be omitted from the final DOS evaluation. Our calculations were performed in the  $u$ -basis of dimension  $L = 30$ , keeping then only  $L = 25$  levels of the reconstructed recursion coefficients for the DOS evaluations.

#### 4. Discussion

The only approximation we have made in our scheme (within the approach of the recursion method itself) is the random initial vector approximation to the TDOS (16). Let us discuss the consequences and some ways to improve the scheme within and beyond (16).

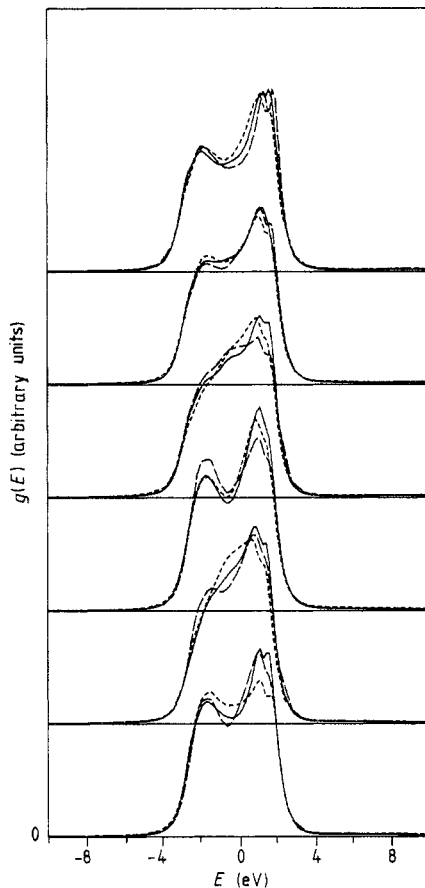
The natural way to cope with the stochastic character of the vector (16) is to average the results over several different random initial vector sets. The effect of this averaging is, however, not as straightforward as for the pure  $g(E)$  evaluation. In the process of decomposition calculation spurious statistically non-vanishing terms may occur which were not present in the pure DOS calculation. This can also explain the fact that increasing  $n_i$  over a certain value (in our test systems  $n_i \approx 30$  for LDOS and  $n_i \approx 5$  for the PDOS cases, see §3) does not further improve the decomposed curves. The notable difference between the two attempts at the LDOS decomposition in figure 2 might also be due to the same reason. Evidently, the selected random initial vector choice suppresses some terms which are present in the simple random initial vector case.

Increasing the cluster size appeared to show a more positive effect (see figure 3). The stochastic terms, which cancel out already before further decomposition processing, vanish faster the larger the basis set is. Thus, while for a simple TDOS calculation the accuracy of the approach (16) is proportional to the product  $n_i \times N$  (Krajčí 1987), the cluster basis set size,  $N$ , seems to be the factor of higher importance in improving our scheme within (16).

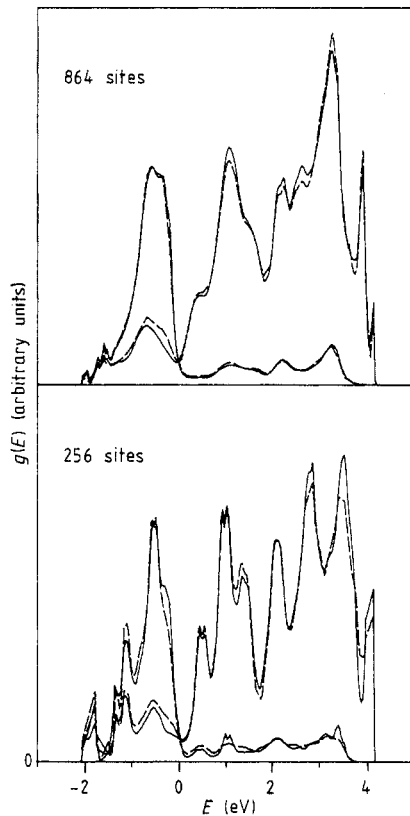
In the limit  $L \rightarrow N$ ,  $\mathbf{U}$  becomes a true unitary transformation matrix and all the results should be independent of the choice of  $|u_0\rangle$ , thus making the problem of the true  $|u_0^{(i)}\rangle$  irrelevant. Increasing the level of truncation  $L$  is, however, far from being an effective way of improving  $|u_0^{(i)}\rangle$ . As can be seen from the dependence of the sum (17) on  $L$  (table 1), the convergence of such an improvement can be expected to be very slow. In addition, for extremely high values of  $L$  tendency to numerical instability may occur.

As has been demonstrated in § 3, while the decomposition into PDOS contributions is in satisfactory agreement also within the approach (16), this does not hold fully for the LDOS evaluations (see figure 2). Notice also that while for our test cases the deviation (18) was found to be very slight for the PDOS evaluations, this was not the case for the LDOS. This indicates that (18) can be considered as a simple criterion of applicability of our scheme. Evidently, attempts to calculate local quantities such as local charges, bond





**Figure 2.** Comparison of the reference (full curve), decomposed (random  $u_0$ ) (broken) and decomposed (selected random  $u_0$ ) (dotted) d-LDOS on several sites of the a-Fe system.



**Figure 3.** Site-type decomposed PDOS for two sizes of the model FCC cluster: reference (full curve) and decomposed (broken).

orders etc within our scheme must be performed very carefully, bearing in mind the possible inadequacy. Notice that the quantities  $\langle \alpha | \varphi_n^* \rangle$  are the LCAO coefficients in our scheme. Hence, if we had a better approach to  $|u_0^{(j)}\rangle$ , quantities otherwise inaccessible within the recursion method (e.g. the participation ratio (Bell and Dean 1970)) could be evaluated as well.

A simple estimate shows that the use of our scheme reduces the number of calculations even for a small number of component-DOS evaluations. The ratio of the extra CPU time spent on the expansion (11),  $\tau_E$ , to the amount of time spent on the recursion transformation (4),  $\tau_R$ , is approximately  $\tau_E/\tau_R = L/N_n$  where  $N_n$  is the average number of basis functions within the interaction sphere. For typical cases ( $N_n \approx 50$ – $100$  at least) even the simplest decomposition of the TDOS into two PDOS contributions is faster than performing transformation (4) twice.

Let us examine now the possibility of improving the  $|u_0^{(j)}\rangle$  beyond (16). Krajčí (1987)

set down the explicit form

$$|u_0^{(l)}\rangle = \frac{1}{\sqrt{N}} \sum_n^N |\Phi_n\rangle \quad (19)$$

for the exact TDOS projection vector which is, unfortunately, of no practical use as we do not know any effective way to construct the eigenfunctions of the full Hamiltonian within the recursion method. Moreover, as has been pointed out in the quoted work, taking the eigenfunctions  $|\varphi_n\rangle$  of the truncated Hamiltonian instead of  $|\Phi_n\rangle$  in (19) fails to give satisfactory results, since the product  $|\langle\varphi_n|u_0^{(l)}\rangle|^2$  is evidently not the  $n$ -dependent  $w_n^{(0)}$  as required for the truncated case (see §2.2). However, employing the renormalized eigenfunction (14) in the truncated analogy of (19)

$$|u_0^{(l)}\rangle = \sum_n^L |\varphi_n^*\rangle = \sum_n^L (w_n^{(0)})^{1/2} |\varphi_n\rangle \quad (20)$$

does not suffer from the above shortcoming and has the correct behaviour for both the  $L \ll N$  and  $L \rightarrow N$  cases.

Unfortunately, though (20) has a correct form and can be easily evaluated, it cannot be considered as a scheme to construct an approach to  $|u_0^{(l)}\rangle$  beyond (16) since by means of the equation (20) the initial vector of the recursion transformation  $|u_0\rangle$  merely reproduces itself because

$$\sum_n |\varphi_n^*\rangle = \sum_n |\varphi_n\rangle \langle\varphi_n|u_0\rangle = |u_0\rangle. \quad (21)$$

Nevertheless, we will make use of property (21) below. In addition, we use the above equations to point out the correspondence between the analogous equations referring to the full and truncated Hamiltonians, respectively. Suppose we have the true  $|u_0^{(l)}\rangle$ . Then for the recursion coefficient  $a_0$  follows

$$a_0 = \frac{1}{N} \sum_n^N E_n. \quad (22)$$

The analogy of (22) for the truncated case is, however,

$$a_0 = \sum_n^L w_n^{(0)} e_n \quad (23)$$

which follows immediately from (A1) in the appendix.

Considering now the pairs of equations (19)–(20) and (22)–(23) we get the following correspondence. Obviously, the sets  $\{E_n, |\Phi_n\rangle\}$  correspond to  $\{e_n, |\varphi_n\rangle\}$ , but less evident is that the analogy of the constant factor  $1/N$  for the full Hamiltonian is the weight  $w_n^{(0)}$  in the truncated case. This also supports our notion that the normalization (14) is a property inherent to the truncation.

Finally, we briefly present an attempt to improve  $|u_0^{(l)}\rangle$ , based on minimizing the local deviations (see (18)):

$$\delta_\alpha = \sum_n w_n^\alpha - \frac{1}{N}. \quad (24)$$

Making use of the self-reproducing property of  $|u_0\rangle$  (21) we derived the following iterative improvement scheme:

$$|u_0^{(l)}\rangle_{j+1} = |u_0^{(l)}\rangle_j \left(1 - \gamma \delta_\alpha / \sum_n w_n^\alpha\right)^{1/2} \quad j = 0, 1, \dots \quad (25)$$

where  $\delta_\alpha$  is defined by (24) and  $\gamma$  is a convergence parameter,  $\gamma < 1$  ensuring that the square root in (25) is real. Though the scheme (25) had a positive effect on reducing the deviations (24) it did not improve the TDOS. This failure becomes evident since any new initial vector of the form (25) generates again the same subspace  $\Gamma_L$  as the initial  $|u_0^{(0)}\rangle_0$  did. Obviously, a more sophisticated scheme incorporating also subspaces beyond  $\Gamma_L$  would be desirable.

## 5. Conclusions

We have proposed a simple decomposition scheme within the tight-binding recursion method which makes it possible to obtain all the projected densities of states within a single run of the recursion procedure. We have reasons to believe that our method is exact for the correct choice of initial projection vector. Our test calculations show that the random initial vector approach to the TDOS appears to be a highly sufficient approximation for a working decomposition scheme when PDOS evaluations only are required. The proposed scheme is, in principle, a fast tool for the complete LCAO analysis; however, this must be attempted with care within our approach to the TDOS, bearing in mind the possible lower reliability of results for evaluation of local quantities. A search for an improvement beyond the random initial vector approach appears to be highly acute in this context. Nevertheless, already in the approach used, the scheme can be successfully employed to speed up at least some electronic structure calculations within the recursion method.

## Acknowledgment

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## Appendix

The algorithm for reconstruction of the recursion coefficients set  $\{a_n, b_n\}$  from the set of eigenvalues and weights  $\{e_n, w_n\}$ ,  $n = 0, \dots, L - 1$  is described here.

The quantities  $a_n, b_n$  are the matrix elements of the truncated Hamiltonian  $\mathbf{h}$  (4); the latter can be expressed (see (5)) as

$$\mathbf{h} = \mathbf{p}\mathbf{e}\mathbf{p}^\dagger. \quad (\text{A1})$$

The elements of the eigenvalue matrix  $e_n$  are all known ( $\mathbf{e}$  is diagonal), while only the first-row elements of the eigenfunction matrix are available.

From (9) their value follows:

$$p_0^n = \langle u_0 | \varphi_n \rangle = |w_n|^{1/2}. \quad (\text{A2})$$

Thus,  $h_{00} = a_0$  can immediately be obtained from (A1). Considering the recurrence relation (see e.g. Heine *et al* 1980)

$$\begin{aligned} b_{k+1}p_{k+1}^n &= (e_n - a_n)p_k^n - b_k p_{k-1}^n \\ p_{-1}^n &= 0 \quad n = 0, \dots, L - 1 \quad k = 0, \dots, L - 1 \end{aligned} \quad (\text{A3})$$

the next row of  $p$ -matrix elements is evaluated; at the same time  $b_{k+1}$  follows from the normalization (7).

Now (A1) is applied to evaluate the next diagonal element of  $\mathbf{h}$  and the whole procedure is repeated until all the  $L$  values of  $a_n, b_n$  are known. Moreover, notice that all the eigenfunction matrix elements have been reconstructed as a byproduct of the procedure as well.

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