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Density of states from the continued fraction expansion: an accelerated convergence approach

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Abstract. In this paper different methods for the calculation of densities of states and other physical quantities by their continued fraction expansions are compared, and a new technique is presented. Continued fraction expansions truncated at different orders are considered as the terms of a sequence convergent to a limiting value. The philosophy of the method is the acceleration of such a sequence by means of appropriate algorithms. Operating in this way, we observe a net reduction of spurious unphysical features of numerical origin in the results.

1. Introduction

The continued fraction method [1, 2] is a very powerful tool for the evaluation of properties of physical systems. Nevertheless, in applying it to practical cases a number of problems arise; among these, the most important is termination. In fact, although a continued fraction is in general made of infinite levels, we can deal only with a finite number of coefficients. So the quantity calculated is an approximation, and we meet the problem of how to make this approximation the best.

In some cases so many coefficients are available that the result is in practice the same as we could obtain with an infinite number of recursion levels [3, 4], but in general this is not possible. When we have only a few parameters and we try to evaluate the continued fraction we obtain in the result a number of features with an unphysical origin. In order to overcome this difficulty, and to extract the maximum physical information from a given set of coefficients, a number of approximations have been proposed.

In what follows we will consider as the quantity of interest the electronic density of states (DOS) of a solid. If it is possible to individuate one or more connected bands the introduction of a terminator (whose analytical form is given in terms of the band limits) is possible [5]. More generally, a terminating procedure, based on orthogonal polynomials to approximate a density of states with an arbitrary number of connected bands with van Hove singularities, has been proposed [6]. This class of methods can be easily extended to systems made up of single components with well defined band limits, building average terminators [7, 8]. In an equivalent way we can evaluate a sequence of asymptotical coefficients and append them to the continued fraction. Such a sequence may be extrapolated by the knowledge of the first pairs of exact coefficients [9, 10]. Operating in this way further improvement is possible by choosing the appending procedure in an appropriate way [11]. Extrapolation techniques may be also applied directly to the continued fraction itself, represented by means of some orthogonal polynomials (e.g. Chebyshev polynomials [12]).

Another approach to the problem of truncation of continued fractions is the so-called maximum entropy procedure [13–15], in which we obtain the DOS by maximizing the entropy of the information contained in the coefficients at our disposal.

The method proposed in this paper is based on the convergence acceleration of the sequence of values of the DOS calculated with different numbers of continued fraction levels by means of a procedure derived in the framework of the Padé approximant theory: the ϵ -univariate algorithm [16]. The use of Padé approximants to improve the convergence of the expansion of physical quantities has already been used in the literature. In particular, if we use the moments of the Hamiltonian to expand the Green function as a power series, quadratic Padé approximants of the density of states may be calculated [17, 18].

The present paper is organized as follows. A critical analysis of different techniques of termination is given in section 2. Section 3 is devoted to a presentation of the accelerated convergence procedure, and in section 4 its application to the calculation of densities of states is considered. Section 5 contains conclusions.

2. Different methods for the determination of the density of states

2.1. Termination procedures based on a knowledge of some features of the density of states

We briefly recall the definition of the continued fraction termination procedure: the substitution of a continued fraction by a smaller one whose n th level has the form

$$E - a_n - b_n^2 t_n(E). \quad (1)$$

The function $t_n(E)$ is called the terminator of the continued fraction. In many cases additional physical information can be used in the determination of the density of states; this information is essentially the position of band edges and the presence of van Hove singularities. Turchi and co-workers [5] have shown the relation between the position of the band edges and the asymptotic behaviour of the continued fraction coefficients. This fact may be used to write down the explicit form of analytical terminators in the case of densities of states composed of one or more connected bands. For example, in the simplest case of one single connected band it follows that the coefficients a_n and b_n follow damped oscillations around their asymptotic values a and b , so the one-band terminator is given by the solution of the equation

$$t(E) = \frac{1}{E - a - b^2 t(\bar{E})}. \quad (2)$$

Equation (2) is quadratic, and therefore has two solutions; we choose the solution which gives the correct behaviour for $E \rightarrow \pm\infty$. In more complex cases of several connected bands the oscillations of the coefficients are not damped, but an analytical expression for the terminator is still possible. As an example, in figure 1 we present the density of states of silicon calculated with 150 exact levels of the continued fraction and the two bands terminator.

Following this line of thought, the next step is to exploit other known features of the density of states (such as internal van Hove singularities). Operating this way [6] it is possible to obtain more accurate results. In practice, the procedure is the following: suppose we have only the first n coefficients of a continued fraction expansion; first we construct a model density of states having known physical features (e.g. band limits and van Hove singularities) and by means of orthogonal polynomials we derive the coefficients of its continued fraction expansion, and the analytical tail. Then, the terminator so calculated is appended to the 'true' continued fraction. In figure 2 we report the density of states for GaAs, which is a three-band system; the continued fraction is terminated with a tail

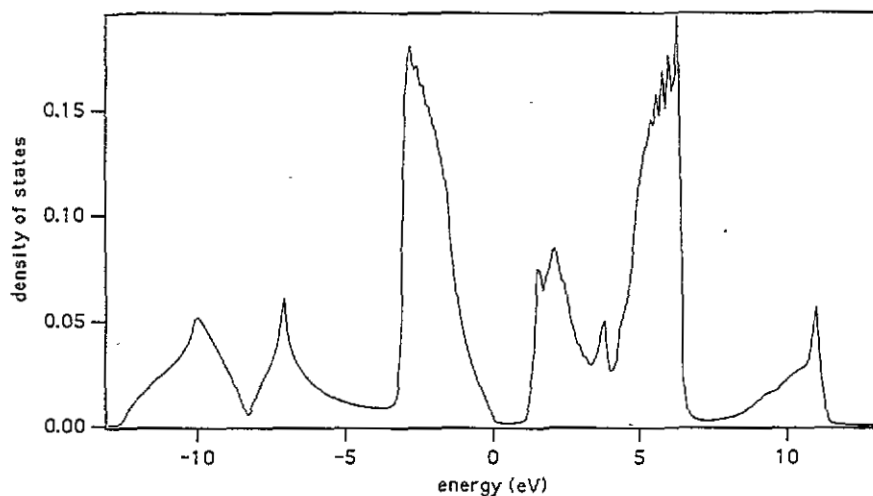


Figure 1. Density of states for silicon calculated with 150 exact levels of the continued fraction and a two-band terminator.

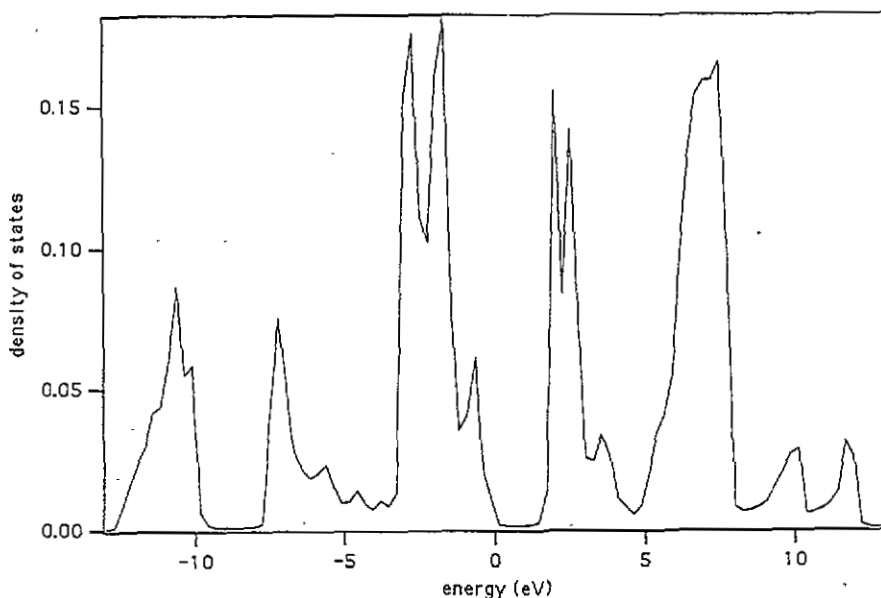


Figure 2. Density of states for gallium arsenide calculated with 100 exact levels of the continued fraction and the terminator of [6].

generated by knowledge of the band limits and assuming a square-root behaviour for the van Hove singularities at the band edges.

This class of method is based upon the assumption that the continued fraction coefficients show an asymptotic trend, so the introduction of the tail does not bring about a strong deviation from the exact behaviour. Moreover, independent information about the density of states is required in order to obtain a more correct and realistic terminator. In many cases one or both of these requests are not satisfied; let us consider, as an example, the density

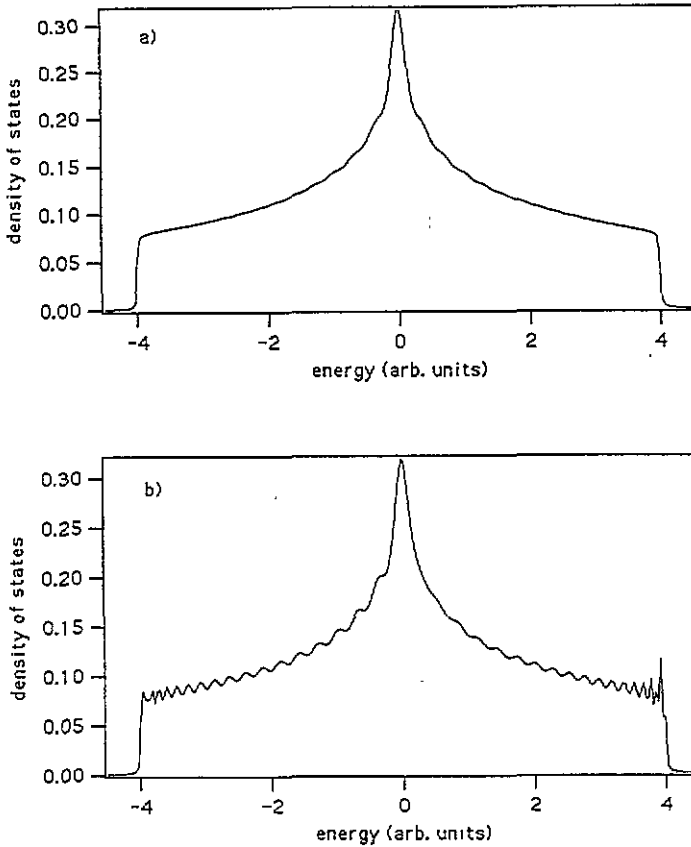


Figure 3. Density of states for the simple square lattice calculated with 40 exact levels of the continued fraction and the single-band terminator evaluated with: (a) the correct band limits $(-4, 4)$ and (b) slightly incorrect band limits $(-4.1, 5.9)$.

of states of a simple model system, the bidimensional square lattice, and suppose that we do not exactly know the band limits. Figure 3(a) represents the correct density of states, while in figure 3(b) we have the result of a termination calculated using incorrect band limits. The lack of knowledge about band limits and/or asymptotic behaviour of continued fraction coefficients is a common situation in the study of heterostructures and disordered systems. As an example, let us consider the surface projected density of states for the one-dimensional binary ordered alloy ABABAB... (figure 4); the Saxon-Hunter theorem [19] tells us which are the maximum allowable limits for the density of states, but the effective limits are smaller and cannot be evaluated. In the case of a disordered alloy the situation is even worse. For this kind of problem different techniques of termination, not based on previous knowledge of the features of the density of states, are required.

2.2. Calculations based only on information contained in the continued fraction

We have seen that in many cases there is no additional information other than the one contained in the continued fraction coefficients, or, in an equivalent way, the moments of the Hamiltonian. In the technique of the quadratic Padé approximants [17, 18] the diagonal matrix element of the Green function is expanded in a formal power series:

$$G_{00}(E) \equiv \left\langle \phi \left| \frac{1}{E - H} \right| \phi \right\rangle = (1/E) \sum_{n=0}^{\infty} \langle \phi | H^n | \phi \rangle (1/E^n) \quad (3)$$

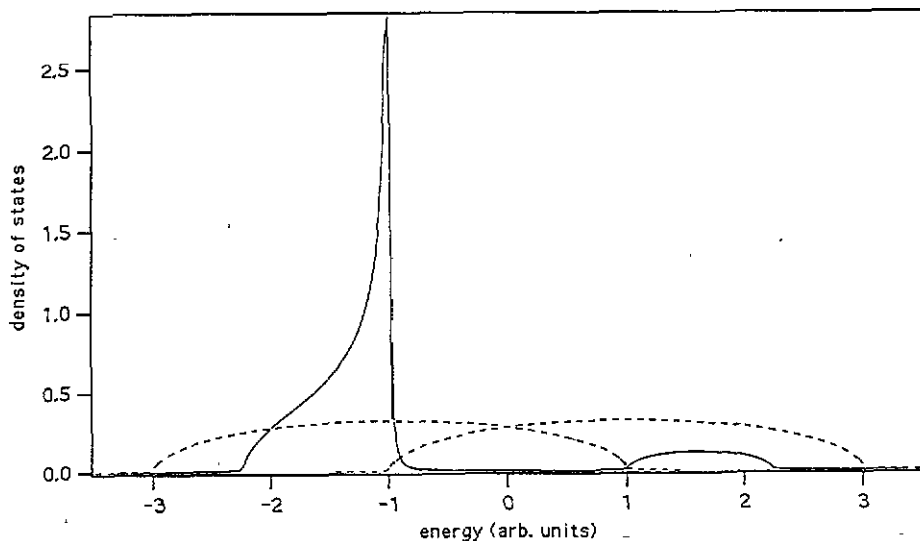


Figure 4. Surface-site-projected density of states for the one-dimensional regular alloy ABABAB... having diagonal energies 1 and -1 (full curve) and surface-site-projected for the pure A and pure B lattices (broken curves).

where H is the Hamiltonian of the system and $|\phi\rangle$ is the state of interest on which we want to calculate the projected density of states, defined as

$$n(E) = -\frac{1}{\pi} \lim_{\eta \rightarrow 0^+} \text{Im} \langle \phi | (E + i\eta - H)^{-1} | \phi \rangle. \quad (4)$$

After indicating the n th moment of the Hamiltonian $\langle \phi | H^n | \phi \rangle$ by μ_n , and the argument $1/E$ by x , we define the power series

$$G(x) = \sum_{n=1}^{\infty} \mu_{n-1} x^n. \quad (5)$$

If we consider three polynomials $P_1^{(n_1)}(x)$, $P_2^{(n_2)}(x)$ and $P_3^{(n_3)}(x)$ of degrees n_1 , n_2 and n_3 such as

$$P_1^{(n_1)}(x)G^2(x) + P_2^{(n_2)}(x)G(x) + P_3^{(n_3)}(x) = o(x^{n_1+n_2+n_3+2}) \quad (6)$$

we obtain an approximation for $G_{00}(E)$ to order $n_1 + n_2 + n_3 + 2$. In fact, having defined

$$p_j^{(n)}(E) \equiv E^n P_j^{(n)}(1/E) \quad j = 1, 2, 3 \quad (7)$$

the solution $g(E)$ of the equation

$$p_1^{(n_1)}(E)g^2(E) + p_2^{(n_2)}(E)g(E) + p_3^{(n_3)}(E) = 0 \quad (8)$$

is coincident with $G_{00}(E)$ up to order $n_1 + n_2 + n_3 + 2$. So we have explicitly

$$g(E) = \frac{-p_2^{(n_2)}(E) \pm \sqrt{r(E)}}{2p_1^{(n_1)}(E)} \quad (9a)$$

with

$$r(E) = (p_2^{(n_2)}(E))^2 - 4p_1^{(n_1)}(E)p_3^{(n_3)}(E). \tag{9b}$$

It is possible to demonstrate that the corresponding value for the density of states is

$$n(E) = |\sqrt{-r(E)}/(2\pi p_1^{(n_1)}(E))| \quad r(E) < 0 \tag{10a}$$

$$n(E) = 0 \quad \text{otherwise.} \tag{10b}$$

For example, in the case of the square lattice the moments are given by the simple relation

$$\mu_{2n} = \binom{2n}{0} \quad \mu_{2n+1} = 0 \tag{11}$$

and the density of states calculated up to degree $n = 5$ is reported in figure 5 (a comparison is possible with figure 3(a)).

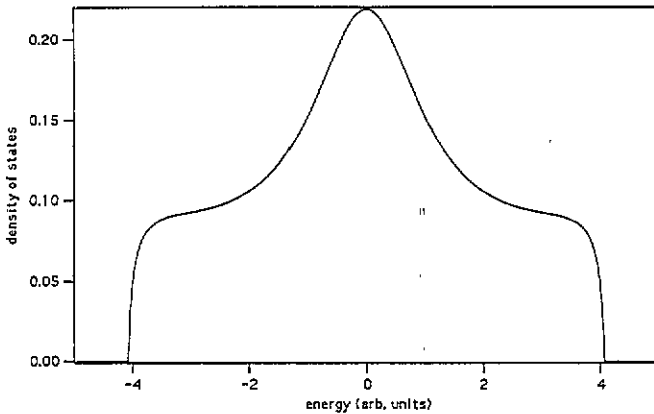


Figure 5. Density of states for the simple square lattice calculated using the method of [18] with $n = 15$.

The quadratic Padé approximant is not the only procedure that gives the density of states starting from the knowledge of the Hamiltonian moments without any extra hypothesis about the density of states itself; an alternative way to treat the problem is one based on the maximum entropy technique [13–15]. According to this approach one looks for a density of states $n(E)$ which maximizes the value of the entropy functional, defined as

$$S[n(E)] = - \int n(E) \ln[n(E)]dE \tag{12}$$

under the constraints

$$\int E^k n(E)dE = \mu_k. \tag{13}$$

It can be shown that the maximum entropy density of states must be of the form

$$n(E) = \exp[f(E)] \tag{14}$$

with

$$f(E) = \sum_{i=0}^M \lambda_i E^i \tag{15}$$

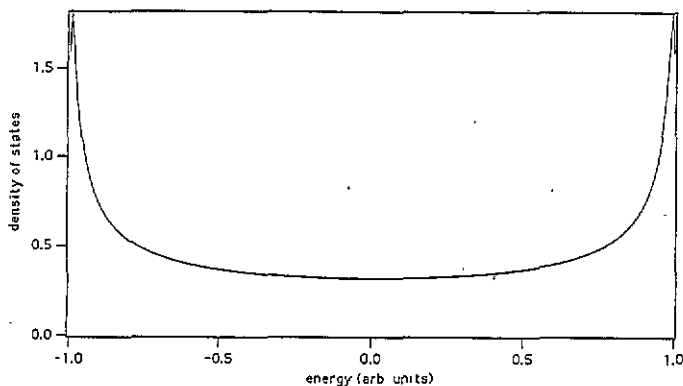


Figure 6. Density of states for the one-dimensional chain calculated with the maximum entropy method using a 9th-order polynomial.

where M is the number of known moments of the Hamiltonian, which is related to the number N of continued fraction coefficients by the relation

$$M = 2N - 1. \quad (16)$$

As an example, in figure 6 we report the density of states for the Hamiltonian of the one-dimensional chain with one orbital per site calculated in the framework of the maximum entropy formalism.

Finally, we consider the quadrature method [20]. This is essentially a technique for the evaluation of integrals with respect to a density of states $n(E)$ of the type

$$\int f(E)n(E)dE \quad (17)$$

by orthogonal polynomials generated using the continued fraction coefficients. In particular, if we consider the indefinite integral with $f(E) = 1$ we obtain the integrated density of states

$$N(E) = \int^E n(E')dE' \quad (18)$$

and by differentiating this last expression we get the density of states $n(E)$. A comparison between quadrature and termination has been also made [21], showing the superiority of the second technique, at least when the internal singularities are sufficiently weak.

Although of great utility in cases in which one cannot employ any further information than the calculated recursion coefficients, the methods presented in this subsection are subject to the strong limitations of numerical instability. In fact we are dealing with polynomials, and due to the finite precision of computers after a certain degree (for double precision calculations typically 20) the largest terms in the polynomial cannot be compared with the smallest ones. So, in the case of quadratic Padé approximants, the results quoted in the literature [18] are obtained using extended precision. Moreover, in the case of the maximum entropy approach, the functional form of the exponential of a polynomial for the density of states allows the possibility of overflows when the range $[-1; 1]$ for the energy is exceeded.

From the previous discussion it is clear that there are a number of cases in which neither the termination, quadratic Padé approximant, nor the maximum entropy approaches are appropriate for the calculation of the density of states. This may happen when we are dealing with complex systems, such as alloys, for which nothing can be said about the main features of the density of states, and we have at our disposal a number of continued fraction

coefficients that is sufficiently large to overcome the range of numerical stability of the methods based on polynomials but not enough to allow the individuation of an asymptotic behaviour of the coefficients. In such unlucky cases the best thing to do seems to be the direct resummation of the continued fraction truncated at a given order, adding a small imaginary part to the energy. Nevertheless in doing so a number of spurious oscillations in the density of states are introduced. The situation can be improved to a certain degree by the application of a technique presented in this paper, and based upon the following concept: if we consider the values for the density of states calculated at a given energy using continued fractions truncated at different orders, we obtain a numerical sequence approaching the exact value as the number of levels in the continued fraction goes to infinity. So, for every energy, this limiting value can be extrapolated by the use of some accelerated convergence procedures. The simplest of these procedures is indeed the averaging over a given number of values, but it is formally correct only in the case of oscillating sequences, and in any case it gives rather rough results. Instead, good results can be obtained by the use of the so-called ϵ -univariate algorithm, derived in the framework of the Padé approximant theory.

3. Acceleration convergence procedure for numerical sequences

We now consider the continued fraction expansion of the density of states of a Hamiltonian H at a given energy E : $\rho(E)$. We indicate by $\rho_n(E)$ the summation of the continued fraction truncated at the n th level; the exact value for $\rho(E)$ will be

$$\rho(E) = \rho_\infty(E) \equiv \lim_{n \rightarrow \infty} \rho_n(E). \quad (19)$$

For any given value of E , $\{\rho_n(E)\}$ may be considered as a numerical sequence converging to the exact value $\rho(E)$. Now the basic idea of the method proposed here is simply the acceleration of the convergence of the numerical sequence by means of a technique based on the Padé approximant theory.

First, we briefly recall the Padé approximant theory [22, 23]. Let us consider a power series

$$f(x) = c_0 + c_1x + c_2x^2 + \dots \quad (20)$$

and two polynomials

$$p(x) = \sum_{i=1}^m a_i x^i \quad (21a)$$

and

$$q(x) = \sum_{i=1}^n b_i x^i. \quad (21b)$$

We indicate by ∂p the exact degree of the polynomial $p(x)$, and by ωf the order of the power series $f(x)$ (i.e. the degree of the first non-zero term in the series). Then the Padé approximation problem of order (m, n) for the series $f(x)$ consists in finding two polynomials $p(x)$ and $q(x)$ such that

$$\partial p \leq m \quad \partial q \leq n \quad \omega(fq - p) \geq m + n + 1. \quad (22)$$

The meaning of (22) is that in the series $(fq - p)(x)$ the coefficients of x^i for $i = 0, 1, \dots, m + n$ must disappear. Condition (22) generates a set of linear equations for the coefficients a_i and b_i of $p(x)$ and $q(x)$. It is clear that $p(x)/q(x)$ is an approximation for the power series $f(x)$. In terms of $p(x)$ and $q(x)$ the approximant for $f(x)$ of order (m, n) is defined as

$$r_{m,n}(x) \equiv \frac{p(x)}{q(x)}. \tag{23}$$

Now consider a sequence of real or complex numbers $\{a_i\}$ having a limit A :

$$\lim_{i \rightarrow \infty} a_i = A. \tag{24}$$

Our problem is to find another sequence $\{b_i\}$ converging faster to A , i.e.

$$\lim_{i \rightarrow \infty} \frac{|b_i - A|}{|a_i - A|} = 0. \tag{25}$$

To do that we construct the power series

$$f(x) = a_0 + \sum_{i=1}^{\infty} (a_i - a_{i-1})x^i. \tag{26}$$

If we define the partial summations

$$F_k(x) = a_0 + \sum_{i=1}^k (a_i - a_{i-1})x^i \tag{27}$$

then we have

$$F_k(1) = a_k \quad k = 0, 1, \dots \tag{28}$$

We can approximate $f(x)$ with the Padé approximant of order (i, i) : $r_{i,i}(x)$; so we can put

$$b_i = r_{i,i}(1) \quad i = 0, 1, \dots \tag{29}$$

It can be demonstrated [16] that the convergence properties of the sequence $\{b_i\}$ are the same or better than the original sequence $\{a_i\}$. To evaluate the Padé approximants there are several algorithms; the best for this case is the so-called ϵ -algorithm [24]. If we define

$$\epsilon_{(2n)}^{(m-n)} = r_{(m,n)} \tag{30}$$

a recursive relation holds:

$$\epsilon_{(2n)}^{(m-n)} = \epsilon_{(2n-2)}^{(m-n+1)} + \frac{1}{\epsilon_{(2n-1)}^{(m-n+1)} - \epsilon_{(2n-1)}^{(m-n)}}. \tag{31}$$

In our case (31) takes the form

$$\epsilon_{-1}^{(k)} = 0 \quad \epsilon_0^{(k)} = F_k(1) = a_k \quad \epsilon_{k+1}^{(\ell)} = \epsilon_{k-1}^{(\ell+1)} + \frac{1}{\epsilon_k^{(\ell+1)} - \epsilon_k^{(\ell)}} \tag{32}$$

with $k, \ell = 0, 1, \dots$. So we have

$$\epsilon_{2i}^{(0)} = r_{i,i}(1) = b_i. \tag{33}$$

In many cases (32) and (33) give rise to an evident improvement of the convergence properties of the original sequence. As an example, we show in table 1 a comparison between a_i and b_i for the sequence

$$a_i = 1 + \frac{1}{0.5 + i^2}. \tag{34}$$

In the following section we apply these results to the partial summations of a continued fraction expansion.

Table 1. Comparison between the sequence (34) $a_i = (0.5 + i^2)^{-1} + 1$ and the sequence $\{b_i\}$ derived by means of (32) and (33).

b_i	a_i	i
1.666 666 666 666 667	1.222 222 222 222 222	2
1.063 492 063 492 064	1.060 606 606 606 061	4
1.014 921 645 751 388	1.027 397 260 273 973	6
1.005 168 505 576 012	1.015 503 875 968 992	8
1.002 216 006 015 733	1.009 950 248 756 219	10
1.001 064 465 653 520	1.006 920 415 224 914	12
1.000 358 558 836 865	1.005 089 058 524 173	14
1.000 470 647 182 837	1.003 898 635 477 583	16
1.000 272 471 993 237	1.003 081 664 098 613	18
1.000 176 283 706 360	1.002 496 878 901 373	20
1.000 104 075 594 782	1.002 063 983 488 132	22
1.000 110 272 240 315	1.001 734 605 377 277	24
1.000 068 560 075 517	1.001 478 196 600 148	26

4. Application to density of states calculations

The accelerated convergence procedure seen in general in the previous section can be applied to the sequence obtained from a continued fraction expansion truncated at progressive levels. Let us consider as an example the density of states of a cubic regular lattice. The Hamiltonian of the system is

$$H = \sum_i |\phi_i\rangle \varepsilon \langle \phi_i| + \sum_{i \neq j}^{nn} |\phi_i\rangle t \langle \phi_j| \quad (35)$$

where $\{\phi_i\}$ is a basis of localized states and the second summation is extended to the nearest neighbours. The density of states for this system is theoretically well known [25] so it represents a good test for the termination procedures.

The exact density of states for a simple cubic lattice is shown in figure 7(a). Now, if we have at our disposal only a limited number of continued fraction coefficients, we can simply truncate the continued fraction expansion by adding to the energy a small imaginary part (figure 7(b)), obtaining a number of spurious oscillations. To eliminate these oscillations one can increase the imaginary part of the energy, but operating in this way the other features of the spectrum are lost. As a first correction to the direct truncation we can introduce a semi-empirical averaging procedure. Suppose that we have N coefficients at our disposal; we calculate at every energy E the values $\rho_i(E)$ where the index i runs from a certain $n < N$ to N , then we take the average:

$$\bar{\rho}_i(E) = \sum_{i=n}^N \frac{\rho_i(E)}{N - n + 1}. \quad (36)$$

The density of states for the simple cubic lattice calculated with this procedure, and with the same number of coefficients and imaginary part of the energy as the one of figure 7(b), is shown in figure 7(c). A strong reduction of spurious oscillations is evident.

Finally, we apply the technique presented in the previous section for the convergence acceleration. As in the case of the average we take the last values of ρ_i from $i = n$ to $i = N$ and then try to find the correct limit of the numerical sequence so obtained. The density of states for the simple cubic lattice calculated this way with the same parameters as figure 7(c) is presented in figure 7(d); a further reduction of spurious oscillations is now evident.

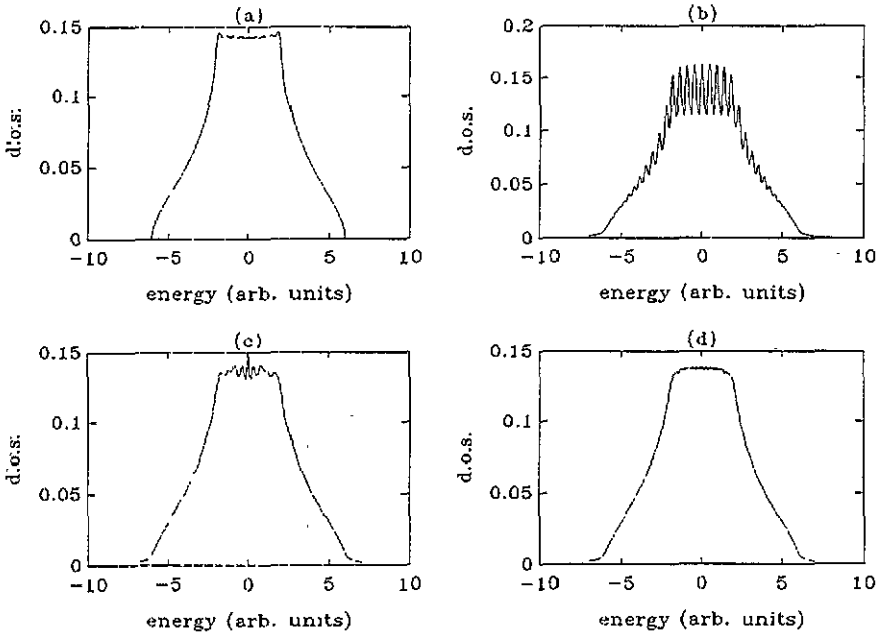


Figure 7. Density of states for the simple cubic lattice: (a) exact; (b) truncated at $N = 39$ coefficients of the continued fraction, the imaginary part of the energy is 0.18; (c) calculated with the average procedure of (36) with $n = 19$ and $N = 39$; (d) calculated with the convergence acceleration procedure by means of the ϵ -univariate algorithm with $n = 19$ and $N = 39$. In (c) and (d) the imaginary part of the energy is still 0.18.

5. Conclusions

In this paper we have presented an original procedure for the termination of continued fraction expansions based on an accelerated convergence algorithm derived in the framework of the Padé approximant theory. We have focused our attention on the calculation of density of states, but the method can be applied to the continued fraction expansion of other quantities of interest. Considering the expansion to order n , ρ_n , as a term in a numerical sequence we use the ϵ -univariate algorithm to extrapolate the limit ρ_∞ , i.e. by hypothesis the exact value of the quantity ρ . As well as the other termination procedures, the method presented in this paper is a mathematical tool to extract the maximum physical information from a given set of continued fraction parameters; it reveals its utility in those cases in which no additional information about the density of states is at our disposal, and the number of continued fraction coefficients is too large to apply techniques based on orthogonal polynomials, but not large enough to individuate an asymptotical trend in the coefficients themselves.

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