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# On the generation of continuous approximate spectral densities from moments

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**Abstract.** We propose to apply the method of moments not to the spectral density itself but rather to one of its derivatives. The spectral density obtained by integration is therefore continuous or smooth depending on the order of the derivative which is used. The problems arising from the fact that the derivatives of the spectral function are generally not positive definite have been resolved. An additional advantage of the method is its ability to reproduce singular spectral densities (e.g. van Hove singularities) as is shown for three illustrative examples.

## 1. Introduction

The methods of moments or Padé approximants and of continued fractions (for a review see Haydock 1980, Kelly 1980 and references cited therein) have been used extensively for the calculation of spectral densities. Provided that the first moments of a spectral density are known, these methods approximate the true spectral density in the sense that the given moments are reproduced.

There are several methods for the determination of a spectral function from moments. The most straightforward procedure is the transformation of the problem of moments to a problem of continued fractions (Gaspard and Cyrot-Lackmann 1973). It turns out that this transformation is numerically unstable. The instability does not depend on this particular evaluation method, but is inherent in the problem of moments and other evaluation techniques are affected in a similar manner. It is the recursion method (Haydock 1980, Kelly 1980) which overcomes this basic difficulty. Although it is mathematically equivalent to the method of moments, the explicit use of the moments is avoided by tridiagonalisation of the operator of which the spectral density is to be calculated. This formulation of the problem allows for numerically stable recurrence relations for the coefficients of the same continued fraction as determined from the moments.

A finite set of moments, of course, only determines a finite number of coefficients of the continued fraction. For the derivation of the spectral function from the continued fraction, two different procedures are commonly used.

In the first method the continued fraction is truncated thus representing a rational function. It can be proved that for the true spectral function being positive definite, this rational function determines an approximate spectral function which consists of a series of $\delta$-functions. In order to get a continuous spectrum, additional smoothing procedures are required (Nex 1978, Gaspard and Cyrot-Lackmann 1973). There is

  

a great deal of freedom in the choice of a smoothing method. It is only restricted by the condition that the given moments must not be changed.

In the second method, the subsequent smoothing procedure is circumvented by a theory on the asymptotic behaviour of the coefficients of the continued fraction. By this theory the asymptotic behaviour of the coefficients is extrapolated from the known coefficients (Gaspard and Cyrot-Lackmann 1973) so that an analytic expression can be derived from the continued fraction from which a continuous spectral density is deduced.

Both methods introduce an additional ingredient into the method of moments and can lead to difficulties in the vicinity of true singularities of the density of states. If the smoothing is too weak, band edges and van Hove singularities often produce spurious oscillations in the approximated density of states; if it is too strong, the structure of the spectrum is destroyed.

Therefore it seems desirable to find a method which, on the one hand, is able to generate continuous approximants to the true spectral density, and which, on the other hand, remains flexible enough to produce the true singularities of the spectrum in an adequate manner.

The aim of the present paper is to propose such a method which fulfils both conditions. Continuous approximants to the spectral density are generated by applying the continued fraction method using moments not to the spectral density itself but rather to its derivatives. For the derivation of the spectral function we take the truncated continued fraction which is terminated according to the number of given moments. In general, the remaining rational function yields a spectral function consisting of a series of $\delta$-functions. Approximating for instance the second derivative by a series of $N$ $\delta$-functions yields a piecewise linear continuous spectral density with $N$ points of discontinuity of the derivative. Although the moments of the spectral function are trivially related to the moments of its derivatives (§ 2), the application of the method of moments to the derivatives needs further consideration.

First, a procedure which in analogy to the recursion method produces a continued fraction avoiding the use of moments does not seem to exist for this case. In order to exploit the advantages of the recursion method we transform the problem of moments to a problem of continued fractions in § 3. It is this transformation where the numerical instability of the method of moments comes into play. As long as the moments are known exactly and can be represented to a sufficient degree of accuracy on the calculator, this difficulty can be circumvented by multiple precision calculations. This is the case for our calculations. If, however, the moments are only known approximately, the applicability of the method becomes limited. Secondly, difficulties with this method arise from the fact that the derivatives are, of course, not positive definite. Therefore, it can happen that the terminated continued fraction has poles outside the real axis, which means that the problem has no solution in the strict mathematical sense since some of the values for the position of the $\delta$-functions become complex. In this case the approximant for the spectral density consists of steps, $\delta$-functions, and derivatives of $\delta$-functions besides the continuous contribution. However, our numerical examples indicate that these additional parts are of less importance than one would expect at first sight. Although for these examples the true spectral densities even have singularities, reasonable approximate solutions to the problem are obtained.

These examples show an important advantage of our new method. It admits very easily the generation of discontinuous steps in the approximate spectral density.

Therefore no problems arise with van Hove singularities, which introduce the spurious oscillations, known from other methods, in the approximate spectral density.

## 2. The method

Consider the spectral density $n(x)$. By a Cauchy-type integral we define the function

$$f(z)=\int_{-\infty}^{+\infty}\frac{\mathrm{d}x}{\pi}\,\frac{n(x)}{z-x} \tag{2.1}$$

of the complex variable $z$. It is analytic in the upper and lower complex plane, provided that $n(x)$ decays fast enough at infinity. The asymptotic expansion of this function at large $z$ is given by

$$f(z)\sim\frac{1}{\pi}\sum_{l=0}^{\infty}\frac{M_l}{z^{l+1}} \tag{2.2}$$

where the coefficients $M_l$ are the moments of $n(x)$ of order $l$,

$$M_l=\int_{-\infty}^{+\infty}\mathrm{d}x\,x^l n(x). \tag{2.3}$$

In many situations it is relatively easy to calculate the moments of a spectral density though $n(x)$ is not known. Therefore one can ask whether it is possible to determine $n(x)$ from the moments. There are two ways for tackling the problem. First one can ask for a function $f(z)$ with correct analytic properties which has the asymptotic expansion (2.2), or secondly one can ask for the solution of equation (2.3) for a given number of moments $M_l$. Both questions are intimately related. The latter is the subject of the method of moments.

The conventional problem of moments is the following (Akhiezer 1965, Shohat and Tamarkin 1963). Given an infinite set of numbers $\mathfrak{M}=\{M_0, M_1, M_2, \ldots\}$, is it possible to find a non-decreasing function $\sigma(x)$ so that for all elements of $\mathfrak{M}$

$$M_l=\int_{-\infty}^{+\infty}x^l\,\mathrm{d}\sigma(x) \tag{2.4}$$

holds (Hamburger's problem of moments)? There is a unique solution of the problem if and only if all the determinants

$$D_l=\begin{vmatrix} M_0 M_1 & \ldots & M_l \\ M_1 M_2 & \ldots & M_{l+1} \\ & \ldots & \\ M_l M_{l+1} & \ldots & M_{2l} \end{vmatrix} \qquad l=0,1,\ldots, \tag{2.5}$$

are positive. Using only the first $2N$ moments $\{M_0, M_1, \ldots, M_{2N-1}\}$ one can determine exact upper and lower bounds on the integrated spectral density $\sigma(x)$. In this case the spectral density $\sigma'(x)=\mathrm{d}\sigma/\mathrm{d}x$ can be represented by a series of $N$ $\delta$-functions

$$\sigma'_N(x)=\sum_{i=1}^{N}p_i\delta(x-x_i). \tag{2.6}$$

This series approximates the true $\sigma'(x)$ in the sense that the first $2N$ moments of $\sigma'_N(x)$,

$$M_l[\sigma'_N(x)] = \int_{-\infty}^{+\infty} \mathrm{d}x\, x^l \sigma'_N(x), \qquad l = 0, 1, \ldots, 2N-1, \tag{2.7}$$

agree with those of $\sigma'(x)$ and that $\sigma_N(x)$, a step function, converges to the true integrated spectral density $\sigma(x)$ for $N \to \infty$.

In physical applications the number of available moments is limited, and frequently it is not the integrated density of states but rather the density of states itself which is to be determined. Representing a continuous density of states by a series of $\delta$-functions is a poor approximation in such cases. Therefore additional smoothing procedures which are not inherent in the method of moments must be introduced (Nex 1978).

In the present paper we suggest a different and more direct way of generating smooth approximate spectral functions from the moments. This method relies basically on the fact that the moments of a spectral function $n(x)$, (2.3), are closely related to the moments of the derivatives of $n(x)$

$$M_l^{(\nu)} = \int_{-\infty}^{+\infty} \mathrm{d}x\, x^l n^{(\nu)}(x). \tag{2.8}$$

Provided that all moments exist, it follows from partial integration of equation (2.8) that

$$M_l^{(\nu)} = [x^{l+1} n^{(\nu)}(x)/(l+1)]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \mathrm{d}x\, x^{l+1} n^{(\nu+1)}(x)/(l+1). \tag{2.9}$$

The first term vanishes because $n(x)$ and its derivatives decrease at least exponentially at infinity; otherwise the moments of all orders would not exist. Comparing equations (2.8) and (2.9) we obtain

$$M_l^{(\nu)} = -lM_{l-1}^{(\nu-1)}. \tag{2.10}$$

This relation implies

$$\begin{aligned} M_l^{(\nu)} &= (-l)(-l+1)\ldots(-1)M_0^{(\nu-1)} \\ &= (-l)(-l+1)\ldots(-1)\int_{-\infty}^{+\infty} \mathrm{d}x\, n^{(\nu-l)}(x) \qquad (2.11a) \\ &= 0 \end{aligned}$$

for $l < \nu$, and

$$M_l^{(\nu)} = (-l)(-l+1)\ldots(-l+\nu-1)M_{l-\nu}^{(0)} \tag{2.11b}$$

for $l \geqslant \nu$, respectively.

Of course, we have to assume that $n(x)$ is differentiable $\nu$ times. This assumption is, however, no serious restriction on the class of allowed spectral functions, because it is always possible to modify a function which has a finite number of irregular points in such a way that it becomes differentiable up to a given order while the changes in the moments remain arbitrarily small.

Knowing the moments of the derivatives of $n(x)$, we no longer try to approximate $n(x)$ but rather its $\nu$th derivative $n^{(\nu)}(x)$ by a series of $N$ $\delta$-functions so that the first $2N$ moments of $n^{(\nu)}(x)$ are exactly represented. Provided that this problem has a solution, the approximate spectral function, which by construction reproduces exactly

the first $2N$ moments, is obtained by integrating the sum of $\delta$-functions $\nu$ times. Hence the resulting $n_N(x)$ is continuous for $\nu = 2$ or differentiable $(\nu - 2)$ times for $\nu > 2$, respectively.

The problem we are faced with can be stated as follows. Given a set of numbers $\{m_0, m_1, \ldots, m_{2N-1}\}$, the first $2N$ non-trivial moments of $n^{(\nu)}(x)$, is it possible to find a sum of $N$ $\delta$-functions

$$g(x) = \sum_{j=1}^{N} p_j \delta(x - x_j) \tag{2.12}$$

so that the relations

$$\begin{aligned} m_l &= \int_{-\infty}^{+\infty} \mathrm{d}x\, x^l g(x), \\ &= \sum_{j=1}^{N} p_j x_j^l, \qquad l = 0, 1, \ldots, 2N-1, \end{aligned} \tag{2.13}$$

hold? At first sight the problem looks very similar to the common problem of moments. There is, however, one essential difference. The basic requirement for the theory of the classical problem of moments, namely $\sigma'(x)$ to be non-negative, is, in general, not fulfilled for $n^{(\nu)}(x)$. Therefore the conventional theory for the existence of $\delta$-approximants is no longer applicable. At this stage we cannot decide whether a solution of our problem with real $p_j$ and $x_j$ actually exists. It seems to be very difficult to find out the necessary conditions on the set $\{m_0, m_1, \ldots, m_{2N-1}\}$.

The following theorem, the proof of which is given in the appendix, states that at least a unique solution with complex values for $p_j$ and $x_j$ exists. Of course, in the case of complex $x_j$ the expression (2.12) becomes meaningless. However, as we shall see later, it is possible to generalise the expression (2.12) in such a way that complex solutions are also admitted.

*Theorem.* We are given a set of $2N$ complex numbers $\{m_0, m_1, \ldots, m_{2N-1}\}$, for which the determinant

$$D_N = \begin{vmatrix} m_0, & m_1, & \ldots & m_{N-1} \\ m_1, & m_2, & \ldots & m_N \\ & & \ldots & \\ m_{N-1}, & m_N, & \ldots & m_{2N-1} \end{vmatrix} \neq 0. \tag{2.14}$$

Then in almost all cases a set of $N$ pairs of complex numbers $\{(p_1, x_1), (p_2, x_2), \ldots, (p_N, x_N)\}$ exists so that the nodes $x_j$ are all different and the following equations hold:

$$m_l = \sum_{j=1}^{N} p_j x_j^l, \qquad l = 0, 1, \ldots, 2N-1. \tag{2.15}$$

By the term 'in almost all cases' we want to exclude the somewhat more complicated situations for which some of the $x_j$ are equal. The case of such accidental degeneracies is not considered here.

In physical applications spectral densities are real and therefore the $m_l$ are real as well. Then, as can be deduced from equation (2.15), the nodes $x_j$ are either real or pairwise complex conjugate. Accordingly we have to distinguish two different cases.

(i) All the nodes $x_j$ turn out to be real. Then the amplitudes $p_j$ are real as well. We obtain

$$m_l = \sum_{j=1}^{N} p_j x_j^l = \int_{-\infty}^{+\infty} \mathrm{d}x\, x^l g(x) \tag{2.16}$$

where $g(x)$ as defined by equation (2.12) is the desired $\delta$-approximation of $n^{(\nu)}(x)$. The problem is solved.

(ii) There are pairs of complex conjugate nodes $x_j$ and $x_{j'} = x_j^*$. For the corresponding amplitudes we get the relation

$$p_j = p_{j'}^*. \tag{2.17}$$

For this case it is not possible to express the $m_l$ as moments of a sum of $\delta$-functions as in equation (2.12). Hence a rigorous solution does not exist in the sense stated above. For the second case there is, however, a way for obtaining at least an approximate solution. For this purpose we consider the contribution $m_l(j, j')$ of a pair of complex conjugate nodes $x_j$ and $x_{j'} = x_j^*$ to the moment of the $l$th order:

$$m_l(j, j') = p_j x_j^l + p_j^* (x_j^*)^l. \tag{2.18}$$

Decomposing $x_j$ and $p_j$ into their real and imaginary parts

$$x_j = x_j' + \mathrm{i}x_j'', \qquad p_j = p_j' + \mathrm{i}p_j'', \tag{2.19}$$

respectively, we obtain

$$m_l(j, j') = 2p_j' \sum_{k=0}^{2k \leq l} \binom{l}{2k} (-1)^k x_j'^{l-2k} x_j''^{2k} - 2p_j'' \sum_{\substack{k=0 \\ 2k<l}} \binom{l}{2k+1} (-1)^k x_j'^{l-2k-1} x_j''^{2k+1}. \tag{2.20}$$

This contribution can be interpreted as resulting from a term $g(x)$ in equation (2.12) of the form

$$g(x; j, j') = 2p_j' \sum_{k=0}^{\infty} \frac{x_j''^{2k}(-1)^k}{(2k)!} \delta^{(2k)}(x - x_j') + 2p_j'' \sum_{k=0}^{\infty} \frac{x_j''^{2k+1}(-1)^k}{(2k+1)!} \delta^{(2k+1)}(x - x_j'). \tag{2.21}$$

In this case the derivative of the spectral density does not only contain $\delta$-functions, but also its derivatives. In principle this is an infinite series. Since we consider only the first $2N$ moments, we can truncate the series and retain only the finite sum

$$g_N(x; j, j') = 2p_j' \sum_{k=0}^{N-1} \frac{x_j''^{2k}(-1)^k}{(2k)!} \delta^{(2k)}(x - x_j') + 2p_j'' \sum_{k=0}^{N-1} \frac{x''^{2k+1}(-1)^k}{(2k+1)!} \delta^{(2k+1)}(x - x_j') \tag{2.22}$$

which reproduces the correct contributions to the first $2N$ moments.

Since in the applications the spectral density is found by integrating $n_N^{(\nu)}(x)$ $\nu$ times, the derivatives of the $\delta$-functions of low order (less than $\nu - 1$) yield smooth contributions to $n_N(x)$, while the derivatives of higher order cause 'steps', $\delta$-peaks, and derivatives of $\delta$-peaks. Thus one would at first think that the method does not work

if complex solutions occur. But this is not the case. In our example the imaginary parts $x_j''$ turned out to be small so that the contributions of the $\delta$-functions and their derivatives were negligible and smooth spectral densities were obtained. The contribution of step functions, on the other hand, turned out to be significant in the vicinity of the van Hove singularities. But since the introduction of steps is suitable for the approximation of these singularities, the occurrence of complex solutions to equations (2.15) even improves the flexibility of the method. However, it may not always be true that the $x_j''$ are small. Therefore the validity of this approximation depends on the actual problem.

Nothing can be said about the convergence of this procedure when more and more moments are taken into account. The proofs on the convergence behaviour usually require the positiveness of the spectral function which is to be determined. Since $n^{(\nu)}(x)$ is certainly not positive, the proofs are not applicable in this context. Our test calculations, however, show good convergence, even in the most unfavourable cases, where the spectral density is singular. As compared with the conventional methods which rely on additional smoothing procedures, our method turns out to work even better because the well known spurious oscillations in the vicinity of the singularities do not occur.

## 3. Transformation to a continued fraction

Instead of attempting to solve equations (2.13) for the nodes $x_j$ and amplitudes $p_j$ directly, it is more convenient to approximate $f(z)$ of equation (2.1) and to determine the $x_j$ as the poles of a rational function $h(z)$ of the complex variable $z$ for which the first $2N$ coefficients $m_l'$ of its asymptotic expansion

$$h(z) \sim \frac{1}{\pi} \sum_{l=0}^{\infty} \frac{m_l'}{z^{l+1}} \tag{3.1}$$

agree with the set of numbers $m_0, m_1, \ldots, m_{2N-1}$ (Wall 1948, Shohat and Tamarkin 1963). As we shall show later this can be achieved immediately by constructing a truncated continued fraction. The rational function obtained in this way has $N$ poles $z_j$, which can be complex, and can be written as

$$h(z) = \frac{1}{\pi} \sum_j \frac{p_j}{z - z_j}. \tag{3.2}$$

For the sake of simplicity we again confine ourselves to the case that all the $z_j$ are different. The asymptotic expansion of expression (3.2) yields

$$m_l' = \sum_j p_j z_j^l \tag{3.3}$$

with $m_l' = m_l$ for $l = 0, \ldots, 2N-1$, so that the poles of $h(z)$ and the corresponding residues give the solution of equations (2.13).

If all the $z_j$ turn out to be real, $h(z)$ is analytic in the upper and lower half-planes as is the function $f(z)$ defined by equation (2.1). If there are, however, some complex $z_j$, $h(z)$ has not the correct analytic properties corresponding to $f(z)$. In this case one first has to determine $g_N(x)$ according to equation (2.22). Then the Cauchy-type

integral

$$\tilde{h}(z)=\int \frac{\mathrm{d}x}{\pi}\,\frac{g_N(x)}{z-x}, \tag{3.2a}$$

which is a rational function, has the desired analytic properties and asymptotic expansion.

We now determine the continued fraction for an approximation of $f(z)$. In the examples we approximate the spectral density by a function which is piecewise linear by applying the method to the second derivative of the spectral density. Therefore we have $m_0=m_1=0$ and $m_2\neq 0$ according to (2.11). For the general case let $m_{l_0}$ be the first non-zero element of the set $m_0,\ldots,m_{2N-1}$. Then $h(z)$ decreases asymptotically as $1/z^{l_0+1}$. It can be represented in the form

$$h(z)=\frac{1}{\pi}\,\frac{A}{\sum_{\mu=0}^{l_0+1}A_\mu z^\mu - r_1(z)} \qquad \text{with } A_{l_0+1}=1 \tag{3.4a}$$

for $l_0$ even or

$$h(z)=\frac{1}{\pi}\,\frac{A-z}{\sum_{\mu=0}^{l_0+2}A_\mu z^\mu - r_1(z)} \qquad \text{with } A_{l_0+2}=1 \tag{3.4b}$$

for $l_0$ odd, where $r_1(z)$ is asymptotically of the order $1/z$. Because both cases are similar we only discuss the first ($l_0$ even). Equating the asymptotic expansion (3.1) of $h(z)$ with $m'_l=m_l$ for $l=0,1,\ldots,2N-1$ to the expression (3.4$a$) and comparing equal powers of $z$ after multiplying by the denominator of (3.4$a$), we obtain

$$\begin{aligned} &A=m_{l_0},\\ &\sum_{\mu=l}^{l_0+1}A_\mu m_{\mu-l-l_0}=0 \qquad \text{for } l=0,\ldots,l_0 \end{aligned} \tag{3.5}$$

and

$$r_1(z)\sum_{n=0}^{\infty}a_n/z^n=\sum_{n=0}^{\infty}b_n/z^{n+1} \tag{3.6}$$

where

$$a_n=m'_{n+l_0}, \qquad b_n=\sum_{\mu=0}^{l_0+1}A_\mu m'_{n+\mu+1+l_0}. \tag{3.7a, b}$$

Equations (3.5) allow for a successive determination of $A_\mu$ and $A$. In equation (3.6) we introduce

$$r_1(z)=\alpha_1/(z-\lambda_1-r_2(z)) \tag{3.8}$$

where $r_2(z)$ is asymptotically of the order $1/z$. Multiplying by the denominator of (3.8) and comparing equal powers of $z$ yields

$$\begin{aligned} &\alpha_1=b_0/a_0, \qquad \lambda_1=b_1/b_0-a_1/a_0,\\ &r_2(z)\sum_{n=0}^{\infty}a'_n/z^n=\sum_{n=0}^{\infty}b'_n/z^{n+1},\\ &a'_n=b_n, \qquad b'_n=b_{n+2}-\lambda_1 b_{n+1}-\alpha_1 a_{n+2}. \end{aligned} \tag{3.9}$$

The equation for $r_2(z)$ is of the same form as that for $r_1(z)$, (3.6). Therefore the last step leading to equations (3.9) can be repeated as often as needed. In this way a continued fraction for $r_1(z)$ is generated. By the common methods the poles and the residues of the truncated continued fraction are determined, and from those $n_N^{(\nu)}(x)$ is calculated. By integration $n(x)$ is obtained.

As is well known the generation of a continued fraction from the moments is numerically unstable. As far as the moments are given exactly, which is the case for our applications, the difficulties are avoided by multiple precision calculations. In contrast to the usual situation where the spectral density itself is approximated by $\delta$-functions and where the numerically stable recursion method works, there seems to be no analogue for the determination of approximants to the derivatives of the spectral function.

## 4. Examples

In order to test the method developed in the preceding sections we apply it to three examples for which the spectral density is known. We calculate the electronic density of states for a tight-binding Hamiltonian with only nearest-neighbour transfer matrix elements (i) for a one-dimensional crystal, (ii) for a two-dimensional square lattice and (iii) for a three-dimensional simple cubic lattice.

(*i*) *One-dimensional crystal*

For a one-dimensional tight-binding crystal the density of states per atom is

$$n(x) = 1/\pi(1-x^2)^{1/2} \tag{4.1}$$

where the transfer matrix element is equal to $\frac{1}{2}$. For the moments we obtain in terms of the binomial coefficients

$$M_{2l} = \binom{-1/2}{l}, \qquad M_{2l+1} = 0. \tag{4.2}$$

We want to represent the density of states by a continuous piecewise linear function. Hence we must approximate the second derivative of $n(x)$ by a series of $\delta$-functions. From equations (2.11) we obtain

$$\begin{aligned} &m_0 = M_0^{(2)} = 0, \\ &m_{2l} = M_{2l}^{(2)} = 2l(2l-1)M_{2l-2} \qquad \text{for } l \geqslant 1, \\ &M_{2l+1} = M_{2l+1}^{(2)} = 0. \end{aligned} \tag{4.3}$$

Since all moments of odd order are equal to zero, the nodes $x_j$ are distributed symmetrically with respect to the origin of the $x$ axis and the corresponding amplitudes $p_j$ are equal. This can be taken into account by writing

$$n''(x) = \sum_{j=1}^{N} 2p_j x_j \delta(x^2 - x_j^2) + p_0 \delta(x) \tag{4.4}$$

instead of (2.12), where $x_j > 0$ and $N$ is the number of non-trivial moments. The equivalent of equation (2.13) reads

$$m_0 = \sum_{j=1}^{N} p_j + p_0, \tag{4.5a}$$

$$m_{2l} = \sum_{j=1}^{N} p_j (x_j^2)^l = \sum_{j=1}^{N} q_j (x_j^2)^{l-1}, \qquad l = 1, \ldots, N. \tag{4.5b}$$

Equations (4.5*b*) represent a problem of moments for the nodes $x_j^2$ and the amplitudes $q_j = p_j x_j^2$ with the moments $\bar{m}_l = m_{2(l-1)}$. After solving this problem $p_0$ is determined by (4.5*a*).

The results of our calculations for $N = 8$, 14 and 20 are represented in figure 1. For $N = 14$ and $N = 20$ the agreement of our approximation and the exact result is rather good. For all $N \leq 20$ the nodes $x_j$ turned out to be real with the exception of the node $x_{j_1}$ which is closest to 1. There is always a small imaginary part in $x_{j_1}$ which decreases with increasing $N$. For $N = 20$ we find $x_{j_1} = 1 + 0.004\mathrm{i}$. This imaginary part is important, for it produces the finite step of appreciable size (figure 1) which models the singularity of the density of states. Nevertheless the intimately related $\delta$-contribution only little affects the density of states. For $N = 20$ this $\delta$-contribution to $n(x)$ has a factor of 0.001 and is negligible. The same is true for the derivatives of the $\delta$-function. It is only the recalculation of the moments of high order for which the imaginary parts become important.

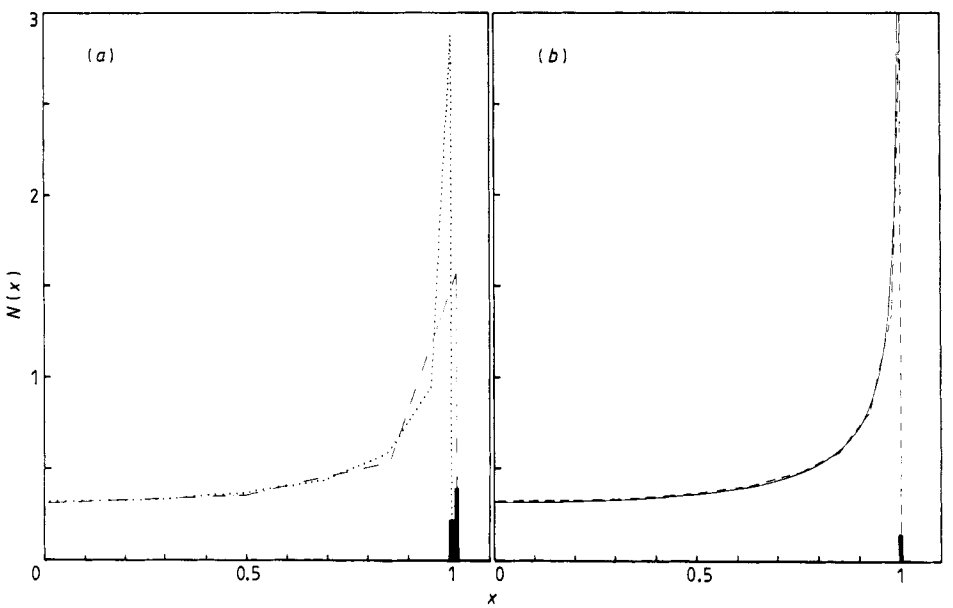


**Figure 1.** The density of states of a one-dimensional crystal at different stages of approximation. The area contained in the $\delta$-contributions is indicated by the filled rectangles at their respective positions. (*a*): $N = 8$ (– · – · – · –), $N = 14$ (· · · · · · ·). (*b*): $N = 20$ (– – – – – –), exact result (———).

(*ii*) *Two-dimensional square lattice*

The density of states per atom for a square lattice with transfer matrix elements of $\frac{1}{4}$ between nearest neighbours is given by

$$n(x) = \frac{4}{\pi^2(1+x)} F\left(\frac{1-x}{1+x}, \frac{\pi}{2}\right). \tag{4.6}$$

Here $F(k, \pi/2)$ denotes the complete elliptic integral of the first kind

$$F(k, \pi/2) = \int_0^{\pi/2} \frac{\mathrm{d}\psi}{(1-k^2 \sin^2 \psi)^{1/2}}. \tag{4.7}$$

The density of states shows a logarithmic singularity at $x = 0$ and a finite step at $x = 1$.

Since the local density of states is related to the Green function by

$$n(x) = (-1/\pi) \lim_{y \to 0^+} \operatorname{Im} G_{00}(x + \mathrm{i}y) \tag{4.8}$$

its moments are conveniently calculated from the asymptotic expansion of the Green function which can be derived from its equation of motion

$$zG_{ij}(z) - \sum_l \Delta_{il} G_{lj}(z) = \delta_{ij}. \tag{4.9}$$

$\Delta_{il}$ denotes the transfer matrix elements

$$\Delta_{il} = \begin{cases} \frac{1}{4} & \text{for nearest neighbours,} \\ 0 & \text{otherwise.} \end{cases}$$

Because the system is translationally invariant the global density of states is equal to the local density of states. For the moments we obtain

$$M_{2l} = \sum_{\substack{l_1, l_2 \\ l_1 + l_2 = l}} \frac{(2l)!}{(l_1!)^2 (l_2!)^2}, \qquad M_{2l+1} = 0. \tag{4.10}$$

For the calculation of the density of states we proceed as in the first example. The results are shown in figure 2 for $N = 10$, 14 and 20. For all cases the agreement

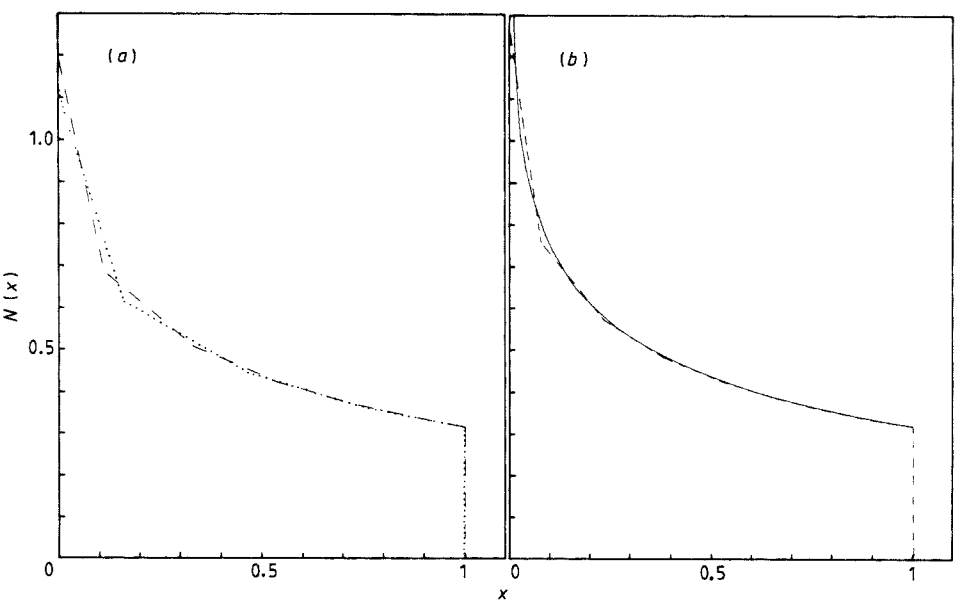


**Figure 2.** The density of states of a square lattice at different stages of approximation. (*a*): $N = 10$ (– · – · – · –), $N = 14$ (· · · · · · ·). (*b*): $N = 20$ (– – – – – – –), exact result (———).

between the exact result and the polygon is good with the possible exception of the region near $x = 0$. However, it is seen from the figure for $N = 20$ that the modelling of the logarithmic singularity is at any rate acceptable.

It is only the region of $x = 1$ where imaginary parts occur. This is again an indication that imaginary parts are related to singularities in the true spectrum. Though the imaginary part is necessary for the generation of the step, its $\delta$-contribution remains negligible. At $x = 0$, which is a node by the prescription (4.4) and not as a consequence of the evaluation of (4.5*b*), no imaginary parts were found. Nevertheless the behaviour of the true density of states is met by the polygon approximation to a sufficient degree.

(*iii*) *Three-dimensional simple cubic crystal* ('*cubium*')

There is no analytical expression for the density of states of cubium. However, numerical values are available (Wolfram and Callaway 1963). Using the same procedure as for the two-dimensional case, however with $\Delta_{ij} = \frac{1}{6}$ for nearest neighbours, we obtain

$$M_{2l} = \sum_{\substack{l_1,l_2,l_3 \\ l_1+l_2+l_3=l}} \frac{(2l)!}{(l_1!)^2(l_2!)^2(l_3!)^2}, \qquad M_{2l+1} = 0. \tag{4.11}$$

Our results for the density of states are represented in figure 3 for $N = 8$, 14, 20 and 26. For $N \geq 14$ we find close agreement with the exact $n(x)$. Even the van Hove singularities at $x = \frac{1}{3}$ and at $x = 1$ are well reproduced. There are no spurious oscillations in the vicinity of these singularities which arise from other methods.

In table 1 we list the complex nodes in dependence on $N$. In all cases these nodes are close to the van Hove singularities or band edges. However, the occurrence of

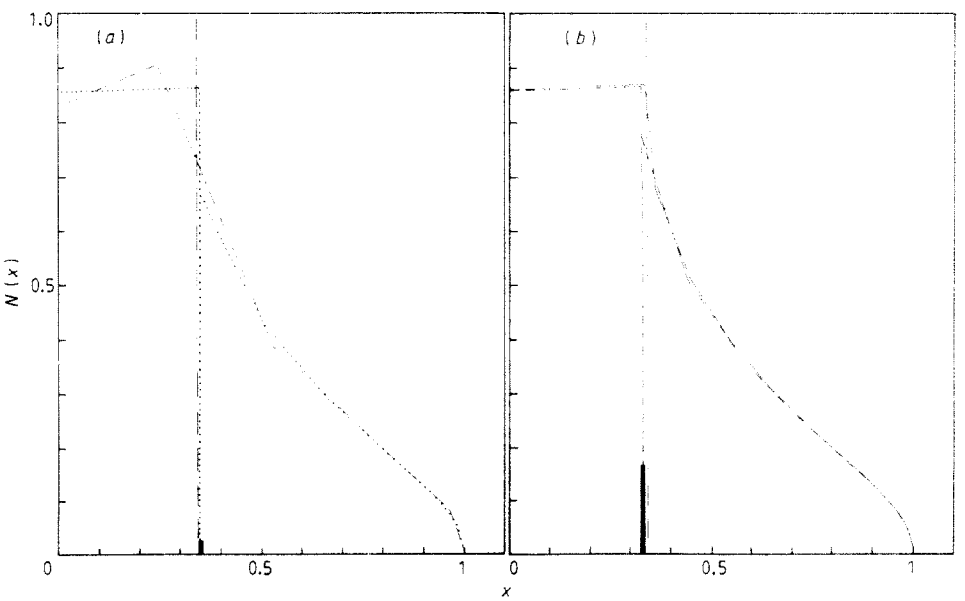


**Figure 3.** The density of states of cubium at different stages of approximation. The broken lines denote the position of the van Hove singularity. The area contained in the $\delta$-contributions is indicated by the filled rectangles at their respective positions. (*a*): $N = 8$ (– · – · – · –), $N = 14$ (· · · · ·). (*b*): $N = 20$ (– – – – – – –), $N = 26$ (———). For $N = 8$ and $N = 26$ there is no $\delta$-contribution.

**Table 1.** List of complex nodes and the weights $w$ of their corresponding $\delta$-functions which occurred for values $2 \leq N \leq 26$ for cubium.

| $N$ | $x_1$ | $w_1$ | $x_2$ | $w_2$ |
|---|---|---|---|---|
| 6 | $0.5904 \pm 0.3745i$ | $-5.6 \times 10^{-3}$ | — | |
| 10 | $0.3094 \pm 0.1058i$ | $7.4 \times 10^{-3}$ | — | |
| 12 | $0.9984 \pm 0.0063i$ | $-2.2 \times 10^{-5}$ | — | |
| 14 | $0.3465 \pm 0.0144i$ | $1.6 \times 10^{-4}$ | — | |
| 18 | $0.3058 \pm 0.0321i$ | $1.4 \times 10^{-3}$ | — | |
| 20 | $0.3257 \pm 0.0328i$ | $1.2 \times 10^{-3}$ | $0 \pm 0.3464i$ | $4.8 \times 10^{-7}$ |
| 22 | $0.9996 \pm 0.0020i$ | $4 \times 10^{-6}$ | | |

complex nodes does not seem to be systematic; for certain values of $N$, all nodes turn out to be real. As in the former examples, the $\delta$-contributions to the density of states due to the imaginary parts are negligible. For $N = 20$, besides the node at $x = 0$ which is introduced by construction, a pair of complex poles with real part $x_j' = 0$ is found. The weight of the corresponding $\delta$-function is $5 \times 10^{-7}$ and does not influence the shape of the spectrum. Occasionally nodes occur which are distinctly beyond the limits of the exact spectrum. In all cases their amplitudes are extremely small and they can be neglected.

## 5. Conclusion

In the present paper we developed a new method for the generation of a continuous approximation to the density of states when its moments are known. The basic idea is to solve the problem of moments not for the density of states but rather for a derivative of a given order. This approach has the advantage that continuous curves are obtained. Although the essential requirement of positive definiteness is not met for the derivatives of spectral functions, a method is found to circumvent the difficulties arising from the non-definiteness. In three typical examples we demonstrated the application of the method. In these examples the true density of states shows singularities of different type. In other methods, singularities frequently introduce spurious oscillations in the approximants of the density of states. But here such difficulties do not arise. This is because our method remains sufficiently flexible to incorporate singular points of the spectra in quite a simple manner. Thus it appears to be well suited for the calculation of spectral densities.

## Acknowledgment

I wish to thank Professor Dr J Jäckle for his continuous interest and many helpful discussions.

## Appendix

In this appendix we prove the thorem of § 2. Consider the polynomial

$$P_0(z) = a_0 + a_1 z + a_2 z^2 + \ldots + a_N z^N \tag{A1}$$

where $a_N = 1$ and the other coefficients $a_j$ $(0 \leq j \leq N-1)$ are still undetermined. Multiplying (A1) by $z^l$ $(0 < l < N-1)$ we get the polynomials

$$P_l(z) = a_0 z^l + a_1 z^{l+1} + a_2 z^{l+2} + \ldots + a_N z^{l+N}. \tag{A2}$$

These polynomials span a linear vector space for which we define a linear functional $\Phi$ assigning the number $m_k$ to each power $z^k$:

$$\Phi[z^k] = m_k, \qquad \text{for } k = 0, 1, \ldots, 2N-1. \tag{A3}$$

On the vector space we demand

$$\Phi \equiv 0. \tag{A4}$$

This implies the following system of linear equations for the $a_j$ $(0 \leq j \leq N-1)$:

$$\begin{aligned} &m_0 a_0 + m_1 a_1 + \ldots + m_{N-1} a_{N-1} = -m_N, \\ &m_1 a_0 + m_2 a_1 + \ldots + m_N a_{N-1} = -m_{N+1}, \\ &\qquad \ldots \\ &m_{N-1} a_0 + m_N a_1 + \ldots + m_{2N-2} a_{N-1} = -m_{2N-1}. \end{aligned} \tag{A5}$$

According to the assumption of the theorem the determinant of the system of equations is non-zero. Hence the $a_j$ are uniquely determined.

The polynomial $P_0(z)$ possesses $N$ uniquely determined, possibly complex zeros, $z_1, z_2, \ldots, z_N$. For the sake of simplicity we confine ourselves to the case that $z_j$ are all distinct. Let $F_j(z)$ be the polynomial of degree $N-1$ for which

$$F_j(z_i) = \delta_{ij}, \qquad i, j \in \{1, 2, \ldots, N\} \tag{A6}$$

holds. For an arbitrary function $f(z)$ the Lagrangian interpolation polynomial which agrees with $f(z)$ in $z_1, z_2, \ldots, z_N$ is given by

$$F(z) = \sum_{j=1}^{N} f(z_j) F_j(z). \tag{A7}$$

Its degree is not higher than $N-1$. Choose especially $f(z) = z^l$. For $0 \leq l \leq N-1$, $F(z)$ and $f(z)$ are identical; for $N \leq l \leq 2N-1$ we find

$$f(z) - F(z) = P(z) P_0(z) \tag{A8}$$

where $P(z)$ is a polynomial of degree not higher than $N-1$. The system of equations (A5) implies

$$\Phi[f(z) - F(z)] = 0. \tag{A9}$$

Using the linearity of the functional and the explicit form of $f(z)$ we finally get

$$\begin{aligned} \Phi[z^l] = m_l &= \Phi[F(z)] \\ &= \sum_{j=1}^{N} z_j^l \Phi[F_j(z)] = \sum_{i=1}^{N} p_j z_j^i \end{aligned} \tag{A10}$$

where we introduced

$$p_j = \Phi[F_j(z)]. \tag{A11}$$

The proof can be generalised to the case in which some of the zeros are of higher order. We omit it, because the proof becomes clumsy and this case is not of practical importance.

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