Reconstruction of the density of states from its moments

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The problem of the reconstruction of a non-negative spectral density from its low-order power moments is reexamined. With the assumption that the parameters of the continued-fraction representation of the Green's function obey a certain analytic expression, we derive an extrapolation procedure for them. This procedure leads to significantly improved results and is simple to implement. Several relevant examples of its application are provided and show the advantages of our method, which works adequately both for the translationally invariant case (i.e., when Van Hove singularities are present) and also in the general disordered situation. The method is particularly useful in trying to estimate the position of the effective band edges (Lifshitz limits), for which it yields quite accurate values.

I. INTRODUCTION

The problem of obtaining a reliable reconstruction of a non-negative spectral density from a finite number of its low-order power moments has been investigated since the last century.[1,2] In spite of its long history there are many aspects of it that remain without a unique answer. On the other hand, methods of moments have found a wide range of applications in several branches of physics[3–7] and chemistry,[8,9] mainly related to the widespread use of fast computers.

In particular in solid-state theory power moments can be related to the geometry and composition of the crystal structure.[8,10] This reduces their evaluation to a problem of counting paths on a lattice. In fact, the number of all possible paths which start and end at a lattice point after n steps is related to the nth power moment.

However, the problem which remains open is that once a finite number of moments is known, no unique most efficient procedure to reconstruct the density of states does exist. A good number of authors[11–13] have addressed this question within the context of solid-state theory, each time refining the available methods.

In this paper we formulate a new procedure which takes as its starting point a conjecture of Gaspard and Cyrot-Lackmann,[13] later proved by Hodges.[14] In fact, for the translationally invariant case, the parameters associated with the continued-fraction representation of the Green's function follow a simple damped oscillatory behavior in the asymptotic region, where their index becomes large. Our conjecture is that these parameters can be fitted by an analytic expression in most possible cases, that is, from the translationally invariant extreme (which implies the presence of Van Hove singularities) to the fully disordered situation.

This way, we proceed to obtain the density of states from the moments without a preconception about its features. When Van Hove singularities are present they do appear as a natural consequence of our procedure, which contains the conjecture of Gaspard and Cyrot-Lackmann[13] as a special case. When there is no translational invariance our method works just as well.

This follows the lines of what we denominate a "fair fit." That is, a fit which yields the density of states on the basis of a general procedure, which is totally free of assumptions about characteristics of the results and which works adequately in all possible circumstances.

Our method is particularly useful in providing the position of the effective band edges (Lifshitz limits), that is, the values of the energies below and above which the density of states becomes negligibly small. This information turns out to be quite relevant, since a wrong value of the bandwidth leads to the appearance of spurious peaks when the density of states is obtained from its power moments.

The remainder of this paper is organized as follows: In Sec. II the analytic derivation of the procedure is presented in precise detail. In Sec. III our method is applied to several illustrative cases and its results are discussed. Finally, Sec. IV closes this paper with a summary and relevant conclusions are drawn.

II. ANALYTIC FORMULATION

The density of states is obtained[3,13] from the Green's function $G(z)$ with the use of

$$D(x)=-\frac{1}{\pi}\,\mathrm{Im}G(x+i0^{+})\ . \tag{2.1}$$

In turn, $G(z)$ is related to the power moments of $D(x)$ through the expansion

$$G(z)=\sum_{n=0}^{\infty}\frac{\mu_n}{z^{n+1}}\ , \tag{2.2}$$

where the elements in the moment sequence $\{\mu_n\}$ are defined as

$$\mu_n=\int_{-\infty}^{\infty}D(x)x^n dx\ . \tag{2.3}$$

For computation purposes it is convenient to use the continued-fraction form of $G(z)$ given by

$$G(z)=\cfrac{1}{z-a_1-\cfrac{b_1}{z-a_2-\cfrac{b_2}{z-a_3-\cdots}}}\ , \tag{2.4}$$

where

$$a_n=\alpha_{2n-1}+\alpha_{2n}\quad (n>1) \tag{2.5a}$$

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$$b_n=\alpha_{2n}\alpha_{2n+1}\,, \tag{2.5b}$$

and $a_1=\alpha_2$. The set $\{\alpha_n\}$ is obtained from

$$\alpha_{2n}=\frac{\Delta_{n-2}}{\Delta_{n-1}}\frac{\Delta'_{n-1}}{\Delta'_{n-2}}\,, \tag{2.6a}$$

$$\alpha_{2n+1}=\frac{\Delta_n}{\Delta_{n-1}}\frac{\Delta'_{n-2}}{\Delta'_{n-1}}\,, \tag{2.6b}$$

and Δ_n and Δ'_n are related to the moments through

$$\Delta_n\equiv\det\begin{vmatrix}\mu_0 & \mu_1 & \cdots & \mu_n\\ \mu_1 & \mu_2 & \cdots & \mu_{n+1}\\ \mu_2 & \mu_3 & \cdots & \mu_{n+2}\\ \vdots & \vdots & & \vdots\\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n}\end{vmatrix}>0\,, \tag{2.7a}$$

$$\Delta'_n\equiv\det\begin{vmatrix}\mu_1 & \mu_2 & \cdots & \mu_{n+1}\\ \mu_2 & \mu_3 & \cdots & \mu_{n+2}\\ \mu_3 & \mu_4 & \cdots & \mu_{n+3}\\ \vdots & \vdots & & \vdots\\ \mu_{n+1} & \mu_{n+2} & \cdots & \mu_{2n+1}\end{vmatrix}, \tag{2.7b}$$

with $\Delta_{-1}=1=\Delta'_{-1}$ and $\Delta_{-2}=-1=\Delta'_{-2}$.

The asymptotic values of a_n and b_n yield important physical information; in fact, a_∞ is the position of the center of the energy band, while the bandwidth is obtained from b_∞ through

$$W=4(b_\infty)^{1/2}\,. \tag{2.8}$$

Gaspard and Cyrot-Lackmann[13] observed that in the presence of Van Hove singularities (i.e., when the system is translationally invariant), the parameters $\{b_{2n}\}$ and $\{b_{2n+1}\}$ coincide with the values that two damped oscillatory functions (which are out of phase by π) take for integer values of their arguments. This observation was formally proved to hold by Hodges.[14]

On the other hand, Baker[3] gives the following expression for the asymptotic value of Δ_n/Δ_{n-1}:

$$\frac{\Delta_n}{\Delta_{n-1}}\underset{n\gg1}{\longrightarrow}2\pi\left[\frac{E_u-E_l}{4}\right]^{2n+1}\times\exp\left[\frac{1}{\pi}\int_{E_l}^{E_u}\frac{\ln D(x)dx}{[(E_u-x)(x-E_l)]^{1/2}}\right], \tag{2.9}$$

where E_l and E_u are the lower and upper band edges of $D(E)$, respectively. An identical expression holds for the ratio Δ'_n/Δ'_{n-1}; both are valid provided $D(E)$ has no gaps in the (E_l,E_u) domain.

Our conjecture, based on the observation of Gaspard and Cyrot-Lackmann,[13] the results of Hodges,[14] and Eq. (2.9) is that the asymptotic behavior of Δ_n/Δ_{n-1}, and, consequently, because of Eqs. (2.5), (2.6), and (2.7), of a_n and b_n, can always be adequately fitted by

$$\Delta_N/\Delta_{N-1}=W_0z_0^N+W_1z_1^N+\cdots+W_pz_p^N\,, \tag{2.10}$$

where the $\{W_i,z_i\}$ are arbitrary complex variables. They can be obtained from the sequence $\{\mu_n\}$ through the use of (2.5) and (2.6).

When this procedure is applied, and all z_i's turn out to be real and smaller than unity, the limit $n\to\infty$ is reached monotonically, which is the observed behavior of densities of states of systems with no translational invariance. On the contrary, if $D(E)$ shows a Van Hove singularity a pair of W and z's are complex conjugate and thus

$$Wz^N+W^*z^{*N}=2\,|\,W\,|\,\,|\,z\,|^N\cos(N\omega+\phi)\,, \tag{2.11}$$

which is the damped oscillatory behavior obtained by Hodges.[14]

In consequence, our ansatz (2.10) is applicable in most circumstances, from the translationally invariant to the fully disordered cases, without any preconception about characteristic behavior of $D(E)$. This way, the information contained in the moment sequence $\{\mu_n\}$ is processed satisfying the criteria of a "fair fit," as enunciated in Sec. I.

The next step in our line of reasoning is to observe that (2.10) can be interpreted as the solution of a homogeneous linear difference equation. And since Eqs. (2.5) and (2.6) provide a relation between Δ_n/Δ_{n-1} and the parameters a_n and b_n, we postulate the existence of a recurrence relation for the $\{a_i\}$ and $\{b_i\}$ sequences, both of them of the form

$$b_{n+k+1}+c_kb_{n+k}+c_{k-1}b_{n+k-1}+\cdots+c_1b_{n+1}+c_0b_n=0\,, \tag{2.12}$$

valid for $n=1,2,3,\ldots$.

Since according to Eqs. (2.8) and (2.10) b_n tends asymptotically to a constant value for $n\gg1$, it is important to realize that some z_i must equal 1 and thus

$$\sum_{i=0}^{k}c_i=-1\,. \tag{2.13}$$

The implementation of the method is now very simple. Let us assume for convenience that $(4k+3)$ moments are known: $\mu_0,\mu_1,\ldots,\mu_{4k+2}$. Use of Eqs. (2.5)–(2.7) allows one to evaluate the first $(2k+1)$ values of the sequences $\{a_i\}$ and $\{b_i\}$. To obtain the $(k+1)$ coefficients c_i of Eq. (2.12) we have to solve the linear system

$$\begin{bmatrix}1 & 1 & \cdots & 1\\ b_1 & b_2 & \cdots & b_{k+1}\\ b_2 & b_3 & \cdots & b_{k+2}\\ \vdots & \vdots & & \vdots\\ b_k & b_{k+1} & \cdots & b_{2k}\end{bmatrix}\begin{bmatrix}c_0\\ c_1\\ c_2\\ \vdots\\ c_k\end{bmatrix}=-\begin{bmatrix}1\\ b_{k+2}\\ b_{k+3}\\ \vdots\\ b_{2k+1}\end{bmatrix}. \tag{2.14}$$

The set $\{c_i\}$ thus obtained is substituted back in Eq. (2.12) to generate recursively the extrapolated values of the parameters b_i. A perfectly analogous procedure is carried out to obtain the set $\{a_i\}$.

The density of states is obtained numerically from Eqs. (2.1) and (2.4) by setting $b_p=b_{p+1}=\cdots=b_\infty$ and $a_p=a_{p+1}=\cdots=a_\infty$. The criterion to determine p is that within the precision one is working with, both $a_p=a_{p+1}$ and $b_p=b_{p+1}$. The value of p when computing with 16 digit accuracy, is typically of the order of 50. This procedure leads to a quadratic equation, as was shown[13] by Haydock *et al.* For example, if 15 exact moments

$(\mu_0,\mu_1,\ldots,\mu_{14})$ of the density of states are known [i.e., $a_1,a_2,\ldots,a_7$ and $b_1,b_2,\ldots,b_7$ are obtained using Eqs. (2.5)–(2.7)], we only have to solve two linear systems of four equations with four unknowns each to obtain the $\{c_i\}$ coefficients of Eqs. (2.12)–(2.14).

After the set $\{c_i\}$ is known the recurrence relations (2.12) are used to generate $a_8,a_9,\ldots,a_p$ and $b_8,b_9,\ldots,b_p$. This constitutes an extremely simple procedure and in most cases it leads to significant improvements in the densities of states. At the same time taking $a_p=a_\infty$ and $b_p=b_\infty$ provides [with the aid of Eq. (2.8) and the fact that a_∞ gives the position of the band center] accurate estimates of the values of the effective band edges, as will be shown in the next section.

III. REPRESENTATIVE NUMERICAL EXAMPLES

In this section we present some illustrative numerical results of the extrapolation procedure outlined above. Emphasis is placed on the difference in values obtained by continuing recursively the $\{a_i\}$ and $\{b_i\}$ sequences, as compared with those obtained following the usual procedure of setting $a_{2k+n}=a_\infty$ and $b_{2k+n}=b_\infty$, where $2k$ is the index of the last given element in the sequence and $n=0,1,2,\ldots$.

Certainly moment methods are not well suited to treat translationally invariant configurations, where Bloch's theorem provides a more powerful tool. However, the simple cubic structure density of states has become a sort of "acid test" for the performance[13] of a reconstruction procedure. Thus in Fig. 1 we display plots of $D(E)$, obtained without and with extrapolation, based on knowing 15 and 39 exact moments of the simple cubic structure, respectively. It is apparent that the spurious oscillations near the kink are strongly quenched, while the Van Hove singularity is reproduced with greater accuracy. Moreover, the bandwidth, which is obtained with an accuracy of 0.3 and 0.2% without extrapolation, is obtained with a precision of 1 part in 10^4 and 2 parts in 10^6 using our procedure with 15 and 39 exact moments, respectively.

A requirement that a valid reconstruction procedure also must satisfy is to accurately simulate narrow peaks of the density of states. The two-dimensional simple quadratic lattice provides such an example, since it has a divergent Van Hove singularity located at the center of the band. In Fig. 2 we display the results obtained using only 11 moments. While without extrapolation a qualitatively incorrect picture does emerge, our procedure manages to strongly suppress spurious oscillations near the band edges and provides a basically correct general picture.

We also applied the extrapolation method to a Bethe lattice[15] with coordination $c=3$ and with first- and second-nearest-neighbor interactions $V_1=1/\sqrt{2}$ and $V_2=0.1$, respectively. The density of states is given[15] by

$$D(E)=\frac{(1-E^2)^{1/2}}{(4E+5)(1-8E^2/9)} . \tag{3.1}$$

In spite of its smooth form, polynomial reconstruction yields poor results, while using extrapolation of the continued-fraction parameters allows to obtain $D(E)$ from only eleven moments with and accuracy of better than 1 part in 10^4.

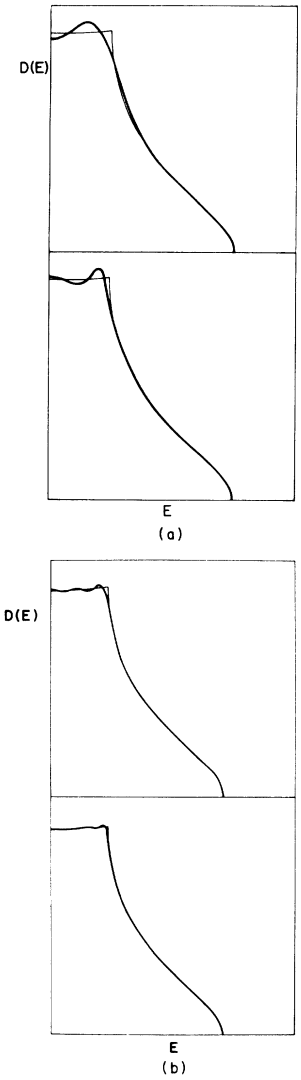

FIG. 1. (a) Density of states of the simple cubic structure for the upper half of its energy domain. The bold lines depict the calculated results, obtained without (upper figure) and with (lower figure) extrapolation, on the basis of 15 given moments. The thin lines are the exact values. (b) Same as (a), but obtained on the basis of 39 exact moments.

We have studied an academic example which exhibits some relevant features of an alloy electron density of states, but which has the advantage of allowing to contrast our results with the exact ones. In fact, we have chosen

$$D(E)=E^j(1-E)^k\sin^2(m\pi E) , \tag{3.2}$$

for which the exact moments are easily evaluated analytically when j, k, and m are integers and it has maxima and band-edge behavior similar to typical metallic alloys. The results for the case $j=k=m=2$, again obtained with only eleven moments, are displayed in Fig. 3. Once more we observe a very substantial improvement when the extrapolation procedure is employed.

This last example was chosen because the exact result is available to compare with. Real disordered binary alloys are more difficult to study, not only because exact densities of states are not available, but also because the exact

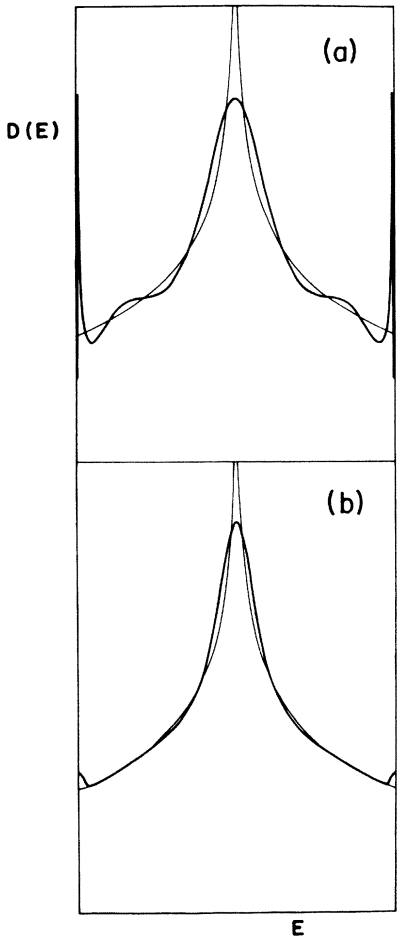

FIG. 2. Density of states of the simple quadratic structure. The bold lines depict the calculated results, obtained without (a) and with (b) extrapolation on the basis of 11 moments. The thin lines are the exact values.

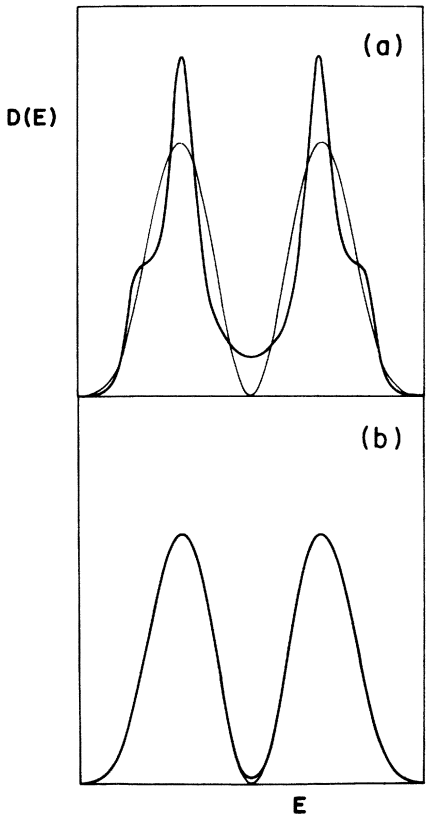

FIG. 3. Reconstruction of the function $E^2(1-E)^2\sin^2(2\pi E)$. The bold lines depict the calculated results, obtained without (a) and with (b) extrapolation and obtained from 11 given moments. The thin lines are the exact values.

moments are hard to obtain.[13] On the other hand, for the simpler problem of a one-dimensional binary disordered alloy (where in principle exact[16] densities of states can be obtained numerically), it is well known that the density of states presents a large number of peaks.[17] Obviously, these peaks will not be resolved through an extrapolation procedure based on a few moments of the density of states. Our present method in addition is useful to obtain b_∞, and thus the effective bandwidth, which is not known *a priori* in the case of disordered alloys. Use of an incorret value of b_∞ in the termination of the continued fraction yields spurious oscillations of the density of states, which might be confused with its real features.

IV. SUMMARY AND CONCLUSIONS

A method to improve the reconstruction of the density of states from a finite number of its low-order power moments, has been presented. It is based on the assumption that the parameters a_n and b_n of the continued-fraction representation for the Green's function (2.4) are analytic functions of n, when n is continued to all positive and real values. This assumption allows one to establish a recursion relation, which in turn allows one to obtain extrapolated values of the a_n's and b_n's beyond the given ones. With these extrapolated parameters included in Eq. (2.4), we obtain using (2.1) significantly improved results for the density of states. The procedure was tested for several representative situations, showing noticeable advantages over the commonly used method, at a cost of modest additional numerical labor.

We have found no problems of numerical stability with the extrapolation procedure proper, provided sufficiently precise values of the given (nonextrapolated) a_n and b_n parameters are fed in. Since, as it is well known,[13] the procedure which generates the latter [Eqs. (2.5)—(2.7)] is ill conditioned, we had to resort to infinite precision arithmetic (i.e., algebraic manipulation) in some instances to obtain these input parameters.

The performance of our procedure when gaps or localized (discrete) states are present in the spectral density has not been examined in this paper. In addition, it also would be interesting to carry out a detailed numerical comparison with the methods of reconstruction of the density of states developed by Corcoran and Langhoff,[8] and by Wheeler *et al.*,[12] in order to accurately assess the relative merits of each of these procedures as well as their shortcomings.

The main successes of our method are to quench spurious oscillations around the exact results; to simulate Van Hove singularities whenever they are present, which no

truncation procedure is capable of doing; to provide an excellent estimate of the position of the band edges, and in general, to improve the results of the reconstruction procedure at the cost of very little additional computation effort. It is most convenient and effective when only few exact moments of the density of states are known.

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