Orthogonalized-moments method

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I propose a method to compute the local density of electronic states in disordered systems. The method makes use of a particular form of the generalized moments of Lambin and Gaspard. It leads to an exact derivation of orthogonalized moments which are simply related to the coefficients of the continued-fraction representation of the density of states. It is numerically stable and analytically equivalent to the recursion method of Haydock.

I. INTRODUCTION

Several real-space techniques have been developed to calculate the local density of electronic states.[8] The recursion method of Haydock[1] is known to be numerically stable. The recursion coefficients are intrinsically nonlinear functions of the local density of states (LDOS), so they do not have simple averaging properties. The generalized-moments method of Lambin and Gaspard[2] sought to combine the advantages of the moment method[3] in averaging over configurations with the numerical stability of the recursion method. In practice, their method involves an iterative procedure which leads also to numerical instabilities. In fact, it is impossible to keep the linearity of the moments in the LDOS and to retain the numerical stability.

The orthogonalized-moments method makes use of a particular form of the generalized moments[2] that is numerically stable. The linearity of the moments in the LDOS is lost, but, since this procedure leads in a numerically stable way to the recursion coefficients, small changes in the moments do not lead to large changes in the computed LDOS—unlike the standard-moments method[3] using Hankel determinants. The final averaging of the LDOS is therefore numerically better convergent.

The principles and main formulas of the continued-fraction method are briefly reviewed. Consider a one-electron tight-binding Hamiltonian $\mathscr{H}$. The LDOS on the local orbital $|O\rangle$ is

$$n(E)=\langle O|\delta(E-\mathscr{H})|O\rangle=\frac{1}{\pi}\lim_{\epsilon\to 0^+}\mathrm{Im}R(z)|_{z=E-i\epsilon} .$$

The resolvent $R(z)$ can be written as

$$R(z)=\langle O|(z-\mathscr{H})^{-1}|O\rangle=\sum_{i=0}^{\infty}\frac{\mu_i}{z^{i+1}} ,$$

with the power moments[3] $\mu_i=\langle O|\mathscr{H}^i|O\rangle$, and the expansion holds if $|z|>||\mathscr{H}||$. To calculate the LDOS at $z=E-i\epsilon$, one needs the analytic continuation inside the circle of radius $||\mathscr{H}||$. This can be achieved by expanding the resolvent $R(z)$ in a continued fraction of the J form[4,5]

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

with a_i,b_i, real and b_i positive. The relation between the moments and the coefficients of the continued fraction is given by ratios of Hankel determinants Δ_i and $\bar{\Delta}_i$.[2] The elements of these Hankel matrices $H_i,\bar{H}_i$ are the power moments.[2,4,5] In practice, the computation of the determinants requires many operations and the calculation is ill conditioned.[6]

II. GENERALIZED-MOMENTS METHOD

In the generalized-moments method[2] one defines polynomial moments, which theoretically are linear on the LDOS like the power moments, but are better conditioned than the latter. The method suggested by Lambin and Gaspard[2] essentially makes use of the following theorem.

Let $n(E)$ be an arbitrary density. Thus, $n(E)$ is a positive real function, and there exist values $\alpha>0$ and $\gamma<\infty$ such that $n(E)<\gamma\exp(-\alpha|E|)$. Under these conditions one can construct a set of orthogonal polynomials $p_i(E)=\sum_{s=0}^{i}A_{is}E^s$ of degree i with $A_{ii}=1$ uniquely.

Starting from such a polynomial sequence one can denote the generalized moments by

$$\nu_{i,j}=\int_{-\infty}^{\infty}dE\,n(E)p_i(E)p_j(E) .$$

Theorem. If a sequence of polynomials $\{p_i(E)\}$ is orthogonal with respect to a LDOS $n(E)$, i.e.,

$$\int_{-\infty}^{\infty}dE\,n(E)p_i(E)p_j(E)=\delta_{i,j}\nu_{i,i} .$$

Then one can conclude (i)

$$p_{i+1}(E)=Ep_i(E)-c_{i+1}p_i(E)-d_ip_{i-1}(E) , \quad (1)$$

for $i\geq 1$, $p_{-1}\equiv 0$, $p_0\equiv 1$, c_i and d_i real. (ii) The recurrence coefficients $\{c_i,d_i\}$ are given by the J-fraction coefficients of the resolvent $R(z)$ corresponding to $n(E)$. Thus,

$$c_i=a_i \text{ and } d_i=b_i . \quad (2)$$

If one could construct the polynomial sequence $\{p_i(E)\}$ to be orthogonal to the *a priori* unknown LDOS $n(E)$, one would have solved the problem: The polynomial sequence $\{p_i(E)\}$ is uniquely determined by its sequence of recurrence coefficients $\{c_i,d_i\}$ and these are just the desired continued-fraction coefficients $\{a_i,b_i\}$ due to (2).

The authors[2] showed how to get rid of the calculation of the Hankel determinants $\Delta_i,\bar{\Delta}_i$. They introduced Gram matrices G_i and $\bar{G}_i$ whose elements are generalized moments

instead of power moments, but their determinants are equal to the determinants of the Hankel matrices. In the orthogonal case the Gram matrix G_i turns out to be diagonal and $\bar{G}_i$ to be tridiagonal. This gives a stable method to calculate the corresponding determinants Δ_i and $\bar{\Delta}_i$. They found[2]

$$a_i = \frac{1}{\bar{\Delta}_{i-2}} \left(\nu_{i-1,i-1} \bar{\Delta}_{i-3} + \frac{\bar{\Delta}_{i-1}}{\nu_{i-1,i-1}} \right) , \tag{3}$$

with $i \geq 2$, $a_1 = \mu_1$, and

$$b_i = \frac{\nu_{i,i}}{\nu_{i-1,i-1}} \quad \text{with } i \geq 1 . \tag{4}$$

The $\bar{\Delta}_j$ are calculated by use of a three-term recurrence relation which involves the input coefficients $\{c_1, d_1, \ldots, c_{j+1}, d_{j+1}\}$. I would like to stress that formulas (3) and (4) are valid only if one knows already the polynomial sequence $\{p_i(E)\}$ which is orthogonal on the unknown LDOS.

Lambin and Gaspard, however, used formulas (3) and (4) with a sequence of input coefficients, or, equivalently, a sequence of polynomials $\{p_i'(E)\}$, which are not orthogonal on $n(E)$. In fact, they calculated

$$\nu_{ij}' = \int_{-\infty}^{\infty} dE\, n(E) p_i'(E) p_j'(E) . \tag{5}$$

Thus, $\nu_{i,j}' \neq 0$ for $i \neq j$, and obviously the inaccuracy of using (5) is crucially dependent on their choice of $\{c_i', d_i'\}$. It is, in fact, an uncontrolled approximation, and they give no general rules for the choice of the input coefficients.

They wrote that $\{p_i'(E)\}$ must be taken "close enough" to the polynomial sequence $\{p_i(E)\}$ orthogonal on $n(E)$. So, one could think of an iteration procedure where one starts with $\{c_i'^{(1)}, d_i'^{(1)}\}$ and calculates $\{c_i'^{(2)}, d_i'^{(2)}\}$ by use of (3) and (4), and so on. Then "orthogonality" would be indicated when $c_i'^{(l)} - c_i'^{(l-1)} < \epsilon_i$ and $d_i'^{(l)} - d_i'^{(l-1)} < \eta_i$ for sufficiently small ϵ_i and η_i. However, this iteration procedure can be numerically unstable, for example, in the problem of the calculation of the LDOS in a randomly substituted alloy.

III. ORTHOGONALIZED-MOMENTS METHOD

The use of generalized moments and its success in getting rid of the calculation of determinants lies essentially in a simplification of the structure of the underlying Hankel matrices. The elements of the Gram matrices G_i and $\bar{G}_i$ are defined by

$$\begin{aligned} (G_i)_{s,t} &= \int_{-\infty}^{\infty} dE\, n(E) p_s(E) p_t(E) = \nu_{s,t} , \\ (\bar{G}_i)_{s,t} &= \int_{-\infty}^{\infty} dE\, n(E) p_s(E) E p_t(E) , \end{aligned} \tag{6}$$

with $0 \leq s,t \leq i$. It is easy to show[2] that

$$\det G_i = \Delta_i \quad \text{and} \quad \det \bar{G}_i = \bar{\Delta}_i .$$

As I will consider the orthogonal case from now on, let me simplify the notation of $\nu_{i,j}$:

$$\nu_{i,j} = \nu_i \delta_{i,j} .$$

The Gram matrices have a much simpler structure than the Hankel matrices due to the orthogonality of the polynomials:

$$G_i = \begin{pmatrix} \nu_0 & 0 & 0 & & \\ 0 & \nu_1 & 0 & & \\ 0 & 0 & \nu_2 & & \\ & & & \ddots & \\ & & & & \nu_i \end{pmatrix} ,$$

thus $\Delta_i = \prod_{s=0}^{i} \nu_s$,

$$\bar{G}_i = \begin{pmatrix} c_1\nu_0 & \nu_1 & & & & & \\ \nu_1 & c_2\nu_1 & \nu_2 & & & & \\ & \nu_2 & \ddots & \ddots & & & \\ & & \ddots & & d_j\nu_{j-1} & & \\ & & & \nu_j & c_{j+1}\nu_j & d_{j+1}\nu_j & \\ & & & & \ddots & \ddots & \\ & & & & \nu_{j+1} & \ddots & \\ & & & & & & c_{i+1}\nu_i \end{pmatrix} . \tag{7}$$

The off-diagonal elements for G_i and $\bar{G}_i$ are zero.

I want to show now that it is indeed possible to construct a sequence of polynomials $\{p_i(E)\}$ which is orthogonal to an *a priori* unknown LDOS. The point is that (3) contains the input coefficients $\{c_i', d_i'\}$ implicitly by the three-term recurrence relation for $\bar{\Delta}_i$. But it is possible to derive another three-term recurrence relation for $\bar{\Delta}_i$, where $\{c_i', d_i'\}$ do not appear. If one introduces

$$\bar{\nu}_i = \int_{-\infty}^{\infty} dE\, n(E) p_i^2(E) E , \tag{8}$$

from (6)–(8) one gets

$$\bar{G}_i = \begin{pmatrix} \bar{\nu}_0 & \nu_1 & 0 & & \\ \nu_1 & \bar{\nu}_1 & \nu_2 & & \\ 0 & \nu_2 & \bar{\nu}_2 & \ddots & \\ & & \ddots & \ddots & \\ & & & & \bar{\nu}_i \end{pmatrix} ,$$

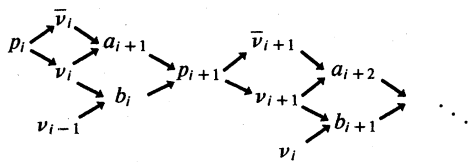
leading to a different three-term recurrence relation for $\bar{\Delta}_i$, namely,

$$\bar{\Delta}_i = \bar{\nu}_i \bar{\Delta}_{i-1} - \nu_i^2 \bar{\Delta}_{i-2} . \tag{9}$$

But from (3) and (9) one gets

$$a_i = \frac{1}{\bar{\Delta}_{i-2}} \left(\nu_{i-1} \bar{\Delta}_{i-3} + \frac{\bar{\nu}_{i-1}}{\nu_{i-1}} \bar{\Delta}_{i-2} - \nu_{i-1} \bar{\Delta}_{i-3} \right) = \frac{\bar{\nu}_{i-1}}{\nu_{i-1}} . \tag{10}$$

Equation (10) together with (4) determines a calculational procedure that gives the exact values of the higher coefficients a_i, b_i just from the power moments μ_j, $j \leq i$. The algorithm is as follows:



by use of

$$\nu_i = \sum_j |\langle O|p_i(\mathscr{H})|j\rangle|^2 \ ,$$

$$\bar{\nu}_i = \sum_{j,l} \langle O|p_i(\mathscr{H})|j\rangle\langle j|\mathscr{H}|l\rangle\langle l|p_i(\mathscr{H})|O\rangle \ ,$$

and

$$a_{i+1} = \frac{\bar{\nu}_i}{\nu_i}, \quad b_i = \frac{\nu_i}{\nu_{i-1}} \ ,$$

$$p_{i+1}(E) = Ep_i(E) - a_{i+1}p_i(E) - b_i p_{i-1}(E) \ .$$

To start the procedure one needs as input $p_1(E)$ and ν_0. But $\nu_0 = 1$ and

$$p_1(E) = E - a_1 = E - \langle O|\mathscr{H}|O\rangle \ .$$

In the Appendix the stability of this algorithm will be discussed in connection with the recursion method.[1]

Another way to look at this orthogonalized-moments method takes the recursion relation directly into account. The scalar product is denoted by

$$(p_i \cdot p_j) \equiv \int_{-\infty}^{\infty} dE\, n(E) p_i(E) p_j(E) \ .$$

Orthogonality means, due to (1) and (2),

$$p_{i+1}(E) = Ep_i(E) - a_{i+1}p_i(E) - b_i p_{i-1}(E) \ , \tag{11}$$

or, equivalently,

$$Ep_{i-1}(E) = p_i(E) + a_i p_{i-1}(E) + b_{i-1}p_{i-2}(E) \ . \tag{12}$$

From (11), orthogonality gives

$$b_i(p_{i-1}\cdot p_{i-1}) = (p_{i-1}\cdot Ep_i) = (Ep_{i-1}\cdot p_i) \ ,$$

and from (12) it gives

$$b_i(p_{i-1}\cdot p_{i-1}) = (p_i \cdot p_i) \ ,$$

thus, $b_i = \nu_i/\nu_{i-1}$. Similarly,

$$a_i(p_{i-1}\cdot p_{i-1}) = (p_{i-1}\cdot Ep_{i-1}) \ ,$$

so $a_i = \bar{\nu}_{i-1}/\nu_{i-1}$.

IV. APPLICATION

In the following I examine a model of a three-dimensional ordered alloy and apply the orthogonalized-moments method to calculate the LDOS $n^{(l)}(E)$ and the total DOS $N(E) = 1/N\sum_l n^{(l)}(E)$. Consider a simple cubic (sc) lattice with alternating A and B sites which form two interpenetrating fcc lattices. A model Hamiltonian for such a system is

$$\mathscr{H} = \sum_{k,\sigma} [\epsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \Delta c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\kappa,\sigma}] \ ,$$

with $c^\dagger_{\mathbf{k}\sigma}$ as electron creation operator, 2Δ as the on-site energy shift between A and B sites,

$$\epsilon(\mathbf{k}) = 2t(\cos k_x + \cos k_y + \cos k_z) \ ,$$

with t as the hopping matrix element between nearest neighbors and $\kappa = \pi(1,1,1)$. Diagonalization yields

$$\mathscr{H} = \sum_{k,\sigma} \tilde{\epsilon}(\mathbf{k}) \tilde{c}^\dagger_{\mathbf{k}\sigma} \tilde{c}_{\mathbf{k}\sigma}, \quad \tilde{\epsilon}(\mathbf{k}) = \mathrm{sgn}[\epsilon(\mathbf{k})]\sqrt{\Delta^2 + \epsilon^2(\mathbf{k})} \ .$$

This leads to a total DOS with an energy gap of width 2Δ centered around the origin and to square-root divergences at $\pm\Delta$. In the presence of an energy gap undamped oscillations of the coefficients occur.[7] To test the method I calculated 12 exact moments and truncated the expansion by use of a square-root terminator which takes these oscillations into account

$$\lim_{i\to\infty} a_i = a + \delta a(-1)^i, \quad \lim_{i\to\infty} b_i = b \ :$$

$$R_\infty(z) = \frac{1}{z - a - \delta a - \dfrac{b}{z - a + \delta a - bR_\infty(z)}} \ ,$$

$$R_\infty(z) = \frac{1}{2b}\left\{ z - a + \delta a + i\left[4b\frac{z-a+\delta a}{z-a-\delta a} - (z-a+\delta a)^2\right]^{1/2}\right\} \ .$$

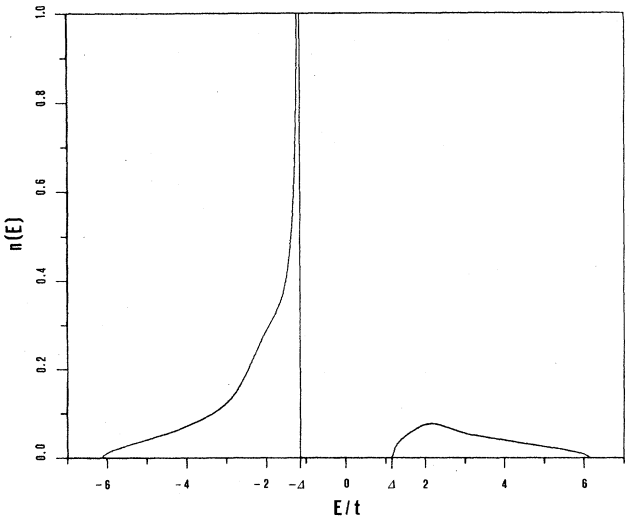


FIG. 1. LDOS calculated by the use of 12 exact moments with a square-root terminator taking into account undamped oscillations of the asymptotic coefficients.

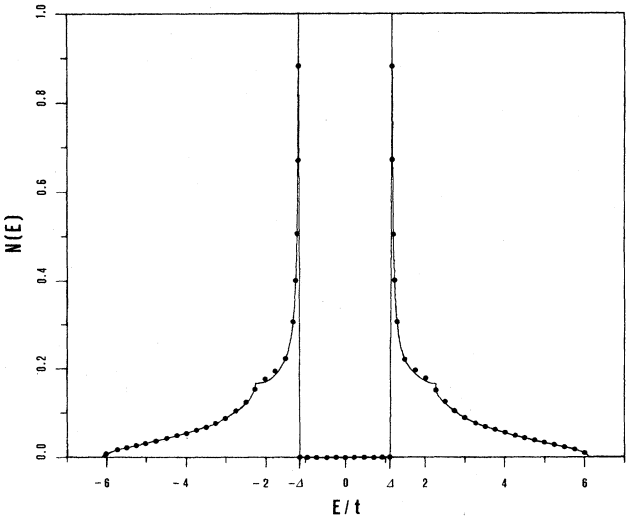


FIG. 2. Exact total DOS for the sc lattice in the presence of a gap. The dotted curve is the approximation by use of the orthogonalized-moments method.

Figure 1 shows the LDOS and Fig. 2 the total DOS. Also, Fig. 2 makes clear that the use of the orthogonalized-moments method reflects all important features of $N(E)$.

V. CONCLUSIONS

In this paper I have presented a simple and exact procedure to go from the power moments to the coefficients of the continued-fraction representation of the resolvent. This procedure was found to be numerically stable. The orthogonalized-moments method makes explicit the link between the moments method and the recursion method, which has been an important problem (e.g., the comments by Weaire[8]). It is equivalent to generating a set of orthogonal but not orthonormal basis vectors using the recursion method.

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APPENDIX

This Appendix is devoted to the analytic equivalence of the orthogonalized-moments method and the recursion method. The recursion method has been extensively discussed by Haydock.[1] Within this scheme the LDOS for a basis orbital $|u_0\rangle \equiv |O\rangle$ is determined by a sequence of environments described by orthonormal states $|u_i\rangle$, where $|u_i\rangle$ is a linear combination of basis orbitals $|l\rangle$. The $|u_i\rangle$ must satisfy the condition that

$$\mathscr{H}|u_i\rangle = A_i|u_i\rangle + B_{i+1}|u_{i+1}\rangle + B_i|u_{i-1}\rangle \ ,$$

where $\mathscr{H}$ is the Hamiltonian of the model. The parameters A_i and B_i describe the coupling of each environment to itself and its neighbors. Such a semi-infinite chain model[1] is equivalent to expressing the matrix of $\mathscr{H}$ as a tridiagonal matrix. One therefore can calculate the zero-zero element of the inverse of the matrix $(\mathscr{H}-E1)$ easily and one gets a J-fraction expansion for the resolvent. The corresponding coefficients are just the chain parameters.[1] Looking at eigenstates of a chain

$$H\sum_{i=0}^{\infty} P_i|u_i\rangle = E\sum_{i=0}^{\infty} P_i|u_i\rangle \ ,$$

one finds a three-term recurrence relation for the $\{P_i\}$:

$$EP_i = A_iP_i + B_{i+1}P_{i+1} + B_iP_{i-1} \ .$$

It is convenient to make the eigenstates have coefficient 1 on $|u_0\rangle$. This makes the $\{P_i\}$ a unique set of polynomials in E,

$$B_{i+1}P_{i+1}(E) = (E-A_i)P_i(E) - B_iP_{i-1}(E) \ ,$$

and

$$P_{-1}(E) \equiv 0, \quad P_0(E) \equiv 1 \ .$$

So, in both methods the fundamental concept is that of the polynomials determined by a three-term recurrence relation. For the chain, the polynomials are orthonormal and

$$R(z) = \frac{1}{z-A_0} - \frac{B_1^2}{z-A_1} - \frac{B_2^2}{z-A_2} - \cdots \ ,$$

$$B_{i+1}P_{i+1}(E) = (E-A_i)P_i(E) - B_iP_{i-1}(E) \ ,$$

$$\int_{-\infty}^{\infty} dE\, n(E)P_i(E)P_j(E) = \delta_{i,j} \ ,$$

$$A_i = \langle u_i|\mathscr{H}|u_i\rangle, \quad B_{i+1} = |(\mathscr{H}-A_i)|u_i\rangle - B_i|u_{i-1}\rangle| \ .$$

In the case of the orthogonalized moments the polynomials are orthogonal but not orthonormal. In this case

$$R(z) = \frac{1}{z-a_1} - \frac{b_1}{z-a_2} - \frac{b_2}{z-a_3} - \cdots \ ,$$

$$p_{i+1}(E) = (E-a_{i+1})p_i(E) - b_ip_{i-1}(E) \ ,$$

$$\int_{-\infty}^{\infty} dE\, n(E)p_i(E)p_j(E) = \delta_{i,j}\nu_i \ ,$$

$$a_i = \frac{\overline{\nu}_{i-1}}{\nu_{i-1}}, \quad b_i = \frac{\nu_i}{\nu_{i-1}} \ .$$

The construction of a chain model is based on a starting vector $|u_0\rangle$ upon which one repeatedly operates with $\mathscr{H}$. Since the chain model is just the representation of $\mathscr{H}$ in terms of a different basis, one can relate the moments to the chain parameters. The recursion method is analytically equivalent to computing orthogonalized moments.

This also makes clear that the stability of the orthogonalized-moments method is the same as that of the recursion method, which has been discussed previously.[1]

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