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Estimation of integrals with respect to a density of states

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Abstract. A method is presented for estimating definite and indefinite integrals over a density function, such as a local density of states, defined by a three-term recurrence relation. This may be generated, for example, by the 'recursion method' applied to some Hamiltonian, and properties of the approximation are given, and the results derived, in that context.

1. Introduction

In this paper we describe a method for estimating integrals over the density function ('density of states') obtained from an operator using the recursion method (Haydock *et al* 1972). The results are essentially those known already for the classical moment problem (see Akhiezer 1965), but reformulated so as to be applicable directly to the tridiagonalisation of an operator, and extended to include non-positive functions. We derive expressions involving only the recursion coefficients, and obtain these directly, rather than using the theory of moments and its consequent numerical problems. We present the results for the general (two-sided) method and indicate the simplifications that occur when the operator is Hermitian and the density of states is positive.

We first briefly describe the recursion method and show the relationship of the coefficients in the tridiagonalisation to the local density of states. We then indicate how the definite and indefinite integrals over this function may be estimated, indicating the relationship of these results to those known for the corresponding moment problem (for the equivalence of these see e.g. Akhiezer 1965). We finally comment on the use of this method and give a simple example as an illustration.

2. The recursion method

The general recursion method associated with the real eigenproblem

$$H\Psi_i = E_i\Psi_i \tag{1a}$$

$$H^\dagger\Phi_i = E_i\Phi_i \tag{1b}$$

may be stated as follows.

Given 'starting' vectors $\tilde{\psi}_0$ and $\tilde{\phi}_0$ define

$$\tilde{\psi}_{n+1} = b_{n+1}^{1/2}\psi_{n+1} = (H - a_n)\psi_n - b_n b_n^{-1/2}\psi_{n-1} \tag{2a}$$

and

$$\tilde{\phi}_{n+1} = b_{n+1} b_{n+1}^{-1/2} \phi_{n+1} = (H^{\dagger} - a_n)\phi_n - b_n^{1/2} \phi_{n-1} \tag{2b}$$

where initially $\psi_0 = b_0^{-1/2} \tilde{\psi}_0$; $\phi_0 = b_0^{1/2} b_0^{-1} \tilde{\phi}_0$; $\phi_{-1} = \psi_{-1} = 0$ ($b^{1/2}$ is taken to mean $|b|^{1/2}$ here and throughout the paper). The coefficients in the recurrence are computed from

$$a_n = \langle \phi_n, H\psi_n \rangle \tag{3a}$$

$$b_n = \langle \tilde{\phi}_n, \tilde{\psi}_n \rangle \tag{3b}$$

where $\langle \cdot, \cdot \rangle$ denotes the usual inner product.

This is the recursion method as defined in Haydock (1977) and in the closely related Lanczos method (see e.g. Wilkinson 1965), particularly as formulated in Paige (1972) for the symmetric case $H = H^{\dagger}$. In the latter case if $\tilde{\phi}_0 = \tilde{\psi}_0$ then $\psi_n = \phi_n$ and $b_n > 0$ for all n. A consequence of this construction is the bi-orthogonality of the vectors $\{\phi_n\}$ and $\{\psi_m\}$:

$$\langle \phi_n, \psi_m \rangle = \delta_{nm}. \tag{4a}$$

3. The local density of states

A subset of the eigenvectors of H and the vectors generated in the recursion method form alternative bases for the subspace generated by H and the starting vectors. We assume also that the eigenvectors of H satisfy the orthogonality condition:

$$\langle \Phi_n, \Psi_m \rangle = \delta_{nm}. \tag{4b}$$

We may thus make the expansions

$$\tilde{\psi}_0 = \sum_i \alpha_i \Psi_i \tag{5a}$$

$$\tilde{\phi}_0 = \sum_j \beta_j \Phi_j \tag{5b}$$

and define the local density function as

$$n(E) = \sum_i \alpha_i \beta_i \delta(E - E_i)$$

where the $\{E_i\}$ are the eigenvalues of the operator H.

If we truncate H in a suitable way to an $N \times N$ matrix, we may define a density function

$$n^N(E) = \sum_{i=1}^{N} \alpha_i^N \beta_i^N \delta(E - E_i^N) \tag{6}$$

in a corresponding way. Then, in the sense of integrals over the density function, we may say

$$\lim_{N \to \infty} n^N(E) = n(E).$$

If H is a symmetric Hamiltonian and $\tilde{\phi}_0 = \tilde{\psi}_0$ then $n(E)$ is the local density of states of interest in many applications of the recursion method (Haydock *et al* 1972):

$$n(E)=\sum_i \alpha_i^2\delta(E-E_i)$$

and integrals with respect to $n(E)$, both definite and indefinite are required.

4. Definite integrals over the density function

In this section we derive a method of estimating the integral

$$\int_{-\infty}^{\infty} f(E)n(E)\,\mathrm{d}E$$

for suitable functions $f(E)$, from the tridiagonalisation coefficients obtained in the recursion method. We do this by obtaining expressions for $\alpha_i^N\beta_i^N$ in the definition of the density function.

As the recursion method constructs a set of vectors spanning the subspace generated by the starting vectors and H, we may expand the eigenvectors of H in that subspace in terms of the tridiagonal basis and write it in the form:

$$\Psi_i=v(E_i)\sum_m p_m(E_i)\psi_m \tag{7a}$$

$$\Phi_i=w(E_i)\sum_n q_n(E_i)\phi_n. \tag{7b}$$

By substituting these expressions into equations (1) and using the definition of the recursion (2), it is straightforward to show, using the bi-orthogonality of $\{\psi_m\}$ and $\{\phi_n\}$, that

$$b_{k+1}b_{k+1}^{-1/2}p_{k+1}(E)=(E-a_k)p_k(E)-b_k^{1/2}p_{k-1}(E) \tag{8a}$$

$$b_{k+1}^{1/2}q_{k+1}(E)=(E-a_k)q_k(E)-b_kb_k^{-1/2}q_{k-1}(E) \tag{8b}$$

with $q_0=b_0^{-1/2}$, $p_0=b_0^{1/2}b_0^{-1}$, and $p_{-1}=0=q_{-1}$. From the normalisation of the eigenfunctions $(4b)$ it may be seen that

$$v(E_i)w(E_i)=\left(\sum_l p_l(E_i)q_l(E_i)\right)^{-1}. \tag{9}$$

By taking inner products of the expansions (5) with the appropriate eigenvector and substituting in equation (7) we obtain

$$\alpha_k=w(E_k) \tag{10a}$$

$$\beta_k=v(E_k). \tag{10b}$$

Hence we obtain the desired result:

$$n^N(E)=\sum_i \alpha_i^N\beta_i^N\delta(E-E_i^N) \tag{11}$$

where

$$\alpha_i^N\beta_i^N=\left(\sum_{l=0}^{N} p_l(E_i^N)q_l(E_i^N)\right)^{-1}.$$

The $\{E_i^N\}$ are the eigenvalues of H truncated by terminating the tridiagonalisation at N 'levels', or in other words, the eigenvalues of the tridagonal matrix T, where

$$T = \begin{bmatrix} a_0 & b_1 & & & \\ 1 & a_1 & b_2 & & \\ & 1 & a_2 & b_3 & \\ & & \cdot & \cdot & \cdot \end{bmatrix}.$$

If the $b_n > 0$ ($H^\dagger = H$) the matrix

$$\begin{bmatrix} a_0 & b_1^{1/2} & & & \\ b_1^{1/2} & a_1 & b_2^{1/2} & & \\ & b_2^{1/2} & a_2 & b_3^{1/2} & \\ & & \cdot & \cdot & \cdot \end{bmatrix}$$

also has eigenvalues E_i^N and is more appropriate computationally. The E_i^N may be readily found using the QR algorithm (Wilkinson 1965) or, in the symmetric case, by use of the Sturm sequence property of such matrices. This now provides us with a method of estimating integrals:

$$\int f(E) n(E)\, \mathrm{d}E \simeq \int f(E) n^N(E)\, \mathrm{d}E = \sum_{i=1}^{N} f(E_i^N) w_i^N \tag{12a}$$

where

$$w_i^N = \alpha_i^N \beta_i^N = \left(\sum_{l=0}^{N} p_l(E_i^N) q_l(E_i^N) \right)^{-1}. \tag{12b}$$

In the symmetric case this is the well known (see e.g. Akhiezer 1965) result of Gaussian quadrature, with

$$w_i^N = \left(\sum_{l=0}^{N} p_l^2(E_i^N) \right)^{-1}.$$

5. Properties of the integral approximation

Here we derive directly properties corresponding to the usual results for Gaussian quadrature, but which do not depend on a positive weight function.

Evidently the $p_n(E)$ and $q_n(E)$ are polynomials in E of degree n, and from the bi-orthogonality (4a) of the tridiagonal basis it may be seen that the polynomials satisfy the orthogonality relationship

$$\sum_{i=1}^{N} \alpha_i^N \beta_i^N p_m(E_i^N) q_n(E_i^N) = \delta_{mn}$$

for $\forall$ with $m, n < N$, and thus in the limit $N \to \infty$

$$\int p_m(E) q_n(E) n(E)\, \mathrm{d}E = \delta_{mn}.$$

A consequence of this (see appendix 1 for the method of proof) is that the approximate quadrature (12) is exact when the integrand $f(E)$ is a polynomial of degree less than or equal to $2N - 1$.

The correspondence to orthogonal families of polynomials is general and we may write (see e.g. Cheney 1966):

$$a_n = \int Ep_n(E)q_n(E)n(E)\,\mathrm{d}E, \tag{12c}$$

$$b_n^{1/2} = \int Ep_n(E)q_{n-1}(E)n(E)\,\mathrm{d}E. \tag{12d}$$

6. Practical computation of the integration formula

The expression (12*b*) for the weights in the integration formula is rather sensitive to the precision of the roots $\{E_i^N\}$ of $p_N(E)$ (equivalent to the eigenvalues of the tridiagonal matrix); we therefore give an alternative expression for them. This is given in Cheney (1966) for Gaussian quadrature corresponding to our symmetric case, but it is possible to derive it directly in the context of the general recursion method (see appendix 2). We find

$$\alpha_i^N\beta_i^N = \left(\sum_{l=0}^{N} p_l(E_i^N)q_l(E_i^N)\right)^{-1} = r_{N-1}(E_i^N)/p'_N(E_i^N) \tag{13}$$

where $r_N(E)$ is a polynomial of degree N satisfying the recurrence relation

$$b_{k+1}b_{k+1}^{-1/2}r_k(E) = (E-a_k)r_{k-1}(E) - b_k^{1/2}r_{k-2}(E) \tag{14}$$

with the initial conditions $r_0 = (b_0b_1)^{1/2}b_1^{-1}$, $r_{-1} = 0$.

7. Indefinite integrals of the local density of states

In the following sections we restrict our attention to positive density functions and the symmetric recursion method. Thus all eigenvalues $\{E_i^N\}$ are real and $b_i > 0$ for all i and N. We will generalise the method of the preceding sections in a way which corresponds to the solution of the classical moment problem (Akhiezer 1965), but which does not involve a direct knowledge of the moments.

To estimate the indefinite integral

$$\int^{E^*} f(E)n(E)\,\mathrm{d}E$$

we force a quadrature node to be at $E = E^*$ (in other words postulate an eigenvalue of H is E^*) and examine the consequence.

We assume that the recursion method has been applied to H, and we know b_0 and $\{a_i, b_i; i = 0, \ldots, N-1\}$. If we now define

$$a_N^* = E^* - b_N^{1/2}\frac{p_{N-1}(E^*)}{p_N(E^*)} \tag{15}$$

and use superscript * to denote the modified functions, we obtain $b_{N+1}^{1/2}p_{N+1}^*(E)$ by recurrence such that $p_{N+1}^*(E^*) = 0$, and we may proceed with the quadrature as before. We obtain an estimate of the indefinite integral by taking as integrand $f^*(E)$

the function

$$f^*(E)=\begin{cases} f(E); & E<E^* \\ \tfrac{1}{2}f(E); & E=E^* \\ 0; & E>E^*. \end{cases}$$

Then, writing $E_L^* = E^*$, the indefinite integral is estimated as

$$\int^{E^*} f(E)n(E)\,\mathrm{d}E \simeq \sum_{i=1}^{L} \alpha_i^*\beta_i^* f(E_i^*) - \tfrac{1}{2}\alpha_L^*\beta_L^* f(E_L^*). \tag{16}$$

It may be seen (see appendix 3) that the definite quadrature obtained by using (16) over the whole range is exact for $f(E)$ a polynomial of degree less than or equal to $2N$. This demonstrates that the restriction of one eigenvalue of H to a specific value does not adversely affect the estimation of the moments of the calculated density function and, together with the positivity of $\alpha_i\beta_i$, leads to the well known moment problem result (Akhiezer 1965) giving the bounds:

$$\sum_{i=1}^{L-1} \alpha_i^*\beta_i^* \leqslant \int^{E^*} n(E)\,\mathrm{d}E \leqslant \sum_{i=1}^{L} \alpha_i^*\beta_i^*. \tag{17}$$

This may be seen by constructing two polynomials $p^+(E)$ and $p^-(E)$ of degree $2N$ (which are integrated exactly) which bound the unit step function $H(E^*-E)$ above and below. These have the defining conditions

$$p^{\pm}(E_i^*)=1, \quad i<L; \qquad p^{\pm}(E_i^*)=0, \quad i>L; \qquad p^{\pm\prime}(E_i^*)=0, \quad i\neq L$$
$$p^+(E^*)=1; \qquad p^-(E^*)=0.$$

8. The density of states

While for quantitative work it is almost always appropriate to use the integration formulae (13) or (16), it is sometimes useful for comparisons to be able to estimate the density of states itself. The approximation we have made to the integrated density function is differentiable, although the density of states is not necessarily so and we do not demand that it is for the quadrature formula. Nevertheless we obtain a useful indication of the density of states by differentiating our approximation to obtain

$$n(E)\simeq\tilde{n}(E)=\sum_{i=1}^{L}\frac{\mathrm{d}w_i}{\mathrm{d}E}-\frac{1}{2}\frac{\mathrm{d}w_L}{\mathrm{d}E}. \tag{18}$$

It should be noted that the approximation does not satisfy some usual properties of analytic functions, as it is strictly a pointwise approximation to the integrated density of states. Thus if

$$\epsilon(E)=\int^{E} en(e)\,\mathrm{d}e \qquad \text{and} \qquad N(E)=\int^{E} n(e)\,\mathrm{d}e$$

and $\tilde{\epsilon}$ and $\tilde{N}$ are our approximations to those functions (via equations (13) and (16)) we have

$$\frac{\mathrm{d}\epsilon(E)}{\mathrm{d}E}=En(E), \qquad \text{but} \qquad \frac{\mathrm{d}\tilde{\epsilon}(E)}{\mathrm{d}E}\neq E\tilde{n}(E).$$

It should be emphasised that the quantitative work is best done with the integration formulae which do possess useful convergence properties.

9. Application of the method

To illustrate the use of the method, we apply it here to the density function $n(E)=(1-E^2)^{1/2}$ for $-1 \leqslant E \leqslant 1$ for which the recursion coefficients are

$$a_i = 0, \qquad b_i = \tfrac{1}{2}; \qquad i \neq 0 \text{ and } b_0 = \pi/2.$$

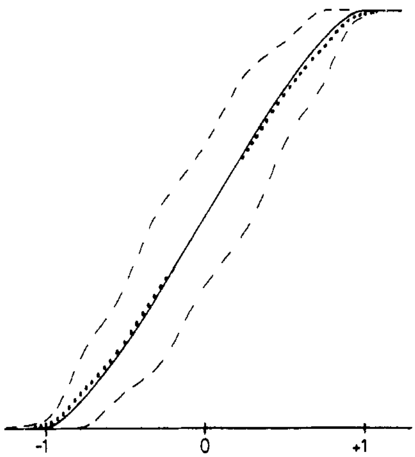

Figure 1. The integrated density of states: full curve, the analytic function $\int_{-1}^{E} (1-e^2)^{1/2}\, de$; broken curve, the computed bounds for $N = 4$; dotted curve, the approximate function for $N = 4$.

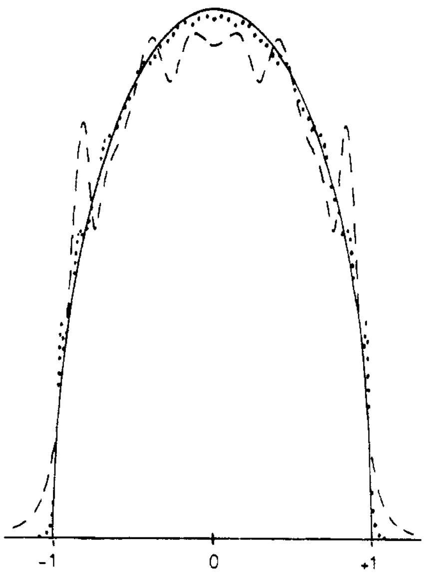

Figure 2. The density of states: full curve, the analytic function $(1-E^2)^{1/2}$; broken curve, approximations with $N = 4$; dotted curve, $N = 10$.

The graph of figure 1 shows the bounds (17) and the approximation (15) to the integrated density of states for $N = 5$ and those of figure 2 provide a comparison of $n(E)$ and $\tilde{n}(E)$ (from equation (18)) for various N. It will be noticed that the error in the integrated density of states is considerably less than the width of the bounds might suggest, and in practice this is generally true, as the bounds are rigorous mathematical extrema. As the number of levels increases, both approximations tend to the respective analytic functions, as may be seen by considering the width of the bounds (17) for the integrated density of states.

10. Conclusions

We have here given a direct formulation of a method of obtaining the integrated density of states, and related functions of interest, from the recursion method of Haydock *et al* (1972). It is readily computable and provides a useful tool in the application of their ideas, and has already been used in several such applications (Gallagher and Haydock 1977, Meek 1976, Terakura 1978).

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Appendix 1. The definite quadrature

In this section we present a method of proof that the quadrature (12) is exact for polynomials of degree less than or equal to $2N-1$. We first show the exactness for polynomials of degree less than N and then extend this to the desired result, after initially making some remarks on the orthogonality of the polynomials $\{q_n(E)\}$ and $\{p_n(E)\}$.

Evidently

$$\psi_n = q_n(H)\tilde{\psi}_0 \qquad \text{and} \qquad \phi_m = p_m(H^\dagger)\tilde{\phi}_0. \tag{A.1}$$

Substituting these identities into the orthogonality relation (4*a*) of the tridiagonal basis and using the expansion (5) of $\tilde{\psi}_0$ and $\tilde{\phi}_0$ in terms of the eigenfunctions $\{\Psi_i\}$ and $\{\Phi_j\}$ leads to the polynomial orthogonality:

$$\sum_{i=1}^{N} \alpha_i^N \beta_i^N p_m(E_i^N) q_n(E_i^N) = \delta_{mn} \tag{A.2}$$

for $m, n < N$; and in the limit $N \to \infty$

$$\int p_m(E) q_n(E) n(E)\, \mathrm{d}E = \delta_{mn}. \tag{A.3}$$

Any polynomial $f_n(E)$, of degree $n < N$, may be written as a linear combination of the $\{p_j(E)\}$:

$$f_n(E) = \sum_{j=0}^{n} \gamma_j p_j(E)$$

and from the orthogonalities (A.2) and (A.3)

$$q_0 \int f_n(E) n(E)\,\mathrm{d}E = \gamma_0 = \sum_{i=1}^{N} \alpha_i^N \beta_i^N f_n(E_i^N)$$

which proves the exactness of the quadrature (12) for polynomials of degree less than N.

To extend this result to polynomials f_n of degree $n \leq 2N-1$, it is only necessary to note that we may write

$$f_n(E) = p_N(E) s(E) + r(E)$$

where r and s are polynomials of degree at most $N-1$. Then, from the orthogonality of p_N to all polynomials of degree less than N, it follows that

$$\int f_n(E) n(E)\,\mathrm{d}E = \int r(e) n(E)\,\mathrm{d}E$$

and, as $p_N(E_i^N) = 0$, that:

$$\sum_{i=1}^{N} \alpha_i^N \beta_i^N f_n(E_i^N) = \sum_{i=1}^{N} \alpha_i^N \beta_i^N r(E_i^N).$$

As r is a polynomial of degree less than N, the integral and sum give the same value, and the desired result is obtained.

Appendix 2. Computation of the weights

The formula (13) for the weights, using the recurrence (14), results from a generalisation of the Christoffel–Darboux formula, and also from an integral identity for the polynomials $\{r_n(E)\}$. We first state these two results and then apply them in deriving the expression (13).

A.2.1. The generalised Christoffel–Darboux identity

$$\sum_{i=0}^{n} p_i(x) q_i(y) = \frac{b_{n+1} p_{n+1}(x) q_n(y) - |b_{n+1}| q_{n+1}(y) p_n(x)}{b_{n+1}^{1/2}(x-y)}. \qquad \text{(A.4)}$$

This identity may be proved by induction, using the recurrence relation (8) to substitute into the right-hand side of (A.4). The special case $x = y$ leads to the corollary

$$\sum_{i=0}^{n} p_i(x) q_i(x) = \frac{1}{b_{n+1}^{1/2}} (b_{n+1} p'_{n+1}(x) q_n(x) - |b_{n+1}| p'_n(x) q_{n+1}(x)) \qquad \text{(A.5)}$$

where $p'_n(x)$ is the derivative of $p_n(x)$ with respect to x.

A.2.2. An integral identity

If we define

$$r_k(x)=\int \frac{p_{k+1}(t)-p_{k+1}(x)}{t-x}n(t)\,\mathrm{d}t \tag{A.6}$$

where $\{p_k\}$ are the polynomials defined earlier (8*a*), then obviously

$$r_{-1}=0 \qquad \text{and} \qquad r_0=(b_0b_1)^{1/2}/b_1$$

and if we substitute the recurrence (8*a*) for p_{k+1} we obtain the recurrence (14) for $r_k(x)$.

A.2.3. The expression for the weights

The identity (A.5) may be substituted into the expression (12*b*) for the weights and, noting that $p_N(E_i^N)=0=q_N(E_i^N)$, we obtain

$$w_i^N=\alpha_i^N\beta_i^N=\left(\sum_{j=0}^{N-1} p_j(E_i^N)q_j(E_i^N)\right)^{-1}=\frac{b_N^{1/2}}{b_Np'_N(E_i^N)q_{N-1}(E_i^N)}. \tag{A.7}$$

We now use the integral identity (A.6) to show that

$$\frac{b_N^{1/2}}{b_Nq_{N-1}(E_i^N)}=r_{N-1}(E_i^N). \tag{A.8}$$

From (A.6) we see that

$$r_{N-1}(E_i^N)=\int \frac{p_N(t)}{t-E_i^N}n(t)\,\mathrm{d}t \tag{A.9}$$

and, putting $y=E_i^N$ and $x=t$ in (A.4), we obtain

$$\frac{b_Nq_{N-1}(E_i^N)}{b_N^{1/2}}\frac{p_N(t)}{t-E_i^N}=\sum_{j=0}^{N-1} p_j(t)q_j(E_i^N).$$

Using this to substitute into (A.9) for $p_N(t)$ gives

$$r_{N-1}(E_i^N)=\frac{b_N^{1/2}}{b_Nq_{N-1}}(E_i^N)\sum_{j=0}^{N-1} q_j(E_i^N)\int p_j(t)n(t)\,\mathrm{d}t.$$

This, by the orthogonality of $\{p_m\}$, reduces to (A.8), which in turn may be substituted into (A.7) to give the result:

$$w_i^N=\frac{r_{N-1}(E_i^N)}{p'_N(E_i^N)}.$$

Appendix 3. The indefinite quadrature

The exactness of the quadrature (16), taking the integral over the whole range:

$$\int f(E)n(E)\,\mathrm{d}E=\sum_{i=1}^{N+1}\alpha_i^*\beta_i^*f(E_i^*) \tag{A.10}$$

may be deduced in a similar manner to that of appendix 1 for the definite quadrature. We first prove the result for polynomials of degree equal to or less than N, and then extend it to those of degree less than or equal to $2N$. Taking the expression for p^*_{N+1}

$$\frac{b_{N+1}}{b^{1/2}_{N+1}} p^*_{N+1}(E) = (E - a^*_N) p_N(E) - b_N^{1/2} p_{N-1}(E),$$

we observe that p^*_{N+1} is orthogonal to q_k for $k \leq N-1$. The case of $k = N-1$ follows from the knowledge of b_N. As in § 5 the polynomials also satisfy the summation orthogonality and consequently (as in appendix 1), the quadrature (A.10) is exact for $f(E)$ a polynomial of degree less than or equal to N. Again if f is now a polynomial of degree less than or equal to $2N$ we may write

$$f(E) = p^*_{N+1}(E)s(E) + r(E),$$

where s is a polynomial of degree less than or equal to $N-1$ and r of degree less than or equal to N. From the exactness of (A.10) for polynomials of degree less than or equal to N and the orthogonality (with respect to integrals over $n(E)$) we may deduce the exactness of (A.10) for $f(E)$ a polynomial of degree less than or equal to $2N$.

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