Modified-Moments Method: Applications to Harmonic Solids*

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Appropriately chosen modified moments of the frequency distribution provide valuable information about harmonic solids. They contain the same information as exact power moments but much more efficiently. They stably determine quadrature formulas which have been shown to give thermal and dynamic properties of harmonic solids with great accuracy. They can be calculated either directly or from exact power moments when these are available. In this paper we give the motivation for a particularly suitable choice of modified moments for harmonic solids and show how the modified moments can be obtained from exact power moments for solids with finite-ranged forces. The modified moments can be stably transformed to power moments and to other choices of modified moments by methods which are described. We show how these transformations can be used to obtain the recursion coefficients of the orthogonal polynomials defined by the frequency distribution. We use the recursion coefficients to obtain the various Gaussian-quadrature formulas of use in the harmonic-solid problem. The transformation from modified moments to quadrature formulas is extremely stable, in striking contrast to the behavior encountered with power moments for which the transformation is exponentially ill conditioned. A particularly useful feature of the modified-moments method for harmonic solids is that *additional information* about the form of the spectral density function can be incorporated in order to improve the accuracy of averages of singular functions without loss of stability. We illustrate this feature of the method by presenting new results for singular averages such as inverse-power moments.

I. INTRODUCTION

Gaussian-quadrature techniques have been shown to be a powerful and practical tool for obtaining very accurate approximations to weighted averages

$$\langle F(\tau, x)\rangle = \int F(\tau, x)G(x)\,dx \tag{1.1}$$

of a known function $F(\tau, x)$ over an unknown nonnegative weight function $G(x)$, provided that a limited number of power moments $\mu_k = \langle x^k\rangle$ of the weight function are known.[1] Such averages and unknown weight functions arise frequently in theoretical chemistry and physics, and these and related techniques have been applied successfully to a variety of problems.[2-14] In particular, thermal and dynamic properties of crystalline solids in the harmonic approximation can be expressed as weighted averages over an unknown frequency distribution. Substantial numbers of power moments of the frequency distributions for a variety of model solids are available.[15-20] Wheeler and Gordon[10,11] have shown that Gaussian quadratures are capable of producing extremely precise upper and lower bounds for thermodynamic properties of simple three-dimensional harmonic solids from these moments.

The approximations are obtained by replacing the integral in (1.1) with a weighted sum and an error term,

$$\langle F(\tau, x)\rangle = \sum_{i=1}^{n} w_i F(\tau, x_i) + \Delta\ , \tag{1.2}$$

where the abscissas x_i and weights w_i are determined by the requirement that they give a specified number $N(n)$ of moments correctly. That is,

$$\sum_{i=1}^{n} w_i x_i^k = \mu_k\ ,\quad k = 0, 1, \ldots, N(n)\ . \tag{1.3}$$

The form of the error, Δ, made in such quadratures is known and, for a certain class of functions $F(\tau, x)$, is of known sign for all $\tau > 0$.[10] By an appropriate choice of quadrature formulas, two approximations with errors of opposite sign may be obtained. This provides upper and lower bounds to the average.

A serious limitation to these quadrature techniques is that the determination of the abscissas and weights of the quadrature formulas from the power moments is generally exponentially ill conditioned. Double-precision or, if a large number of moments is known, multiple-precision arithmetic must be used in the computations, and the moments themselves must be known exactly or with extremely high precision.

Recently, Sack and Donovan[21] and Gautschi[22] have observed that if, instead of the power moments μ_k, one knows *modified moments* $\nu_k = \langle p_k\rangle$, where the $p_k(x)$ are polynomials of degree k orthogonal with respect to some weight function $H(x)$, distinct

from but defined on the same interval as $G(x)$, then the problem of determining the quadrature formulas may be very well conditioned. In this case, however, the transformation from the μ_k to the ν_k is generally ill conditioned.

In this paper we reexamine the harmonic-solid problem in the light of this new development. We show that for simple harmonic solids a particularly suitable choice of modified moments can be found, such that the transformation to the abscissas and weights is extremely well conditioned, while, simultaneously, the ill-conditioned transformation from the power moments to the modified moments is easily accomplished with no loss of information. In addition, these modified moments can be computed directly for simple harmonic solids without recourse to the power moments. We have shown this elsewhere.[23] Here we give procedures for transforming from the exact power moments, when they are known, to exact modified moments and show how modified moments can be used to determine accurate thermodynamic properties for harmonic solids.

In Sec. II we motivate our choice of modified moments and show how they can be obtained exactly from power moments in the case of simple harmonic solids with nearest-neighbor force constants. We compare the power moments and modified moments for nearest-neighbor cubic-close-packed and hexagonal-close-packed solids, and give a procedure for transforming modified moments back to power moments and to other choices of modified moments.

In Sec. III we outline the transformation from the modified moments to the recursion coefficients α_k, β_k of the polynomials $\pi_k(x)$ orthogonal with respect to $G(x)$, and then to the abscissas and weights of quadrature formulas. When, as is the case for harmonic solids, $G(x)$ is nonzero on only a finite interval, it is useful to employ four distinct quadrature formulas in which zero, one, or two abscissas are fixed at the ends of the interval.[10,11] By the methods outlined in Sec. III and detailed in the Appendix, we show how all four of these quadratures can be obtained directly from the recursion coefficients α_k, β_k. This represents a significant improvement over the methods employed by Wheeler and Gordon in which "shifted moments" were used to obtain two of the quadratures. We also examine in Sec. III the stability of the transformations from modified moments to recursion coefficients and then to abscissas and weights. We find that they are remarkably stable, there being virtually no buildup of error either in the recursion coefficients or in the abscissas and weights, even when limited-precision arithmetic is used.

For harmonic solids with nearest-neighbor central forces the moments can be expressed exactly as integers by a suitable change of scale. For longer- but finite-ranged forces and noncentral forces the moments can be expressed as polynomials (or multinomials) in the force-constant ratios with integer coefficients. A substantial number of such moments are becoming available.[17,18] In Sec. IV we show how such polynomial power moments can be transformed exactly to polynomial modified moments. The stability of the transformations from these modified moments to the recursion coefficients and the abscissas and weights is examined. We find, again, that once the modified moments are known to a given accuracy, the abscissas and weights are determined to essentially the same accuracy regardless of the choice of force-constant ratios.

The quadrature methods developed by Wheeler and Gordon for harmonic solids were greatly strengthened by the incorporation of *additional information* about the weight function $G(x)$ in the form of series expansion coefficients for $G(x)$ at $x=0$. In Sec. V we show how additional information about the density function, such as bounds to series expansion coefficients for $G(x)$ or even simply knowledge of the *functional form* of $G(x)$ at some point, can be used with modified moments to obtain improved estimates for averages. We also present some new results on inverse-power moments for harmonic solids to illustrate the power of this technique.

In Sec. VI we summarize the advantages of the modified-moments technique and indicate some of the possibilities for its further development.

II. MODIFIED MOMENTS

It is easy to see qualitatively why the transformation from the power moments to the abscissas and weights of the quadrature formulas is so ill conditioned. The function x^n [which, averaged over $G(x)$, is the moment μ_n] weights large values of x more and more heavily as n increases. If $G(x)$ is nonzero only on a finite interval, say, $[0,1]$, then for large n the most significant figures in μ_n describe the behavior of $G(x)$ very near $x=1$, while information about $G(x)$ on the rest of the interval is hidden in the less significant figures. The abscissas and weights, on the other hand, are sensitively related to the behavior of $G(x)$ on the entire interval and thus depend upon the information which lies in these less significant figures of μ_n.

It might be expected that averages of polynomials, appropriately chosen to sample the entire interval, would determine quadrature formulas more stably. In this section we introduce such polynomials and show how their averages can be determined from the power moments of harmonic solids with nearest-neighbor central forces.

A. Choice of Modified Moments

Any non-negative weight function $G(x)$ uniquely defines a set of (monic) orthogonal polynomials $\pi_k(x)$, $k=0, 1, 2, \cdots$:

$$\langle \pi_k \pi_l \rangle \equiv \int \pi_k(x)\pi_l(x)G(x)\,dx = \delta_{lk}\langle \pi_k \pi_k \rangle , \qquad (2.1)$$

which satisfies a three-term recursion relation of the form

$$\pi_{k+1}(x) = (x-\alpha_k)\pi_k(x) - \beta_k \pi_{k-1}(x) \quad (\pi_0 \equiv 1,\ \pi_{-1} \equiv 0) . \qquad (2.2)$$

These orthogonal polynomials sample the entire interval, and the quadratures can be determined stably when they are known (Sec. III). Unfortunately, the orthogonal polynomials cannot be determined stably directly from the power moments. They do suggest a form for other polynomials which sample the entire interval.

If we could find a *known* weight function $H(x)$ with the properties that it is nonzero on the same interval as $G(x)$, that it is, in some sense, similar to $G(x)$, and that its own orthogonal polynomials $p_k(x)$ are known, then we would expect the "modified moments"

$$\nu_n = \langle p_n(x) \rangle = \int G(x)p_n(x)\,dx , \quad n=0,1,2,\cdots \qquad (2.3)$$

to be much more sensitive to the behavior of $G(x)$ than the corresponding power moments and to determine the quadrature formulas stably. This is the motivation for the introduction of modified moments. These expectations have been justified theoretically[22] and found to be borne out in practice with classical weight functions.[21,22] For physical applications, where $G(x)$ is unknown, there remains one problem: the polynomials p_k must be chosen so that the (ill-conditioned) transformation from power moments to modified moments can be accomplished accurately.

The distribution function for a harmonic solid in three dimensions is known to vary proportionally to $x^{1/2}$ near $x=0$ and to $(1-x)^{1/2}$ near $x=1$.[24] The weight function

$$H(x) = (8/\pi)[x(1-x)]^{1/2} \qquad (2.4)$$

has these properties and, in addition, the important advantage that the recursion coefficients a_n and b_n for *its* orthogonal polynomials $p_n(x)$ are constants, independent of n:

$$p_{n+1}(x) = (x-a_n)p_n(x) - b_n p_{n-1}(x) \qquad (a_n = \tfrac{1}{2},\ b_n = \tfrac{1}{16}) . \qquad (2.5)$$

The polynomials p_n are shifted Chebyshev polynomials of the second kind,[25] and the power moments of $H(x)$ are given by

$$\mu_n = 8\,\frac{(2n+1)!!}{(2n+4)!!} , \quad n=0,1,2,\cdots . \qquad (2.6)$$

The moments of this distribution function are, in fact, similar to those for harmonic solids. In Table I we compare several power moments of $H(x)$ with those for the cubic-close-packed (ccp) and hexagonal-close-packed (hcp) harmonic solids with nearest-neighbor radial force constants only.

It is a feature of harmonic crystals with only one force constant that the moments can be expressed exactly as integers by a suitable change of scale. For example, the moments μ_n of the ccp solid in Table I become integers when multiplied by 16^n. This corresponds to a change of scale in the variable x by a factor of 16, so that $G(x)$ becomes nonzero on the interval $[0,16]$. The corresponding scale change applied to the weight function (2.4) has the result that the recursion coefficients also become integers: $a_n = 8$ and $b_n = 16$. For the hcp solid the appropriate scale factor is 48, with corresponding recursion coefficients $a_n = 24$ and $b_n = 144$. In general, for our choice of $H(x)$, if the interval is scaled to $[0, L]$, then

$$a_n = \tfrac{1}{2}L , \quad b_n = (\tfrac{1}{4}L)^2 . \qquad (2.5a)$$

B. Transformation from Power Moments to Modified Moments

The modified moments can be determined from the power moments as follows. Consider the matrix $\underline{Y}$ with elements

$$Y_{kl} = \langle p_k(x)x^l \rangle , \quad k,l = 0,1,2,\cdots . \qquad (2.7)$$

The first row of $\underline{Y}$ consists of the power moments; the first column consists of the modified moments:

$$\begin{aligned} Y_{0,l} &= \langle x^l \rangle = \mu_l , \quad l=0,1,2,\cdots , \\ Y_{k,0} &= \langle p_k(x) \rangle = \nu_k , \quad k=0,1,2,\cdots . \end{aligned} \qquad (2.8)$$

Given the first row of $\underline{Y}$, the remaining rows can be determined by using the recursion relation (2.5) for the polynomials p_n to obtain the equation

$$Y_{k+1,l} = Y_{k,l+1} - a_k Y_{k,l} - b_k Y_{k-1,l} \quad (Y_{0,l} = \mu_l ,\ Y_{-1,l} \equiv 0) . \qquad (2.9)$$

TABLE I. Power moments (rounded) for $H(x)$ in Eq. (2.4) and for the nearest-neighbor ccp and hcp solids.

	μ_n		
n	$H(x)$	ccp[a]	hcp[b]
0	1.0	1.0	1.0
1	0.5	0.5	0.5
2	0.3125	0.3125	0.3125
3	0.21875	0.22265625	0.22265625
4	0.1640625	0.17163086	0.17156304
5	0.12890625	0.13882446	0.13867611
6	0.10473633	0.11578751	0.11558643
7	0.08728027	0.098589778	0.09837381
8	0.07418823	0.085196208	0.08499683

[a]See Ref. 15. [b]See Ref. 17.

Given N power moments, a triangular portion of $\underline{Y}$ is generated containing all elements $Y_{k,l}$ with $k+l \leq N$. The first N modified moments appear in the first column of $\underline{Y}$. This method for obtaining the modified moments from the power moments has the useful property that the integers encountered in the transformation from μ_k to ν_k never grow significantly larger than μ_k itself. Thus, the transformation can be carried out exactly whenever the arithmetic used is of sufficient precision to represent the power moments exactly.

Using this procedure, we have transformed the exact power moments available for the nearest-neighbor ccp and hcp solids into modified moments. In each case, the modified moments are much smaller than the corresponding power moments. They contain the same information about $G(x)$ as do the power moments, but much more efficiently. The magnitudes of the modified and power moments for the ccp and hcp solids are compared in Tables II and III, respectively. In Table II we have included results obtained from the *direct computation*[23] of 40 modified moments for the ccp solid. The exact modified moments have appeared elsewhere.[23] Exact power moments have been computed from them and are available on request. The modified moments for the hcp solid have not appeared previously and are given exactly in Table III.

As noted earlier, the transformation from the power moments to the modified moments is itself ill conditioned. If μ_{20} for the ccp solid were known to only 12 significant figures, ν_{20} would be completely undetermined. It is only because we can perform the transformation exactly that no information is lost. In fact, as we shall see in Sec. III, all of the ill-conditioned nature of the transformation from the power moments to the quadrature formulas is contained in this step. Once the modified moments are known to a given accuracy, the abscissas and weights can be determined with the same accuracy.

TABLE II. Modified moments and power moments for nearest-neighbor solid.

n	$\nu_n \times 16^{n}$ [a]	$\mu_n \times 16^{n}$ [b]
0	1.0	1.0
1	0.0	8.0
2	0.0	8.0×10^{1}
3	1.6×10^{1}	9.12×10^{2}
4	-1.6×10^{1}	1.12×10^{4}
5	-2.24×10^{2}	1.46×10^{5}
6	-1.92×10^{2}	1.94×10^{6}
7	2.24×10^{2}	2.65×10^{7}
8	1.84×10^{3}	3.66×10^{8}
9	1.92×10^{4}	5.12×10^{9}
10	4.04×10^{4}	7.22×10^{10}
15	5.20×10^{7}	4.43×10^{16}
20	-5.63×10^{9}	3.04×10^{22}
25	-2.13×10^{13}	2.24×10^{28}
30	-8.14×10^{15}	1.75×10^{34}
35	1.59×10^{19}	1.43×10^{40}
39	3.30×10^{21}	7.90×10^{44}

[a]Rounded. See Ref. 23 for exact values.

[b]Rounded. Exact power moments can be computed from the exact modified moments. Isenberg (Ref. 17) and Salsburg and Huckaby (Ref. 18) have previously obtained the first 20 power moments exactly by other procedures. Forty exact power moments are available from the authors on request.

TABLE III. Modified moments and power moments for nearest-neighbor hcp solid.

n	$\nu_n \times 48^{n}$ [a]	$\mu_n \times 48^{n}$ [b]
0	1	1.0
1	0	2.4×10^{1}
2	0	7.2×10^{2}
3	432	2.46×10^{4}
4	−1656	9.11×10^{5}
5	−49032	3.53×10^{7}
6	−7236	1.41×10^{9}
7	−8 55360	5.78×10^{10}
8	−81 07992	2.40×10^{12}
9	6116 31000	1.00×10^{14}
10	33893 23608	4.25×10^{15}
11	−4 23837 40320	1.82×10^{17}
12	−7 87518 47052	7.79×10^{18}
13	−99 66590 96328	3.37×10^{20}
14	−6476 60374 55244	1.46×10^{22}
15	33287 75251 30080	6.37×10^{23}
16	9 90648 62014 55400	2.79×10^{25}
17	−38 85459 39834 86232	1.23×10^{27}

[a]Exact.

[b]Rounded. See Ref. 20 for exact values.

C. Transformations of Modified Moments

The modified moments can be easily transformed back to the power moments by using the recurrence relation (2.9) to compute the matrix $\underline{Y}$ from its first column. More generally, it is easy to transform from any one set of modified moments ν_k, defined by the polynomials p_k with recursion coefficients a_k and b_k, to any other set ν'_k, defined by the polynomials p'_k with recursion coefficients a'_k and b'_k. The matrix $\underline{Y}$ with elements $Y_{k,l} = \langle p'_k p_l \rangle$ [of which (2.7) is a special case] can be generated recursively from its first row. Applying Eq. (2.5) twice, the elements $Y_{k,l}$ are seen to satisfy the recursion relation

$$Y_{k+1,l} = Y_{k,l+1} - (a'_k - a_l) Y_{k,l} - b'_k Y_{k-1,l} + b_l Y_{k,l-1}$$
$$(Y_{0,l} = \nu_l, \quad Y_{-1,l} \equiv 0) . \qquad (2.10)$$

Given N elements of the first row, $Y_{0,l} = \nu_l$, a triangular portion of $\underline{Y}$ is obtained, the first column of which contains the first N modified mo-

ments ν_k'. Using this procedure it is possible to transform from one set of modified moments to another without going through the (much larger) power moments.

Another indication of the efficiency with which modified moments store the information about $G(x)$ is that the transformation from modified moments to other modified moments or to power moments via Eq. (2.10) is extremely stable, in total contrast to the transformation from power moments to modified moments. Approximate modified moments can be transformed to approximate power moments via Eq. (2.10) with essentially no loss in accuracy.

III. TRANSFORMATION FROM MODIFIED MOMENTS TO QUADRATURE FORMULAS

A. Transformation to Orthogonal Polynomial Recursion Coefficients

As remarked in Sec. II, the quadrature formulas can be determined stably when the orthogonal polynomials belonging to $G(x)$ are known. The transformation from power moments to quadrature formulas proceeds through the modified moments to the recursion coefficients α_k and β_k of these orthogonal polynomials and then to the abscissas and weights. We have seen how to obtain the modified moments exactly from the power moments. The recursion coefficients α_k and β_k can be obtained from the modified moments by applying the transformation (2.10) from one set of moments ν_k to another set ν_k' in the special case where the polynomials $p_k'(x)$ are the orthogonal polynomials $\pi_k(x)$, so that $a_k' = \alpha_k$, $b_k' = \beta_k$. The matrix $\underline{Z}$ with elements $Z_{k,l} = \langle \pi_k p_l \rangle$ contains the modified moments as its first row, that is, $Z_{0,l} = \nu_l$ ($l = 0, 1, 2, \cdots$). By orthogonality, it must have zero entries below the diagonal, that is, $Z_{k,l} = 0$ ($k > l$). The elements of $\underline{Z}$ satisfy the recursion relation

$$Z_{k+1,l} = Z_{k,l+1} - (\alpha_k - a_l) Z_{k,l} - \beta_k Z_{k-1,l} + b_l Z_{k,l-1}$$
$$(Z_{-1,k} \equiv Z_{k,-1} \equiv 0, \quad k = 0, 1, 2, \cdots) . \quad (3.1)$$

When the kth and $(k-1)$th rows of $\underline{Z}$ are known, the requirements that $Z_{k+1,k-1} = Z_{k+1,k} = 0$ determine α_k and β_k to be

$$\beta_k = \frac{Z_{k,k}}{Z_{k-1,k-1}}, \quad (\beta_0 = \mu_0)$$
$$\alpha_k = a_k + \frac{Z_{k,k+1}}{Z_{k,k}} - \frac{Z_{k-1,k}}{Z_{k-1,k-1}} . \quad (3.2)$$

Once α_k and β_k are known, the remaining elements $Z_{k+1,l}$ ($l > k$) of the $(k+1)$th row can be determined. When an even number ($2n$) of modified moments, $\nu_0, \nu_1, \ldots, \nu_{2n-1}$, are known, one obtains n α's and n β's, $\alpha_0, \beta_0, \ldots, \alpha_{n-1}, \beta_{n-1}$, where $\beta_0 = \mu_0$ and $\alpha_0 = \mu_1$. If an odd number ($2n+1$) of moments are known, one obtains $n+1$ β's but only n α's.

The procedure given above is essentially the same as one proposed by Sack and Donovan,[21] although the derivation given here is somewhat more straightforward. Our expression for β_k is simpler in form because of the simple form of our polynomial recursion formulas. Gautschi[22] employed a different method in which the Gram matrix with elements $\langle p_k p_l \rangle$ is first formed using the recursion (2.10), and then factored by the Cholesky method into the product of two triangular matrices. [If, instead of the Cholesky factorization into matrices which are the transpose of one another, one factors the Gram matrix into a left triangular matrix $\underline{L}$ with unit diagonal and a right triangular matrix $\underline{R}$, then $\underline{R}$ is identical with $\underline{Z}$ in Eq. (3.1). The α's and β's can then be determined using Eq. (3.2).]

The transformation from the modified moments to the recursion coefficients α_k and β_k is extremely well conditioned and can be carried out using limited precision arithmetic with virtually no build-up of error. For example, when 40 modified moments for the ccp solid[23] were used to determine the first 20 α's and β's, using first double-precision and then single-precision arithmetic, we found that the single-precision results were reliable to full single-precision accuracy (11 significant figures) for all 20 recursion coefficients.

In sharp contrast to this stability is the behavior encountered when the power moments are transformed directly to the α's and β's. This can be done by applying the method following (3.1) with $a_l = b_l = 0$ and $\nu_l = \mu_l$.[26] Between one and two significant figures are lost for each pair α_k, β_k, which are determined. Thus 40 modified moments, even when known only to limited accuracy, determine the α's and β's to the *same accuracy*, whereas 40 power moments cannot be used, even when known to *double-precision* accuracy, because all 25 significant figures are lost before the 40th moment is reached. Similar behavior is encountered in the hcp case.

In Table IV we give the first few recursion coefficients for the ccp case, normalized to the interval $[0, L]$ with $L = 16$. As n increases, α_n and β_n approach $a_n = 8 = \frac{1}{2}L$ and $b_n = 16 = (\frac{1}{4}L)^2$, respectively. The first few α's and β's are themselves integers, or close to integers, which are not 8 and 16. It might be supposed that, by choosing the first few coefficients a_n and b_n to be integers other than 8 and 16, we might further reduce the size of the modified moments. The first few modified moments can, indeed, be made smaller by this device, but no systematic reduction in the size of the higher-order modified-moments results, nor any change in the stability of the transformation to α's and β's. Similarly, transformation of the mod-

TABLE IV. Recursion coefficients for nearest-neighbor ccp solid orthogonal polynomials on the interval [0,16].

n	α_n [a]	β_n [a]
0	8.0	1.0
1	9.0	16.0
2	7.2142857	14.0
3	8.1205190	15.025510
4	8.2062831	17.375851
5	7.9327746	15.660066
6	7.8354061	15.730480
7	8.2144437	16.141563
8	7.8501701	16.057087
9	8.0570572	15.718632
10	8.0310605	16.448207

[a]The recursion coefficients have been rounded to eight significant figures. They were obtained to machine accuracy (about 25 significant figures on the CDC 3600).

ified moments for the ccp solid, via Eq. (2.10), to shifted Chebyshev modified moments of the *first* kind,[25] with recursion coefficients $a_k = \frac{1}{2}L$ $(k=0, 1, \cdots)$, $b_1 = 2(\frac{1}{4}L)^2$, and $b_k = (\frac{1}{4}L)^2$ $(k=2, 3, \cdots)$ [see Eq. (2.5)], resulted in no significant changes either in the size of the moments or in the stability of the transformations.

Once the recursion coefficients α_k and β_k are known, the abscissas and weights of each of the four quadrature formulas used by Wheeler and Gordon[10] can be determined by diagonalizing a real symmetric tridiagonal matrix. For the case in which all of the abscissas are undetermined and for that in which one abscissa is fixed at the origin, the matrices are exactly those given by Gordon.[1] Wheeler and Gordon[10,11] used a set of "shifted" moments to obtain the remaining quadratures, but this method required recomputing the recursion coefficients. In fact, all four of the quadratures are easily obtained directly from the recursion coefficients α_k and β_k. We summarize the procedure below; details and proofs are given in the Appendix.

B. Determination of Quadrature Formulas

When $2n$ moments are given so that $\alpha_0, \beta_0, \cdots, \alpha_{n-1}, \beta_{n-1}$ are known, the abscissas for the n-point quadrature formula with no fixed abscissas are the eigenvalues of the matrix $\underline{M}^{(n)}$:

$$\underline{M}^{(n)} = \begin{pmatrix} \alpha_0 & -\sqrt{\beta_1} & & & \\ -\sqrt{\beta_1} & \alpha_1 & -\sqrt{\beta_2} & & \\ & -\sqrt{\beta_2} & \alpha_2 & -\sqrt{\beta_3} & \\ & & & & -\sqrt{\beta_{n-1}} \\ & & & -\sqrt{\beta_{n-1}} & \alpha_{n-1} \end{pmatrix} . \tag{3.3}$$

The weights are the squares of the first elements of the corresponding normalized eigenvectors, multiplied by μ_0. To obtain the quadratures with one or two fixed abscissas, we make use of the functions $\gamma_k(z) \equiv \pi_k(z)/\pi_{k+1}(z)$, which are determined recursively by

$$\begin{aligned} &\gamma_0(z) = 1/(z-\alpha_0) \\ &\gamma_k(z) = 1/[z-\alpha_k-\beta_k\gamma_{k-1}(z)], \quad k=1,2,\cdots . \end{aligned} \tag{3.4}$$

If only $2n-1$ moments are given so that α_{n-1} is undetermined (though β_{n-1} is known), the n-point quadrature formula with one abscissa fixed at x_0 is obtained from $M^{(n)}$ in the same manner as above except that α_{n-1} is replaced by

$$\alpha_{n-1}^{\dagger}(x_0) = x_0 - \beta_{n-1}\gamma_{n-2}(x_0) . \tag{3.5}$$

Useful quadratures are obtained when x_0 is chosen as either the left or right endpoint of the interval. Finally, if $2n$ moments are given, the $(n+1)$-point quadrature formula with two fixed abscissas x_1 and x_2 is determined from the $(n+1)\times(n+1)$ matrix $\underline{M}^{(n+1)}$ in which β_n and α_n are replaced by

$$\beta_n^{\ddagger} = (x_1 - x_2)/[\gamma_{n-1}(x_1) - \gamma_{n-1}(x_2)] ,$$

$$\alpha_n^{\ddagger} = x_1 - \beta_n^{\ddagger}\gamma_{n-1}(x_1) . \tag{3.6}$$

A useful quadrature is obtained when x_1 and x_2 are chosen to be the ends of the interval $[0, L]$ on which $G(x)$ is nonzero. Golub[27] has given an equivalent procedure which expresses $\alpha_n^{\dagger}$, $\alpha_n^{\ddagger}$, and $\beta_n^{\ddagger}$ in terms of solutions of systems of linear equations.

We have tested the stability of this procedure by comparing results using single- and double-precision arithmetic to obtain abscissas and weights for all four quadrature formulas. In no case was there any detectable buildup of error for $n \leq 20$. Thus, the 40 modified moments of the ccp lattice, even if known to only single-precision accuracy, determine the abscissas and weights of the quadrature formulas to that same accuracy. Similar stability was observed in the hcp case.

IV. TRANSFORMATION TO MODIFIED MOMENTS WHEN THE POWER MOMENTS ARE FUNCTIONS OF FORCE-CONSTANT RATIOS

In Sec. II we showed how the power moments of the frequency distributions of harmonic solids with only nearest-neighbor force constants could be

transformed exactly to modified moments. In that case the power moments could be expressed exactly as integers. When longer- but finite-ranged forces or noncentral forces are present, the power moments become functions of ratios of force constants and cannot, in general, be expressed as integers. However, the power moments can be expressed as polynomials (or multinomials) in the force-constant ratios with integer coefficients. The kth-power moment is written as a polynomial of degree k. It is possible to transform these kth-degree polynomial power moments exactly to kth-degree polynomial modified moments.

When the power moments are polynomials in a force-constant ratio r, the length L of the appropriately scaled interval of definition of $G(x)$ becomes a first-degree polynomial in r. From Eq. (2.5a), the recursion coefficients a_n and b_n become polynomials in r of degree one and two, respectively. For example, for the ccp solid with nearest- and next-nearest-neighbor interactions, the appropriate scaling is $L=16+4r$, and the recursion coefficients are $a_n=8+2r$ and $b_n=16+8r+r^2$.

The transformation from polynomial power moments to polynomial modified moments proceeds in the same way as for simple integer moments. The recursion formula (2.9) now involves products of polynomials. The element $Y_{i,j}$ of $\underline{Y}$ is a polynomial of degree at most $i+j$. Isenberg[17] has reported exact polynomial power moments for a number of model solids. These power moments were transformed into polynomial modified moments. As in the simple integer case, we found that the coefficients in the polynomial elements of the matrix $\underline{Y}$ along an upward sloping diagonal joining the kth modified moment to the kth-power moment never grow significantly larger than those in the power moment, and that the modified moments are much smaller than the corresponding power moments.

If the polynomial modified moments are evaluated for a particular choice of the force-constant ratio, the methods of Sec. III can be applied to obtain abscissas and weights for the appropriate quadrature formulas. We have investigated the stability of this procedure for a variety of lattices and force-constant ratios and have found that, as in the simple integer case, the transformation is strikingly stable. No detectable loss of accuracy occurs in single-precision arithmetic in the transformation of the modified moments to the abscissas and weights for any of the lattices or force-constant ratios which we have tried.

V. USE OF ADDITIONAL INFORMATION ABOUT THE SPECTRAL DENSITY

If the function $F(\tau,x)$ in Eq. (1.1) is singular at one end of the interval—as is the case for some of the functions of interest in the harmonic-solid problem—then the bounds obtained from moments alone may converge slowly or there may be no bound on $\langle F(\tau,x)\rangle$ in one direction. Wheeler and Gordon found that additional information about the spectral density, in the form of series expansion coefficients for $G(x)$ near $x=0$, could be used to greatly improve upon the bounds obtained from moments alone. The same procedure can be adapted to improve the bounds obtained from *modified* moments without causing serious loss in the stability of the transformation from modified moments to quadratures.

A. Improved Bounds from Series Coefficients

The spectral density for a three-dimensional harmonic solid typically has the form near $x=0$,

$$G(x)=\tfrac{1}{2}\sqrt{x}\,C(x) \qquad [x=(\omega/\omega_{\max})^2]\,, \tag{5.1}$$

where $C(x)$ is a smoothly varying function which has a Taylor-series expansion

$$C(x)=\sum_{n=0}^{\infty} c_n x^n \qquad (c_0>0)\,, \tag{5.2}$$

with nonzero radius of convergence R. If lower bounds c_n^L to the coefficients c_n are known, as well as a lower bound R_L to the radius of convergence, then the lower bound to $G(x)$ defined by

$$\begin{aligned} G^L(x)&=\tfrac{1}{2}\sqrt{x}\left(\sum_n c_n^L x^n\right)\equiv\tfrac{1}{2}\sqrt{x}\,C^L(x) \quad (0\le x<R_L)\\ &=0 \qquad\qquad\qquad\qquad\qquad\qquad (R_L\le x\le 1)\,, \end{aligned} \tag{5.3}$$

can be subtracted from G leaving a non-negative weight function

$$\hat{G}(x)=G(x)-G^L(x)\,. \tag{5.4}$$

[One need not, of course, actually know an infinite sequence of coefficients c_n^L. Any lower bound $C^L(x)$ to $C(x)$ can be used. In practice, examination of the behavior of the first few coefficients usually allows one to replace the infinite series in Eq. (5.2) with an appropriate polynomial.] The power moments of $\hat{G}$ are simply the differences of the power moments of G and G^L, and the average of $F(\tau,x)$ is the sum of the averages over $\hat{G}$ and G^L separately;

$$\langle F(\tau,x)\rangle=\int_0^1 F(\tau,x)\hat{G}(x)\,dx+\int_0^1 F(\tau,x)G^L(x)\,dx\,. \tag{5.5}$$

The quadrature formulas may be used to evaluate the average over $\hat{G}$, while the average over G^L can be computed directly. If the bound $C^L(x)$ is close to $C(x)$ near $x=0$, the bounds to $\langle F(\tau,x)\rangle$ will generally be improved. This improvement can be quite striking if $F(\tau,x)$ varies rapidly near $x=0$ or diverges there.

It is clear that this procedure can be used with modified moments. The contribution to the nth

modified moment from $G^L(x)$ is additive:

$$\nu_n = \hat{\nu}_n + \nu_n^L \ , \tag{5.6}$$

where

$$\nu_n^L = \int_0^{R_L} G^L(x) p_n(x)\, dx \ .$$

The $\hat{\nu}_n$ are modified moments of a non-negative weight function and determine the quadrature formula appropriate to $G(x)$ by the procedure described in Sec. III.

These modified moments cannot, however, be obtained stably by transforming the $\hat{\mu}_n$ to $\hat{\nu}_n$ via Eq. (2.9). Because of the exponentially ill-conditioned character of that transformation, the non-integer $\hat{\mu}_n$ cannot be reliably transformed to $\hat{\nu}_n$ in finite-precision arithmetic. Instead, the contribution to ν_n from $G^L(x)$ must be computed directly and subtracted from the exact modified moment to give $\hat{\nu}_n$. This is easily accomplished by using a Gaussian-quadrature formula appropriate to the weight function $h(x) = \frac{1}{2}\sqrt{x}$ on the interval $[0, R_L]$ to integrate the function $(\sum_n c_n^L x^n) p_k(x)$. Because $C^L(x)$ is generally a smoothly varying function on $[0, R_L]$, it is sufficient to use a quadrature of high enough degree to integrate $p_k(x)$ exactly. We have found in practice that the recursion relation (2.5) may be used to evaluate the polynomial $p_k(x)$ at the abscissas, and that the quadrature for ν_k^L is independent of the number of points used and of the degree of $C^L(x)$, provided only that the number of points is at least $\frac{1}{2}k$.

Once the modified moments $\hat{\nu}_k$ have been determined precisely, the transformation to the corresponding recursion coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$ and abscissas and weights proceeds by the methods of Sec. III. However, the stability of this transformation is now somewhat dependent upon the choice of $G^L(x)$. The extreme stability of the transformation from the modified moments to the recursion coefficients observed in Secs. III and IV resulted from the fact that $G(x)$ and $H(x)$ are nonzero on the same interval and have similar behavior, at least near the ends of that interval. If $G^L(x)$ is very close to $G(x)$ on a substantial portion of the interval of definition of G, then $\hat{G}(x)$ and the $H(x)$ function do not have this similar behavior. It may be expected that the transformation from the $\hat{\nu}_k$ to the α's and β's will be less stable. While use of series coefficients does result in some loss of stability, it is relatively minor for useful choices of $G^L(x)$, and the modified-moments procedure remains vastly more stable than the direct transformation from the power moments.

To illustrate both the power and the limitations of this technique, let us return to the ccp solid with nearest-neighbor force constants for which Isenberg has computed a large number of series coefficients.[28] The coefficients for this model are all positive, so that the series for $C(x)$ in Eq. (5.2) can simply be truncated and the coefficients rounded down to provide the lower bound $C^L(x)$. The radius of convergence of the series for $C(x)$ is known to be $R = \frac{1}{4}$ when $G(x)$ is defined on $[0, 1]$.

The averages of various inverse and half-integral powers of x,

$$\mu_{-1} = \langle 1/x \rangle, \quad \mu_{-1/2} = \langle x^{-1/2} \rangle, \quad \mu_{1/2} = \langle x^{1/2} \rangle,$$

are required in the calculation of thermal properties and correlation functions of harmonic crystals. The moment $\mu_{1/2}$ is just twice the zero-point internal energy of vibration U_0 in appropriate units, while μ_{-1} and $\mu_{-1/2}$ are required in the calculation of the classical and quantum limits of the position autocorrelation function. In addition, the average

$$\mathfrak{L} = \langle \ln(x^{1/2}) \rangle$$

contributes to the free energy and entropy of a harmonic solid at finite temperatures and is of interest when considering the relative thermodynamic stability of two alternative crystalline forms of a solid. We have computed rigorous upper and lower bounds to each of these averages using a technique described in Sec. VI of Ref. 10 in which the left-hand side fixed point of the quadratures is fixed at some nonzero x_0, rather than at $x = 0$, and the sign of the error is checked directly. Using all 30 of Isenberg's coefficients (rounded down to 20 significant figures) and placing x_0 at 0.1 (on the interval $[0, 1]$), we find with 40 modified moments that

$$\mu_{-1} = 3.35882615\,36^{32}_{10} \ ,$$

$$\mu_{-1/2} = 1.63590789\,055^{58}_{47} \ ,$$

$$-\mathfrak{L} = 0.42886956\,6196^{71}_{62} \ ,$$

$$U_0/3Nh\omega_{\max} = \tfrac{1}{2}\mu_{1/2} = 0.34088722\,029172^{25}_{02} \ ,$$

with a precision of one part in 10^{11}, 10^{12}, 10^{13}, and 10^{14}, respectively.

By comparing the results in single- and double-precision arithmetic of the transformation from the modified moments $\hat{\nu}_k$ to the recursion coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$ and abscissas and weights, we have found that when 30 low-frequency coefficients are used to give $G^L(x)$ up to $R^L = 0.1$, about seven significant figures are lost in α_{20}, and about six figures are lost in the values of the points and weights for the quadrature formulas using 40 modified moments. Thus, with 25-significant-figure arithmetic the α's and β's and the abscissas and weights should be reliable to between 17 and 19 significant figures. This may be compared to the results if the power moments are used directly, in which case we cannot even *use* more than about 35 moments with 25-significant-figure arithmetic.

The results reported assume that Isenberg's coefficients determine $G(x)$ to an accuracy of at least

one part in 10^{12} on the interval $[0, 0.1]$. This seems quite reasonable; even if there were a systematic buildup of error in the higher-order coefficients, this error would not seriously affect the accuracy of $G^L(x)$ because of our conservative choice of $R_L = 0.1$.

If we attempt to use Isenberg's full 30-term series all the way up to the radius of convergence R, however, we find that all 25 double-precision significant figures are lost after only 30 moments are used. If only three coefficients (to 20 significant figures) are used to provide a lower bound $G^L(x)$ all the way up to $R_L = R = \frac{1}{4}$, only four significant figures are lost in the α's and β's by the time n reaches 40, and only three significant figures are lost in the abscissas and weights. Lower bounds to μ_{-1}, $\mu_{-1/2}$, and $-\mathfrak{L}$ and both upper and lower bounds to $\mu_{+1/2}$ can then be determined. The lower bound to μ_{-1} is

$$\mu_{-1} = 3.35882597 ,$$

which is correct to one part in 10^7. When six series coefficients are used to give $G^L(x)$ up to $x = R_L = R$, about six significant figures are lost in α_{20} and β_{20}, and about five in the abscissas and weights for $n = 40$. The lower bound to μ_{-1} then has a fractional error of only 1×10^{-10}.

The incorporation of additional information about $G(x)$ in the form of low-frequency series expansion coefficients can dramatically strengthen the quadrature methods. Knowledge of even a few low-frequency coefficients is sufficient to provide extremely accurate estimates of averages of even the most singular integrands. The application of this technique is presently limited to some extent by difficulties in obtaining the low-frequency coefficients. At present, substantial numbers of very accurate coefficients are available for only one model solid[28]; however, further advances in this area appear to be likely.[29]

B. Improved Bounds from Knowledge of Functional Form of $G(x)$

Even when *no* information is available about the numerical values of the series coefficients, the mere knowledge of the existence and form of the expansion of $G(x)$ near $x = 0$ can be used to improve the bounds obtained from moments. We emphasized in Sec. II that the most significant figures in the power moments contain information about the end of the interval. Similarly, the "shifted" moments $\mu_n' = \langle (1-x)^n \rangle$ contain information about the behavior of $G(x)$ near $x = 0$. Using the functional form of $G(x)$ expressed in Eqs. (5.1) and (5.2), we can write

$$2\mu_n' = \sum_{k=0}^{\infty} c_k \int_0^{1/4} x^{k+1/2}(1-x)^n \, dx + \int_{1/4}^{1} (1-x)^n G(x)\, dx$$

$$= \sum_{k=0}^{\infty} c_k B_{1/4}(k+\tfrac{3}{2}, n+1) + \int_{1/4}^{1} (1-x)^n G(x)\, dx , \tag{5.7}$$

where $B_x(p, q)$ is the incomplete beta function,

$$B_x(p, q) = \int_0^x t^{p-1}(1-t)^{q-1}\, dt . \tag{5.8}$$

Dividing by $B_{1/4}(\frac{3}{2}, n+1)$ we obtain the result

$$\mu_n^* \equiv \frac{2\mu_n'}{B_{1/4}(\frac{3}{2}, n+1)} = \sum_{j=0}^{\infty} c_j K_j(n) + R_n , \tag{5.9}$$

where

$$K_j(n) = \frac{B_{1/4}(j+\frac{3}{2}, n+1)}{B_{1/4}(\frac{3}{2}, n+1)} \quad (K_0 \equiv 1) . \tag{5.10}$$

$K_j(n)$ is of order n^{-j} as $n \to \infty$ and the remainder term,

$$R_n = \frac{\int_0^{1/4} (1-x)^n G(x)\, dx}{B_{1/4}(\frac{3}{2}, n+1)} , \tag{5.11}$$

is at most $O[n^{3/2}(\frac{3}{4})^n]$ as $n \to \infty$. Thus, the sequence μ_n^* is monotone decreasing toward c_0 for large n. Examination of the dependence of $K_j(n)$ and R_n upon n shows that the sequence of extrapolations,

$$\mu_n^* - K_1(n)\, \frac{\mu_n^* - \mu_{n-1}^*}{K_1(n) - K_1(n-1)} ,$$

tends to c_0 from below with an asymptotic error of order n^{-2}. Using 40 moments for the ccp solid in this way we obtain the bounds

$$2.565 < c_0 < 2.798 .$$

The correct value is $2.603457\cdots$, less than 2% larger than the lower bound.

The bounds to c_0 obtained in this way can be used to improve the bounds from moments to averages of singular functions. For example, if 40 modified moments are used alone to determine a lower bound to μ_{-1}, the result is low by almost 3%:

$$\mu_{-1} \geq 3.26 .$$

If we used the lower bound to c_0 determined from the moments, the bound is low by less than one part in 10^3:

$$\mu_{-1} \geq 3.3567 .$$

Thus, even knowledge only of the existence and form of the expansion for $G(x)$ is sufficient to dramatically improve upon the bounds obtained from moments alone.

VI. DISCUSSION

We have seen that appropriately defined modified moments provide particularly valuable information about the spectral density functions of harmonic solids. First, they store the information about the density function more efficiently than do the power moments. They are much smaller than the power moments and are more sensitive to the be-

havior of $G(x)$ on its interval of definition. When the modified moments are known, even only to limited accuracy, the power moments can be determined to the same accuracy, whereas the converse is not true. Second, the modified moments determine with great accuracy and stability the abscissas and weights of quadrature formulas which can be used to obtain properties of harmonic solids with extreme accuracy. This stability is not limited to a single system but is found for a variety of crystal structures and force-constant ratios. Third, the modified moments can be used in conjunction with additional information about the spectral density function with little loss in the stability of the procedure.

We have used the great stability of the modified-moments method to reexamine the bounds on thermal properties of harmonic solids obtained directly from the power moments by Wheeler and Gordon. They claimed that their bounds were reliable because the instabilities in that procedure appeared to introduce errors in the bounds which were always several orders of magnitude less than the difference between the bounds. We find that this is essentially correct. However, it should be noted that that procedure cannot be used with the number of moments now available.

The reason why the bounds found by Wheeler and Gordon are not particularly sensitive to errors in the abscissas and weights is probably that they are averages of rather smooth monotone functions. The average of a rapidly oscillating function may be more sensitive. The momentum and position autocorrelation functions of harmonic solids are such averages and show somewhat greater sensitivity to errors in the abscissas and weights. The autocorrelation functions also illustrate the value of a quadrature method which allows the stable use of large numbers of moments, as the time to which these correlation functions are accurately determined is proportional to the number of moments which can be used.[30]

In view of the useful characteristics of modified moments for harmonic solids detailed above, a procedure for the computation of modified moments directly from the dynamical matrix, without recourse to power moments, is desirable. We have presented such a procedure[23] and have shown that it is a practical method for the computation of modified moments.

It would seem that, for most model solids, direct computation of the modified moments is preferable to the computation of power moments followed by transformation to modified moments as described in Sec. II. For example, we computed[23] 40 exact modified moments for the nearest-neighbor ccp solid directly from the dynamical matrix. This is more than twice the number of exact power moments which had previously been obtained. Exceptions occur when the power moments are already known exactly or when, as in some simple models, it is possible to obtain a closed-form expression for the power moments enabling them to be computed much more easily than by standard methods. For example, the power moments of a simple model analyzed by Montroll[31] can be so expressed and 200 exact power moments can easily be computed and transformed to modified moments.[32] This is roughly four times the number of modified moments which could practically be obtained by the methods of Ref. 23.

The direct computational method will be particularly valuable for more complex solids in which the moments are functions of force-constant ratios. Because modified moments need to be known only approximately in order to accurately determine properties of solids, the direct computation of modified moments can be carried out using limited-precision arithmetic for a specific choice of force-constant ratios. (We have computed such approximate modified moments for model solids with both the nearest-neighbor and next-nearest-neighbor force constants for a variety of force-constant ratios. Comparison with exact modified moments determined by the methods of Sec. IV indicates that the direct computation is both stable and accurate, the moments being determined to essentially machine accuracy in every case with no detectable buildup of error.) In contrast, because power moments must be known essentially exactly, they must be expressed as multinomials in the force-constant ratios. The bookkeeping involved in the computation of the multinomial coefficients, as well as in their transformation to multinomial modified moments, becomes extremely cumbersome as the number of force-constant ratios grows. The advantage of having a general expression for the moments as functions of force-constant ratios is soon outweighed by this fact.

We believe that the advantages of the modified-moments method for harmonic solids with short-ranged forces are established. The methods for computing modified moments—either from known power moments or directly from the dynamical matrix—are straightforward. Once modified moments are known, the procedures described in Secs. III–V provide a simple method for obtaining bounds to many properties of physical interest. It seems likely that the utility of the modified-moments method can be extended to harmonic solids with long-ranged forces such as occur in ionic and dipolar crystals and in metals. The exact computation of moments in such cases seems unlikely. However, the modified moments need not be known exactly for most purposes, and it should be possible to devise approximate methods for moment

computation which are sufficiently accurate to provide valuable bounds to the properties of such systems. Other systems in which we expect the modified-moments concept to be useful are disordered solids and solids with impurities. We are presently investigating these possibilities.

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APPENDIX

We show here how to obtain the abscissas and weights for quadrature formulas in which zero, one, or two abscissas are fixed, directly from the recursion coefficients α_k and β_k of the orthogonal polynomials of $G(x)$. We deal first with the case in which none of the abscissas is fixed. The solution for this case was given by Gordon,[1] but the derivation given here in terms of orthogonal polynomials lays the foundation for the remaining cases and, we feel, is somewhat more straightforward than that given by Gordon in terms of continued fractions. We then derive the results when one or two abscissas are fixed in somewhat less detail.

The monic orthogonal polynomials $\pi_k(x)$ belonging to $G(x)$ are defined by the equation

$$\langle \pi_k \pi_l \rangle \equiv \int G(x)\pi_k(x)\pi_l(x)\,dx = \delta_{kl}\langle \pi_k \pi_k \rangle , \qquad \text{(A1)}$$

where δ_{kl} is the standard Kronecker δ symbol. They satisfy the three-term recursion relation

$$\pi_{k+1}(x) = (x-\alpha_k)\pi_k(x) - \beta_k \pi_{k-1}(x) \quad (\pi_0 \equiv 1,\ \pi_{-1} \equiv 0) \qquad \text{(A2)}$$

The normalization constant $\langle \pi_k \pi_k \rangle$ can be found in terms of the β's by multiplying (A2) by π_{k-1} and averaging over $G(x)$. Making use of orthogonality, one then obtains

$$\beta_k \langle \pi_{k-1}\pi_{k-1} \rangle = \langle \pi_{k-1} x \pi_k \rangle = \langle \pi_k \pi_k \rangle , \qquad \text{(A3)}$$

from which follows

$$\langle \pi_k \pi_k \rangle = \beta_0 \beta_1 \cdots \beta_k \quad (\beta_0 = \mu_0;\ k = 0, 1, 2, \cdots) . \qquad \text{(A4)}$$

Dividing Eq. (A2) by $(\beta_0\beta_1\cdots\beta_k)^{1/2}$, we find that the *orthonormal* polynomials, $\pi_k^*(x)$, belonging to $G(x)$ satisfy the three-term recursion relation

$$\beta_{k+1}^{1/2}\pi_{k+1}^*(x) = (x-\alpha_k)\pi_k^*(x) - \beta_k^{1/2}\pi_{k-1}^*(x) . \qquad \text{(A5)}$$

The first n of these equations can be written in matrix form as follows:

$$(\underline{\mathbf{M}}^{(n)} - \underline{\mathbf{I}}x)\begin{pmatrix} \pi_0^* \\ \pi_1^*(x) \\ \\ \pi_{n-1}^*(x) \end{pmatrix} = \beta_n^{1/2}\begin{pmatrix} 0 \\ 0 \\ 0 \\ \pi_n^*(x) \end{pmatrix} , \qquad \text{(A6)}$$

where the matrix $\underline{\mathbf{M}}^{(n)}$ is given in Eq. (3.3). Inspection of Eq. (A6) reveals that the roots $x_1, x_2, \ldots, x_n$ of $\pi_n^*(x)$ are the *eigenvalues* of $\underline{\mathbf{M}}^{(n)}$ and that the *eigenvectors* of $\underline{\mathbf{M}}^{(n)}$ are of the form $[\pi_0^*, \pi_1^*(x_i), \ldots, \pi_{n-1}^*(x_i)]$ $(i = 1, \ldots, n)$. Because the roots $x_1, \ldots, x_n$ of π_n^* are distinct[33] and $\underline{\mathbf{M}}^{(n)}$ is real and symmetric, the eigenvectors are mutually orthogonal. The $n \times n$ matrix $\underline{\mathbf{S}}$ of *normalized* eigenvectors with elements

$$S_{k,i} = \pi_k^*(x_i)\left(\sum_{k=0}^{n-1}[\pi_k^*(x_i)]^2\right)^{-1/2}$$

$$(k = 0, 1, \ldots, n-1;\ i = 1, 2, \ldots, n) \qquad \text{(A7)}$$

is therefore unitary.

It is now easy to show that the eigenvalues $x_1, \ldots, x_n$ of $\underline{\mathbf{M}}^{(n)}$ are the abcissas, and that the squares of the first elements of the normalized eigenvectors, multiplied by $\beta_0 = \mu_0$,

$$w_i = \mu_0 S_{0,i}^2 = \mu_0\left(\sum_{k=0}^{n-1}[\pi_k^*(x_i)]^2\right)^{-1} , \qquad \text{(A8)}$$

are the weights of the Gaussian quadrature which gives the first $2n$ moments correctly. We observe that any power of x up to x^n can be expressed as a linear combination of the orthogonal polynomials $\pi_0^*, \pi_1^*, \ldots, \pi_n^*$, so that it is sufficient to verify that the proposed quadrature correctly evaluates all of the averages

$$\langle \pi_k^* \pi_l^* \rangle = \delta_{kl} \quad (k = 0, 1, \ldots, n-1;\ l = 0, 1, \ldots, n) . \qquad \text{(A9)}$$

That is, we require that

$$\sum_{i=1}^{n} w_i \pi_k^*(x_i)\pi_l^*(x_i) = \delta_{kl}$$

$$(k = 0, 1, \ldots, n-1;\ l = 0, 1, \ldots, n) . \qquad \text{(A10)}$$

When $l = n$, the sum is zero because the x_i are the roots of $\pi_n^*(x)$. The remaining sums are simply products of the rows of the (unitary) matrix $\underline{\mathbf{S}}$, which are orthonormal. This completes the proof for the case when none of the abscissas are predetermined. Exactly $2n$ moments are required for the construction of the matrix $\underline{\mathbf{M}}^{(n)}$. Note that while β_n appeared formally in Eq. (A6), its *value* was not required. Thus the n-abscissa quadrature formula can be constructed from exactly $2n$ moments.

Quadrature with One Abscissa Fixed

If $2n+1$ moments are known, so that β_n can be determined in addition to $\alpha_0, \beta_0, \ldots, \alpha_{n-1}, \beta_{n-1}$, then in addition to the orthogonal polynomials $\pi_0, \pi_1, \ldots, \pi_n$ we can construct the (monic) *quasi-orthogonal* polynomial $\pi_{n+1}^\dagger(x)$ defined by the requirement that it be orthogonal [over $G(x)$] to all polynomials of degree $n-1$ or less and have a root at a prescribed point x_0. From the orthogonality of $\pi_{n+1}^\dagger$ to all polynomials of degree $n-1$ or less, it

is easy to show that it must satisfy a three-term recursion relation in terms of the π's of the form

$$\pi^{\dagger}_{n+1}(x) = (x - \alpha^{\dagger}_n)\pi_n - \beta_n \pi_{n-1} ,$$

where β_n is the known recursion coefficient for the orthogonal polynomials and $\alpha^{\dagger}_n$ can be determined from the requirement that $\pi^{\dagger}_{n+1}(x_0) = 0$, as follows. The equation

$$\pi^{\dagger}_{n+1}(x_0) = 0 = (x_0 - \alpha^{\dagger}_n)\pi_n(x_0) - \beta_n \pi_{n-1}(x_0) \qquad \text{(A11)}$$

implies that

$$\alpha^{\dagger}_n = x_0 - \beta_n \left(\frac{\pi_{n-1}(x_0)}{\pi_n(x_0)} \right) . \qquad \text{(A12)}$$

It is useful to define the sequence of functions

$$\gamma_k(z) = \pi_k(z)/\pi_{k+1}(z) \quad (k = 0, 1, 2, \cdots) . \qquad \text{(A13)}$$

They may be determined recursively by applying Eq. (A2) to $\pi_{k+1}(z)$ to obtain

$$\gamma_k(Z) = 1/[z - \alpha_k - \beta_k \gamma_{k-1}(z)] \quad (k = 0, 1, 2, \cdots)$$
$$[\gamma_{-1}(z) \equiv 0] . \qquad \text{(A14)}$$

Then Eq. (A12) for $\alpha^{\dagger}_n$ is just

$$\alpha^{\dagger}_n = x_0 - \beta_n \gamma_{n-1}(x_0) . \qquad \text{(A15)}$$

Dividing Eq. (A6) by $(\beta_0 \cdots \beta_n)^{1/2}$, we can write the equations for π^*_0, π^*_1, ..., π^*_n and $\pi^{\dagger}_{n+1}$ in the matrix form

$$(\underline{M}^{\dagger} - \underline{I}\, x) \begin{pmatrix} \pi^*_0 \\ \pi^*_1(x) \\ \vdots \\ \pi^*_n(x) \end{pmatrix} = (\beta_0 \beta_1 \cdots \beta_n)^{-1/2} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \pi^{\dagger}_{n+1}(x) \end{pmatrix} , \qquad \text{(A16)}$$

where $\underline{M}^{\dagger}$ is the real symmetric $(n+1)\times(n+1)$ tridiagonal matrix $\underline{M}^{(n+1)}$ defined by Eq. (3.3), except that the last element is $\alpha^{\dagger}_n$ instead of α_n. Again, the eigenvalues of $\underline{M}$ are the roots of $\pi^{\dagger}_{n+1}$, one of which must lie at x_0. The argument that the abscissas and weights of the quadrature which gives μ_0, μ_1, ..., μ_{2n} correctly are the eigenvalues of $\underline{M}$ and the squares of the first elements of the normalized eigenvectors proceeds exactly as before.

Quadrature with Two Abscissas Fixed

When only $2n$ moments are known, we can still define, in addition to the orthogonal polynomials π_0, ..., π_n, a generalization of the quasi-orthogonal polynomial which is of degree $n+1$, but which is orthogonal [over $G(x)$] only to polynomials of degree $n-2$ and less, and which has two prescribed roots x_1 and x_2. This polynomial is uniquely defined by these requirements if the leading coefficient is taken as unity. It satisfies a recursion relation of the form

$$\pi^{\ddagger}_{n+1}(x) = (x - \alpha^{\ddagger}_n)\pi_n(x) - \beta^{\ddagger}_n \pi_{n-1}(x) , \qquad \text{(A17)}$$

where $\alpha^{\ddagger}_n$ and $\beta^{\ddagger}_n$ are determined by the equations

$$\begin{aligned} \pi^{\ddagger}_{n+1}(x_1) &= 0 = (x_1 - \alpha^{\ddagger}_n)\pi_n(x_1) - \beta^{\ddagger}_n \pi_{n-1}(x_1) , \\ \pi^{\ddagger}_{n+1}(x_2) &= 0 = (x_2 - \alpha^{\ddagger}_n)\pi_n(x_2) - \beta^{\ddagger}_n \pi_{n-1}(x_2) . \end{aligned} \qquad \text{(A18)}$$

Solving for $\alpha^{\ddagger}_n$ in terms of $\beta^{\ddagger}_n$ and the α_0, β_0, ..., α_{n-1}, β_{n-1} in the same manner as for the case with one fixed abscissa, we obtain the two equations

$$\begin{aligned} \alpha^{\ddagger}_n &= x_1 - \beta^{\ddagger}_n \gamma_{n-1}(x_1) \\ &= x_2 - \beta^{\ddagger}_n \gamma_{n-1}(x_2) , \end{aligned} \qquad \text{(A19)}$$

where $\gamma_{n-1}(z)$ is defined by Eq. (A13). The coefficient $\beta^{\ddagger}_n$ is then given by the equation

$$\beta^{\ddagger}_n = (x_1 - x_2)/[\gamma_{n-1}(x_1) - \gamma_{n-1}(x_2)] . \qquad \text{(A20)}$$

Once $\alpha^{\ddagger}_n$ and $\beta^{\ddagger}_n$ are determined, the abscissas and weights are again given by the eigenvalues and eigenvectors of the real symmetric $(n+1)\times(n+1)$ tridiagonal matrix $\underline{M}^{\ddagger}$, which is identical to $\underline{M}^{(n+1)}$ except that α_n and β_n are replaced by $\alpha^{\ddagger}_n$ and $\beta^{\ddagger}_n$.

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