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MODIFIED MOMENTS AND GAUSSIAN QUADRATURES*

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A number of the speakers at this conference have referred to or made use of the close connection between Padé approximants, continued fractions, moment theory, orthogonal polynomials, and (Gaussian) quadrature formulas. I want to discuss an application of a recent development in the theory (and practice) of Gaussian quadratures which may well have repercussions in other of these areas, namely, the *modified moments procedure* discussed recently by Sack and Donovan [14] and Gautschi [1].

1. **The Quadrature Problem.** In the language of Gaussian quadratures, the central problem I want to consider is the following: Given a finite number $(N+1)$ of *power* moments, $\mu_0, \mu_1, \cdots, \mu_N$ of an *unknown* probability density $G(x)$:

$$\mu_k \equiv \langle x^k \rangle \equiv \int_a^b x^k G(x)\, dx \quad (-\infty \leqq a < b \leqq +\infty), \tag{1.1}$$

estimate or bound the average of a *known* function $F_\tau(x)$:

$$\langle F_\tau(x) \rangle \equiv \int_a^b F_\tau(x)\, G(x)\, dx, \tag{1.2}$$

where $F_\tau(x)$ may depend on a parameter τ as well as upon x. This is accomplished by replacing the integral by a quadrature formula:

$$\langle F_\tau(x) \rangle = \sum_1^n w_i F_\tau(x_i) + \Delta \tag{1.3}$$

where the abscissas x_i and weights w_i are determined by the condition that they give the moments correctly:

$$\sum_{i=1}^n w_i x_i^k = \mu_k \quad (k = 0, \cdots, N). \tag{1.4}$$

When both a and b in (1.1) and (1.2) are finite, four distinct quadratures are useful: with no preassigned abscissas (Gauss), with one abscissa fixed at either a or b (Radau), or with abscissas fixed at both a and b (Lobatto). The number of abscissas and weights is chosen

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so that the moment constraints uniquely determine the weights and unassigned abscissas. The error term Δ can be expressed in terms of the unknown density function:

$$\Delta = \int_a^b F_\tau^{(n)}[\xi(x)] \prod_u \prod_p (x - x_u)^2(x - x_p)\, G(x)\, dx \tag{1.5}$$

where the index p runs over the preassigned abscissas (if any), the index u over the unassigned abscissas, and where $\xi(x)$ lies in the interval (a, b). If the derivatives $F_\tau^{(n)} \equiv (\partial^n F/\partial x^n)_\tau$, are of constant sign on (a, b), then the error Δ is of known sign and both upper and lower bounds on $\langle F_\tau(x)\rangle$ are determined from any given number of moments.

In the case when $F_\tau(x) = 1/(1 + x\tau)$ the average may be expanded as a series of Stieltjes, and the quadrature becomes a Padé approximant:

$$\langle F_\tau(x)\rangle = \int_a^b \frac{G(x)\,dx}{1 + x\tau} = \sum_0^\infty \mu_k(-x\tau)^k \cong \sum_1^n w_i\left(\frac{1}{1 + x_i\tau}\right). \tag{1.6}$$

If no abscissas are preassigned, the quadrature is the $[n - 1/n]$ Padé approximant to $\langle F_\tau(x)\rangle$; if one abscissa is fixed at $x = 0$, then the $[n - 1/n - 1]$ approximant is obtained.

All four of the quadratures above, as well as the Padé approximants and continued fractions to series of Stieltjes can be obtained if we know the *recursion coefficients*, α_k, β_k, for the *orthogonal polynomials*, $\pi_n(x)$, defined by $G(x)$:

$$\langle \pi_k \pi_\ell \rangle = \int_a^b \pi_k(x)\pi_\ell(x) G(x)\, dx = \delta_{k\ell}\langle \pi_k \pi_k \rangle \tag{1.7}$$

$$\pi_{k+1}(x) = (x - \alpha_k)\pi_k - \beta_k \pi_{k-1}(x) \quad (\pi_0 \equiv 1, \pi_{-1} \equiv 0). \tag{1.8}$$

Orthogonality guarantees that β_k is positive:

$$\langle \pi_k x \pi_{k-1}\rangle = \langle \pi_k \pi_k\rangle = \beta_k \langle \pi_{k-1}\pi_{k-1}\rangle \tag{1.9}$$

The recursion coefficients can be obtained from the power moments by the following variation of an algorithm attributed to Chebyshev [5, 17]. Consider the matrix Z with elements $Z_{k,\ell} = \langle \pi_k x^\ell \rangle$, which must be zero if $k > \ell$ and which satisfy $Z_{-1,\ell} = 0$, $Z_{0,\ell} = \mu_\ell$. Equation (9) implies that the elements of Z satisfy the recursion relation:

$$Z_{k+1,\ell} = Z_{k,\ell+1} - \alpha_k Z_{k,\ell} - \beta_k Z_{k-1,\ell}. \tag{1.10}$$

Given k rows of Z, then α_k and β_k are determined:

$$\begin{aligned} Z_{k+1,k-1} = 0 &\Rightarrow \beta_k = Z_{k,k}/Z_{k-1,k-1} \quad (\beta_0 \equiv \mu_0) \\ Z_{k+1,k} = 0 &\Rightarrow \alpha_k = Z_{k,k+1}/Z_{kk} - Z_{k-1,k}/Z_{k-1,k-1}. \end{aligned} \tag{1.11}$$

The rest of row $k + 1$ can then be obtained from (1.10). In this way the coefficients α_k, β_k can be generated recursively from the moments.

The Chebyshev algorithm has the advantage over Rutishauser's [13] QD and Gordon's [4] PD algorithms that it cannot fail as a result of symmetries in $G(x)$. It requires only the nonnegativity of $G(x)$. In practice it seems to be slightly more stable than either the QD or PD algorithms.

Once the recursion coefficients α_k, β_k are known, all four quadrature formulas can be determined stably and rapidly by diagonalization of a real, symmetric, tridiagonal matrix [2, 3, 18]. Continued fractions to series of Stieltjes can also be determined [4]. The *associated* continued fraction of even order to the series of Stieltjes $\sum_{n=1}^{\infty} \mu_n(-z)^n$ is just given by

$$A_n^e(z) = \frac{\beta_0}{1 + \alpha_0 z} - \frac{\beta_1}{1 + \alpha_1 z} - \frac{\beta_2}{1 + \alpha_2 z} - \cdots. \tag{1.12}$$

The coefficients in the corresponding continued fraction:

$$C(z) = \frac{c_0}{1} + \frac{c_1 z}{1} + \frac{c_2 z}{1} + \cdots,$$

are easily obtained recursively from α_k, β_k by the relations

$$\begin{aligned} c_0 &= \beta_0 = \mu_0, \quad & c_{2n} &= \beta_n / c_{2n-1}, \\ c_1 &= \alpha_0 = \mu_1/\mu_0, \quad & c_{2n+1} &= \alpha_n - c_{2n}, \end{aligned} \tag{1.13}$$

while the associated continued fraction of *odd* order is obtained by replacing the last α_n in (1.12) by c_{2n} in (1.13).

2. **Illustrative Example.** The estimation of averages by quadratures obtained from power moments is quite successful when relatively few moments are known. One example of a physical problem in which quadrature methods have proven useful is that of the harmonic solid [19, 20]. In this case, the density $G(x)$ is known analytically for only a few special cases [10] whereas substantial numbers of exact power moments can be computed for many cases [6–8, 15]. $G(x)$ always possesses singularities in slope (the van Hove singularities [16]) and may even have integrable divergences due to accidental symmetries [11, 12].

Some typical functions $F_r(x)$ which are of interest in the harmonic solids problem and the physical properties which they determine are the following:

$F_\tau(x)$	*Property*
$\ell n[(\sqrt{x}/2\tau)^{-1}\sinh(\sqrt{x}/2\tau)]$	free energy, $f(\tau)$
$(1/2)\sqrt{x}\coth(\sqrt{x}/2\tau)$	internal energy $u(\tau)$
$[(\sqrt{x}/2\tau)/\sinh(\sqrt{x}/2\tau)]^2$	heat capacity $C(\tau)$
$(1/2)\sqrt{x}$	zero point energy $u(0)$
$(1/2)\ell n\, x$	singular part of f

where τ is a normalized temperature. (τ is measured in units of the maximum frequency times Planck's constant, which is roughly in units of the Debye temperature of the solid.) Each of these functions has the property that its derivatives $F_\tau^{(n)}(x)$ are constant in sign on $x \in [0, 1]$ [19], so that rigorous bounds are obtained.

Gaussian quadratures determine the thermodynamic properties of harmonic solids with extreme precision. As an example, consider the cubic-close-packed (ccp) solid with nearest-neighbor interactions. A substantial number of moments have been calculated for this model by several investigators [6, 8, 15, 21]. The bounds to the zero point energy $u(0) = \langle(1/2)\sqrt{x}\rangle$ for this model from only 4 moments already agree to better than 4% [20]. With 10 moments, the fractional error is less than 1×10^{-3}; with 20 moments, 1×10^{-4}; and with 30 moments about 2×10^{-5}. For less singular functions the bounds are much tighter. Thirty moments determine $u(\tau)$ to better than 1 part in 10^{10} whenever τ is greater than .06, and 12 moments determine $u(\tau)$ to better than 1 part in 10^8 for $\tau \geqq 0.14$ [19].

Several points are worth emphasizing about the utility of the quadrature technique for this problem. First, the *same set* of abscissas and weights, x_i, w_i, serves for *all* of the thermodynamic functions, and for all temperatures. The thermodynamic properties are given as weighted sums of a few simple functions of temperature and are easily evaluated as functions of τ. Second, the quadratures give upper and lower bounds at all τ for most thermodynamic properties which are the *best bounds possible* given only the moments (This follows from the *constructive* nature of the bounds [19, 20]). Third, additional information about $G(x)$ in the form of series expansion coefficients near $x = 0$ can be incorporated into the procedure in order to improve the bounds. For example, the knowledge of three approximate series expansion coefficients for $G(x)/\sqrt{x}$ near $x = 0$ enabled us [20] to improve the bounds on $u(0)$ to an error of 3×10^{-7} from 20 moments and 1×10^{-8} from 30 moments, and to obtain a single simple quadrature for the heat capacity which is correct to better than 1 part in

10^7 at all temperatures. When many coefficients are known to high precision, averages even of singular functions such as $\ell n\, x$ and x^{-1} can be bounded both above and below with great precision [18, 19].

Difficulties with the quadrature technique arise, however, when attempts are made to use large numbers of power moments or limited precision arithmetic in the computation of quadratures, or when the function $F_\tau(x)$ is sufficiently rapidly varying. The transformation from power moments to orthogonal polynomial recursion coefficients is generally exponentially ill conditioned. In practice (for the harmonic solid) one or two significant figures are lost for each pair α_k, β_k determined. Even with 25-significant figure arithmetic, for example, the transformation breaks down at about μ_{35}. Even when the transformation does not break down completely, the recursion coefficients contain a steadily growing error which is propagated to the abscissas and weights.

An example of an average for which these problems arise is the momentum autocorrelation function for harmonic solids. The classical or high temperature limit of this function is just a Fourier transform of the frequency spectrum: $\langle \boldsymbol{p}(0) \cdot \boldsymbol{p}(t) \rangle = \langle \cos t\sqrt{x} \rangle$. Despite the fact that the derivatives of $F_t(x) = \cos(t\sqrt{x})$ are not constant in sign, bounds to $\langle \boldsymbol{p}(0) \cdot \boldsymbol{p}(t) \rangle$ can be obtained [22] which determine it accurately out to a time $t_{\max}$ which is *proportional* to the number of moments available: $t_{\max} \approx (4/e)N$. In addition, because of the rapidly oscillating nature of $\cos(t\sqrt{x})$ for large t, the average is more sensitive to errors in the abscissas and weights than are the thermodynamic properties.

3. **Modified Moments.** The reason for the ill-conditioned nature of the transformation from power moments to quadrature formulas is fairly obvious: the function x^n samples $G(x)$ only near $x = 1$ for large n. Averages of functions like $\cos(n\pi x)$ or suitably chosen polynomials which sample the entire interval would be preferable. Sack and Donovan [14] and Gautschi [1] have observed that polynomials $p_n(x)$ satisfying a *known* recursion relation:

$$(3.1) \qquad p_{k+1}(x) = (x - a_k)p_k(x) - b_k p_{k-1}(x) \quad (p_0 = 1 \quad p_{-1} = 0),$$

and orthogonal to a *known* density $H(x)$ which is nonzero on the same interval as $G(x)$ and is in some sense similar to it, provide a particularly suitable choice. Modified moments, defined as averages of these polynomials:

$$\nu_n \equiv \langle p_n(x) \rangle = \int_a^b p_n(x) G(x)\, dx \tag{3.2}$$

determine the recursion coefficients stably [1]. Unfortunately, the transformation from power moments to modified moments is then necessarily ill conditioned. Thus, we must either find a method for the direct computation of modified moments or find a way to carry out the ill-conditioned transformation from power moments to modified moments sufficiently accurately. Both of these approaches have proved successful for the harmonic solid problem.

The transformation from power moments to modified moments can be carried out recursively by construction of the matrix Y with elements $Y_{k,\ell} = \langle p_k x^\ell \rangle$ from its first row which consists of the power moments. From (3.1) it follows that the elements of Y satisfy the recursion relation

$$\begin{aligned} &Y_{k+1,\ell} = Y_{k,\ell+1} - a_k Y_{k,\ell} - b_k Y_{k-1,\ell} \\ &(Y_{-1,\ell} = 0,\ Y_{0,\ell} = \mu_\ell). \end{aligned} \tag{3.3}$$

Given N power moments, a triangular portion of Y can be constructed with the first N modified moments appearing in the first column. More generally any one set of modified moments ν_k corresponding to polynomials p_k with recursion coefficients a_k, b_k can be transformed to any other set ν_k' with corresponding p_k', a_k', b_k', by recursive construction of the matrix Y with elements $\langle p_k' p_\ell \rangle$ from its first row. Applying (3.1) first to the primed polynomials, then to the unprimed, we see that the elements of Y must satisfy the recursion relation

$$\begin{aligned} &Y_{k+1,\ell} = Y_{k,\ell+1} - (a_k' - a_k) Y_{k,\ell} - b_k' Y_{k-1,\ell} + b_k Y_{k,\ell-1} \\ &(Y_{k,-1} = Y_{-1,\ell} = 0;\quad Y_{0,\ell} = \nu_\ell,\quad Y_{k,0} = \nu_k') \end{aligned} \tag{3.4}$$

of which (3.3) is a special case.

For the harmonic solid problem, a very natural choice of modified moments can be found for which it is possible to carry out the transformation from power to modified moments entirely within the field of integer arithmetic so that exact modified moments can be easily obtained from exact power moments despite the ill conditioned nature of the problem. The density $H(x) = (8/\pi)[x(1-x)]^{1/2}$ $(0 \leqq x \leqq 1)$ is nonzero on the same interval as $G(x)$ and has similar behavior to $G(x)$ at the ends of the interval [9]. It defines the shifted Chebyshev polynomials of the second kind with recursion coefficients [cf. (3.1)] $a_k = 1/2$, $b_k = 1/16$, independent of k. (For the harmonic solid, these are the limiting values of α_k, β_k, respectively, in (1.8).) For solids with finite-ranged forces, it is possible to rescale the variable x so that all

of the moments as well as a_k and b_k become either integers or polynomials in force constant ratios with integer coefficients [18]. For the nearest-neighbor ccp solid considered in section 2, the appropriate scale factor, L, is 16. For the nearest-neighbor hexagonal-close-packed solid, the scale factor is $L = 48$. For solids with longer-ranged forces the scale factor is a polynomial (or multinomial) of degree one in the force constant ratios. Multiplication of μ_n by L^n results in an integer or a polynomial with integer coefficients, while a_k and b_k are scaled to $L\,a_k$, $(L/2)^2 b_k$.

The transformation (3.2) from power moments to modified moments has the computational advantage that the elements of Y along the diagonal connecting μ_n to ν_n never grow significantly larger than μ_n itself so that exact modified moments can be obtained whenever sufficient precision is available to represent the power moments exactly.

As an example, we compare in Table 1 the power moments and modified moments for the nearest-neighbor ccp solid. The modified moments are much smaller than the corresponding power moments. In fact, the envelope of the ratio $|\nu_n|/\mu_n$ falls off as 4^{-n} for large n. More precisely, $|\nu_n|/\mu_n = o[(1/4 + \epsilon)^n]$ for all $\epsilon > 0$. (Unpublished calculation). The transformation from power moments is thus exponentially ill conditioned. Only because we are able to carry out the transformation *exactly* do we obtain useful information.

The transformation from modified moments to the recursion coefficients α_k, β_k, can be carried out in a variety of ways. Gautschi [1] proceeded through the Gram matrix with elements $\langle p_k p_\ell \rangle$ by Cholesky factorization. We prefer a simpler route, very similar to that employed by Sack and Donovan [14] which is essentially a modification of the Chebyshev algorithm discussed in section 1. Consider the matrix Z with elements $Z_{k,\ell} = \langle \pi_k p_\ell \rangle$ which must be zero if $k > \ell$. The elements of Z satisfy the recursion relation (3.4) with $a_k' = \alpha_k$, $b_k' = \beta_k$ [cf. (1.10)]. Given k rows of Z, α_k and β_k are determined [cf. (1.11)]

$$
\begin{aligned}
Z_{k+1,k-1} = 0 \;&\Rightarrow \beta_k = Z_{k,k}/Z_{k-1,k-1} \quad (\beta_0 \equiv \mu_0) \\
Z_{k+1,k} = 0 \;&\Rightarrow \alpha_k = a_k + Z_{k,k+1}/Z_{k,k} - Z_{k-1,k}/Z_{k-1,k-1}.
\end{aligned} \tag{3.5}
$$

The rest of row $k + 1$ can then be generated using (3.4). This "modified Chebyshev algorithm" is closely related to Gautschi's method: if, instead of the Cholesky factorization into the product of a lower left triangular matrix and its transpose, one employs an $L - R$ factorization into a lower left triangular matrix L with *unit diagonal* and a right triangular matrix R, then $Z = R$.

Modified moments enjoy a number of significant advantages over power moments. They contain the same information as power moments, but much more efficiently. One evidence of this is their smaller size, noted above. Another, is that *approximate* modified moments can be transformed *stably* to power moments as well as to other modified moments via (3.4), whereas the transformation from power- to modified moments is exponentially ill conditioned. Most importantly the modified moments determine the recursion coefficients α_k, β_k and thereby the quadrature formulas with *extreme stability*. For example, when forty modified moments for the nearest-neighbor ccp solid were used to determine twenty α's and β's, there was no detectable buildup of error using 12-figure arithmetic. [By contrast, even with 25-figure arithmetic, no more than about 35 power moments could be used because of complete loss of accuracy.] Finally, the techniques developed by Wheeler and Gordon [19] for using additional information about $G(x)$ in the form of expansion coefficients can be incorporated into the modified moments technique with little loss in the extraordinary stability of the method [18].

Direct computation of modified moments for harmonic solids, without passing through the power moments, is also possible [21]. The computation of power moments proceeds by taking the trace of the nth power of the dynamical matrix, D [6, 7, 8, 9, 15]. Instead of taking powers of D, define a sequence of matrices by the recursion formula [cf. (3.1)],

$$P_{k+1} = (D - a_k 1)P_k - b_k P_{k-1} \quad (P_0 \equiv 1, P_{-1} = 0) \tag{3.6}$$

where 1 is the unit matrix. The modified moment ν_n is then given by the trace of P_n. We have obtained 40 exact modified moments for the nearest-neighbor ccp solid in this way, which is more than twice the number of power moments previously computed for this solid. More importantly, the direct computation of modified moments is *stable* when carried out in limited precision arithmetic. As a result, approximate modified moments can be calculated for solids in which the dynamical matrix depends on force constant ratios. We hope to extend the direct computation of approximate modified moments to systems with long-ranged forces where exact moments are difficult or impossible to obtain.

Modified moments appear to be a powerful tool for characterizing distribution functions. They determine quadrature formulas as well as Padé approximants and continued fraction to series of Stieltjes with great stability. It seems likely that they will prove useful in other problems of mathematical physics as well as the harmonic solid considered here.

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TABLE 1. Modified Moments and Power Moments for Nearest Neighbor ccp Solid

n	(a) $\nu_n \times 16^n$	(b) $\mu_n \times 16^n$
0	1	1
1	0	8
2	0	80
3	16	912
4	−16	11248
5	−224	145568
10	4.04×10^4	7.22×10^{10}
20	-5.63×10^9	3.04×10^{22}
30	-8.14×10^{15}	1.75×10^{35}
39	3.30×10^{21}	7.90×10^{44}

[a]Moments after ν_5 are rounded. Exact values for all modified moments up to ν_{39} are given in reference 21.

[b]Moments after μ_5 are rounded. Exact power moments can be computed from the exact modified moments. Isenberg [8] and Salsburg and Huckaby [15] have previously obtained the first twenty power moments exactly by other procedures. Forty exact power moments are available from the author on request.