JOURNAL OF COMPUTATIONAL PHYSICS 5, 125–138 (1970)

# Methods of Evaluating $N$-Dimensional Integrals with Polytope Bounds

W. G. RUDD,* Z. W. SALSBURG, AND L. M. MASINTER

*Department of Chemistry, Rice University, Houston, Texas 77001*

Received June 13, 1969

Three algebraic methods of evaluating integrals of the form,

$$\mathscr{I} = \int \cdots \int P(\mathbf{x}^N) \sum_{i=1}^{K} H\left(a_{i0} + \prod_{j=1}^{N} a_{ij}x_j\right) dx_1 ,..., dx_N ,$$

where $H(x)$ is the unit Heaviside function and $P(\mathbf{x}^N)$ is a polynomial in the $N$ integration variables are described. Emphasis is placed on computer implementation of the integration techniques.

## I. INTRODUCTION

In recent investigations of the statistical thermodynamics of rigid disk and sphere solids [1], we found it necessary to evaluate configuration space integrals of the form

$$\mathscr{I} = \int \cdots \int d\mathbf{x}^N \, P(\mathbf{x}^N) \prod_{i=1}^{K} H(L_i^{(N)}), \tag{1.1}$$

where $H(x)$ is the unit Heaviside function,

$$H(x) = \begin{cases} 1 & x \geqslant 0 \\ 0 & x < 0, \end{cases} \tag{1.2}$$

$P(\mathbf{x}^N)$ is a polynomial in the $N$ integration variables

$$\begin{aligned} \mathbf{x}^N &= (x_1 ,..., x_N) \quad \text{and} \\ L_i^{(N)} &= a_{i0} + \mathbf{a}_i^N \cdot \mathbf{x}^N, \end{aligned} \tag{1.3}$$

where the $\mathbf{a}_i^N$ are $N$ vectors of constants, $i = 1,..., K$. The $(N-1)$-dimensional hyperplanes defined in Eq. (1.3) enclose an $N$-dimensional polytope, $\mathscr{R}$, which is

* Present address: Department of Chemistry, State University of New York at Albany, Albany, New York.

the region of integration in Eq. (1.1). Since $\mathscr{I}$ must be finite, $\mathscr{R}$ is bounded, and, since $\mathscr{R}$ is the intersection of (convex) $N$-dimensional half-spaces, $\mathscr{R}$ is convex [2].

Numerical integration techniques for evaluating such integrals were rejected as impractical for the degree of accuracy we require. The methods described below are thus completely algebraic, with accuracy limited only by computer round-off error.

In Section II we outline the Bounds Pair method, which is perhaps the most straight-forward procedure, and a geometrical approach. The Parts method is described in detail in Section III. A recently developed means of avoiding cumbersome polynomial manipulation is to be found in Section IV, followed by a discussion of practical considerations in Section V. The Appendix contains the evaluation of a simple integral by all the techniques described herein.

## II. The Bounds Pair Method and a Geometrical Approach

### *The Bounds Pair Method*

After integrating over the first $i$ variables, Eq. (1.1) has the form

$$\mathscr{I} = \sum_q \int \cdots \int d\mathbf{x}^{N-i}\, P_q(\mathbf{x}^{N-i}) \prod_{j=1}^{K_q} H(L_{j,q}^{(N-i)}), \tag{2.1}$$

where the sum includes all the polynomials and associated products of Heaviside functions which have arisen from integration over the first $i$ variables. In order to integrate over $x_{i+1}$ for a given $q$, one now separates out those Heaviside functions which define a bound on $x_{i+1}$. One then integrates over $x_{i+1}$ using all possible pairs of upper and lower bounds on $x_{i+1}$ in succession. In principle, for each pair of bounds, one obtains a pair of new polynomials and corresponding products of Heaviside functions, each involving $N - i - 1$ variables. That is, each term in the sum (2.1) leads to a new sum of the form (2.1), with $N - i$ replaced by $N - i - 1$. Some of the terms in this new sum, which form the origins of new branches in the tree structure thus formed, can be eliminated using the testing procedures described in Section III. The reader may find it helpful to refer to the Appendix for a sample calculation.

### *A Geometrical Approach*

A simplex is the simplest possible $N$-dimensional polytope; its vertices are $N + 1$ points, not all of which lie in an $(N - 1)$-plane. The $N$ volume, or content, of a simplex is given by [3]

$$V_s = (N!)^{-1} \left| \det \begin{pmatrix} \mathbf{r}_1 \\ \vdots \\ \mathbf{r}_N \end{pmatrix} \right| \tag{2.2}$$

where $\mathbf{r}_j$ is a vector from one of the vertices of the simplex, taken as the origin, to the $j$th vertex. C. A. Rogers [4] has shown that it is possible to cover a closed convex polytope with simplices. An algorithm based on his proof was coded for the Rice computer, but the method was discarded as impractical [5].

## III. Integration by Parts

### General Description

The result of integrating over $i$ variables in (1.1) is again of the form (2.1). Consider

$$\mathscr{I}_p = \int \cdots \int d\mathbf{x}^{N-i}\, P_p(\mathbf{x}^{N-i}) \prod_{j=1}^{K_p} H(L_{j,p}^{(N-i)}), \tag{3.1}$$

the $p$th term in (2.1). In the usual formula

$$\int_a^b u\, dv = uv \Big|_a^b - \int_a^b v\, du \tag{3.2}$$

for integration by parts, we let

$$u = \prod_{j=1}^{K_p} H(L_{j,p}^{(N-i)}) \tag{3.3}$$

and

$$dv = P_p(\mathbf{x}^{N-i})\, dx_{i+1} \tag{3.4}$$

Using [6]

$$dH(ax) = a\, \delta(ax)\, dx, \tag{3.5}$$

where $\delta(x)$ is the Dirac delta function, and

$$H(x)\, \delta(x) \equiv \delta(x), \tag{3.6}$$

we find (dropping the subscript $p$)

$$du = \sum_{\ell=1}^{K} a_{\ell,i+1}\, \delta(L_\ell^{(N-i)}) \prod_{j=1}^{K} H(L_j^{(N-i)})\, dx_{i+1}, \tag{3.7}$$

and

$$v = \tilde{P}(\mathbf{x}^{N-i}), \tag{3.8}$$

in which $\tilde{P}$ is the indefinite integral resulting from integrating $P$ over $x_{i+1}$. Since the polytope is a bounded region of space,

$$uv \Big|_{-\infty}^{\infty} \equiv 0. \tag{3.9}$$

Hence

$$\mathscr{I}_p = -\sum_{\ell=1}^{K_p} a_{\ell,i+1} \int \cdots \int d\mathbf{x}^{N-i-1}\, dx_{i+1}\, \delta(L_{\ell,p}^{(N-i)}) \prod_{j=1}^{K_p} H(L_{j,p}^{(N-i)})\, \tilde{P}(\mathbf{x}^{N-i}). \tag{3.10}$$

Using the fact that

$$\int_{-\infty}^{\infty} f(x)\, \delta(ax)\, dx = f(0)/|\, a \,| \tag{3.11}$$

we do the $x_{i+1}$ integration to obtain

$$\mathscr{I}_p = -\sum_{\ell=1}^{K_p} \sin(a_{\ell,i+1}) \int \cdots \int d\mathbf{x}^{N-i-1} \prod_{j=1}^{K_p} H(L_{j,\ell}^{(N-i-1)})\, \tilde{P}_\ell(\mathbf{x}^{N-i-1}) \tag{3.12}$$

where we have defined

$$\sin(x) = \begin{cases} x/|\, x \,|, & x \neq 0 \\ 0, & x = 0, \end{cases} \tag{3.13}$$

and $\tilde{P}_\ell(\mathbf{x}^{N-i-1})$ and the $L_{j,\ell}^{(N-i-1)}$ are the results of setting

$$x_{i+1} = -\frac{1}{a_{\ell,i+1}} \left(a_{\ell,0} + \sum_{k=i+2}^{N} a_{\ell,k} x_k\right) \tag{3.14}$$

into the corresponding terms in (3.10).

Hence, the integration over $x_1$ yields, in general, several new $(N-1)$-dimensional integrals of the form (1.1), each with its own polynomial and corresponding set of Heaviside function bounds. Each of these yields, upon integration over $x_2$, a new set of integrals of the form (1.1). The result is a tree structure with $N$ levels and many branches. Some of the branches can be eliminated immediately, reducing the complexity of the calculations.

Thus, the Parts integration procedure involves three basic steps:

(1) indefinite integration of the current polynomial;

(2) substitution of the value of the integration variable, obtained from the delta functions, into the polynomial and Heaviside functions; and

(3) testing of the resulting sets of bounds to eliminate redundant ones and to determine if the remaining bounds enclose a nonzero volume.

The procedure in steps (1) and (2) is straightforward; we now describe the testing methods.

### *Elimination of Redundant Bounds and Noncontributing Cases*

After integrating over $i$ variables down one branch of the tree, the resulting bounds are of the form

$$\prod_{\ell=1}^{m} H(a_{\ell,0} + \sum_{k=i+1}^{N} a_{\ell,k}x_k). \tag{3.15}$$

For the purpose of discussion, and for machine calculations, it is convenient to regard each bound as forming a column in the matrix

$$\mathbf{A} = \begin{bmatrix} a_{1,i+1} & a_{2,i+1} & \cdots & a_{m,i+1} \\ a_{1,i+2} & & & \vdots \\ \vdots & \vdots & & \\ a_{1,N} & & \cdots & a_{m,N} \\ a_{1,0} & a_{2,0} & \cdots & a_{m,0} \end{bmatrix}, \tag{3.16}$$

in which the constants $a_{\ell,0}$ form the last row.

The tests, in the order in which they are applied, are as follows [7]:

(1) CBNDS—check for "constant" bounds;

(2) PARCH—check for parallel bounds; and

(3) LP —linear programming test.

The result of substitution into the Heaviside functions in the preceding levels of integration may leave one or more bounds with $a_{\ell,k} = 0, k = i + 1,..., N$; hence the result is $H(a_{\ell,0})$. CBNDS detects these conditions and, if $a_{\ell,0} \geqslant 0$, the bound is eliminated as being redundant [8]; if $a_{\ell,0} < 0$, the entire case is thrown out, since the Heaviside function is zero.

PARCH tests for pairs of bounds which form parallel planes. If a pair of parallel planes is detected, there are three possibilities:

(1) The pair of bounds restricts the range of integration to lie between the two planes (Fig. 1a). Both bounds are then valid, and, indeed, necessary.

(2) The pair of bounds restricts the range of integration to lie on the same side of the parallel planes (Fig. 1b). The bound which restricts the range of integration the most is retained, the other is eliminated as being redundant [9].

(3) The bounds restrict the range of integration to regions on opposite sides of the parallel planes (Fig. 1c). It is obvious that this case can contribute nothing further to the integral, and the entire case and the branches it generates are eliminated.

Thus, CBNDS and PARCH eliminate constant and redundant bounds and some cases which can contribute nothing further to the integral. If the current set of

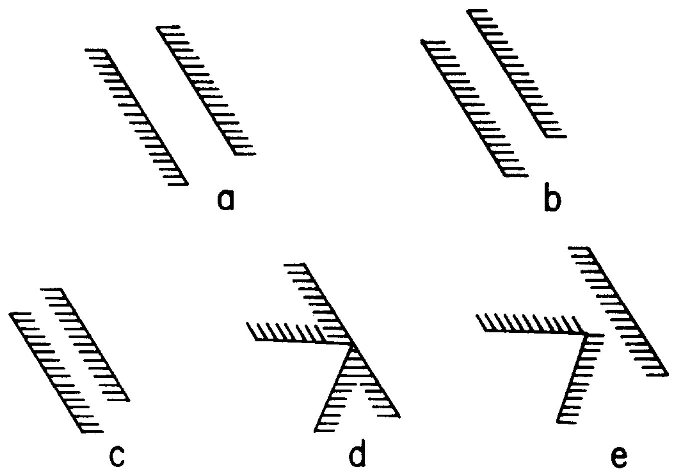


FIG. 1. Illustrating the configurations of bounds detected by the parallel bounds and linear programming tests. The range of integration lies on the unshaded sides of the planes in each case.

bounds passes these tests, we apply the linear programming test, which detects situations such as in Figs. 1d and 1e, which are not detectable by the other means described above.

The basic problem is: given a set of linear constraints of the form,

$$\sum_{j=1}^{n} a_{ij}x_j + a_{i,0} \geqslant 0, \qquad i = 1,..., m, \tag{3.17}$$

determine whether or not the polytope defined by these constraints has a nonzero content. In order to do this, we insert an additional variable, $x_0$, into each of the above constraints to find

$$\sum_{j=1}^{n} a_{ij}x_j + a_{i,0} \geqslant x_0 \tag{3.18}$$

or

$$\sum_{j=1}^{n} (-a_{ij})\, x_j + x_0 \leqslant a_{i,0}, \qquad i = 1,..., m. \tag{3.19}$$

Now we maximize $x_0$ (minimize $-x_0$) subject to the constraints (3.19) and note that if $\max(x_0) > 0$, the content of the polytope defined by (3.18) must be nonzero, while if $\max(x_0) \leqslant 0$, the result of integration over $x_1 ,..., x_n$ will vanish.

The problem of maximizing $x_0$ subject to the constraints (3.19) is simply the dual problem to the usual (primal) linear programming problem [10]. The first feasible solution for this extended problem (3.19) is chosen to be

$$x_0 = \min_i \{a_{i0}\}, \qquad x_1 = \cdots = x_n = 0. \tag{3.20}$$

For our purposes, it is not always necessary to complete the entire maximization procedure for $x_0$. The linear programming subroutine [11] is exited whenever the current value of $x_0$ is positive nonzero (indicating nonzero volume) or when the maximum value of $x_0$ is found to be negative. The test described above can be used as a test for a feasible solution in the general linear programming problem.

We have described three basic methods for computing integrals of the form (5.1). A discussion of the relative merits of these methods is to be found in Section V. We turn now to an investigation of a recently discovered means of avoiding the cumbersome and time-consuming polynomial manipulations which arise in the application of the Bounds Pair and the Parts integration procedures.

## IV. Exponential Polynomials

For the present, we let the polynomial $P(\mathbf{x}^N) = 1$ in Eq. (1.1) [12]. We then have

$$\mathscr{I} = \int \cdots \int d\mathbf{x}^N \prod_{j=1}^{K} H(L_j^{(N)}) = \lim_{S\to 0} \int \cdots \int e^{S\boldsymbol{\alpha}^N \cdot \mathbf{x}^N} \prod_{j=1}^{K} H(L_j^{(N)})\, d\mathbf{x}^N, \tag{4.1}$$

where $\boldsymbol{\alpha}^N$ is an $N$ vector of arbitrary, nonzero constants, $S$ is a real number, and the $L_j^{(N)}$, as defined in Eq. (1.3), form the bounding planes of the convex polytope which is the bounded region of integration $\mathscr{R}$. Upon integrating over $x_1$ in the right side of Eq. (4.1), we have, using the Parts integration procedure [see Eq. (3.10)]

$$\mathscr{I} = -\lim_{S\to 0} \sum_{\ell=1}^{K} \frac{\operatorname{sgn}(a_{\ell,1})}{S\alpha_1}\, e^{-S(a_{\ell,0}/a_{\ell,1})\alpha_1} \int \cdots \int d\mathbf{x}^{N-1}\, e^{S\boldsymbol{\alpha}_\ell^{N-1}\cdot\mathbf{x}^{N-1}} \prod_{j=1}^{K} H(L_{j,\ell}^{(N-1)}) \tag{4.2}$$

$$= \lim_{S\to 0} \mathscr{I}(S) \tag{4.3}$$

where $\boldsymbol{\alpha}_\ell^{(N-1)}$ is the $(N-1)$ vector of constants which result from setting

$$x_1 = -\frac{1}{a_{\ell,1}} \left(a_{\ell,0} + \sum_{k=2}^{N} a_{\ell,k} x_k\right) \tag{4.4}$$

into the exponential in Eq. (4.1) for each $\ell$ in the sum (4.2) and the $L_{j,\ell}^{(N-1)}$ are obtained similarly. The remaining $(N-1)$-dimensional integrals in (4.2) are again of the form of Eq. (4.1).

The result of integration over all $N$ variables in (4.1) is thus

$$\mathscr{I} = \lim_{S\to 0} \sum_{\tau} \frac{c_\tau \, e^{S\mathbf{q}_\tau^{(0)}\cdot\boldsymbol{\alpha}^N}}{S^N \prod_{j=1}^{N} (\mathbf{q}_\tau^{(j)} \cdot \boldsymbol{\alpha}^N)}, \tag{4.5}$$

where $\mathbf{q}_\tau^{(0)}$ is an $N$ vector of constants, $\mathbf{q}_\tau^{(j)}$ is an $N$ vector of constants, the last $N - j$ of which are zero, and $c_\tau$ is a constant depending on the coefficients in the Heaviside functions.

At first glance, it appears that the limit (4.5) does not exist. However, since we know $\mathscr{I}$ to be finite, all divergent terms in a Maclauren series expansion of the *sum* must cancel, provided that none of the $\mathbf{q}_\tau^{(j)} \cdot \boldsymbol{\alpha}^N = 0$. The latter possibility can be avoided by proper choice of the initial vector $\boldsymbol{\alpha}^N$ [13].

In order to evaluate the limit (4.3) we apply the residue theorem, with the simple result

$$\mathscr{I} = \frac{1}{2\pi i} \oint_\Gamma \frac{\mathscr{I}(S)}{S}\, dS = \frac{1}{N!} \sum_\tau c_\tau \frac{(\mathbf{q}_\tau^{(0)} \cdot \boldsymbol{\alpha}^N)^N}{\prod_{j=1}^{N} (\mathbf{q}_\tau^{(j)} \cdot \boldsymbol{\alpha}^N)}. \tag{4.6}$$

For some applications [14], it is desirable to find polynomial expressions for the results of integrals of the form (1.1) after integrating over just $i < N$ variables. The exponential polynomials can be transformed into the usual polynomial form through

$$P(\mathbf{x}^{N-i}) = \frac{c}{i!} \frac{(\mathbf{q}^{(0)} \cdot \boldsymbol{\alpha}^N)^i}{\prod_{j=1}^{i} (\mathbf{q}^{(j)} \cdot \boldsymbol{\alpha}^N)}, \tag{4.7}$$

where the $\mathbf{q}^{(j)}$ are defined as above and $\mathbf{q}^{(0)}$ is an $N$ vector of the form

$$\mathbf{q}^{(0)} = (b_1, b_2, ..., b_i, b_{i+1}x_{i+1}, ..., b_N x_N), \tag{4.8}$$

where the $b_j$ are constants.

Finally, for a nonconstant polynomial $P(\mathbf{x}^N)$ in (1.1), such as

$$P(\mathbf{x}^N) = \sum_j a_j \prod_{i=1}^{N} x_i^{n_{ij}} \tag{4.9}$$

the integral $\mathscr{I}$ can be computed as [15]

$$\mathscr{I} = \lim_{S\to 0} \sum_j a_j \prod_{i=1}^{N} \frac{\partial^{n_{ij}}}{\partial \alpha_i^{n_{ij}}} \int \cdots \int \frac{e^{S\boldsymbol{\alpha}^N \cdot \mathbf{x}^N}}{S^{n_{ij}}} \prod_{l=1}^{K} H(L_l^{(N)})\, d\mathbf{x}^N. \tag{4.10}$$

Hence

$$\mathscr{I}(S) = \sum_j a_j \prod_{i=1}^{N} \frac{\partial^{n_{ij}}}{\partial \alpha_i^{n_{ij}}} \sum_\tau c_\tau \frac{e^{S\mathbf{q}_\tau^{(0)}\cdot\boldsymbol{\alpha}^N} S^{-N-n_{ij}}}{\prod_{\ell=1}^{N} (\mathbf{q}_\tau^{(\ell)} \cdot \boldsymbol{\alpha}^N)}, \tag{4.11}$$

and the limit $S \to 0$ can be obtained from the residue theorem.

It is interesting to note that the final answers are independent of the choice of $\boldsymbol{\alpha}^N$. This is related to the fact that the choice of the contour $\Gamma$ in Eq. (4.6) is arbitrary, so long as $\Gamma$ encloses the point $S = 0$.

## V. Practical Considerations

We have described three basic methods of handling the bounds in integrals of the form (1.1) and have indicated a means by which one can avoid polynomial manipulations in computing such integrals. In this final section we discuss some aspects of our experience in computer implementation of these algorithms.

All three of the basic procedures described above have been coded and run on the Rice computer. The geometrical approach was discarded as being totally impractical; it was estimated that one of the simpler polytopes of interest contained more than one billion simplices [16].

The Bounds Pair method was the first to be programmed. Using this method, a relatively simple integral, involving nine variables with thirty-five bounding planes, required approximately two hundred hours computing time [17]. The most complicated case then under consideration was run for about fifty hours with no nonzero contributions. The addition of the linear programming test to this package reduced the running time for the simple case described above to about fifty hours.

We next coded the Parts method with the linear programming test, and found the normal running time to be reduced by a factor of five.

Finally, one can sometimes split a complicated cluster into two "loosely connected" pieces, obtaining the integral as a function of the variables common to both pieces. One then multiplies the resulting polynomials and Heaviside functions together and integrates over the remaining variables. Hence, for example, instead of a single nine-dimensional integral, one computes perhaps five thousand three-dimensional integrals.

The two methods we have actually used, the Bounds Pair and the Parts methods, require large and variable memory allocation for the polynomials which arise in the intermediate computations. In order to do these calculations, a dynamic storage allocation system is necessary. Such a system, called STEX, is available at the Rice computer, and is ideally suited for our calculations. Under STEX control, areas of storage no longer needed by the program are freed for use in later calculations.

When necessary, the free space is compacted into one large block, to facilitate the finding of available space.

In order to eliminate the time wasted in unnecessary polynomial manipulations and to make it possible to carry out these calculations on a computer with essentially fixed storage allocation, one of us (Masinter) has recently coded the Parts method with exponential polynomials for the Burroughs 5500 computer at Rice University. The recursive nature of the Algol system is well suited to the inherently recursive procedures described above. Unfortunately, the difference in speeds of the two computers prohibits an exact estimate of the improved efficiency of the exponential polynomial procedure, but we feel that running times for complicated integrals should be reduced by a factor of five.

In summary, we have tried several methods of evaluating, algebraically, integrals of the form (5.1). The Parts procedure with exponential polynomials is the most efficient algorithm we have yet been able to devise.

## Appendix

In order to illustrate the integration techniques described above, we apply each of the methods to a very simple example (Fig. 2):

$$\mathscr{I} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_1\, dx_2\, H(1 - x_1)\, H(1 + x_1)\, H(1 - x_2)\, H(1 + x_2) \\ \times H(1 - x_1 + x_2)\, H(1 + x_1 - x_2). \tag{A-1}$$

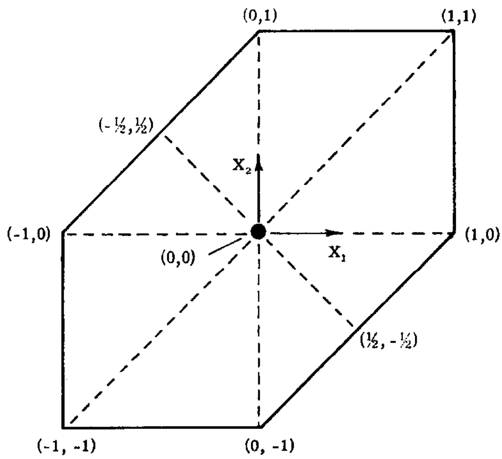


FIG. 2. The region of integration for Eq. (A-1). The dashed lines partition the region into simplices.

This example is too simple to permit a comparison of the relative merits of the integration techniques.

*The Bounds Pair Method*

The bounds on $x_1$ are

$$\left.\begin{matrix} -1 \\ x_2 - 1 \end{matrix}\right\} \leqslant x_1 \leqslant \left\{\begin{matrix} 1 \\ x_2 + 1 \end{matrix}\right. \tag{A-2}$$

or

$$\begin{array}{rcl} -1 \leqslant x_1 & \text{if} & x_2 \leqslant 0 \\ x_2 - 1 \leqslant x_1 & \text{if} & x_2 > 0 \\ 1 \geqslant x_1 & \text{if} & x_2 > 0 \\ x_2 + 1 \geqslant x_1 & \text{if} & x_2 \leqslant 0. \end{array} \tag{A-3}$$

Thus we have

$$\mathscr{I} = \int_{-1}^{1} dx_2 \Big[\int_{-1}^{1} dx_1\, H(-x_2)\, H(x_2) + \int_{-1}^{x_2+1} dx_1\, H(-x_2)$$
$$+ \int_{x_2-1}^{1} dx_1\, H(x_2) + \int_{x_2-1}^{x_2+1} dx_1\, H(x_2)\, H(-x_2)\Big]. \tag{A-4}$$

Since

$$H(x)\, H(-x) \equiv 0,$$

the integration over $x_1$ yields

$$\mathscr{I} = \int_{-1}^{0} (2 + x_2)\, dx_2 + \int_{0}^{1} (2 - x_2)\, dx_2 = 3, \tag{A-5}$$

as expected.

Thus the $x_1$ integration yields two contributing branches, one for positive $x_2$ and one for negative $x_2$. If this example were a more complicated integral in a higher number of dimensions, integration over $x_2$ would yield, in general, several new branches for each of the two branches generated by the $x_1$ integral.

*The Geometrical Method*

Reference to Fig. 2 shows that the area of the figure is one half the sum of the absolute values of the following determinants (Eq. 2.2):

$$\begin{vmatrix} \frac{1}{2} & -\frac{1}{2} \\ 1 & 0 \end{vmatrix}, \quad \begin{vmatrix} \frac{1}{2} & -\frac{1}{2} \\ 0 & -1 \end{vmatrix}, \quad \begin{vmatrix} 0 & -1 \\ -1 & -1 \end{vmatrix}, \quad \begin{vmatrix} -1 & 0 \\ -1 & -1 \end{vmatrix}$$
$$\begin{vmatrix} -\frac{1}{2} & \frac{1}{2} \\ -1 & 0 \end{vmatrix}, \quad \begin{vmatrix} -\frac{1}{2} & \frac{1}{2} \\ 0 & 1 \end{vmatrix}, \quad \begin{vmatrix} 0 & 1 \\ 1 & 1 \end{vmatrix}, \quad \begin{vmatrix} 1 & 0 \\ 1 & 1 \end{vmatrix}. \tag{A-6}$$

The general procedure for partitioning an $N$-dimensional polytope into simplices is too lengthy to describe here.

*Integration by Parts*

In this case, Eq. (3.10) becomes

$$\mathscr{I} = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\, B(x_1, x_2)[\delta(1 - x_1) - \delta(1 + x_1) + \delta(1 - x_1 + x_2) - \delta(1 + x_1 - x_2)], \tag{A-7}$$

where

$$B(x_1, x_2) = x_1 H(1 - x_1)\, H(1 + x_1)\, H(1 - x_2)\, H(1 + x_2) \times H(1 - x_1 + x_2)\, H(1 + x_1 - x_2). \tag{A-8}$$

The $x_1$ integration yields

$$\begin{aligned}\mathscr{I} = \int_{-\infty}^{\infty} dx_2[&H(0)\, H(2)\, H(1 - x_2)\, H(1 + x_2)\, H(x_2)\, H(2 - x_2)\\ &+ H(2)\, H(0)\, H(1 - x_2)\, H(1 + x_2)\, H(2 + x_2)\, H(-x_2)\\ &+ (1 + x_2)\, H(-x_2)\, H(2 + x_2)\, H(1 - x_2)\, H(1 + x_2)\, H(0)\, H(2)\\ &+ (1 - x_2)\, H(2 - x_2)\, H(x_2)\, H(1 - x_2)\, H(1 + x_2)\, H(2)\, H(0)].\end{aligned} \tag{A-9}$$

Application of the CBNDS test removes all Heaviside functions whose arguments are constants:

$$\begin{aligned}\mathscr{I} = \int_{-\infty}^{\infty} dx_2\, H(1 - x_2)\, H(1 + x_2)[&H(x_2)\, H(2 - x_2) + H(2 + x_2)\, H(-x_2)\\ &+ (1 + x_2)\, H(-x_2)\, H(2 + x_2) + (1 - x_2)\, H(2 - x_2)\, H(x_2)].\end{aligned} \tag{A-10}$$

PARCH removes all redundant parallel bounds, with the result

$$\begin{aligned}\mathscr{I} &= \int_{-\infty}^{\infty} dx_2[H(x_2)\, H(1 - x_2) + H(1 + x_2)\, H(-x_2)\\ &\qquad + (1 + x_2)\, H(-x_2)\, H(1 + x_2) + (1 - x_2)\, H(x_2)\, H(1 - x_2)]\\ &= \int_{-1}^{0} (2 + x_2)\, dx_2 + \int_{0}^{1} (2 - x_2)\, dx_2 = 3\end{aligned} \tag{A-11}$$

*Exponential Polynomials*

Let $\boldsymbol{\alpha}^2 = (1, \pi)$. Then Eq. (4.2) becomes

$$\mathscr{I}(S) = \int_{-\infty}^{\infty} \frac{dx_2}{S} [H(x_2)\, H(1 - x_2)\, e^{S(1+\pi x_2)} - H(1 + x_2)\, H(-x_2)\, e^{S(-1+\pi x_2)}$$
$$+ H(-x_2)\, H(1 + x_2)\, e^{S(1+(1+\pi)x_2)} - H(x_2)\, H(1 - x_2)\, e^{S(-1+(1+\pi)x_2)}]. \tag{A-12}$$

The $x_2$ integral yields

$$\mathscr{I}(S) = \frac{1}{S^2} \Big[ \frac{1}{\pi} (e^{S(1+\pi)} - e^S - e^{-S} + e^{-S(1+\pi)})$$
$$+ \frac{1}{1+\pi} (e^S - e^{-\pi S} - e^{S\pi} + e^{-S}) \Big], \tag{A-13}$$

and application of the residue theorem gives the desired result.

## Acknowledgments

Much of this work was carried out with the financial support of the Robert A. Welch Foundation of Houston, Texas, the National Science Foundation through Grant GP-6447, and the Phillips Petroleum Company. The U. S. Atomic Energy Commission, through Contract AT-(40-1)-1825, The Shell Development Company, and the Humble Oil Company provided funds for the original construction of the Rice Computer. The U. S. Atomic Energy Commission, through Contract AT-(40-1)-2572, has supported a research program that has produced improvements in hardware and solftware which greatly increased the power of the Rice Computer for these calculations. We also wish to thank the staffs of the Rice Computer and the Burroughs 5500 for their invaluable assistance.

## References

1. See, for example, W. G. Rudd, Z. W. Salsburg, A. P. Yu, and F. H. Stillinger, Jr., *J. Chem. Phys.* **49**, 4857 (1968).
2. For a more complete discussion of the nature of $R$, see Frank H. Stillinger, Jr., and Zevi W. Salsburg, Limiting polytope geometry for rigid rods, disks, and spheres, (to be published).
3. See, for example, P. M. Y. Sommerville, "An Introduction to the Geometry of $N$ Dimensions," p. 124, Dover Publications, Inc., New York, 1958.
4. C. A. Rogers, "Packing and Covering," Cambridge University Press, Cambridge, England, 1964.
5. The reviewer has pointed out that Stroud [*Mathematics of Computation* **18**, 590 (1964)] has given formulas for the integrals of monomials over a standard $N$-simplex. Stroud's results can be extended to include integrals of arbitrary polynomials $P(\mathbf{x}^N)$ as in Eq. (1.1).

6. Eq. (3.5) is to be interpreted in the sense of symbolic differentiation as in B. FRIEDMAN, "Principles and Techniques of Applied Mathematics," pp. 137–143, John Wiley and Sons, Inc., New York, 1956.
7. The names are those of the computer programs written to carry out the tests.
8. The elimination of these bounds is not logically necessary, but does save memory space and computer time.
9. Observe that, if both bounds were retained, CBNDS would later eliminate all results which arose from using the redundant bound.
10. See, for example, SAUL I. GASS, "Linear Programming Methods and Applications," McGraw-Hill, Inc., New York, 1958; G. B. DANTZIG, "Linear Programming and Extension," Princeton University Press, Princeton, N. J.; W. W. COOPER, A. HENDERSON, AND A. CHARNES, "An Introduction to Linear Programming," John Wiley and Sons, Inc., New York, 1953.
11. G. SITTON has coded a modified version of the revised Simplex algorithm for the Rice computer.
12. With $P(\mathbf{x}^N) = 1$, $\mathscr{I}$ is simply the content of the polytope $\mathscr{P}$.
13. In practice, we use $\alpha_i = (ke)^i$, which insures that the contour $\Gamma$ does not cross any poles in the integrand of (4.6). We chose $k$ to be a rational constant such that $k^N$ is of the order of magnitude of the value of $\mathscr{I}$. This is done to minimize round-off error. Thus we can do integrals in which the coefficients in the $L_j^{(N)}$ are algebraic numbers.
14. For example, RUSSELL D. LARSEN, AND Z. W. SALSBURG, *J. Chem. Phys.* **45**, 4190 (1966).
15. Eq. (4.10) arises from writing

$$P(\mathbf{x}^N)\, e^{S\alpha^N\cdot\mathbf{x}^N} = \sum_j a_j \prod_{i=1}^{N} S^{-n_{ij}}(\partial^{n_{ij}}/\partial\alpha^{n_{ij}})\, e^{S\alpha^N\cdot\mathbf{x}^N}$$

and interchanging the processes of integration and differentiation.
16. For a discussion of the surprising complexity of these polytopes, see [2].
17. The computer times quoted here are for the Rice computer, which is comparable in speed to the IBM 7040.