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On some definite multiple integrals

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Abstract. We study definite integrals over the ordinary three-dimensional space of $\prod_{ij} f(r_{ij}) \prod_j W(r_j)$, where $f(r_{ij})$ is a function only of the distance r_{ij} between points $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ and $W(r)$ is either a Gaussian or any other function which ensures the convergence of the integral. No analytical formula for them in general is known at present. The method is based on a multipole expansion for angular integrations and a transfer matrix approach for radial integrations. It can be generalized for any number of dimensions. A detailed study is presented for the case of $f(r) = r$ and $W(r) = \exp(-r^2/2)$, for three and one dimensions. To illustrate the generality of the method, the same integrals in one dimension are calculated with $W(r)$ as a step function. Comparison with the analytical solutions then provides a family of identities.

1. Introduction

Let

$$\overline{F} = \int \mathrm{e}^{-(r_1^2+r_2^2+\cdots)/2} F(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots) \prod_j \frac{\mathrm{d}^3\boldsymbol{r}_j}{(2\pi)^{3/2}} \tag{1.1}$$

where $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots,$ are vectors in the ordinary three-dimensional space, the function $F(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots)$ is some product of functions $\prod_{ij} f(r_{ij})$ depending only on the distances $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$, the integral is taken over all the space, and the normalization is chosen such that $\overline{1} = 1$. Zeische came across the particular integrals [1]

$$\begin{aligned} &X_1 = \overline{r_{12}} = \frac{4}{\sqrt{\pi}} && X_2 = \overline{r_{12}r_{23}} = 2 + \frac{6\sqrt{3}}{\pi} \\ &X_3 = \overline{r_{12}r_{23}r_{34}} = ? && X_n = \overline{r_{12}r_{23}\ldots r_{n\,n+1}} = ? \end{aligned} \tag{1.2}$$

$$\begin{aligned} &Y_2 = \overline{r_{12}r_{21}} = 6 && Y_3 = \overline{r_{12}r_{23}r_{31}} = ? \\ &Y_4 = \overline{r_{12}r_{23}r_{34}r_{41}} = ? && Y_n = \overline{r_{12}r_{23}r_{34}\ldots r_{n1}} = ? \end{aligned} \tag{1.3}$$

If one replaces the r_{ij} by an even power of them, then the integrations are simpler [1].

Doing a multipole expansion in terms of spherical harmonics one can do angular integrations. Only radial integrations then remain, which can be reduced to the solutions of Fredholm integral equations. Curiously, the problem is less difficult in d dimensions when d is odd, than for even dimensions where it is more difficult. We have not been able to solve the integral equations. Radial integrations can be done by direct calculation with increasing complexity as n number of vectors increases. There seems to be no simple closed formula for X_n or Y_n. The kernels of the integral equations play a role similar to a transfer matrix

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as, for example, in the study of the Ising model in statistical mechanics. These kernels are real symmetric and the traces of their first few powers can easily be computed. The largest eigenvalues dominate which yield the approximate formulae

$$X_n = A_1\lambda_1^n(0) + A_2\lambda_2^n(0) + A_3\lambda_3^n(0) \tag{1.4}$$

$$Y_n = \lambda_1^n(0) + \lambda_2^n(0) + \lambda_3^n(0) + 3\lambda_1^n(1) \tag{1.5}$$

where the constants have the approximate values

$$A_1 = 0.965\,282 \qquad A_2 = 0.033\,892 \qquad A_3 = 0.000\,712 \tag{1.6}$$

$$\lambda_1(0) = 2.344\,693 \qquad \lambda_2(0) = -0.192\,339 \qquad \lambda_3(0) = -0.017\,291$$
$$\lambda_1(1) = -0.387\,100. \tag{1.7}$$

Such integrals can conveniently be represented by graphs. Thus X_n is an open chain with n links while Y_n is a loop with n links. All angular integrations can be performed by our method of multipole expansion for graphs having either no loop (tree structure) or one loop. For graphs involving two or more loops, angular integrations can again be done but they involve the Wigner 3-j or 6-j symbols (Racah coefficients) familiar in the quantum theory of angular momentum. Then only the radial integrations will remain. The method of multipole expansion and integral equations can also be used when the exponentials in (1.1) are replaced by the weight $\prod_i W(r_i)$, $W(r)$ decreasing fast enough for the integral to exist. This is the case, for example, when the variables are confined inside the unit sphere, i.e. $W(r) = 1$ for $r \leqslant 1$ and $W(r) = 0$ for $r > 1$.

This paper is organized as follows. In section 2 we explain the multipole expansion for three dimensions. Angular integrations are performed in section 3. Section 4 is devoted to the integral equations related to radial integrations. In section 5 we compute the radial integrals directly. All considerations until now were for three dimensions. The generalization to other dimensions is given in section 6. The special case where $d = 1$ is treated in section 7. In section 8 the same integrals are calculated for a step function $W(r)$ instead of the Gaussian weight used previously. The appendix gives relevant information for the general d-dimensional case.

2. Multipole expansion

Denoted by θ_{ij} the angle between $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$, $f(r_{ij})$ is a function of r_i, r_j and $x = \cos\theta_{ij}$, symmetric in r_i and r_j,

$$f(r_{ij}) \equiv f[(r_i^2 + r_j^2 - 2r_ir_jx)^{1/2}]. \tag{2.1}$$

Any function $f(r_{ij})$ square integrable in $-1 \leqslant x \leqslant 1$ can be expanded in terms of Legendre polynomials [2] $P_l(x)$, $l = 0, 1, \ldots,$

$$f(r_{ij}) = \sum_{l=0}^{\infty} F_l(r_i, r_j)P_l(x) \qquad (x = \cos\theta_{ij}). \tag{2.2}$$

The orthogonality relation [2]

$$\int_{-1}^{1} P_l(x)P_m(x)\,\mathrm{d}x = h_l\delta_{lm} \qquad h_l = \frac{2}{2l+1} \tag{2.3}$$

allows us to write

$$F_l(r_i, r_j) = \frac{1}{h_l}\int_{-1}^{1} f(r_{ij})P_l(x)\,\mathrm{d}x. \tag{2.4}$$

For the integrals (1.2) and (1.3) we take $f(r_{ij}) = r_{ij}$. In this case, and more generally if $f(r_{ij}) = r_{ij}^{2n+1}$, $n = 0, 1, \ldots$, in order to calculate $F_l(r_i, r_j)$ one can use two other general properties of orthogonal polynomials, namely the existence of a generating function

$$(1 + z^2 - 2xz)^{-1/2} = \sum_{l=0}^{\infty} P_l(x) z^l \qquad |z| \leqslant 1 \tag{2.5}$$

and the linear recurrence relation which relates three consecutive polynomials

$$x P_l(x) = \frac{l}{2l+1} P_{l-1}(x) + \frac{l+1}{2l+1} P_{l+1}(x). \tag{2.6}$$

In particular,

$$r_{ij}^{2n+1} = r_i^{2n+1}(1 + z^2 - 2xz)^{n+1/2} \qquad z = \frac{r_j}{r_i} \tag{2.7}$$

and assuming $z \leqslant 1$, one gets from (2.5)

$$r_{ij}^{2n+1} = r_i^{2n+1}(1 + z^2 - 2xz)^{n+1} \sum_{k=0}^{\infty} P_k(x) z^k \tag{2.8}$$

and from (2.4) for $r_i \geqslant r_j$

$$F_l(r_i, r_j) = \frac{1}{h_l} r_i^{2n+1} \sum_{k=0}^{\infty} z^k \int_{-1}^{1} (1 + z^2 - 2xz)^{n+1} P_l(x) P_k(x)\, \mathrm{d}x. \tag{2.9}$$

Now expanding $(1+z^2-2xz)^{n+1}$ in powers of x and using iteratively the recurrence relation (2.6), each term $x^p P_k(x)$ can be expressed as a linear combination with constant coefficients of the $p + 1$ polynomials $P_{k-p}, P_{k-p+2}, \ldots, P_{k+p-2}, P_{k+p}$. The integration over x can then be performed using the orthogonality relation (2.3). For the case $n = 0$, this procedure gives

$$F_l(r_i, r_j) = r_i \left[\frac{1}{2l+3} \left(\frac{r_j}{r_i} \right)^{l+2} - \frac{1}{2l-1} \left(\frac{r_j}{r_i} \right)^{l} \right] \qquad r_i \geqslant r_j. \tag{2.10}$$

The next step of the multipole expansion method follows from the invariance of r_{ij} under a simultaneous SO(3) rotation of $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$. The spherical harmonics Y_{lm}, $l \geqslant 0$, $-l \leqslant m \leqslant l$, form the standard basis of the irreducible representations of the SO(3) group in the space of square integrable functions defined on the surface of the three-dimensional sphere with the invariant measure $\mathrm{d}\Omega = \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi$. The orthogonality relation reads [3]

$$\int Y_{lm}^*(\Omega) Y_{l'm'}(\Omega)\, \mathrm{d}\Omega \equiv \int_0^{\pi} \mathrm{d}\theta \sin\theta \int_0^{2\pi} \mathrm{d}\phi\, Y_{lm}^*(\theta, \phi) Y_{l'm'}(\theta, \phi) = \delta_{ll'} \delta_{mm'} \tag{2.11}$$

and one special value we need is

$$Y_{00}(\Omega) = \frac{1}{\sqrt{4\pi}}. \tag{2.12}$$

One also has the addition theorem [2, 5]

$$P_l(x) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}^*(\Omega_i) Y_{lm}(\Omega_j) \tag{2.13}$$

where Ω_i stands for the polar angles (θ_i, ϕ_i) of $\boldsymbol{r}_i$.

3. Angular integrations

Doing a multipole expansion of each function $f(r_{ij})$ one can conveniently represent the integrals by introducing a graphical representation as follows. To each function $f(r_{ij})$ there is a link between the points i and j to which is associated a sum over l_{ij}, m_{ij}, a radial function $(4\pi/(2l_{ij}+1))F_{l_{ij}}(r_i, r_j)$, the spherical harmonic $Y^*_{l_{ij}m_{ij}}(\Omega_i)$ at the end i and $Y_{l_{ij}m_{ij}}(\Omega_j)$ at the end j. Each vertex i stands for the radial integration

$$(2\pi)^{-3/2}\int_0^\infty \mathrm{d}r_i r_i^2\,\mathrm{e}^{-r_i^2/2}$$

and the angular integration $\int \mathrm{d}\Omega_i$.

Let us first consider the diagram with a single chain. At each end point there is only one spherical harmonic. From the special value (2.12) and the orthogonality relation (2.11), the integration at the end point $\int \mathrm{d}\Omega$ yields the factor $\sqrt{4\pi}\,\delta_{l0}\delta_{m0}$. Then the integration $\int \mathrm{d}\Omega_i$ for each vertex joined to this end point, using (2.11), propagates the values $l = 0$ and $m = 0$ all along the chain. Thereby one obtains for a chain of length n

$$X_n = \left(\frac{2}{\pi}\right)^{1/2}\int_0^\infty r_1\,\mathrm{e}^{-r_1^2/4}K_0(r_1, r_2)K_0(r_2, r_3)\ldots K_0(r_n, r_{n+1})r_{n+1}\,\mathrm{e}^{-r_{n+1}^2/4}\prod_{j=1}^{n+1}\mathrm{d}r_j \tag{3.1}$$

$$= \langle g|K_0^n|g\rangle \tag{3.2}$$

where for compactness and to emphasize the structure of the expression, we have used bracket notation with

$$K_l(r, r') = \langle r|K_l|r'\rangle = \left(\frac{2}{\pi}\right)^{1/2}\frac{1}{2l+1}F_l(r, r')rr'\,\mathrm{e}^{-(r^2+r'^2)/4} \tag{3.3}$$

$$\langle r|g\rangle = \left(\frac{2}{\pi}\right)^{1/4} r\,\mathrm{e}^{-r^2/4} \qquad \langle g|g\rangle = 1. \tag{3.4}$$

Notice that only the multipole $l = 0$ occurs in X_n.

For one loop diagrams, a similar argument shows that all the links carry the same value of l and m. Since the result of the angular integrations no longer depends on m, one gets a sum over l with a weight $2l + 1$ for the loop. Thus for a loop of n links one gets

$$Y_n = \sum_{l=0}^{\infty}(2l+1)\int_0^\infty K_l(r_1, r_2)K_l(r_2, r_3)\ldots K_l(r_n, r_1)\prod_{j=1}^{n}\mathrm{d}r_j \tag{3.5}$$

$$= \sum_{l=0}^{\infty}(2l+1)\mathrm{Tr}K_l^n. \tag{3.6}$$

The same method applies to any graph having either no loop (tree structure) or one loop. Indeed the $l = 0$ and $m = 0$ values propagate along each branch from the external end point to a vertex where it reaches either a loop or another branch. For graphs involving two or more loops, the l values carried by each incoming link at a bifurcation have to be recoupled according to the usual angular momentum algebra. The angular integration over each Ω_i implies the invariance of the result under any individual rotation of $\boldsymbol{r}_i$. Therefore, all the incoming l values at a vertex must be recoupled to zero. This recoupling scheme involves Wigner 3-j or 6-j symbols (Racah coefficients) familiar in the quantum theory of angular momentum.

Notice that the above discussion is valid for any function $f(r_{ij})$ depending only on the distance r_{ij} and for any weight $W(r)$ replacing the Gaussian.

4. Radial integrations

Consider now the integral equation

$$\int_0^\infty K_l(r,r')\psi_j(r',l)\,\mathrm{d}r' = \lambda_j(l)\psi_j(r,l) \tag{4.1}$$

with $K_l(r,r')$ given by (3.3) above. The kernel $K_l(r,r')$ is real symmetric and the trace of its square for $f(r_{ij}) = r_{ij}$

$$\int_0^\infty K_l^2(r,r')\,\mathrm{d}r\,\mathrm{d}r' = \frac{4}{\pi(2l+1)^2}\int_{0\leqslant r\leqslant r'<\infty}\left[\frac{1}{2l+3}\frac{r^{l+3}}{r'^{l}} - \frac{1}{2l-1}\frac{r^{l+1}}{r'^{l-2}}\right]^2 \times \mathrm{e}^{-(r^2+r'^2)/2}\,\mathrm{d}r\,\mathrm{d}r' \tag{4.2}$$

is finite. According to a theorem of Fredholm [4], the eigenvalues $\lambda_j(l)$ are discrete and their only point of accumulation may be zero. The eigenvalues $\lambda_j(l)$ lie on a finite part of the real line and the eigenfunctions $\psi_j(r,l)$ can be chosen to be real orthonormal

$$\int_0^\infty \psi_j(r,l)\psi_k(r,l)\,\mathrm{d}r = \delta_{jk}. \tag{4.3}$$

The eigenvalues can be supposed to be ordered in decreasing absolute value. One can therefore write the spectral decomposition

$$K_l(r,r') = \sum_j \lambda_j(l)\psi_j(r,l)\psi_j(r',l) \tag{4.4}$$

and hence

$$X_n = \left(\frac{2}{\pi}\right)^{1/2}\sum_j \lambda_j^n(0)\left(\int_0^\infty \psi_j(r,0)r\,\mathrm{e}^{-r^2/4}\,\mathrm{d}r\right)^2 = \sum_j \lambda_j^n(0)\langle\psi_j|g\rangle^2 \tag{4.5}$$

$$Y_n = \sum_{l=0}^{\infty}(2l+1)\sum_j \lambda_j^n(l). \tag{4.6}$$

The traces of the first two powers of $K_l(r,r')$ are

$$T_1(l) = \mathrm{Tr}K_l = \int_0^\infty K_l(r,r)\,\mathrm{d}r = -\left(\frac{2}{\pi}\right)^{1/2}\frac{8}{(2l-1)(2l+1)(2l+3)} \tag{4.7}$$

$$T_2(l) = \mathrm{Tr}K_l^2 = \int_0^\infty K_l^2(r,r')\,\mathrm{d}r\,\mathrm{d}r' = \frac{4}{\pi(2l+1)^2}\left(\frac{1}{(2l+3)^2}I_{l+3} - \frac{2}{(2l-1)(2l+3)}I_{l+2} + \frac{1}{(2l-1)^2}I_{l+1}\right) \tag{4.8}$$

where

$$I_l = \int_0^\infty \mathrm{d}r\,r^{2l}\,\mathrm{e}^{-r^2/2}\int_r^\infty \mathrm{d}r'\,r'^{6-2l}\,\mathrm{e}^{-r'^2/2} = 48\int_0^1 \frac{t^{2l}}{(t^2+1)^4}\,\mathrm{d}t. \tag{4.9}$$

The last expression, obtained by a change of variables $u = rr'$, $t = r/r'$, shows that $I_{l+1} < I_l$. Replacing the t^2+1 in the denominator by 2 or $2t$ one obtains bounds for I_l

$$\frac{3}{2l+1} < I_l < \frac{3}{2l-3} \qquad l \geqslant 2. \tag{4.10}$$

A rough upper bound for $T_2(l)$ is thus given by

$$T_2(l) < \frac{4}{\pi(2l+1)^2}\left(\frac{1}{(2l+3)^2} + \frac{2}{(2l-1)(2l+3)} + \frac{1}{(2l-1)^2}\right) I_{l+1}$$
$$= \frac{16}{\pi(2l+3)^2(2l-1)^2} I_{l+1} \tag{4.11}$$

i.e. $T_2(l)$ decreases at least as fast as l^{-5} with l. For example

$$I_1 = \frac{3\pi}{4} + 1 \qquad I_2 = \frac{3\pi}{4} - 1 \qquad I_3 = \frac{15\pi}{4} - 11$$
$$I_4 = 83 - \frac{105\pi}{4} \qquad I_5 = \frac{315\pi}{4} - 247 \qquad I_6 = \frac{2723}{5} - \frac{693\pi}{4} \tag{4.12}$$

giving

$$T_2(0) = \frac{20}{3} - \frac{32}{9\pi} \approx 5.534\,898 \qquad T_2(1) = \frac{224}{75\pi} - \frac{4}{5} \approx 0.150\,686$$
$$T_2(2) = \frac{76}{105} - \frac{24\,992}{11\,025\pi} \approx 0.002\,249 \qquad T_2(3) = \frac{170\,272}{99\,225\pi} - \frac{172}{315} \approx 0.000\,194. \tag{4.13}$$

The kernel $K_0(r, r')$ is positive everywhere, so that among its eigenvalues, one having the largest absolute value is positive and non-degenerate. It is bounded by $\sqrt{T_2(0)}$.

Expressions (1.4) and (1.5) are the truncated forms of (4.5) and (4.6) retaining only three dominant eigenvalues $\lambda_j(0)$, and one dominant eigenvalue $\lambda_1(1)$. The eigenvalues λ_j and the constants A_j were computed by diagonalizing a discrete version of the kernels with 1000 points and step length 0.01. These approximate formulae reproduce the analytical values of X_n for $1 \leqslant n \leqslant 4$ given by (1.2), (5.17) and (5.18) correct up to at least 6 decimal points. Actually two eigenvalues are sufficient for $n \geqslant 2$. To convince ourselves that the other eigenvalues of $K_0(r, r')$ are quite negligible, we did also compute

$$T_3(0) = \mathrm{Tr} K_0^3 = \left(\frac{2}{\pi}\right)^{3/2} \left(\frac{305}{27} - \frac{137\pi\sqrt{2}}{6} + \frac{171\sqrt{2}}{2} \arctan\sqrt{2}\right) \approx 12.883\,024 \tag{4.14}$$

while $\lambda_1^3(0)+\lambda_2^3(0)+\lambda_3^3(0) \approx 12.883\,029$. As $T_1(l)$ is negative and $T_2(l)$ decreases fast with l, we keep only $\lambda_1(1)$. Numerically, the values $\lambda_2(1) = -0.028\,21$ and $\lambda_3(1) = -0.006\,15$ are negligible. Setting $n = 2$ in (1.5) yields $Y_2 \approx 5.984\,418$ instead of the known value 6.

5. Direct calculation of radial integrations

For X_n one needs only $F_0(r_1, r_2)$, so one can successively find with increasing complications

$$f_1(r) = \int_0^\infty F_0(r', r) r'^2 \,\mathrm{e}^{-r'^2/2} \,\mathrm{d}r' \tag{5.1}$$

$$f_{j+1}(r) = \int_0^\infty f_j(r') F_0(r', r) r'^2 \,\mathrm{e}^{-r'^2/2} \,\mathrm{d}r' \qquad j \geqslant 1. \tag{5.2}$$

For $f(r_{ij}) = r_{ij}$, one has

$$f_1(r) = \mathrm{e}^{-r^2/2} + \frac{1}{r}(r^2+1)\varphi(r) \tag{5.3}$$

$$f_2(r) = \frac{5}{3}\,\mathrm{e}^{-r^2} + \frac{1}{3}(r^2+6)\left[\frac{\pi}{2} - \varphi^2(r)\right] - \frac{2}{3r}(r^2+5)\varphi(r)\,\mathrm{e}^{-r^2/2} + \frac{\sqrt{2}}{3r}(6r^2+7)\varphi(r\sqrt{2}) \tag{5.4}$$

with $\varphi(r)$ the error function

$$\varphi(r) = \int_0^r \mathrm{e}^{-r'^2/2}\,\mathrm{d}r'. \tag{5.5}$$

From $f_1(r)$ and $f_2(r)$ one obtains

$$X_1 = \frac{2}{\pi}\int_0^\infty r^2\,\mathrm{e}^{-r^2/2} f_1(r)\,\mathrm{d}r \tag{5.6}$$

$$X_2 = \left(\frac{2}{\pi}\right)^{3/2}\int_0^\infty r^2\,\mathrm{e}^{-r^2/2} f_1^2(r)\,\mathrm{d}r = \left(\frac{2}{\pi}\right)^{3/2}\int_0^\infty r^2\,\mathrm{e}^{-r^2/2} f_2(r)\,\mathrm{d}r \tag{5.7}$$

$$X_3 = \left(\frac{2}{\pi}\right)^{2}\int_0^\infty r^2\,\mathrm{e}^{-r^2/2} f_1(r) f_2(r)\,\mathrm{d}r \tag{5.8}$$

$$X_4 = \left(\frac{2}{\pi}\right)^{5/2}\int_0^\infty r^2\,\mathrm{e}^{-r^2/2} f_2^2(r)\,\mathrm{d}r. \tag{5.9}$$

The integrals involved are of the general form

$$I(k, j, \mu) = \int_0^\infty p(r)\varphi^j(r)\,\mathrm{e}^{-\mu^2 r^2/2}\,\mathrm{d}r \tag{5.10}$$

where $p(r)$ is a polynomial of degree k, μ is a real number and j is an integer. Such integrals can be simplified first by decreasing the integer j successively to zero. For this, choose a polynomial $q(r)$ of degree $k-1$ such that

$$\frac{\mathrm{d}}{\mathrm{d}r}(q(r)\,\mathrm{e}^{-\mu^2 r^2/2}) = \mathrm{e}^{-\mu^2 r^2/2}[p(r) + K] \qquad K \text{ constant} \tag{5.11}$$

and integration by parts gives

$$\int_0^\infty p(r)\,\mathrm{e}^{-\mu^2 r^2/2}\varphi^j(r)\,\mathrm{d}r = -K\int_0^\infty \mathrm{e}^{-\mu^2 r^2/2}\varphi^j(r)\,\mathrm{d}r - \int_0^\infty q(r)\,\mathrm{e}^{-(\mu^2+1)r^2/2} j\varphi^{j-1}(r)\,\mathrm{d}r \tag{5.12}$$

the integrated part being zero at both limits if $j > 0$. So (5.12) gives $I(k, j, \mu)$ in terms of $I(0, j, \mu)$, $I(k-1, j-1, \sqrt{\mu^2+1})$ and known functions. Thus $I(k, j, \mu)$ can be expressed in terms of the integrals $I(0, j', \mu')$ and $I(k', 0, \mu')$. The $I(k, 0, \mu)$ are standard integrals involving gamma functions. As for $I(0, j, \mu)$, differentiating with respect to μ and integrating by parts as above, one gets a first-order differential equation in μ

$$\frac{\mathrm{d}}{\mathrm{d}\mu}[\mu I(0, j, \mu)] = -j\int_0^\infty \varphi^{j-1}(r) r\,\mathrm{e}^{-(\mu^2+1)r^2/2}\,\mathrm{d}r = -\frac{\delta_{j1}}{\mu^2+1} - \frac{j(j-1)}{\mu^2+1} I(0, j-2, \sqrt{\mu^2+2}) \tag{5.13}$$

with the solution

$$\mu I(0, j, \mu) = \frac{1}{j+1}\left(\frac{\pi}{2}\right)^{(j+1)/2} - \int_1^\mu \mathrm{d}\mu\left[\frac{\delta_{j1}}{\mu^2+1} + \frac{j(j-1)}{\mu^2+1} I(0, j-2, \sqrt{\mu^2+2})\right] \tag{5.14}$$

since $I(0, j, 1) = (\pi/2)^{(j+1)/2}/(j+1)$. The integrations on the right-hand side of (5.14) are more elementary and can be carried out. For example, one has

$$I(0, 1, \mu) = \int_0^\infty \mathrm{e}^{-\mu^2 r^2/2}\varphi(r)\,\mathrm{d}r = \frac{\pi}{2\mu} - \frac{1}{\mu}\arctan\mu \tag{5.15}$$

$$I(0, 2, \mu) = \int_0^\infty \mathrm{e}^{-\mu^2 r^2/2}\varphi^2(r)\,\mathrm{d}r = \frac{1}{\mu}\left(\frac{\pi}{2}\right)^{3/2} - \frac{\sqrt{2\pi}}{\mu}\arctan\frac{\mu}{\sqrt{\mu^2+2}}. \tag{5.16}$$

Of course, the effort needed to compute X_n increases fast with n. For example, we get from (5.6)–(5.9) X_1 and X_2 as given in (1.2), and

$$X_3 = \frac{56\sqrt{2}}{3\pi\sqrt{\pi}} - \frac{216}{\pi\sqrt{\pi}}\arctan(\sqrt{2}) + \frac{238}{3\sqrt{\pi}} \approx 12.442\,385 \tag{5.17}$$

$$X_4 = \frac{232}{45} + \frac{56}{\pi\sqrt{3}} - \frac{3140}{9\pi} + \frac{260\sqrt{5}}{9\pi^2} + \frac{912}{\pi^2}\arctan\sqrt{5} + \frac{224}{\pi^2\sqrt{3}}\arctan\sqrt{\frac{5}{3}} \approx 29.174\,181. \tag{5.18}$$

There seems to be no general closed formula.

To compute Y_n needs even more effort as one needs integrals over products of $F_l(r_i, r_j)$ for all l and finally a sum over l. Again there seems to be no general formula.

6. Number of dimensions other than one or three

The generalization of the definite integral (1.1) in a d-dimensional space, with the same normalization $\overline{1} = 1$, reads

$$\overline{F} = \int \mathrm{e}^{-(r_1^2+r_2^2+\cdots)/2} F(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots) \prod_j \frac{d^d \boldsymbol{r}_j}{(2\pi)^{d/2}}. \tag{6.1}$$

The multipole expansion method of section 2 can be adapted here. The choice of the orthogonal set of polynomials (Legendre for $d = 3$) is related to the irreducible representations of the rotation group in d-dimensional Euclidean space in order that one can write an addition theorem similar to (2.13). In general, for any given d let $\mathcal{P}_l(x)$ denote the suitable complete set of polynomials orthogonal on $(-1, 1)$ with the weight $w(x)$

$$\int_{-1}^{1} \mathcal{P}_l(x)\mathcal{P}_k(x)w(x)\,\mathrm{d}x = h_l \delta_{lk}. \tag{6.2}$$

Any square integrable function $f(r_{ij})$ with the weight function $w(x)$ can be expanded in terms of these $\mathcal{P}_l(x)$

$$f(r_{ij}) = \sum_{l=0}^{\infty} F_l(r_i, r_j)\mathcal{P}_l(x) \tag{6.3}$$

where $x = \cos\theta_{ij}$ and $F_l(r_i, r_j)$, symmetric in r_i and r_j, is given by

$$F_l(r_i, r_j) = \frac{1}{h_l}\int_{-1}^{1} f(r_{ij})\mathcal{P}_l(x)w(x)\,\mathrm{d}x. \tag{6.4}$$

To calculate $F_l(r_i, r_j)$ for special functions $f(r_{ij})$, one may take advantage of the existence of a generating function of the type (2.5) and the existence of a recurrence relation

$$x\mathcal{P}_l(x) = a_l \mathcal{P}_{l-1}(x) + b_l \mathcal{P}_{l+1}(x) \tag{6.5}$$

as in the case $d = 3$. The next step is to consider the generalized spherical harmonics $\mathcal{Y}_{l\{m\}}$. For each non-negative integer l they are [5]

$$n_l = \frac{(2l + d - 2)(l + d - 3)!}{(d - 2)!l!} \tag{6.6}$$

in number and are characterized by a set of integers $m_1, m_2, \ldots, m_{d-2}$ with the restrictions

$$l \geqslant m_1 \geqslant m_2 \geqslant \cdots \geqslant m_{d-3} \geqslant |m_{d-2}| \geqslant 0. \tag{6.7}$$

They form a standard orthonormal basis of the irreducible representations of the rotation group SO(d) in the space of square integrable functions defined over the surface of the d-dimensional unit sphere with the invariant measure [6]

$$\mathrm{d}\Omega = (\sin\theta_1)^{d-2}(\sin\theta_2)^{d-3}\ldots\sin\theta_{d-2}\,\mathrm{d}\theta_1\ldots\mathrm{d}\theta_{d-2}\,\mathrm{d}\phi \qquad 0 \leqslant \theta_j \leqslant \pi \qquad 0 \leqslant \phi \leqslant 2\pi. \tag{6.8}$$

The $\mathcal{Y}_{l\{m\}}$ are orthonormal

$$\int \mathcal{Y}^*_{l\{m\}}(\Omega)\mathcal{Y}_{l'\{m'\}}(\Omega)\,\mathrm{d}\Omega = \delta_{ll'}\delta_{\{m\}\{m'\}} \tag{6.9}$$

and the special value we need is

$$\mathcal{Y}_{0\{0\}}(\Omega) = S_d^{-1/2} \tag{6.10}$$

where

$$S_d = \frac{2\pi^{d/2}}{\Gamma(d/2)} \tag{6.11}$$

is the surface area of the d-dimensional unit sphere. So we have the addition theorem [7]

$$\mathcal{P}_l(x) = c_l S_d \sum_{\{m\}} \mathcal{Y}^*_{l\{m\}}(\Omega_i)\mathcal{Y}_{l\{m\}}(\Omega_j) \tag{6.12}$$

where Ω_i denotes the direction of the unit vector $\boldsymbol{r}_i/r_i$ and the sum $\{m\}$ is over all integers satisfying the inequalities (6.7).

Now doing a multipole expansion of each function $f(r_{ij})$, exactly as described previously for the case $d = 3$, allows us to do the angular integrations, and one obtains for X_n and Y_n expressions similar to (3.2) and (3.6)

$$X_n = \langle g|K_0^n|g\rangle \tag{6.13}$$

$$Y_n = \sum_{l=0}^{\infty} n_l \mathrm{Tr} K_l^n \tag{6.14}$$

where the kernels K_l and the normalized $|g\rangle$ are given by

$$K_l(r, r') = \langle r|K_l|r'\rangle = k_d c_l F_l(r, r')(rr')^{(d-1)/2}\,\mathrm{e}^{-(r^2+r'^2)/4} \tag{6.15}$$

$$\langle r|g\rangle = \sqrt{k_d}\, r^{(d-1)/2}\,\mathrm{e}^{-r^2/4} \qquad \langle g|g\rangle = 1 \tag{6.16}$$

and

$$k_d = \frac{S_d}{(2\pi)^{d/2}}. \tag{6.17}$$

Continuing to use bracket notation, we consider now the eigenvalue equation

$$K_l|\psi_j(l)\rangle = \lambda_j(l)|\psi_j(l)\rangle. \tag{6.18}$$

As in the case $d = 3$, for any l the kernel $K_l(r, r')$ is real symmetric for any square integrable function $f(r_{ij})$, and due to the exponential factors in (6.15), the trace of its square is finite. Therefore, the spectrum of this Fredholm kernel is discrete, real and bounded, the only possible accumulation point being zero. Thus one can write the spectral decomposition

$$K_l = \sum_j \lambda_j(l)|\psi_j(l)\rangle\langle\psi_j(l)| \tag{6.19}$$

where the eigenstates $|\psi_j(l)\rangle$ are chosen to be real orthonormal

$$\langle\psi_j(l)|\psi_{j'}(l)\rangle = \delta_{jj'} \qquad \langle r|\psi_j(l)\rangle \text{ real} \tag{6.20}$$

and the eigenvalues are supposed to be ordered in decreasing absolute value. So from (6.13) and (6.14) one gets for X_n and Y_n expressions like (4.5) and (4.6)

$$X_n = \sum_j \lambda_j^n(0)\langle\psi_j(0)|g\rangle^2 \tag{6.21}$$

$$Y_n = \sum_{l=0}^{\infty} n_l \sum_j \lambda_j^n(l). \tag{6.22}$$

In the appendix we indicate the set of appropriate polynomials $\mathcal{P}_l(x)$ orthogonal on $(-1, 1)$, the weight $w(x)$, the normalization constant h_l, the generating function, the constants a_l, b_l, c_l, appearing in equations (6.5), (6.12) and (6.15), and some other information. The graphical representation of the integrals, X_n as a chain with n links, Y_n as a loop with n links, etc and the remarks about angular integrations made for the case $d = 3$ are valid with minor changes. Let us remark that for any d a direct calculation of X_1 and Y_2 using the integration variables $\boldsymbol{r}_1 \pm \boldsymbol{r}_2$ in (6.1) yields

$$X_1 = \frac{2\Gamma((d+1)/2)}{\Gamma(d/2)} \qquad Y_2 = 2d. \tag{6.23}$$

For the case $d = 1$ the group SO(1) of rotations in one dimension is a discrete group with only two elements, identity and the parity operation. For this reason the above considerations are much simplified for $d = 1$, and we briefly discuss this case in section 7.

7. Case of one dimension

For the particular case of one dimension there are no angular integrations but the variables r_i run over $(-\infty, \infty)$. Although the considerations are valid for any square integrable function $f(r_{ij})$, we give here the details only for r_{ij}. The kernel in the integral equation (4.1) is

$$K(r, r') = (2\pi)^{-1/2}|r - r'|\,\mathrm{e}^{-(r^2+r'^2)/4} \tag{7.1}$$

over the interval $(-\infty, \infty)$. Since $K(r, r')$ is invariant under a simultaneous change of sign of r and r', the eigenfunctions of the integral equation

$$(2\pi)^{-1/2}\int_{-\infty}^{\infty} |r - r'|\,\mathrm{e}^{-(r^2+r'^2)/4}\psi_j(r')\,\mathrm{d}r' = \lambda_j\psi_j(r) \tag{7.2}$$

are either even or odd. The even (odd) eigenfunctions are also eigenfunctions of

$$\int_0^{\infty} K_\pm(r, r')\psi_{j\pm}(r')\,\mathrm{d}r' = \lambda_{j\pm}\psi_{j\pm}(r) \tag{7.3}$$

with

$$K_\pm(r, r') = K(r, r') \pm K(r, -r'). \tag{7.4}$$

Note that a factor 1/2 on the right-hand side of this equation is missing, since the domain of integration is reduced from $(-\infty, \infty)$ to $(0, \infty)$.

These plus or minus kernels, eigenvalues and eigenfunctions correspond respectively to the multipoles $l = 0$ and $l = 1$ of the general case presented in the previous section, which are the only possibilities for one dimension (see the appendix). The traces of powers of $K_\pm(r, r')$ and $K(r, r')$ are related by the simple equation

$$Y_n = \mathrm{Tr}K^n = \mathrm{Tr}K_+^n + \mathrm{Tr}K_-^n. \tag{7.5}$$

One can again calculate these traces $T_{n\pm} = \mathrm{Tr} K_\pm^n$

$$T_{1\pm} = \pm\sqrt{\frac{2}{\pi}} \qquad T_{2\pm} = 1 \pm \frac{2}{\pi} \tag{7.6}$$

$$T_{3\pm} = \frac{3}{2\sqrt{\pi}} \pm \left(\frac{2\sqrt{2}}{\pi\sqrt{\pi}} - \frac{9}{2\sqrt{\pi}} + \frac{18}{\pi\sqrt{\pi}} \arctan\sqrt{2} \right) \tag{7.7}$$

$$T_{4\pm} = \frac{1}{3} - \frac{4}{\pi} + \frac{4\sqrt{3}}{\pi} \pm \left(\frac{4}{\pi^2} + \frac{4\sqrt{3}}{3\pi} \right) \tag{7.8}$$

and

$$X_1 = \frac{2}{\sqrt{\pi}} \qquad X_2 = \frac{1}{3} + \frac{2\sqrt{3}}{\pi} \tag{7.9}$$

$$X_3 = \frac{5}{\sqrt{\pi}} + \frac{4\sqrt{2}}{\pi\sqrt{\pi}} + \frac{2\sqrt{2}}{\pi\sqrt{\pi}} - \frac{12}{\pi^2} \arctan\sqrt{2} \tag{7.10}$$

$$Y_2 = 2 \qquad Y_3 = \frac{3}{\sqrt{\pi}}. \tag{7.11}$$

A numerical estimate of the eigenvalues $\lambda_{j\pm}$ of $K_\pm$ with 1000 discrete integration points and step length 0.01 gives the dominant eigenvalues as

$$\lambda_{1+} = 1.2459 \qquad \lambda_{2+} = -0.2886 \qquad \lambda_{3+} = -0.0619 \qquad \lambda_{4+} = -0.0272 \tag{7.12}$$

$$\lambda_{1-} = -0.5945 \qquad \lambda_{2-} = -0.0897 \qquad \lambda_{3-} = -0.0350 \qquad \lambda_{4-} = -0.0186. \tag{7.13}$$

Compared to the cases $d = 2$ and $d = 3$ they decrease slowly, and to have comparable precision one needs a smaller integration step.

8. Integration inside the unit sphere

To illustrate the general character of our method we will now compute the integrals X_n and Y_n when the variables are restricted to lie inside the unit sphere. This means that we replace the Gaussian weight by the weight $\prod_i W(r_i)$, where $W(r) = 1$ for $r \leqslant 1$ and $W(r) = 0$ for $r > 1$. We will treat only the simpler case $d = 1$. As the X_n and the Y_n can also be computed directly with an effort increasing with n, we get some identities.

In what follows, all the variables are restricted to the interval (0,1). For $d = 1$ we have

$$K_+(r, r') = \max(r, r') \tag{8.1}$$

$$K_-(r, r') = -\min(r, r'). \tag{8.2}$$

The integral equation (7.3) implies that the eigenfunctions $\psi_{j\pm}(r)$ satisfy the following differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2} \psi_{j\pm}(r) = \pm \frac{1}{\lambda_{j\pm}} \psi_{j\pm}(r). \tag{8.3}$$

Its solutions are

$$\psi_{j\pm}(r) = A\, \mathrm{e}^{+r/\sqrt{\pm\lambda_{j\pm}}} + B\, \mathrm{e}^{-r/\sqrt{\pm\lambda_{j\pm}}}. \tag{8.4}$$

The constants A, B and the eigenvalues $\lambda_{j\pm}$ are determined by injecting (8.4) in the integral equation (7.3) which has to be satisfied. The kernel K_+ has only one positive eigenvalue λ_{0+} and all other eigenvalues λ_{j+} are negative. They are given by

$$\sqrt{\lambda_{0+}} = \tanh \frac{1}{\sqrt{\lambda_{0+}}} \qquad -\sqrt{-\lambda_{j+}} = \tan \frac{1}{\sqrt{-\lambda_{j+}}} \qquad j \geqslant 1. \tag{8.5}$$

The kernel K_- has only negative eigenvalues given by

$$\lambda_{j-} = -\frac{4}{\pi^2} \frac{1}{(2j+1)^2} \qquad j \geqslant 0. \tag{8.6}$$

Formula (7.5) gives Y_n as the sum of traces of K_+^n and K_-^n, the second one can be written explicitly as [11]

$$\mathrm{Tr} K_-^n = \frac{(-4)^n}{\pi^{2n}} \sum_{j=0}^{\infty} \frac{1}{(2j+1)^{2n}} = \frac{(-4)^n (4^n - 1)|B_{2n}|}{2(2n)!} \tag{8.7}$$

where B_{2n} are the Bernoulli numbers. Thus (7.5) gives

$$\sum_{j=0}^{\infty} \lambda_{j+}^n = Y_n - \frac{(-4)^n (4^n - 1)|B_{2n}|}{2(2n)!}. \tag{8.8}$$

For X_n given by (6.21), we also need the overlap $\langle \psi_{j+} | g \rangle^2$ between the normalized eigenfunction $\langle r | \psi_{j+} \rangle = \psi_{j+}(r)$ and $\langle r | g \rangle = g(r) = 1$. From (8.4) and (8.5), one finds

$$\langle \psi_{j+} | g \rangle^2 = 2\lambda_{j+}^2 \qquad j \geqslant 0. \tag{8.9}$$

This leads us to

$$X_n = 2 \sum_{j=0}^{\infty} \lambda_{j+}^{n+2}. \tag{8.10}$$

Equations (8.8) and (8.10) give in this case a relation between X_n and Y_n

$$-X_n + 2Y_{n+2} = \frac{(-4)^{n+2}(4^{n+2} - 1)|B_{2n+4}|}{(2n+4)!}. \tag{8.11}$$

If we introduce the new positive variables ρ_0 and ρ_j, $j \geqslant 1$, by

$$\lambda_{0+} = \rho_0^2 \qquad \lambda_{j+} = -\rho_j^2 \qquad j \geqslant 1 \tag{8.12}$$

then (8.8), (8.10) and (8.11) take the simple form ($X_0 \equiv 1$)

$$\rho_0^{2n} + (-1)^n \sum_{j=1}^{\infty} \rho_j^{2n} = Y_n - \frac{(-4)^n (4^n - 1)|B_{2n}|}{2(2n)!} = \frac{1}{2} X_{n-2} \qquad n \geqslant 2 \tag{8.13}$$

where ρ_0 and ρ_j are the positive real roots of the equations

$$\rho_0 = \tanh(1/\rho_0) \qquad -\rho_j = \tan(1/\rho_j) \qquad j \geqslant 1. \tag{8.14}$$

Numerically one has the approximate values,

$$\rho_0 = 0.833\,557 \qquad \rho_1 = 0.357\,349 \qquad \rho_2 = 0.163\,365 \qquad \rho_3 = 0.107\,317. \tag{8.15}$$

Computing X_n and Y_n directly, these provide identities. For example, one has directly

$$X_1 = \frac{2}{3} \qquad X_2 = \frac{7}{15} \qquad X_3 = \frac{34}{105} \qquad X_4 = \frac{638}{2835} \qquad Y_2 = \frac{2}{3} \qquad Y_3 = \frac{4}{15} \tag{8.16}$$

so that

$$\rho_0^4 + \sum_{j=1}^{\infty} \rho_j^4 = \frac{1}{2} \qquad \rho_0^6 - \sum_{j=1}^{\infty} \rho_j^6 = \frac{1}{3} \qquad \rho_0^8 + \sum_{j=1}^{\infty} \rho_j^8 = \frac{7}{30} \qquad \rho_0^{10} - \sum_{j=1}^{\infty} \rho_j^{10} = \frac{17}{105}$$

$$\rho_0^{12} + \sum_{j=1}^{\infty} \rho_j^{12} = \frac{319}{2835} \qquad \text{etc.} \tag{8.17}$$

These are the first members of a family of identities. Direct step by step integrations as in (5.1) and (5.2) yields rational numbers for X_n and Y_n.

A similar computation in three, five or seven dimensions will hopefully give new identities. We expect to come back to this point later.

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Appendix

Polynomials $\mathcal{P}_l(x)$

Tchebichef polynomials [8] $T_l(x)$ for $d = 2$, and Gegenbauer polynomials [9] $C_l^{((d-2)/2)}$ for $d \geqslant 3$ (for $d = 3$, they coincide with the Legendre polynomials [2]).

Weight function

$$w(x) = (1 - x^2)^{(d-3)/2}. \tag{A1}$$

Normalization constant

$$h_l = \frac{\pi}{2}(1 + \delta_{l0}) \qquad d = 2 \tag{A2}$$

$$= \frac{2\sqrt{\pi}\,\Gamma(d + l - 2)\Gamma((d-1)/2)}{(2l + d - 2)l!\Gamma(d-2)\Gamma((d-2)/2)} \qquad d \geqslant 3. \tag{A3}$$

Generating function

$$(1 + z^2 - 2xz)^{1-d/2} = \sum_{l=0}^{\infty} C_l^{((d-2)/2)}(x) z^l \qquad d \geqslant 3 \qquad |z| < 1 \tag{A4}$$

$$-\frac{1}{2}\ln(1 + z^2 - 2xz) = \sum_{l=1}^{\infty} \frac{1}{l} T_l(x) z^l \qquad d = 2 \qquad |z| < 1 \tag{A5}$$

or

$$\frac{1 - z^2}{1 + z^2 - 2xz} = T_0(x) + 2\sum_{l=1}^{\infty} T_l(x) z^l \qquad d = 2 \qquad |z| < 1. \tag{A6}$$

Coefficients in the recurrence relation [8, 9]

$$a_l = b_l = \tfrac{1}{2} \qquad d = 2 \tag{A7}$$

$$a_l = \frac{l + d - 3}{2l + d - 2} \qquad b_l = \frac{l + 1}{2l + d - 2} \qquad d \geqslant 3. \tag{A8}$$

Generalized spherical harmonics $\boldsymbol{\mathcal{Y}}_{l\{m\}}$ [10]

For $d = 2$, the harmonics are simply the exponentials $(1/\sqrt{2\pi})\,\mathrm{e}^{\mathrm{i}m\phi}$, and for $d \geqslant 3$, one has the normalized surface harmonics $N(m_k)^{-1/2}\mathcal{Y}(m_k;\theta_k,\pm\phi)$, (identical to the spherical harmonics $Y_{lm}(\theta,\phi)$ for $d = 3$), where according to Bateman [10] m_k stands for $\{m_0 = l, m_1, \ldots, m_{d-2}\}$ with $m_{d-2} \geqslant 0$, and negative values of m_{d-2} correspond to $-\phi$

$$N(m_0, m_1, \ldots, m_{d-2}) = 2\pi \prod_{k=1}^{d-2} E_k(m_{k-1}, m_k) \tag{A9}$$

$$E_k(m, m') = \frac{\pi 2^{k-2m'-d+2}\Gamma(m + m' + d - k - 1)}{(m + (d - k - 1)/2)(m - m')![\Gamma(m' + (d - k - 1)/2)]^2}. \tag{A10}$$

Coefficient in the addition theorem [7]

$$c_l = \frac{1}{2} \qquad d = 2; \qquad c_l = \frac{d-2}{2l + d - 2} \qquad d \geqslant 3. \tag{A11}$$

For even dimensions d the generating functions are not convenient to calculate $F(r_i, r_j)$ for $f(r_{ij}) = r_{ij}$. For example, when $d = 2$, K_0 involves an elliptic integral

$$K_0(r, r') = \frac{\sqrt{rr'}(r + r')}{\pi}\boldsymbol{E}\left(\frac{2\sqrt{rr'}}{r + r'}\right)\mathrm{e}^{-(r^2+r'^2)/4} \tag{A12}$$

where $\boldsymbol{E}$ is the complete elliptic integral of the second kind,

$$\boldsymbol{E}(k) = \int_0^{\pi/2} (1 - k^2 \sin^2\theta)^{1/2}\,\mathrm{d}\theta. \tag{A13}$$

A numerical diagonalization of the kernel K_0 with 1000 points and step length 0.01 gives the dominant eigenvalues as

$$\lambda_1(0) = 0.903\,4944 \qquad \lambda_2(0) = 0.093\,3744 \qquad \lambda_3(0) = 0.007\,0863. \tag{A14}$$

For one dimension the surface of the unit sphere reduces to two points $+1$ and -1, the polynomials $\mathcal{P}_l(x)$ are only two, $\mathcal{P}_0(x) = 1$ and $\mathcal{P}_1(x) = x$, the integrations in equations (6.2), (6.4) and (6.9) are reduced to a sum of two terms, and the formal structure for general d, though not needed as we saw in section 7, can be maintained.

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