# Box integrals

D.H. Bailey* J.M. Borwein† R.E. Crandall‡

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**Abstract.** By a "box integral" we mean here an expectation $\langle |\vec{r} - \vec{q}|^s \rangle$ where $\vec{r}$ runs over the unit $n$-cube, with $\vec{q}$ and $s$ fixed, explicitly:

$$\int_0^1 \cdots \int_0^1 \left( (r_1 - q_1)^2 + \cdots + (r_n - q_n)^2 \right)^{s/2} \, dr_1 \cdots dr_n.$$

The study of box integrals leads one naturally into several disparate fields of analysis. While previous studies have focused upon symbolic evaluation and asymptotic analysis of special cases (notably $s = 1$), we work herein more generally—in interdisciplinary fashion—developing results such as: (1) analytic continuation (in complex $s$), (2) relevant combinatorial identities, (3) rapidly converging series, (4) statistical inferences, (5) connections to mathematical physics, and (6) extreme-precision quadrature techniques appropriate for these integrals. These intuitions and results open up avenues of experimental mathematics, with a view to new conjectures and theorems on integrals of this type.

*Lawrence Berkeley National Laboratory, Berkeley, CA 94720, dhbailey@lbl.gov. Supported in part by the Director, Office of Computational and Technology Research, Division of Mathematical, Information, and Computational Sciences of the U.S. Department of Energy, under contract number DE-AC02-05CH11231.

†Faculty of Computer Science, Dalhousie University, Halifax, NS, B3H 2W5, Canada, jborwein@cs.dal.ca. Supported in part by NSERC and the Canada Research Chair Programme.

‡Center for Advanced Computation, Reed College, Portland OR, crandall@reed.edu.

## 1 Box integrals as expectations

We define a box integral[1] for dimension $n$ and parameters $\vec{q}, s$ as the expectation, from a fixed point $\vec{q}$, of a certain norm $|r-q|^s$ with point $\vec{r}$ chosen in equidistributed random fashion over the unit $n$-cube:

$$\begin{aligned} X_n(s,\vec{q}) &:= \langle |\vec{r}-\vec{q}|^s \rangle_{r\in[0,1]^n} \\ &= \int_{\vec{r}\in[0,1]^n} |\vec{r}-\vec{q}|^s \, \mathcal{D}\vec{r}, \\ &= \int_0^1 \cdots \int_0^1 \left((r_1-q_1)^2+\cdots+(r_n-q_n)^2\right)^{s/2} \, dr_1\cdots dr_n, \end{aligned} \tag{1}$$

where here and elsewhere $\mathcal{D}\vec{r} := dr_1\cdots dr_n$ is the $n$-space volume element. We also shall denote simply by $r$ the magnitude $|\vec{r}|$.

There are two classically important instances/functionals of the $X$-integrals, namely $B_n$ and $\Delta_n$ defined:

$$\begin{aligned} B_n(s) &:= X_n(s,\vec{0}) = \int_{\vec{r}\in[0,1]^n} r^s \, \mathcal{D}\vec{r} \\ &= \int_0^1 \cdots \int_0^1 \left(r_1^2+\cdots+r_n^2\right)^{s/2} \, dr_1\cdots dr_n, \end{aligned} \tag{2}$$

$$\begin{aligned} \Delta_n(s) &:= \langle X_n(s,\vec{q}) \rangle_{\vec{q}\in[0,1]^n} = \int_{\vec{r},\vec{q}\in[0,1]^n} |\vec{r}-\vec{q}|^s \, \mathcal{D}\vec{r}\,\mathcal{D}\vec{q} \\ &= \int_0^1 \cdots \int_0^1 \left((r_1-q_1)^2+\cdots+(r_n-q_n)^2\right)^{s/2} \, dr_1\cdots dr_n\, dq_1\cdots dq_n. \end{aligned} \tag{3}$$

Note that

1. $B_n(1)$ is the expected distance of a random point from any *vertex* of the $n$-cube,
2. $\Delta_n(1)$ is the expected distance *between* two random points of said cube,
3. $X_n(1,(1/2,1/2,\ldots 1/2)\ )$ is the expected distance of a random point from the *center* of said cube.

These are oft-discussed entities in the literature. There are many others such as the expected distance between points on distinct sides of a cube or hypercube investigated in [8, §1.7] or [6]. We remark that $B_3(1)$ is also known as the *Robbins constant*, after [12]. Note that the third entity here is not genuinely different, because for general $s$ one has the expected norm from center as

$$X_n(s,(1/2,1/2,\ldots 1/2)\ ) = \frac{1}{2^s} B_n(s), \tag{4}$$

[1]Not to be confused with "box integrals" of particle physics, those integrals being scattering-loop contributions, although such entities are indeed $n$-dimensional integrals.

as can be shown quickly from relations (1) by setting $\vec{q} = (1/2, 1/2, \ldots 1/2)$ ), changing to $p_i = (r_i - q_i)/2$, and observing how the integral has scaled. This is one of the various relations we shall develop that hold for all complex $s$; in particular, we shall address analytic continuation. It will turn out, interestingly, that $B_n(s)$ is always analytic in $s$ except for a simple pole at $s = -n$.

There have been interesting modern treatments of the $B_n$ and related integrals, as in [6], [8, p.208], [17], [15]. Related material is also found in [10, 16]. A pivotal, original treatment is the 1976 work of Anderssen et al, [1] who gave a large-$n$ asymptotic series

$$B_n(1) \sim \sqrt{\frac{n}{3}}\left(1 - \frac{n}{10} + \ldots\right), \tag{5}$$

together with a convergent series development for $B_n(1)$ we cite later (and extend to general $s$), and a collection of bounds, derived via statistical theory, such as

$$\sqrt{\frac{n}{4}} \le B_n(1) \le \sqrt{\frac{n}{3}}.$$

This asymptotic is especially interesting when one realizes that the positive unit $n$-ball sector (the intersection of the $n$-ball with the cube $[0,1]^n$) has volume decaying superexponentially fast with $n$. Intuitively speaking, this discrepancy is due to the fact of "so many corners" of the $n$-cube, where integrable matter resides. We shall argue using statistical intuition that for general $s$,

$$B_n(s) \sim \left(\frac{n}{3}\right)^{s/2}. \tag{6}$$

A word here is relevant as to the importance of box integrals in other fields of research. It should be noted first that the Anderssen et al. work [1] was motivated by global-optimization study, which explains why the adroit use of statistical principles is apparent in that effort. Secondly, there are problems of lattice theory—such as derivation of what are called "jellium" potentials, that involve $B_n(s)$ for negative $s$. It is easy to imagine how potential theory for a periodic crystal can involve box integrals. We define and discuss later an $n$-dimensional jellium potential $J_n$ as an expectation $\langle V_n \rangle$ where $V_n$ is a potential relevant to the $n$-dimensional Laplace equation.

As we explain herein, it turns out that both $B_n(s), \Delta_n(s)$ even for large $n$ can be numerically evaluated to extreme precision, in much the same way that Bailey et al. [5] resolved the Ising-class integrals $C_n$ for dimension $n \sim 1000$ to hundreds of decimals. In that previous work, a modified-Bessel kernel was employed in a 1-dimensional representation suitable for numerical quadrature. In our present case, an error-function kernel is appropriate. These high-precision quadratures have motivated some conjectures and subsequent proofs of same.

## 2 Dimensional reduction via vector-field calculus

It turns out that a box integral $X_n(s, \vec{q})$ can be reduced to a suitable integral over the *faces* of a displaced $n$-cube, in some instances reducible yet further to edges, and so on. Let us write

$$X_n(s, \vec{q}) \;=\; \int_{\vec{r}\,\in\,\mathcal{C}} r^s \;\mathcal{D}\vec{r},$$

where $r := |\vec{r}|$ and the integration is over a translated cube

$$\mathcal{C} \;:=\; [0,1]^n - \vec{q}.$$

We may then invoke an elegant procedure from mathematical physics; namely, we attempt to write the (radially symmetric) integrand $r^s$ as the Laplacian of a scalar field. That is, we seek a function $\Phi$ of position, such that

$$\nabla^2\Phi(\vec{r}) \;=\; r^s.$$

A radially symmetric solution will satisfy the radial part of the Laplacian relation, as

$$\frac{1}{r^{n-1}}\frac{\partial}{\partial r}\left(r^{n-1}\frac{\partial}{\partial r}\right) \;=\; r^s,$$

whence there is a solution satisfying

$$\frac{\partial\Phi}{\partial r} \;=\; \frac{1}{n+s}r^{s+1}.$$

The point of these machinations is that we may now utilize the divergence theorem for vector fields, in the form[2]

$$\int_R \nabla\cdot\vec{\mathcal{F}}\;\mathcal{D}\vec{r} \;=\; \int_{\partial R}\vec{\mathcal{F}}\cdot\;\mathcal{D}\vec{a},$$

where $\vec{\mathcal{F}}(\vec{r})$ is a vector field, the left-hand integral is over the interior of a region $R$, the right integral is over the boundary, with $\mathcal{D}\vec{a}$ denoting an area element with vector direction always normal to the surface.

The next step is to consider the vector field defined $\vec{\mathcal{F}} := \nabla\Phi$. Using the above observations, we conclude

$$X_n(s, \vec{q}) \;=\; \frac{1}{n+s}\int_{\vec{r}\,\in\,\partial\mathcal{C}} r^s\;\vec{r}\cdot\hat{\mu}\;da \tag{7}$$

[2]Known classically as the Gauss theorem for vector fields, this integral relation is ubiquitous in electrostatics and hydrodynamics.

where $da$ is the surface element with normal unit vector $\hat{\mu}$. Note that we have hereby reduced the box integral to an integral over the *faces* of a certain, displaced unit cube. For the box integrals $B_n(s)$, so we have offset $\vec{q} = (1/2, \ldots, 1/2)$, we realize there are $2n$ symmetrically situated faces, and our results boils down to the dimensional-reduction relation

$$B_n(s) \;=\; \frac{n}{n+s} \int_{\vec{r}\,\in\,[0,1]^{n-1}} \left(r^2+1\right)^{s/2} \;\mathcal{D}\vec{r}. \tag{8}$$

So for example the 2-dimensional case reduces to a 1-dimensional integral and a final hypergeometric evaluation.

$$\begin{aligned} B_2(s) \;&:=\; \int_{\vec{r}\,\in\,[0,1]^2} r^s \;\mathcal{D}\vec{r} \;=\; \frac{2}{2+s}\int_0^1 (x^2+1)^{s/2}\,dx \\ &=\; \frac{2}{2+s}\;{}_2F_1\left(\frac{1}{2}, -\frac{s}{2}; \frac{3}{2}; -1\right). \end{aligned} \tag{9}$$

This hypergeometric entity is rational when $s$ is a nonnegative even integer, and evidently is always a surd plus the log of a surd for $s$ a nonnegative odd integer (see Section 7 for some closed forms).

For the 3-dimensional case, we are able to reduce one further dimension by employing, after the first reduction step from (8), a 2-dimensional solution to

$$\nabla^2 \Phi \;=\; (r^2+1)^{s/2},$$

which solution has the property

$$r\frac{\partial \Phi}{\partial r} \;=\; \frac{(r^2+1)^{s/2}-1}{s+2},$$

to get a 1-dimensional representation, like so:

$$\begin{aligned} B_3(s) \;&=\; \frac{3}{3+s}\int_{\vec{r}\,\in\,[0,1]^2} (r^2+1)^{s/2}\;\mathcal{D}\vec{r} \\ &=\; \frac{3}{3+s}\frac{2}{2+s}\int_0^1 \frac{(y^2+2)^{s/2}-1}{y^2+1}\,dy \\ &=\; \frac{6}{(3+s)(2+s)}\left(-\frac{\pi}{4} + \int_0^{\pi/4} (1+\sec^2 t)^{s/2+1}\,dt\right). \end{aligned} \tag{10}$$

As with the cases $B_2(s)$, these $B_3(s)$ do enjoy some closed forms, as in Section 7.

# 3 Error-function formalism and combinatorics

We have seen that an $n$-dimensional box integral can be reduced by at least one dimension. It turns out that, for numerical quadrature applications, one may achieve a *one*-dimensional integral representation of either $B_n$ or $\Delta_n$. The procedure runs as follows.[3] We start with a certain representation of complex powers:

$$z^\rho \;=\; \frac{\rho}{\Gamma(1-\rho)} \int_0^\infty t^{-\rho-1}\left(1-e^{-tz}\right)\, dt, \tag{11}$$

valid for $\Re(z) > 0$ and $\Re(\rho) \in (0,2)$. We next define two key functions

$$b(u) \;:=\; \int_0^1 e^{-u^2x^2}\, dx \;=\; \frac{\sqrt{\pi}\,\operatorname{erf}(u)}{2u}, \tag{12}$$

$$d(u) \;:=\; \int_0^1\int_0^1 e^{-u^2(x-y)^2}\, dx\, dy \;=\; \frac{-1+e^{-u^2}+\sqrt{\pi}\, u\, \operatorname{erf}(u)}{u^2}. \tag{13}$$

Now, the defining integrals (2) and (3), and the representation (11), lead to 1-dimensional integrals for each of $B_n, \Delta_n$, like so:

$$B_n(s) \;=\; \frac{s}{\Gamma(1-s/2)} \int_0^\infty \frac{du}{u^{s+1}}\left(1-b(u)^n\right), \tag{14}$$

$$\Delta_n(s) \;=\; \frac{s}{\Gamma(1-s/2)} \int_0^\infty \frac{du}{u^{s+1}}\left(1-d(u)^n\right), \tag{15}$$

both of which being convergent integrals for $\Re(s) \in (0,2)$. Incidentally, these integrals prove immediately that both $B_n, \Delta_n$ for any fixed real $s$ are monotonic increasing in $n$.

We discuss the issue of numerical quadrature of these error-function representations later. For the moment, we give relevant series developments, as these, relevant to computations on $B_n$:

$$b(u) \;=\; \sum_{k=0}^\infty \frac{(-1)^k u^{2k}}{k!(2k+1)} \;=\; e^{-u^2}\sum_{k=0}^\infty \frac{2^k u^{2k}}{(2k+1)!!}, \tag{16}$$

and these for $\Delta_n$ manipulations:

$$\begin{aligned} d(u) \;&=\; \sum_{k=0}^\infty \frac{(-1)^k u^{2k}}{(k+1)!(2k+1)} \\ &=\; e^{-u^2}\sum_{k=0}^\infty u^{2k}\left(\frac{2^{k+1}}{(2k+1)!!}-\frac{1}{(k+1)!}\right). \end{aligned} \tag{17}$$

[3]The present authors developed this technique for $B_n$, with a view to extreme-precision quadrature and subsequent experimental mathematics. We found later that M. Trott had previously applied a similar approach for the $\Delta_n$ [17]. In a sense, the present treatment is an attempt at unification of the ideas, for more general box integrals.

We discuss in Section 8 how these series play key roles in numerical quadrature. For the moment, we analyze properties of the 1-dimensional integral representations (14), and (15). Important relations along these lines will be these two, where coefficients $\beta_{nk}, \delta_{nk}$ are implicitly defined

$$\left(b\left(\sqrt{t/2}\right)e^{t/2}\right)^n \quad =: \quad \sum_{k\geq 0}\beta_{nk}t^k, \tag{18}$$

$$\left(d\left(\sqrt{t/2}\right)e^{t/2}\right)^n \quad =: \quad \sum_{k\geq 0}\delta_{nk}t^k. \tag{19}$$

Inserting these into (14, 15) we obtain two formal series:

$$B_n(s) \quad = \quad n^{s/2}\sum_{k=0}^{\infty}\left(\frac{2}{n}\right)^k(-s/2)_k\beta_{nk}, \tag{20}$$

$$\Delta_n(s) \quad = \quad n^{s/2}\sum_{k=0}^{\infty}\left(\frac{2}{n}\right)^k(-s/2)_k\delta_{nk}, \tag{21}$$

where $(z)_k$ is the *Pochhammer symbol*[4]. Though developed formally, with regard for convergence issues, it can be shown that each series here converges absolutely whenever $\Re(s)+n>0$.

To sketch the convergence argument, we initially focus on combinatorial relations for the $\beta_{nk}$ (the analysis for the $\Delta_n$ series is similar). An elementary observation is in order. First, for $s=2m$ with $m$ a nonnegative integer, the box integral $B_n(2m)$ can always be written as a finite combinatorial sum of rational components, via simple expansion of the defining integrand. Equivalently, series (20) devolves for $s=2m$ an even integer, into a finite sum

$$\begin{aligned} B_n(2m) \quad &:= \quad \int_{\vec{r}\,\in\,[0,1]^n}\left(r_1^2+\ldots r_n^2\right)^m\ \mathcal{D}\vec{r} \\ &= \quad n^m\sum_{k=0}^{m}(-m)_k\left(\frac{2}{n}\right)^k\beta_{nk}. \end{aligned} \tag{22}$$

This representation of $B_n$ at even integers will prove quite useful in further analysis. Next, stemming from the implicit definition (18) one can derive various relations, the first of which being a beautiful reciprocal relation with the finite sums $B_n(2m)$:

$$\beta_{nk} \quad = \quad \frac{n^k}{2^k k!}\sum_{j=0}^{k}\binom{k}{j}\left(\frac{-1}{n}\right)^j B_n(2j). \tag{23}$$

[4]The Pochhammer symbol $(z)_k := z(z+1)\cdots(z+k-1)$ is extended, for $z$ not a positive integer, by $(z)_k := \Gamma(z+k)/\Gamma(z)$, and for all $z$ we define $(z)_0 := 1$.

Other derivable relations are

$$\beta_{nk} = \frac{n^k}{2^k k!}\int_{\vec{r}\,\in\,[0,1]^n}\left(1-\frac{r^2}{n}\right)^k\,\mathcal{D}\vec{r}, \tag{24}$$

$$\beta_{nk} = \sum_{k_1+\ldots k_n=k}\frac{1}{(2k_1+1)!!}\cdots\frac{1}{(2k_n+1)!!},$$

$$\beta_{nk} = \sum_{j=0}^{k}\frac{1}{(2k+1)!!}\beta_{n-1,k-j}. \tag{25}$$

In checking all of these combinatorial relations, it is convenient to know some "starting cases." We define $\beta_{n0} := 1$ if $n = 0$, else 0, and note

$$\beta_{1k} = \frac{1}{(2k+1)!!},\quad \beta_{n1} = \frac{n}{3},\quad \beta_{n2} = \frac{n^2}{18}+\frac{n}{90},$$

$$B_n(0) = 1,\quad B_n(2) = \frac{n}{3},\quad B_n(4) = \frac{n^2}{9}+\frac{4n}{45},$$

and so on. Now to the convergence issue for the general expansion (20). From relation (24) one can show

$$\beta_{nk} \le \frac{n^k}{2^k k!}\max\left(1,(n/k)^{n/2}\right),$$

and one has for the relevant Pochhammer symbol

$$|(-s/2)_k| = O\left(k!k^{-1-\Re(s/2)}\right).$$

Thus the $k$-th summand in (20) is $O(1/k^{n+\Re(s)+1})$ and absolute convergence obtains whenever $n+\Re(s) > 0$.

Using the above analysis for the general series (20)—and after a similar analysis for (21)—we see that several results accrue. We obtain convenient expansions for the even-argument $B_n(2m), \Delta_{2m}$, and an analytic continuation at least for $n+\Re(s) > 0$. There are various additional inferences we may pursue, such as asymptotic behavior (see Section 6), but first we shall describe a more powerful analytic continuation—and more rapidly converging general series—for the $B_n$ in particular.

# 4 Analytic continuations

Remarkably, and perhaps surprisingly, the relation (8) actually leads to a rapidly (linearly) converging general series for $s$, and a subsequent analytic continuation to *all* complex $s$.

Indeed, using the ideas behind (14) we can infer from the dimensional-reduction formula (8) that

$$B_n(s) \quad = \quad \frac{n}{n+s}\frac{s}{\Gamma(1-s/2)}\int_0^\infty \frac{du}{u^{s+1}}\left(1-e^{-u^2}b(u)^{n-1}\right), \tag{26}$$

leading, after term-by-term integration as before, to an efficient general expansion

$$B_n(s) \quad = \quad n^{s/2}\frac{n}{n+s}\sum_{k=0}^{\infty}\left(\frac{2}{n}\right)^k (-s/2)_k\beta_{n-1,k}. \tag{27}$$

The rather innocent-looking modifications here over the generally slower series (20) give a much more efficient series. Indeed, since

$$\left(\frac{2}{n}\right)^k (-s/2)_k\beta_{n-1,k} \quad = \quad O\left((1-1/n)^k k^{-1-\Re(s/2)-n/2}\right)$$

the sum in the general series (27) is linearly convergent for fixed $n$. Thus, (27) *provides an analytic continuation of* $B_n$ *to all complex* $s$ *except for a simple pole at* $s=-n$.

It is not hard to see how analytic continuation works for the box integrals $B_n$. Take the trivial scenario of $n=1$ dimension. Then, formally, $B_1(s)=\int_0^1 x^s\,dx = 1/(s+1)$ and though the integral diverges for $s=-1$, the analytic continuation of $B_1$ is the function $1/(s+1)$. The same kind of thinking reveals that in $n$ dimensions, the integrand $r^s$ does diverge for $s=-n$; yet, there is an analytic continuation to finite $B_n$ values at any other $s$. An example of a continued value—when the literal integral of $r^s$ is infinite—is

$$B_4(-5) \quad = \quad -0.96120393268995345712165978002474521286412992715\ldots,$$

which could well have a closed form but we do not know it; this approximate value was obtained from the series (27). Note in this regard that our previous, hypergeometric-like reductions (9, 10) for $B_2(s), B_3(s)$ respectively are *already* in analytic continuation form.

There is another way to obtain an efficient series and subsequent continuation, which is foreshadowed by the statistical work in [1] where the attention was exclusively on $B_n(1)$. Within our present formalism we can generalize to arbitrary $s$ by contemplating the expectation

$$\langle r^s\rangle_{\vec{r}\in[0,1]^n} \quad = \quad \frac{n}{n+s}\left\langle\left((1+(n-1)/2)+(r^2-(n-1)/2)\right)^{s/2}\right\rangle_{\vec{r}\in[0,1]^{n-1}},$$

where we have written $1+r^2$ in an intentionally cumbersome way in order to invoke the binomial theorem for power $s/2$. After manipulation, we obtain a very efficient series

$$B_n(s) \quad = \quad \left(\frac{n+1}{2}\right)^{s/2}\frac{n}{n+s}\sum_{k=0}^{\infty}\binom{s/2}{k}\frac{\alpha_{n-1,k}}{(n+1)^k}, \tag{28}$$

where the new $\alpha$-coefficients are defined

$$\alpha_{nk} := 2^k \sum_{j=0}^{k} \binom{k}{j} \left(\frac{1-n}{2}\right)^{k-j} B_n(2j).$$

Incidentally, in computations involving the series (28) it is useful to know, as a simple consequence of (8), that

$$B_n(2m) = \frac{n}{n+2m} \sum_{k=0}^{m} \binom{m}{k} B_{n-1}(2k).$$

In this way, numerical evaluation of (28) becomes an exercise in the use of recursion relations.

Again we have a convergent series for all complex $s$ except for the pole at $s = -n$; indeed (28) appears to be the fastest converging series we have, although (27) has certain practical features, such as the appearance of the $\beta$-terms which in turn can be evaluated via fast convolution from (25).

# 5 "Jellium" physics and box integrals

Given an $n$-cube of uniformly charged jelly of total charge $+1$, what is the electrostatic potential energy of an electron (having charge $(-1)$) at the cube center? This question cannot be answered until we settle on suitable potentials in $n$ dimensions. One possibility—which we hereby adopt—is to take the radial potential at distance $r$ from the electron as $V_n(r)$, where

$$V_1(r) := r - 1/2, \tag{29}$$

$$V_2(r) := \log(2r), \tag{30}$$

$$V_n(r) := 2^{n-2} - \left(\frac{1}{r}\right)^{n-2}, \quad n > 2. \tag{31}$$

These potentials are uniquely determined by two requirements a) $V_n$ satisfies the Laplace equation in $n$ dimensions, and b) $V_n$ vanishes on any face-center ($r = 1/2$). (We are free in electrostatic theory to give any potential a constant offset.)

Let us then define the $n$-th *jellium potential* as

$$J_n := \langle V_n(r) \rangle_{\vec{r} \in [-1/2,1/2]^n}.$$

Interestingly, every $J_n$ except $J_2$ is essentially—up to offset—a box integral. We can dispense with exact evaluations for $n = 1, 2$ (see Section 7), and observe that

$$J_n = 2^{n-2}(1 - B_n(2-n)), \quad n > 2. \tag{32}$$

Because the general jellium potential involves negative parameter $s = 2 - n$ for $n > 2$, we are moved to use one of (20, 27, 28) for evaluation. However, reminiscent of relations (14), (15) one may derive an additional error-function representation

$$B_n(s) \quad = \quad \frac{2}{\Gamma(-s/2)} \int_0^\infty \frac{du}{u^{s+1}} b(u)^n, \tag{33}$$

valid for $\Re(s)$ in the negative interval $(-n, 0)$.

# 6 Intuition via the central limit theorem

The *central limit theorem* of classical probability theory tells us that in some appropriate sense, the distribution of the random variable $\chi := \vec{r} \cdot \vec{r}$ over $\vec{r} \in [0,1]^n$ is Gaussian-normal, with mean and variance

$$\begin{aligned} \langle \chi \rangle \quad &= \quad \frac{n}{3}, \\ \langle (\chi - \langle \chi \rangle)^2 \rangle \quad &= \quad \langle (r^2 - n/3)^2 \rangle \quad = \quad \frac{4n}{45}. \end{aligned}$$

Heuristically speaking, then, we should have

$$B_n(s) \quad \sim_n \quad \frac{1}{\sqrt{2\pi v}} \int_{-\infty}^{\infty} (n/3 + x)^s e^{-x^2/(2v)} \, dx,$$

where $v := 4n/45$. Interestingly, even though error terms in central-limit expansions can be problematic, binomial development of the integrand gives

$$B_n(s) \quad \sim_n \quad \left(\frac{n}{3}\right)^{s/2} \left(1 + \frac{s(s-2)}{10n} + \ldots \right).$$

This agrees, at least through the first two parenthetical terms, with the proven asymptotic of Anderssen et al. [1] for their case $s = 1$.

Still thinking statistically and heuristically, there is another intriguing way to infer that $B_n(s) \sim_n (n/3)^{s/2}(1 + c/n)$ for constant $c$, which is to rewrite (24) in the form

$$\beta_{nk} \quad = \quad \frac{n^k}{3^k k!} \int_{\vec{r} \,\in\, [0,1]^n} \left(1 - \frac{3r^2 - n}{2n}\right)^k \mathcal{D}\vec{r}, \tag{34}$$

where we note that there is now a $3^k$ in the denominator. Evidently, then, the $\beta$-coefficient is seen to depend on moments $\mu_m := \langle (r^2 - n/3)^m \rangle$; additionally we have $\mu_0 = 1, \mu_1 = 0, \mu_2 = 4n/45$, and generally $\mu_m = O(1 + m^2/n)$. Now these estimates for $\mu$, when inserted into the converging series (20), can be seen to give the desired asymptotic. We have not made this argument rigorous; however, relation (34) is promising in this regard.

## 7 Various closed forms

We next state some known closed and nearly closed forms. The nearly-closed forms engage four unresolved integrals which are given numerically in a website file [4].

**1. Box integrals as expectations of distance**—or inverse-distance-from-vertex:

$$\begin{aligned}
B_2(-1) &= \log\left(3+2\sqrt{2}\right), \\
B_3(-1) &= -\frac{\pi}{4} - \frac{1}{2}\log 2 + \log(5+3\sqrt{3}), \\
B_1(1) &= \frac{1}{2}, \\
B_2(1) &= \frac{\sqrt{2}}{3} + \frac{1}{3}\log\left(\sqrt{2}+1\right), \\
B_3(1) &= \frac{\sqrt{3}}{4} + \frac{1}{2}\log\left(2+\sqrt{3}\right) - \frac{\pi}{24}, \\
B_4(1) &= \frac{2}{5} + \frac{7}{20}\pi\sqrt{2} - \frac{1}{20}\pi\log\left(1+\sqrt{2}\right) + \log(3) - \frac{7}{5}\sqrt{2}\arctan\left(\sqrt{2}\right) + \frac{1}{10}\mathcal{K}_0,
\end{aligned}$$

where the one unresolved term, namely

$$\mathcal{K}_0 := \int_0^1 \frac{\log(1+\sqrt{3+y^2}) - \log(-1+\sqrt{3+y^2})}{1+y^2}\,dy = 2\int_0^1 \frac{\operatorname{arctanh}\left(\frac{1}{\sqrt{3+y^2}}\right)}{1+y^2}\,dy, \tag{35}$$

is a dilogarithm-like entity that can be evaluated reasonably rapidly, via the 2-dimensional sum

$$\mathcal{K}_0 = \sum_{m,k\geq 0} \frac{2^{k+1}}{2m+1}\frac{I_{m+k}}{3^{m+k+1}} = \frac{2}{3}\sum_{p=0}^{\infty} I_p \left(\frac{2}{3}\right)^p \sum_{n=0}^{p} \frac{1}{2^n\,(2n+1)},$$

where $I_0 := 1/2$ and

$$I_m = \frac{1}{2m+1}\left\{2mI_{m-1} + \left(\frac{3}{4}\right)^m \frac{1}{2}\right\}.$$

Now $\mathcal{K}_0$ can also be recast from this sum in a form revealing more obviously a linear convergence (essentially, by powers of (2/3)):

$$\mathcal{K}_0 = \sum_{n=1}^{\infty} \beta\left(\frac{1}{2}, n\right)\kappa_n \left(\frac{2}{3}\right)^n - \frac{1}{2}\sum_{n=1}^{\infty} {}_2F_1\left(1, n+\frac{1}{2}, n+1, \frac{3}{4}\right)\kappa_n \left(\frac{1}{2}\right)^n$$

where

$$\kappa_n \;:=\; \sum_{m=1}^{n} \frac{1}{(2\,m-1)\,2^m}.$$

The expression for $B_4(1)$ results from two dimension reductions followed by substantial symbolic computation with the remaining two-dimensional integrals, all of which ultimately resolved—via dilogarithms—except for $\mathcal{K}_0$.

**2. Average distance**—or inverse-distance between two points:

$$\begin{aligned}
\Delta_2(-1) &= \frac{2}{3} - \frac{4}{3}\sqrt{2} + 4\log(1+\sqrt{2}),\\
\Delta_1(1) &= \frac{1}{3},\\
\Delta_2(1) &= \frac{1}{15}\left(2+\sqrt{2}+5\log(1+\sqrt{2})\right),\\
\Delta_3(1) &= \frac{4}{105} + \frac{17}{105}\sqrt{2} - \frac{2}{35}\sqrt{3} + \frac{1}{5}\log(1+\sqrt{2}) + \frac{2}{5}\log(2+\sqrt{3}) - \frac{1}{15}\pi,\\
\Delta_4(1) &= \frac{26}{15}\,\mathrm{G} - \frac{34}{105}\,\pi\,\sqrt{2} - \frac{16}{315}\,\pi + \frac{197}{420}\,\log(3) + \frac{52}{105}\,\log\left(2+\sqrt{3}\right)\\
&+ \frac{1}{14}\,\log\left(1+\sqrt{2}\right) + \frac{8}{105}\,\sqrt{3} + \frac{73}{630}\,\sqrt{2} - \frac{23}{135} + \frac{136}{105}\,\sqrt{2}\arctan\left(\frac{1}{\sqrt{2}}\right)\\
&- \frac{1}{5}\,\pi\,\log\left(1+\sqrt{2}\right) + \frac{4}{5}\,\alpha\,\log\left(1+\sqrt{2}\right) - \frac{4}{5}\,\mathrm{Cl}_2\left(\alpha\right) - \frac{4}{5}\,\mathrm{Cl}_2\left(\alpha+\frac{\pi}{2}\right).
\end{aligned}$$

$$\begin{aligned}
\Delta_5(1) &= \frac{65}{42}\,\mathrm{G} - \frac{380}{6237}\,\sqrt{5} + \frac{568}{3465}\,\sqrt{3} - \frac{4}{189}\,\pi - \frac{449}{3465} - \frac{73}{63}\,\sqrt{2}\arctan\left(\frac{\sqrt{2}}{4}\right) - \frac{184}{189}\,\log(2)\\
&+ \frac{64}{189}\,\log\left(\sqrt{5}+1\right) + \frac{1}{54}\,\log\left(1+\sqrt{2}\right) + \frac{40}{63}\,\log\left(\sqrt{2}+\sqrt{6}\right) - \frac{5}{28}\,\pi\,\log\left(1+\sqrt{2}\right)\\
&+ \frac{52}{63}\,\pi\,\log(2) + \frac{295}{252}\,\log(3) + \frac{4}{315}\,\pi^2 + \frac{3239}{62370}\,\sqrt{2} - \frac{8}{21}\sqrt{3}\,\arctan\left(\frac{1}{\sqrt{15}}\right)\\
&- \frac{52}{63}\,\pi\,\log\left(\sqrt{2}+\sqrt{6}\right) + \frac{5}{7}\alpha\,\log\left(1+\sqrt{2}\right) - \frac{5}{7}\,\mathrm{Cl}_2\left(\alpha\right) - \frac{5}{7}\,\mathrm{Cl}_2\left(\alpha+\frac{\pi}{2}\right) + \frac{52}{63}\,\mathcal{K}_1,
\end{aligned}$$

where the unresolved quantity is the integral

$$\mathcal{K}_1 \;:=\; \int_3^4 \frac{\mathrm{arcsec}\,(x)}{\sqrt{x^2-4\,x+3}}\,dx, \tag{36}$$

and where $\alpha := \arcsin\left(2/3 - 1/6\sqrt{2}\right)$, G is the *Catalan constant*, $\mathrm{Cl}_2$ is the order-2 *Clausen function*, $\Psi_n$ is the order-$n$ *polygamma* function, and $\mathrm{Li}_n$ is the *polylogarithm* function—see [8] or [11] for details.

The evaluations for $\Delta_4(1)$ and $\Delta_5(1)$ come from taking those given in [17] and then (i) carefully eliminating dependent terms (which often entails reexpressing logarithms and polylogarithms) and (ii) using the *Kummer formula* [11, eq. (5.5)] to express the remaining polylogarithms as Clausen functions.

**3. Jellium potentials vs. dimension:**

$$\begin{aligned}
J_1 &= -\frac{1}{4}, \\
J_2 &= -\frac{3}{2} + \frac{\pi}{4} + \frac{1}{2}\log 2, \\
J_3 &= 2 + \frac{1}{2}\pi - 3\log\left(2+\sqrt{3}\right), \\
J_4 &= 4 + \pi^2 + 8\,\mathrm{G} - \frac{4}{3}\ln\left(2+\sqrt{3}\right)\pi - 4\,\mathrm{Cl}_2\left(\frac{1}{6}\pi\right) - 4\,\mathrm{Cl}_2\left(\frac{5}{6}\pi\right) - 16\,\mathcal{K}_2 \\
J_5 &= 8 - \frac{5}{3}\pi^2 - 20\ln\left(2+\sqrt{3}\right)\pi + 80\,\mathcal{K}_3.
\end{aligned}$$

The unresolved quantities in the above are given by

$$\begin{aligned}
\mathcal{K}_2 &:= \int_0^{\pi/4} \sqrt{1+\sec^2(a)}\,\arctan\left(\frac{1}{\sqrt{1+\sec^2(a)}}\right) da \\
&= \frac{\pi^2}{16} - \sum_{m=1}^{\infty} \frac{(-1)^m}{2^m} \sum_{k=1}^{m-1} \frac{\binom{-(m-k)}{k}}{2(m-k)+1} \sum_{j=0}^{k-1} \frac{(-1)^j}{2\,j+1} \\
&= 1 - \frac{\pi}{4} + \frac{\pi^2}{16} - \sum_{N=1}^{\infty}\left(\frac{1}{2}\right)^N \sum_{n=1}^{N}\binom{N-1}{n-1}\sum_{m=1}^{N-1}\frac{(-1)^{n+m}}{(2\,m+1)\,(2\,n+1)} \\
&+ \sum_{N=1}^{\infty}\left(\frac{1}{2}\right)^N \sum_{n=1}^{N}\binom{N-1}{n-1}\sum_{m=1}^{n}\frac{(-1)^{n+N-m}}{(2\,N-2\,m+1)\,(2\,n+1)}
\end{aligned} \tag{37}$$

and

$$\begin{aligned}
\mathcal{K}_3 &:= \int_0^{\pi/4}\int_0^{\pi/4}\sqrt{1+\sec^2(a)+\sec^2(b)}\,da\,db \qquad (38)\\
&= -\sqrt{3}\sum_{n=0}^{\infty}\frac{\binom{2\,n}{n}/\left(2\,n-1\right)}{12^n}\sum_{k=0}^{n}\binom{n}{k}\left(\frac{\pi}{4}-\sum_{j=0}^{k-1}\frac{(-1)^j}{2\,j+1}\right)\left(\frac{\pi}{4}-\sum_{j=0}^{n-k-1}\frac{(-1)^j}{2\,j+1}\right).
\end{aligned}$$

The value of $J_4$ was obtained from (8). The even-more partial expansion of $J_5$ was likewise obtained from two polar transformations.

Note again that the dimensions $n = 1, 2$ have special status, as per (29), (30) and (31).

## 8 Extreme-precision quadrature

Using the 1-dimensional integral representations (14), (15) and (33), we were able to generate extreme-precision values of $B_n := B_n(1)$, $\Delta_n := \Delta_n(1)$ and $B_n(2-n)$, respectively, for a selection of $n$. Note that $J_n$ can be readily and accurately evaluated from $B_n(2-n)$ by using (32). These numerical values are given explicitly in Appendix 1, together with values for the unresolved integrals $\mathcal{K}_n$ for $n = 0, 1, 2$ and 3, which we computed using (35), (36), (37) and (38), respectively.

These integrals were computed using the tanh-sinh quadrature scheme. Tanh-sinh quadrature is remarkably effective in evaluating integrals to very high precision, even in cases where the integrand function has an infinite derivative or blow-up singularity at one or both endpoints. It is well-suited for highly parallel evaluation [2], and is also amenable to computation of provable bounds on the error [3]. It is based on the transformation $x = g(t)$, where $g(t) = \tanh[\pi/2 \cdot \sinh(t)]$. In a straightforward implementation of the tanh-sinh scheme, one first calculates a set of *abscissas* $x_k$ and *weights* $w_k$

$$\begin{aligned} x_j &:= \tanh[\pi/2 \cdot \sinh(jh)] \\ w_j &:= \frac{\pi/2 \cdot \cosh(jh)}{\cosh^2[\pi/2 \cdot \sinh(jh)]}, \end{aligned}$$

where $h$ is the interval of integration. Then the integral of the function $f(t)$ on $[-1, 1]$ is performed as

$$\int_{-1}^{1} f(x)\, dx \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\, dt \;\approx\; h \sum_{-N}^{N} w_j f(x_j)$$

where $N$ is chosen so that the terms $w_j f(x_j)$ are sufficiently small that they can be ignored for $j > N$. Full details of a robust implementation are given in [7]. Tanh-sinh quadrature has its roots in a 1969 paper by Schwartz [13], although it was first described in the present form in 1973 by Takahashi and Mori [14].

Computing $B_n$ using (14) requires one to perform two integrals, one with the integrand function $f(u) = (1 - (\sqrt{\pi}/(2u) \cdot \mathrm{erf} u)^n / u^{s+1}$, from 0 to 1, and a second integral of $f(1/u)/u^2$, from 0 to 1. Adding the two together gives the integral from 0 to $\infty$. Computing these integrals is complicated by the fact that in tanh-sinh quadrature, the integrand function must be evaluated to high precision very close to the endpoints, and subtractions or other inaccuracies int he function evaluation can result in quadrature errors (a difficulty first described in 1984 by Evans, Forbes and Hyslop [9]). In this case, it is not sufficient just to compute erf to high relative precision near zero; because of the subtractions here, one must use a Taylor series expansion for the integrand function when the argument is within say $10^{-10}$ of zero. Computing these Taylor series coefficients (which we did using *Mathematica*) turned out to be the most expensive part of the entire computation. Once highly accurate integrand functions were available, the quadrature evaluations for $B_n$ were completed in less than one minute each.

Computing $\Delta_n$ using (15) also required Taylor series expansions, at least for the first of the two integrals to be performed. Again, obtaining these Taylor series coefficients turned out to be the most expensive aspect of the computation. Computing the $B_n(2-n)$ integrals required no Taylor series expansions and was completely straightforward.

Computing $\mathcal{K}_0$, $\mathcal{K}_1$ and $\mathcal{K}_2$ using (35), (36) and (37) was relatively straightforward. However, computing $\mathcal{K}_3$ using (38) requires 2-dimensional quadrature. We were able to do this by a straightforward extension of the 1-dimensional tanh-sinh scheme to two dimensions. However, because many times more function evaluations are required, the run time was correspondingly longer—four hours, as opposed to a few seconds for the others. We also computed $\mathcal{K}_3$ using the nested infinite series given just following (38), but this required even more run time. The two numerical values, however, agreed.

All of our computed values are available on a public website [4].

# 9 Open problems

- Can the jellium potential $J_3$ be generalized for different offset vectors (but still in a 3 dimensional setting), to yield via summation the true jellium potential due to an *infinite* cube of charged jelly?

  This leads to the intriguing research area of obtaining other Madelung and Wigner lattice sums via box integrals with changing offset. Note the fixed point $\vec{q}$ in the very definition of $X_n$ does *not* have to be within the unit cube.

- What is the precise asymptotic behavior of $\Delta_n(s)$?

- The authors of the original treatment [1] pointed out that a series of the type (28) does not seem to be available even for their parameter case of $s = 1$. Nor do we know presently how to convert (27) for the $\Delta_n$ problems. We do have (21) which converges, albeit slowly. So, what is a rapidly converging series for $\Delta_n$?

- How can (7) be used to reduce the dimension—in a convenient way—for some specific $\Delta_n$? We say "convenient" because the many symmetries of the $B_n$ cases allowed us to make practical use of (8).

- How can (34) be used to establish a precise asymptotic expansion for $B_n(s)$? The original reference [1] perhaps contains sufficient clues.

- Which of the $\mathcal{K}_i$ integrals can be further or completely resolved?

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