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Rectangular vesicles in three dimensions

J Ma and E J Janse van Rensburg

Department of Mathematics and Statistics, York University, Toronto, Ontario, M3J 1P3, Canada

E-mail: rensburg@yorku.ca

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Abstract
The phase diagram of a model of rectangular vesicles in three dimensions is examined. The scaling of the generating function is determined in the area–perimeter, volume–area and volume–perimeter ensembles. The results are interpreted within the framework of tricritical scaling, and the crossover exponents associated with the transitions are determined. We identify three phases in the phase diagram, a needle phase, a disc phase and a cubical phase. These phases are separated by three curves of transitions that meet in a multicritical point.

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1. Introduction

Models of partitions and other models of convex polygons in the square lattice have captured the imagination of mathematicians since the publication of the MacMohan conjectures [21]. These conjectures involved diagrammatic representations of partitions of integers, and they inspired many models in combinatorial mathematics including Ferrer's diagrams and a variety of lattice path and convex polygons models. These are now classical models in combinatorics [16–19, 28, 31] and they have received considerable attention in the literature (see, for example, [3, 4, 8]). In three dimensions models of plane partitions have been studied with reference to the alternating sign matrix theorem [32]. Lattice random discs in two dimensions and lattice random surfaces in three dimensions are the undirected versions of these models, and have been studied as models to understand the thermodymical properties of vesicles or of interfaces, see, for example, [1, 2, 11, 12], and references therein.

Lattice vesicles are models of convex polygons in an area–perimeter ensemble. These models are closely related to Ferrer's diagrams and to models of fully and partially directed paths [24, 25], and were also considered by Temperley in the 1950s [30]. In the physics literature, the study of directed and undirected models of lattice paths and vesicles was inspired by efforts to understand and model the entropic nature of polymers.

Models of polyominoes have been studied in the square lattice as models of two-dimensional vesicles, and they have been analysed in particular from a statistical mechanics point of view [2–4, 8]. These models can be analysed using known combinatorial techniques and in some cases one may solve explicitly for the generating function. For example, solutions for models of partition polygons go back many decades to the work of Ramanujan and Hardy [9, 10]. Other models may present difficult mathematical challenges (for example, various models of convex lattice polygons [26, 27, 29]). Generally, the phase diagram of the statistical mechanics model underlying the directed lattice model can be examined by solving the combinatorial problem followed by the examination of the asymtotics of the generating function close to a critical point.

Some models have solutions expressible in terms of well-understood special functions, and in those cases the description of the models is in some sense complete. In other models, such as that presented in this paper, the generating function appears not to be related to a known special function. In such cases the model is examined by finding integral approximations to the generating function. These representations do allow the determination of scaling exponents readily.

In figure 1 several two-dimensional square lattice polygon models of vesicles are shown. Consider such a model of polygons in the square lattice composed of n unit squares and with m perimeter edges. The most basic quantity associated with the model is $c_n(m)$; this is the number of polygons for area n unit area squares and perimeter m unit length edges. The generating function is a two-variable function

$$G(t,q) = \sum_{n\geqslant 0} \left[\sum_{m\geqslant 0} c_n(m) t^m \right] q^n, \tag{1}$$

where t is the 'perimeter generating variable', and q is the 'area generating variable'. In the model of square lattice vesicles in figure 1(a), it has been shown [12, 15] that the generating function is

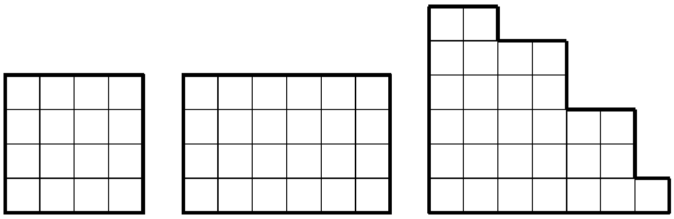
$$\begin{aligned} S(t,q) &= \sqrt{\frac{2\pi(1+qt^4)(1+qt^{-4})}{|\log q^2|}}\, \mathrm{e}^{(\pi^2/6+\mathcal{L}i_2(-qt^4)+\mathcal{L}i_2(-qt^{-4}))/\log q^2} + 1 + O(t^{-4}) \\ &\sim \frac{1}{\sqrt{|\log q^2|}} \mathcal{G}_o\big(|\log t^2|/\sqrt{|\log q^2|}\big) \end{aligned} \tag{2}$$

where $\mathcal{G}_o(x) = \mathrm{e}^{x^2/2}$. It is customary to define *scaling fields*[1] $s = |\log t^2|$ and $g = |\log q^2|$ so that $s \to 0^+$ and $g \to 0^+$ as the singularity at (1, 1) is approached from below. In that case the result above becomes

$$\begin{aligned} S(t,q) &\sim g^{-1/2}\mathcal{G}_o(sg^{-1/2}) \\ &= s^{-1}(sg^{-1/2})\mathcal{G}_o(sg^{-1/2}) \\ &= s^{-1}\mathcal{H}_o(sg^{-1/2}) \end{aligned} \tag{3}$$

where $\mathcal{H}_o(x) = x\mathcal{G}_o(x)$. The appearance of the combination $s/\sqrt{g}$ indicates that $S(t,q)$ have particularly simple behaviour along curves given by $s/\sqrt{g}$ = const. Note also that the crossover from $s = 0$ to $g = 0$ is determined by the combination, and that the power of g plays a particular role. It is the *crossover exponent*.

[1] Standard notation would introduce the scaling fields g and t instead. However, since t is already introduced as a generating variable, the scaling field instead will be denoted by s. Usually, if the critical point is located at (t_c, q_c), then $g = |q - q_c| \approx |\log(q/q_c)|$ and $s = |t - t_c| \approx |\log(t/t_c)|$, or g and s are linear combinations of $|q - q_c|$ and $|t - t_c|$.



(a) (b) (c)

Figure 1. Models of square lattice vesicles. Square and rectangular vesicles are illustrated in (*a*) and (*b*), while (*c*) is a partition vesicle.

A similar result is known for the model of rectangular square lattice vesicles in the area–perimeter ensemble [27]. In particular, the scaling relation of the generating function in this model is [15]

$$R(t,q) \sim t^2 g^{-1} \mathcal{R}_o(sg^{-1}), \tag{4}$$

where the scaling fields are $s = |\log t^2|$ and $g = |\log q|$ and the scaling function $\mathcal{R}_o$ is related to a Lerch–Phi function $L_P(z,a,x) = \sum_{n=0}^{\infty} \frac{z^n}{(x+n)^a}$ by $\mathcal{R}_o(x) = x^{-1} - L_P(t^2q, 1, x)$.

The asymptotic result for $S(t,q)$ in equation (2) is referred to as 'scaling of the generating function', and it is not unexpected. In the most general terms, tricritical scaling theory predicts this scaling result for the generating function of lattice vesicles [8, 12, 25]. In the generic case with generating function $G(t,q)$ and with scaling fields s and g, it is expected that

$$G(t,q) \sim A(t,q) + g^{2-\alpha_t}\mathcal{K}_o(sg^{-\phi}) = A(t,q) + s^{2-\alpha_u}\mathcal{K}_1(sg^{-\phi}) \tag{5}$$

in its asymptotic regime as the scaling fields decrease to zero on approaching the tricritical point at $(s,g) = (0,0)$. The tricritical point is located on the critical curve $q_c(t)$, and this is the radius of convergence of the generating function. In this case one may identify the scaling function $\mathcal{K}_o$ as either $\mathcal{G}_o$ or $\mathcal{R}_o$. Observe that consistency requires that

$$\phi = \frac{2-\alpha_t}{2-\alpha_u} \tag{6}$$

and that $G(t,0) \sim s^{2-\alpha_u}$ while $G(0,q) \sim g^{2-\alpha_t}$. The exponent ϕ describes crossover as the tricritical point is approached from either the s- or g-axes. $A(t,q)$ is an analytic background term. The scaling exponents for square and rectangular vesicles in the square lattice can be read from equations (3) and (4). In particular,

$$\phi = \begin{cases} 1/2, & \text{square vesicles;} \\ 1, & \text{rectangular vesicles.} \end{cases} \tag{7}$$

One may also read of the values of $2-\alpha_u$ and $2-\alpha_t$ for these models.

Crossover exponents are known for a wide class of lattice vesicles and models of directed paths, see, for example, [5, 6, 8, 13, 14, 29]. The well-known partition generating function has similarly been analysed [9, 24, 27] as well as more general two-dimensional models of vesicles, including stack and staircase polygons [4, 27, 31] or partially of fully convex models of lattice vesicles [26, 27].

In this paper we continue the work which began in [15]. In particular, the two simple models of three-dimensional cubic lattice vesicles in figure 1 were examined. Crossover exponents and scaling relations were determined for a model of cubical vesicles and for a model of rectangular box vesicles. The generating function of cubical vesicles is

$$T(t,q,p) = \sum_{n=0}^{\infty} t^{12n} q^{6n^2} p^{n^3} \tag{8}$$

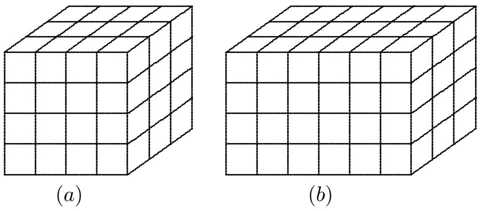


Figure 2. Models of cubic lattice vesicles. Cubical rectangular box vesicles are illustrated in (*a*) and (*b*).

where t generates perimeter, q area and p volume. From the Jacobi triple product it follows that

$$T(1,q,1) = \tfrac{1}{2}(1 + (-q^6, q^{12})^2_\infty (q^{12}, q^{12})_\infty). \tag{9}$$

In this case, $(t,q)_n$ is a q-deformation of the factorial:

$$(t,q)_n = \prod_{m=0}^{n-1} (1 - tq^m). \tag{10}$$

It is shown in [15] that if $\mathcal{G}(x) = \mathrm{e}^{x^2}(1 - \mathrm{erf}(x))$, then

$$T(t,q,1) = \frac{1}{2} + \frac{\sqrt{\pi}}{12s}[\sqrt{6}sg^{-1/2}]\mathcal{G}(\sqrt{6}sg^{-1/2}) + R_1 \tag{11}$$

where $|R_1| \leqslant 6B_2 t^{12} q^6 (|\log t| + |\log q|)$, and $B_2 = 1/6$ is the second Bernoulli number.

A similar result is known for $T(1,q,p)$, the generating function of cubical vesicles in the area–volume ensemble. Let

$$\mathcal{F}(x) = \left|\frac{x}{32}\right|^{1/6} \left[\frac{2\sqrt{3}\pi}{9\Gamma(2/3)} F_{1,1}(1/6, 1/3; x) - \frac{\sigma_x |x/32|^{2/3}}{3} F_{2,2}([1/2, 1], [2/3, 4/3]; x) \right.$$
$$\left. + \frac{\sqrt{\pi}|x/32|^{1/2}}{18} F1, 1(5/6, 5/3; x) \right] \tag{12}$$

where $\sigma_x = 1$ if $x \geqslant 1$ and $\sigma_x = -1$ if $0 < x < 1$, and where $F_{a,b}(\ldots; x)$ are hypergeometric functions in standard notation. Then

$$T(1,q,p) = \tfrac{1}{2} + \tau^{-1}\mathcal{F}(32\sigma_q[\tau\chi^{-2/3}]^3) + R_2, \tag{13}$$

where $\tau = |\log q|$ and $\chi = |\log p|$. The remainder term is bound by

$$|R_2| \leqslant \frac{B_2}{2} \sum_i \left|6r_i^2 \log p + 4r_i \log q\right| p^{r_i^3} q^{r_i^2} \tag{14}$$

and the sum is over all roots of the polynomial in r:

$$9r^4 \log^2 p + 12r^3 \log p \log q + 4r^2 \log^2 q + 6r \log p + 2 \log q = 0. \tag{15}$$

Thus, even in this simple model it is a challenge to verify the expected scaling of the generating function.

Some partial results were obtained for the model of rectangular box vesicles in figure 1(*b*) [15]. This model will be discussed in more detail in the following sections, and in particular, the scaling of the generating function will be examined.

2. Tricritical scaling and rectangular box vesicles

2.1. Tricritical scaling

The statistical mechanics of a model of vesicles involves a partition function

$$Z_n(t) = \sum_{m\geqslant 0} c_n(m)t^m. \tag{16}$$

The thermodynamic properties of the model are described by the limiting free energy (density)

$$\mathcal{F}_p(t) = \lim_{n\to\infty} \frac{1}{n} \log Z_n(t). \tag{17}$$

Phase transitions are non-analytic points in $\mathcal{F}_p(t)$, which can be shown to be convex, and therefore measurable and analytic almost everywhere. In most vesicle models there appears to be exactly one non-analyticity in $\mathcal{F}_p(t)$ at (say) $t = t_c$. A comparison with equation (1) shows that the limiting free energy is in fact related to the radius of convergence $q_c(t)$ of the generating function:

$$\mathcal{F}_p(t) = -\log q_c(t). \tag{18}$$

The critical point is then a non-analyticity in the *critical curve* $q_c(t)$.

Since $q_c(t)$ is a curve of singularities in the generating function, a proper description of the critical point at $t = t_c$ will include a study of the singular structure of $G(t, q)$ along the critical curve $q_c(t)$. This description is provided by *tricritical scaling theory* [8, 20] predicated on the assumption that a generic generating function (or grand partition function) $G(t, q)$ should exhibit certain scaling behaviour in its asymptotic regime close to the tricritical point on $q_c(t)$.

Tricritical scaling introduces scaling fields (or axes) g and s with origin at the tricritical point and with the g-axis tangent to $q_c(t)$ at $t = t_c$, and s transverse to it. In the gs-plane, the critical curve is a phase boundary, and the behaviour of $G(t, q)$ close to the tricritical point is given by equation (5). This introduces the *crossover exponent* ϕ that describes crossover behaviour between the scaling fields g and s. Along the curves $g^{-\phi}s = C_0$ in the gs-plane the generating function has asymptotic behaviour

$$G(t, q) \sim A(t, q) + C_0 g^{2-\alpha_t}, \tag{19}$$

$$G(t, q) \sim A(t, q) + C_1 s^{2-\alpha_u}, \tag{20}$$

and the singular behaviour in $G(t, q)$ at the critical point is described by the exponent $2 - \alpha_t$ or $2 - \alpha_u$ as the tricritical point is approached.

The non-analyticity in $\mathcal{F}_p(t)$ is described by the introduction of an exponent α, and then considering the shape of the limiting free energy close to the critical point:

$$\mathcal{F}_p(t) \sim C_0|t - t_c|^{2-\alpha} + \text{analytic terms}, \qquad \text{as} \quad t \to t_c^+. \tag{21}$$

The exponent α is also called the *specific heat exponent*, and it describes a singularity in the specific heat (the second derivative of $\mathcal{F}_p(t)$ to $\log t$). In this description, the generating function $G(t, q)$ may be interpreted as a generalized *grand potential*, whilst the limiting free energy $\mathcal{F}_p(t)$ includes both entropic and energy contributions (and may be considered a Helmholtz free energy, if considered from a classical thermodynamic point of view). The crossover exponent is related to the specific heat exponent by a hyperscaling relation

$$2 - \alpha = 1/\phi, \tag{22}$$

and this relates the exponents α_u and α_t finally to the thermodynamic properties of the model, tying together the grand canonical (or generating function) approach and the canonical (or free energy) approach into one description of the thermodynamics of the model.

2.2. Rectangular vesicles in three dimensions

The three-dimensional version of rectangular vesicles is a model of vesicles with generating function

$$B(t, q, p) = \sum_{i,j,k>0} t^{4(i+j+k)} q^{2(ij+jk+ki)} p^{ijk}. \tag{23}$$

Partial results were obtained in [15]. In particular, it was shown that

$$B(1, q, 1) = \frac{\sqrt{\pi}}{\sqrt{|\log q^2|}} \int_1^\infty \frac{\mathrm{e}^{-|\log q^2|(y(y+4)/4)}}{1 - \mathrm{e}^{-y|\log q^2|}} \operatorname{erf} i\left(y\sqrt{|\log q^2|}/2\right) \mathrm{d}y + \frac{B_q}{\sqrt{1-q^2}}; \tag{24}$$

$$B(1, 1, p) = \frac{1}{|\log p|} \int_0^p \frac{\log(1-y)}{\log y} \frac{\mathrm{d}y}{y} + \frac{R_p}{1-p}, \tag{25}$$

where B_q can be bounded by a constant for all q in the half-open interval $[q_0, 1)$, and R_q can be bounded by a constant for all points (p, q) in the rectangle $[p_0, 1] \times [q_0, 1]$, and where p_0 and q_0 are arbitrary but fixed in the open interval (0, 1). The integrals in these expressions are divergent; in the first case apparently proportional to $|\log q^2|^{-1}$, and in the second case slower than any inverse power of $|\log p|$. One may attempt to assign values to the critical exponents, and comparison to equations (19) and (20) indicates that $2 - \alpha_u = -3/2$ while $2 - \alpha_t = -1$. These results suggest that $\phi = 2/3$, but an explicit form for the tricritical scaling form of $B(1, q, p)$ is not known, and a scaling function for this model has also not been found. It was conjectured in [15] that $\phi = 2/3$ in this model, and evidence consistent with this conjecture is examined there.

In this paper we examine this model of three-dimensional rectangular vesicles more closely. We re-examine approximations of $B(1, q, 1)$ and $B(1, 1, p)$ and improved asymptotic approximations are found containing a logarithmic integral or iterated logarithms, respectively. The two variable generating function is subsequently studied in the tq-, tp- and qp-ensembles. In these cases we were able to approximate the generating functions by integral expressions that exhibit the expected scaling of the model.

3. Scaling in rectangular vesicles in three dimensions

Consider the generating function $B(t, q, p)$ in equation (23). The phase diagram of this model is three dimensional, and there are phase boundaries separating a bulk phase of 'finite vesicles' (where $B(t, q, p)$ is finite) from a bulk phase of 'infinite vesicles' where vesicles of arbitrary large size make a contribution to $B(t, q, p)$ so that it is divergent. The phase boundary is a surface of critical values of the generating variables in parameter space. This critical surface intersects the surfaces $t = 1, q = 1$ and $p = 1$ in critical curves, and in each case there is a tricritical point located on the critical curve at $t = q = p = 1$. This point is a multicritical point in the three-dimensional phase diagram, where it has complicated scaling properties. We examine these by considering the scaling of the two-variable generating functions $B(1, q, p)$, $B(t, q, 1)$ and $B(t, 1, p)$ in the vicinity of the multicritical point.

In our approaches we rely on the Euler–MacLaurin formula to approximate series by integrals. The advantage is that the error term can be controlled, so that the nature of the approximation is well understood. The resulting approximation allows substitutions that will explicitly exhibit the scaling properties of the model. This gives the critical exponents from which the model can be defined.

Theorem 3.1 (Euler–MacLaurin formula). *Suppose* f *is a* $2m$*-times continuously differentiable function on the interval* $[0, N]$ *(that is,* $f \in C^{2m}[0, N]$*). Then*

$$\sum_{n=1}^{N} f(n) = \int_1^N f(x)\,\mathrm{d}x + \frac{1}{2}[f(1) + f(N)] + \sum_{n=1}^{m-1} \frac{B_{2n}}{(2n)!}[f^{(2n-1)}(N) - f^{(2n-1)}(1)] + R_m.$$

The remainder term R_m *is given by the integral*

$$R_m = \int_1^N [B_{2m} - B_{2m}(x - \lfloor x \rfloor)] \frac{f^{(2m)}(x)}{(2m)!}\,\mathrm{d}x$$

over the Bernoulli polynomials $B_{2m}(x)$ *and the* $2m$th *derivative of* f*.* $B_{2m} = B_{2m}(0)$ *is the* $2m$th *Bernoulli number: in particular* $B_2 = 1/6$.

One may take $N \to \infty$ in the Euler–MacLaurin formula, provided that the error term can be controlled. Putting $m = 1$ and taking $N \to \infty$ then gives the following corollary:

Corollary 3.2. *Suppose* f *is a twice continuously differentiable function on the interval* $[0, \infty)$*. Then*

$$\sum_{n=1}^{\infty} f(n) = \int_1^{\infty} f(x)\,\mathrm{d}x + \frac{1}{2}[f(1) + f(\infty)] + R_1.$$

The remainder term is

$$R_1 = \int_1^{\infty} [B_2 - B_2(x - \lfloor x \rfloor)] \frac{f^{(2)}(x)}{2}\,\mathrm{d}x,$$

and $|R_1| \leqslant ([B_2 f'(x)]/2)|_{x=1}^{\infty}$.

One may directly compute that

$$B(t, 1, 1) = \frac{t^{12}}{(1 - t^4)^3}, \tag{26}$$

so consider next $B(1, q, 1)$ and $B(1, 1, p)$.

3.1. Approximating $B(1, q, 1)$

In equation (26) above, the behaviour of $B(t, 1, 1)$ was examined as $t \to 1^-$. Next, consider $B(1, q, 1)$ as $q \to 1^-$. This function is somewhat complicated, but it is possible to prove that to a first approximation,

$$B(1, q, 1) \sim \frac{\log|\log q^2| + C}{|\log q^2|^{3/2}} \qquad \text{as} \quad q \to 1^-, \tag{27}$$

where C is a finite constant. This is an improvement on equation (24), and the scaling in the scaling field $|\log q|$ is exposed as $q \to 1^-$. The starting point of the calculation is

$$\begin{aligned} B(1, q, 1) &= \sum_{i,j,k>0} q^{2(ij+jk+ki)} = \sum_{i,j>0} \frac{q^{2ij} q^{2(i+j)}}{1 - q^{2(i+j)}} \\ &= 2 \sum_{i>j>0} \frac{q^{2ij} q^{2(i+j)}}{1 - q^{2(i+j)}} + \sum_{k>0} \frac{q^{2k(k+2)}}{1 - q^{4k}} \\ &= 2 \sum_{n=1}^{\infty} \sum_{k=1}^{\infty} \frac{q^{2n(k+1)+2k(k+2)}}{1 - q^{2(n+2k)}} + \sum_{k=1}^{\infty} \frac{q^{2k(k+2)}}{1 - q^{4k}} \end{aligned} \tag{28}$$

where the substitions $j = k$ and $i = k + n$ were made in the summation indices in the last step. This substitution changes the order of terms in the summation—we assume that q is small enough that the series converge absolutely.

The Euler–MacLaurin formula can now be applied by putting $f(x) = (q^{2x(k+1)+2k(k+2)})/(1 - q^{2(x+2k)})$. Expand the denominator as an infinite series, interchange the series and the integral, and then integrate term by term to find that

$$\begin{aligned}\int_1^\infty f(x)\,\mathrm{d}x &= q^{2k(k+2)} \sum_{m=0}^{\infty} q^{4mk} \int_1^\infty q^{2x(m+k+1)} \\ &= \frac{q^{2k(k+2)}}{|\log q^2|} \sum_{m=0}^{\infty} \frac{q^{4mk+2(m+k+1)}}{m+k+1} \\ &= \frac{1}{q^{2k^2}|\log q^2|} \sum_{m=k+1}^{\infty} \frac{q^{2m(2k+1)}}{m}.\end{aligned} \tag{29}$$

These results can be put together with equation (28) to obtain the following: there exists a function R_1 of q such that

$$B(1, q, 1) = \frac{2}{|\log q^2|} \sum_{k=1}^{\infty} \sum_{m=k+1}^{\infty} \frac{q^{2m(2k+1)}}{mq^{2k^2}} + \sum_{k=1}^{\infty} \frac{q^{2k(k+2)}}{1 - q^{4k}} + \sum_{k=1}^{\infty} \frac{q^{2(k^2+3k+1)}}{1 - q^{4k+2}} + R_1. \tag{30}$$

Moreover, R_1 is bounded by

$$\begin{aligned}|R_1| &\leqslant B_2 |\log q| \sum_{k=1}^{\infty} \frac{q^{2(k+1)^2+2k}((k+1)(1 - q^{4k+2}) + q^{4k+2})}{(1 - q^{4k+2})^2} \\ &\leqslant B_2 |\log q^2| \sum_{k=1}^{\infty} \frac{q^{2(k+1)^2}(k(1 - q^{4k+2}) + 1)}{(1 - q^{4k+2})^2}\end{aligned} \tag{31}$$

since $0 \leqslant q \leqslant 1$.

Application of the Euler–MacLaurin formula will produce the approximation in theorem 3.4. The remainder term in equation (31) must also be bound. It follows that

$$|R_1| \leqslant B_2 |\log q^2| \left(\sum_{k=1}^{\infty} \frac{kq^{2(k+1)^2}}{1 - q^{4k+2}} + \sum_{k=1}^{\infty} \frac{q^{2(k+1)^2}}{(1 - q^{4k+2})^2} \right). \tag{32}$$

Consider first the second series in this bound. Since $0 < q < 1$ and $k + 1 \geqslant 2$,

$$\begin{aligned}Q_1 &= \sum_{k=1}^{\infty} \frac{q^{2(k+1)^2}}{(1 - q^{4k+2})^2} \leqslant \sum_{k=1}^{\infty} \frac{q^{4k}}{(1 - q^{4k})^2} \\ &= \frac{q^4}{2|\log q^2|(1 - q^4)} + \frac{q^4}{2(1 - q^4)^2} + S_1(q) \left[\frac{q^4(1 + q^4)|\log q^2|}{(1 - q^4)^3} \right]\end{aligned} \tag{33}$$

and where $|S_1(q)| \leqslant B_2$ is a function of q. In a similar fashion

$$\begin{aligned}Q_2 &= \sum_{k=1}^{\infty} \frac{kq^{2(k+1)^2}}{1 - q^{4k+2}} \leqslant \sum_{k=2}^{\infty} \frac{kq^{2k^2}}{1 - q^6} \\ &= \frac{q^8}{2|\log q^2|(1 - q^6)} + \frac{q^8}{(1 - q^6)} + S_2(q) \left[\frac{q^8(1 - 8|\log q^2|)}{1 - q^6} \right]\end{aligned} \tag{34}$$

where $|S_2(q)| \leqslant B_2$ is a function of q. Since $|R_1| \leqslant 2B_2|\log q|(Q_1 + Q_2)$, these results can be taken together in the following lemma.

Lemma 3.3. *Suppose that $q \in [q_0, 1)$, where $0 < q_0 < 1$. Then there exists a constant C such that the error term in equation (30) is bound by*

$$R_1| \leqslant \frac{C}{|\log q^2|}.$$

Proof. Observe that as $q \to 1^-$, then $Q_1|\log q|^2 \to 3/32 + S_1(1)/16$ and $Q_2|\log q|^2 \to 1/24$. Hence, if $q \in [q_0, 1)$, then there exists an $M > 0$ such that $Q_1 + Q_2 \leqslant M/|\log q^2|^2$. Using this in equation (30) then gives the claimed bound, where C is finite. □

It remains to approximate the remaining terms in equation (30) and to bound the error terms on those. This is done in appendix A and, after much calculation, the final result is theorem 3.4.

Theorem 3.4. *For every $q_0 \in (0, 1)$ there exists a finite constant $C > 0$ and a bounded function α_q $(1 \leqslant \alpha_q \leqslant 6)$ such that for all $q \in (q_0, 1)$*

$$\begin{aligned} B(1, q, 1) &= \sqrt{\frac{\pi}{\alpha_q |\log q^2|^3}} + \frac{2\gamma}{|\log q^2|} + \frac{2\log(\alpha_q |\log q^2|)}{|\log q^2|} \\ &\quad + \frac{4}{|\log q^2|} \sum_{k=1}^{\infty} \frac{(-1)^n}{2nn!} (\alpha_q |\log q^2|)^{n-1/2} \\ &\quad - \frac{4}{|\log q^2|} \sum_{k=1}^{\infty} \frac{(-1)^n}{(2n+1)n!} (\alpha_q |\log q^2|)^n + R_q, \end{aligned}$$

where for every $\epsilon > 0$ the remainder R_q is bounded by

$$|R_q| \leqslant \frac{C}{|\log q^2|^{1+\epsilon}}.$$

In the above, γ is Euler's constant.

This result generalizes the partial result in equation (24), and by comparison to equation (19) it appears that the exponent $2 - \alpha_t$ has been determined: $2 - \alpha_t = -3/2$. A numerical approximation can also be made for $B(1, q, 1)$ as $q \to 1^-$. The result is

$$B(1, q, 1) \approx \frac{2\sqrt{2}|\log(1-q)| - 10}{5|\log q^2|^{3/2}} + \frac{2|\log(1-q)| + \sqrt{\pi/2}}{2|\log q^2|} - 9.488. \tag{35}$$

The dominant term in the approximation of $B(1, q, 1)$ as $q \to 1^-$ in theorem 3.4 is the first term. The first infinite series is in fact a logarithmic integral:

$$\begin{aligned} &\frac{4}{|\log q^2|} \sum_{k=1}^{\infty} \frac{(-1)^n}{2nn!} (\alpha_q |\log q^2|)^{n-1/2} \\ &\qquad = \frac{4}{\sqrt{\alpha_q |\log q^2|^3}} (Li(\alpha_q |\log q^2|) - \gamma - \log(\alpha_q |\log q^2|)). \end{aligned} \tag{36}$$

Since $Li(x) \approx x/\log x$, this is dominated by the iterated logarithm which diverges. The contribution from this term is dominant in the scaling regime. The second series in theorem 3.4 is dominated by the first series: one may for example replace the factor $(2n + 1)$ in the denominator by $(2n)$ and note that this series diverges proportional to $|\log(\alpha_q |\log q^2|)|/|\log q^2|$ as $q \to 1^-$. We take these results together as follows:

Theorem 3.5. *For every* $q_0 \in (0, 1)$ *there exists a finite constant* $C > 0$ *and a bounded function* α_q $(1 \leqslant \alpha_q \leqslant 6)$ *such that for* $q \in (q_0, 1)$

$$B(1, q, 1) = \frac{4|\log(\alpha_q|\log q^2|)| + C}{\sqrt{\alpha_q|\log q^2|^3}} + O\left(\frac{|\log(\alpha_q|\log q^2|)|}{|\log q^2|}\right).$$

The scaling of $B(1, q, 1)$ as $q \to 1^-$ is seen to be $B(1, q, 1) \sim |\log|\log q^2||/|\log q^2|^{3/2}$. This is not a pure powerlaw divergence as we found for $B(t, 1, 1)$, but since the iterated logarithm is only slowly divergent, this will appear close to a powerlaw over small ranges of q. This result is also very similar to the numerical approximation found in equation (35).

3.2. Approximating $B(1, 1, p)$

The generating function $B(1, 1, p)$ is given by the triple summation

$$B(1, 1, p) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} p^{ijk}. \tag{37}$$

As with $B(1, q, 1)$, it is challenging to determine the asymptotic behaviour of $B(1, 1, p)$. We found that for some unknown but bounded functions C_0 and C_1 of $\in [p_0, 1)$,

$$B(1, 1, p) = \frac{|\log|\log p||^2}{2|\log p|} + \frac{C_0|\log|\log p||}{|\log p|} + \frac{C_1}{|\log p|} + R \qquad \text{as} \quad p \to 1^-, \tag{38}$$

where $p_0 > 0$ is fixed, and where the remainder term R is bounded by a constant. Thus, the approximation produces two terms growing at nearly the same rate; the first outperforming the second only by an iterated logarithm.

The approximation proceeds by first partially resolving the triple summation to get

$$B(1, 1, p) = 2\sum_{k=1}^{\infty}\left[\sum_{n=1}^{\infty}\frac{p^{kn+k(k-1)}}{1 - p^{kn+k(k-1)}}\right] - \sum_{k=1}^{\infty}\frac{p^{k^2}}{1 - p^{k^2}}. \tag{39}$$

The resulting series over n is approximated by an integral; this cancels the second series, and the result is that

$$B(1, 1, p) = \frac{2}{|\log p|}\sum_{k=1}^{\infty}\frac{|\log(1 - p^{k^2})|}{k} + R_1,$$

where

$$|R_1| \leqslant B_2|\log p|\sum_{k=1}^{\infty}\frac{kp^{k^2}}{(1 - p^{k^2})^2}. \tag{40}$$

In appendix B these series are examined and approximated; a technicality requires that $p > \mathrm{e}^{-1}$ in the next theorem.

Theorem 3.6. *For every* $p \in (\mathrm{e}^{-1}, 1)$ *there exist constants* A, B *and* C *such that*

$$B(1, 1, p) = \frac{|\log|\log p||^2}{2|\log p|} + R$$

where

$$|R| \leqslant \frac{A|\log(1 - p)|}{|\log p|} + \frac{B}{|\log p|} + C$$

This completes the appromixation to $B(1, 1, p)$, and the result is equation (38). This gives theorem 3.7:

Theorem 3.7. *There exists a* $p_0 > e^{-1}$ *such that for all* $p \in [p_0, 1)$*, there are bounded functions* C_0 *and* C_1 *of* p *so that*

$$B(1, 1, p) = \frac{|\log|\log p||^2}{2|\log p|} + \frac{C_0|\log|\log p||}{|\log p|} + \frac{C_1}{|\log p|} + R$$

where the remainder term R *is bounded by a constant and by decaying terms in* p *as* $p \to 1^-$.

3.3. Approximating $B(1, q, p)$

The generating function $B(1, q, p)$ is given by the triple summation which may be partially summed to get

$$B(1, q, p) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} q^{2(ij+jk+ki)} p^{ijk} = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \frac{(pq^2)^{ij} q^{2(i+j)}}{1 - p^{ij} q^{2(i+j)}}. \tag{41}$$

In appendix C this generating function is approximated by a double integral. In particular, it is shown that

$$B(1, q, p) = 2\int_1^{\infty}\int_1^{\infty} \frac{(pq^2)^{(y+1)(y+x+1)} q^{2(x+2y+2)}}{1 - p^{(y+1)(y+x+1)} q^{2(x+2y+2)}}\,\mathrm{d}x\,\mathrm{d}y + \frac{H(p, q)}{1 - pq^4} + \frac{H'(p, q)}{|\log(pq^4)|} + R \tag{42}$$

where the functions $H(p, q)$ and $H'(p, q)$ and the remainder term R are bounded in the region defined by $p \leqslant 1$, $pq^4 \leqslant 1$ and for a finite $q > q_1 \in (1, \infty)$.

The scaling of $B(1, p, q)$ can be determined by examining the double integral above. In particular, substitute first $x + y$ by z followed by substituting $p^{(y+1)(z+1)}(q^2)^{y+z+2} = 1 - \alpha$, simplifying and then substituting $-y \log p = \beta + \log p + \log(q^2)$. The result is that

$$B(1, q, p) = \frac{\mathrm{e}^{-2\frac{|\log q^2|^3}{|\log p|^2}}}{|\log p|}\int_{|\log p^2 q^2|}^{\infty} \mathrm{e}^{\frac{\beta|\log q^2|^2}{|\log p|^2} + \frac{|\log q^2|^2}{\beta|\log p|^2}} \times \left[\int_{1-\mathrm{e}^{\left(\frac{|\log q^2|^2}{|\log p|} - \beta - \frac{\beta^2}{|\log p|}\right)}}^{1} (1-\alpha)^{\frac{|\log q^2|}{|\log p|}\left(1 - \frac{|\log q^2|}{\beta}\right)} \frac{\mathrm{d}\alpha}{\alpha}\right] \frac{\mathrm{d}\beta}{\beta}. \tag{43}$$

Observe the appearance of the ratio $|\log q^2|^3/|\log p|^2$ and the inverse power of $|\log p|$.

Consider the case that $\frac{|\log q^2|^3}{|\log p|^2} = \text{const}$ as $(p, q) \to (1, 1)^-$. Note that the limits on the integral over α approaches the empty set while the integral over β approaches $(0, \infty)$. Comparing this to the scaling form for $B(1, 1, p)$ in theorem 3.6 suggests that one may expect that

$$B(1, q, p) = C(q, p)\frac{|\log(1 - p)|^2}{|\log p|}\left[\mathrm{e}^{-2\frac{|\log q^2|^3}{|\log p|^2}}\right] \tag{44}$$

where $C(q, p)$ is a function of (p, q) that remains bounded as $(q, p) \to (1, 1)^-$ along the curve $\frac{|\log q^2|^3}{|\log p|^2} = C_t$. Putting $\log q_0 = [C_t|\log p|]^{2/3}$ changes this to

$$B(1, q_0, p)|_{C_t} = C(q_0, p)\frac{|\log(1 - p)|^2}{|\log p|}\,\mathrm{e}^{-2C_t} \tag{45}$$

along the curve $|\log q^2|^3 = C_t|\log p|^2$—in other words, where one has put $\left|\log q_0^2\right| = [C_t|\log p|^2]^{2/3}$. In figure 3 equation (45) is examined by plotting $C(q_0, p) = B(1, q_0, p)\,\mathrm{e}^{2C_t}|\log p|/|\log(1 - p)|^2$ against $p \in (0, 1)$. The curves correspond to the choices $C_t = 1$ and $C_t = 1/2$, and represent the residual corrections to the scaling of $B(1, q, p)$ not taken into account by equation (45).

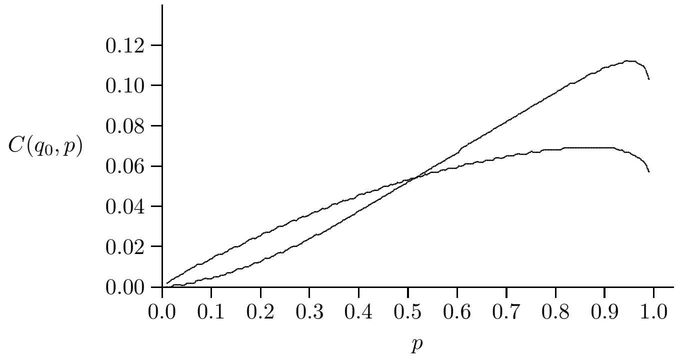


Figure 3. $C(q_0, p) = B(1, q_0, p)e^{2C_t}|\log p|/|\log(1-p)|^2$ against p for $p \in [0, 0.99]$, along the curve $|\log q^2|^3 = C_t|\log p|^2$, for $C_t = 1$ and $C_t = 1/2$ (this curve is lower towards values of p close to 1). In this range of p, $B(1, q_0, p)$ diverges (for $p = 0.99$, $B(1, q_0, p) > 200$), but the values of $C(q_0, p)$ remain modest. This shows that the scaling of $B(1, q, p)$ along curves $|\log q^2|^3 = C_0|\log p|^2$ is described well by equation (45).

3.4. Approximating $B(t, q, 1)$

The generating function $B(t, q, 1)$ is given by the triple summation

$$B(t, q, 1) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} t^{4(i+j+k)} q^{2(ij+jk+ki)} = t^4 \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \frac{(t^4q^2)^{i+j} q^{2ij}}{1 - t^4 q^{2(i+j)}}. \qquad (46)$$

In appendix D this generating function is approximated by a double integral in theorem 4.8: in particular,

$$B(t, q, 1) = 2t^4 \int_1^{\infty}\int_1^{\infty} \frac{(t^4q^2)^{x+2y} q^{2xy+2y^2}}{1 - t^4 q^{2x+4y}}\, dx\, dy + R_0 \qquad (47)$$

where R_0 is a remainder term bounded by

$$|R_0| \leqslant \frac{L_0(t, q)|\log tq|}{(1-tq)^2} + \frac{L_1(t, q)}{|\log tq|} + \frac{L_2(t, q)}{1 - tq} \qquad (48)$$

and the $L_i(t, q)$ are functions bounded by constants for all (t, q) such that $0 \leqslant q \leqslant 1$, $0 \leqslant t \leqslant t_0$ and $0 \leqslant tq \leqslant 1$ for any finite and fixed $t_0 > 1$.

Consider equation (47). Write it as an iterated integral, first to x, and then to y. Substitute x by $x + y = z$ followed by substituting z by $1 - t^4 q^{2z+2y} = \alpha$. Then substitute y by β via $2y^2 \log q = -\beta$. Simplification of the resulting integral gives

$$B(t, q, 1) = \frac{2\, e^{\frac{|\log t^4|^2}{|\log q^2|}}}{\sqrt{|\log q^2|^3}} \int_{|\log q^2|}^{\infty} e^{\beta + \frac{\beta|\log t^4|}{\sqrt{|\log q^2|}}} \times \left[\int_{1 - t^4 q^2 e^{-2\sqrt{\beta|\log q^2|}}}^{1} (1-\alpha)^{\frac{|\log t^4|}{|\log q^2|} + \frac{\sqrt{\beta}}{\sqrt{|\log q^2|}}} \frac{d\alpha}{\alpha}\right] \frac{d\beta}{\sqrt{\beta}} + R_0. \qquad (49)$$

This expression indicates scaling behaviour in $B(t, q, 1)$. In particular, notice the appearance of ratios $\frac{|\log t^4|^2}{|\log q^2|}$ and $\frac{|\log t^4|}{|\log q^2|}$, and one may approach the critical point at $(1, 1)$ along the curve $\frac{|\log t^4|^2}{|\log q^2|} = C_t$. In that case it follows that $\frac{|\log t^4|}{|\log q^2|} \sim \frac{1}{|\log t^4|} \to \infty$ as $(t, q) \to (1, 1)^-$. In equation (49), this shows that the integral over α approaches zero. Comparison to equation (35) shows that

$$B(t, q, 1) = C(t, q) \frac{|\log(1 - q^2)|}{|\log q^2|^{3/2}} \left[e^{\frac{|\log t^4|^2}{|\log q^2|}}\right] + R_0 \qquad (50)$$

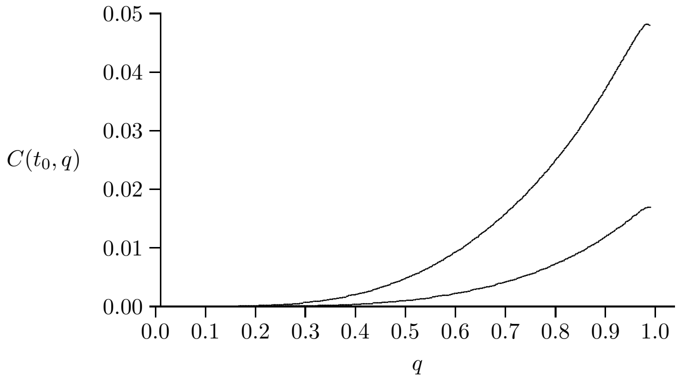


Figure 4. $C(t_0, q) = B(t_0, q, 1)e^{-C_t}|\log q^2|^{3/2}/|\log(1-q^2)|$ against q for $q \in [0, 0.99]$, along the curve $|\log t^4|^2 = C_t|\log q^2|$, for $C_t = 1$ and $C_t = 1/2$ (this is the lower curve). In this range of q, $B(t_0, q, 1)$ diverges (for $q = 0.99$, $B(t_0, q, 1) > 500$), but the values of $C(t_0, q)$ remain modest. The curves appear to approach finite values as $q \to 1^-$, and this indicates that the scaling of $B(t, q, 1)$ along curves $|\log t^4|^2 = C_t|\log q^2|$ is described well by equation (51).

Table 1. Ratios of $C(t_0, q)$ for $C_t = 1$ and $C_t = 1/2$.

q	0.50	0.60	0.70	0.80	0.85	0.90	0.95	0.99
Ratio	4.80	4.13	3.76	3.41	3.28	3.12	2.98	2.81

where $C(t, q)$ is a function of (t, q) that remains bounded as $(t, q) \to (1, 1)^-$ along the curve $\frac{|\log t^4|^2}{|\log q^2|} = C_t$. Putting $\log t_0 = [C_t|\log q^2|]^{1/2}$ changes this to

$$B(t_0, q, 1)|_{C_t} = C(t_0, q)\frac{e^{C_t}|\log(1-q^2)|}{|\log q^2|^{3/2}} + R_0. \tag{51}$$

In figure 4 plots of $C(t_0, q) = e^{-C_t}B(t_0, q, 1)|\log q^2|^{3/2}/|\log(1-q^2)|$ for $C_t = 1$ and $C_t = 1/2$ are presented. This shows that there is still some residual scaling not accounted for by equation (51). Consider on the other hand the ratios of the constants $C(tC_t, q)$ for $C_t = 1$ and $C_t = 1/2$ in table 1. These data show that the ratio between the two curves approaches a constant as $q \to 1^-$.

3.5. Approximating $B(t, 1, p)$

The generating function $B(t, 1, p)$ is given by the triple summation

$$B(t, 1, p) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} t^{4(i+j+k)}p^{ijk} = t^4\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\frac{t^{4(i+j)}p^{ij}}{1-t^4p^{ij}}. \tag{52}$$

In appendix E this generating function is approximated by the double integral in theorem 4.11. In particular

$$B(t, 1, p) = 2t^4\int_1^{\infty}\int_1^{\infty}\frac{t^{4(y+2x)}p^{xy+x^2}}{1-t^4p^{xy+x^2}}\,dx\,dy + R_0 \tag{53}$$

where the remainder terms R_0 are bounded by

$$|R_0| \leqslant \frac{K_0(t, p)|\log(t^4p)|}{(1-t^4p)^2} + \frac{K_1(t, p)}{|\log(t^4p)|} + \frac{K_2(t, p)}{1-t^4p}, \tag{54}$$

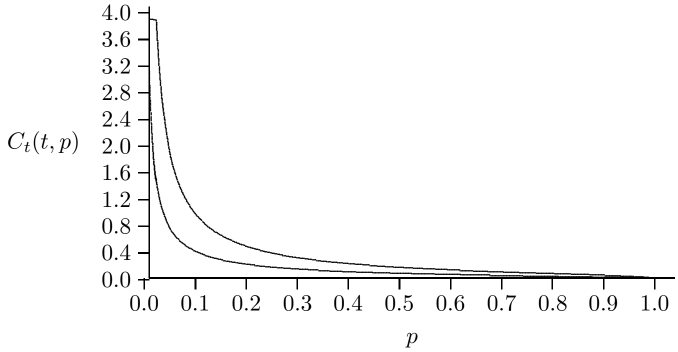


Figure 5. $C_t(t, p) = B(t, 1, p)|\log p|/|\log(1-p)|^2$ against p for $p \in [0, 0.99]$, along the curve $|\log t^4|^3 = C_t|\log p|$, for $C_t = 1$ and $C_t = 1/2$ (this curve is lower towards values of p close to 1.)

where for any finite $t_0 > 0$ the functions $K_i(t, p)$ are bounded by constants for all (t, p) such that $0 \leqslant p \leqslant 1$, $0 \leqslant t^4 p \leqslant 1$ and for all $0 \leqslant t \leqslant t_0$. Thus

$$|R_0| \sim O\left(\frac{1}{1-t^4 p}\right) \qquad \text{as} \quad t^4 p \to 1^-. \tag{55}$$

The scaling in this model may be extracted from equation (53). Substitute the integration in y by $y = z - x$ to get an integral over z. Follow on by substituting the integration in z by $t^4 p^{xz} = 1 - \alpha$ to get an integral over α. Simplify the integral and substitute the integration over x by $t^{\frac{4|\log t^4|}{x|\log p|}} = \mathrm{e}^{-\beta}$. Further simplification gives

$$B(t, 1, p) = \frac{2}{|\log p|} \int_0^{\frac{|\log t^4|^2}{|\log p|}} \mathrm{e}^{\beta - \frac{|\log t^4|^3}{\beta|\log p|}} \left[\int_{1-t^4 \mathrm{e}^{-\frac{|\log t^4|^2}{\beta} - \frac{|\log t^4|^4}{\beta^2|\log p|}}}^1 (1-\alpha)^{\frac{\beta}{|\log t^4|}} \frac{\mathrm{d}\alpha}{\alpha}\right] \frac{\mathrm{d}\beta}{\beta} + R_0. \tag{56}$$

Observe the appearance of the ratios $\frac{|\log t^4|^n}{|\log p|}$ for $n = 2, 3, 4$. Consider the case that $\frac{|\log t^4|^3}{|\log p|} = C_t > 0$. In that event $\frac{|\log t^4|}{|\log p|} = \frac{C_t}{|\log t^4|^2} \to 0^+$ as $t \to \infty$, and $\frac{|\log t^4|^4}{|\log p|} = C_t|\log t^4| \to \infty$ as $t \to 0^+$. In other words, the range of the integrals above approaches [0, 1] over α and [0, 0] over β. Only the ratio $\frac{|\log t^4|^3}{|\log p|}$ is explicitly present in the integrand, and so it appears that the scaling is determined by this ratio.

Consider thus the case that $C_t = \frac{|\log t^4|^3}{|\log p|} > 0$. Then one may consider the scaling of the generating function as the critical point is approached along the curve $\frac{|\log t^4|^3}{|\log p|} = C_t$. In that event, $\frac{|\log t^4|^2}{|\log p|} = \frac{C_t^{2/3}}{|\log p|^{1/3}}$, and $\frac{|\log t^4|^4}{|\log p|} = C_t^{4/3}|\log p|^{1/3}$, and the expression becomes

$$\begin{aligned} B(t, 1, p)|_{C_t} &= \frac{2}{|\log p|} \int_0^{\frac{C_t^{2/3}}{|\log p|^{1/3}}} \mathrm{e}^{\beta - C_t/\beta} \\ &\quad \times \left[\int_{1-t^4 \mathrm{e}^{-\frac{C_t^{2/3}|\log p|^{2/3}}{\beta} - \frac{C_t^{4/3}|\log p|^{1/3}}{\beta^2}}}^1 (1-\alpha)^{\frac{\beta}{C_t^{1/3}|\log p|^{1/3}}} \frac{\mathrm{d}\alpha}{\alpha}\right] \frac{\mathrm{d}\beta}{\beta} + R_0 \\ &\approx \frac{2}{|\log p|} \int_0^\infty \mathrm{e}^{\beta - C_t/\beta} \left[\int_0^1 (1-\alpha)^{\frac{\beta}{C_t^{1/3}|\log p|^{1/3}}} \frac{\mathrm{d}\alpha}{\alpha}\right] \frac{\mathrm{d}\beta}{\beta} + R_0. \end{aligned} \tag{57}$$

It appears that the scaling in this model is determined primarily by the factor $\frac{1}{|\log p|}$ as $(t, p) \to (1, 1)^-$ along a curve determined by C_t. Theorem 3.7 suggests that

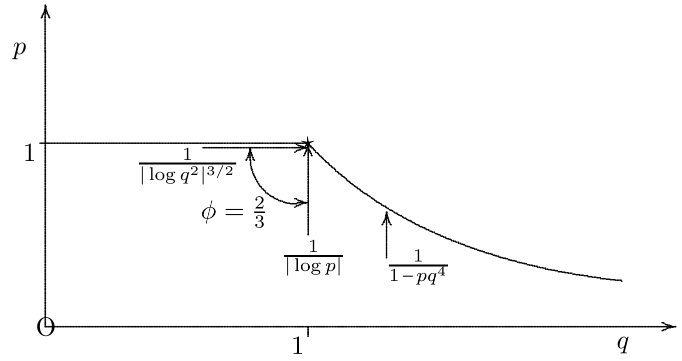


Figure 6. The phase diagram of rectangular vesicles in the qp-ensemble. The critical curve $p(q)$ passes through the tricritical point $p(1) = 1$, and the scaling of the generating function is indicated around this point. The crossover exponent associated with this model has value 2/3. For values of $q > 1$ the critical curve is given by simple poles in the generating function, and this corresponds to a collapse of the vesicle to a linear sequence of unit cubes. For $q < 1$ the vesicle inflates to a cube. At $q = 1$, the relative scaling associated with p and q indicates that the vesicle similarly has a cubical shape, with area increasing as the 2/3-power of volume.

$$B(t, 1, p) \approx \frac{|\log(1-p)|}{|\log p|} C_t(t, p), \qquad \text{along the curve} \quad |\log t^4|^3 = C_t |\log p|, \tag{58}$$

where $C_t(t, p)$ is a function of p. In figure 5 $C_t(t, p)$ is plot against p for $C_t = 1$ and $C_t = 1/2$. It appears that $C_t(t, p)$ approaches zero as $p \to 1^-$ along $|\log t^4|^3 = C_t|\log p|$, but slower than $|\log p|$.

4. Discussion

Consider the scaling in this model in the qp-plane. There is a tricritical point at $(p, q) = (1, 1)$, and the scaling in $B(1, q, 1)$ and $B(1, 1, p)$ as this point is approached is given in theorems 3.5 and 3.7. The crossover from $B(1, q, 1)$ to $B(1, 1, p)$ should involve a ratio $|\log q^2|^3/|\log p|^2$ so that

$$B(1, q, p) \approx \frac{1}{\sqrt{|\log q^2|^3}} \mathcal{G}_{qp}\left(\frac{|\log q^2|}{|\log p|^{2/3}}\right) \tag{59}$$

where $\mathcal{G}_{qp}(x) \sim x^{3/2}$ if $x \to \infty$ and $\mathcal{G}_{qp}(x) \sim C_{qp}$, a constant, if $x \to 0^+$.

In the result in equations (43) and (44) the scaling of the two variable function $B(1, q, p)$ similar to equation (59) was obtained. Observe the appearance of the ratio $\frac{\sqrt{|\log q^2|^3}}{|\log p|}$ in this equation. Other ratios of $|\log q^2|$ and $|\log p|$ are also obtained, but they appear to be dominated by this one, and they are lesser corrections to scaling. In equation (44) we attempt to give the dependence of $B(1, q, p)$ close to the critical point at $(p, q) = (1, 1)$.

One may read off the values of critical exponents from our results. From theorems 3.5 and 3.7 it appear that $2 - \alpha_u = 3/2$ while $2 - \alpha_t = 1$. The crossover exponent is seen from the ratio $\frac{|\log q^2|}{|\log p|^{2/3}}$ to be $\phi = 2/3$, and this satisfies equation (6). In figure 6 these results are summarized. The divergence of the generating function along the curve $1 - pq^4 = 0$ is seen from equation (42), and this is a sequence of simple poles along the critical curve. These values verify the results in [15].

In the tq-ensemble scaling can similarly be determined. The critical curve is $q(t)$, and there is a tricritical point at $q(1) = 1$. We have already indicated that $B(1, q, 1) \sim \frac{1}{|\log q^2|^{3/2}}$ in

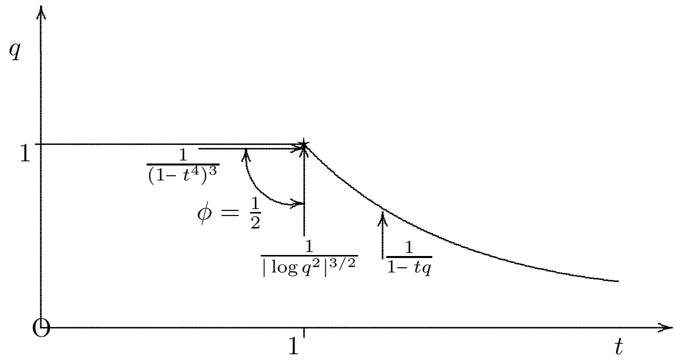


Figure 7. The phase diagram of rectangular vesicles in the tq-ensemble. The critical curve $q(t)$ passes through the tricritical point $q(1) = 1$, and the scaling of the generating function is indicated around this point. The crossover exponent associated with this model has value $1/2$. For values of $t > 1$ the critical curve is given by simple poles in the generating function, and this corresponds to a collapse of the vesicle to a linear sequence of unit cubes. For $t < 1$ the generating function is dominated by terms corresponding to cubes or discs. At $t = 1$, the relative scaling associated with q and t indicates that the vesicle similarly has cubical or disc shape, with perimeter increasing as the $1/2$-power of area.

theorem 3.5. One can also directly show that $B(t, 1, 1) = \frac{t^{12}}{(1-t^4)^3}$. Thus, $2 - \alpha_t = 3/2$ while $2 - \alpha_u = 3$, and the crossover behaviour in the generating function should be given by

$$B(t, q, 1) \approx \frac{1}{|\log t^4|^3} \mathcal{G}_{tq}\left(\frac{|\log t^4|}{|\log q^2|^{1/2}}\right) \tag{60}$$

where $\mathcal{G}_{tq}(x) \sim x^3$ if $x \to \infty$ and $\mathcal{G}_{tq} \sim C_{tq}$, a constant, if $x \to 0^+$.

The proposed scaling form in equation (60) is consistent with the result in equation (49), which also contains lesser corrections to scaling. In equation (50), a proposed scaling form close to the tricritical point is conjectured. The crossover exponent in this ensemble is $\phi = 1/2$, and this value is again consistent with the ratio $\frac{2-\alpha_t}{2-\alpha_u}$ as in equation (6). These results are indicated in figure 7. The divergence of the generating function along the curve $1 - tq = 0$ follows from equation (48). This is a sequence of simple poles in the generating function.

Finally, one may also consider this model in the tp-ensemble. There is a tricritical point at $(t, p) = (1, 1)$, and the scaling in $B(t, 1, 1)$ and $B(1, 1, p)$ as this point is approached is given by the fact that $B(t, 1, 1) = \frac{t^{12}}{(1-t^4)^3}$, and by theorem 3.7. Thus, $2 - \alpha_t = 1$ while $2 - \alpha_u = 3$. The crossover from $B(t, 1, 1)$ to $B(1, 1, p)$ should involve a ratio $\sqrt{|\log t^4|^3}/|\log p|$ so that

$$B(t, 1, p) \approx \frac{1}{|\log t^4|^3} \mathcal{G}_{tp}\left(\frac{|\log t^4|}{|\log p|^{1/3}}\right) \tag{61}$$

where $\mathcal{G}_{tp}(x) \sim x^3$ if $x \to \infty$ and $\mathcal{G}_{tp}(x) \sim C_{tp}$, a constant, if $x \to 0^+$.

The proposed scaling form in equation (61) is consistent with the result in equation (56), which also contains lesser corrections to scaling. In equation (58), a proposed scaling form close to the tricritical point is conjectured. The crossover exponent in this ensemble is $\phi = 1/3$, and this value is again consistent with the ratio $\frac{2-\alpha_t}{2-\alpha_u}$ as in equation (6). These results are indicated in figure 8. The divergence of the generating function along the curve $1 - t^4 p = 0$ follows from equation (54). This is a sequence of simple poles in the generating function.

The full phase diagram of the model is given by a critical surface in the three-dimensional tqp-space. Figures 6, 7 and 8 are cuts through this critical surface, putting either t, or p or q

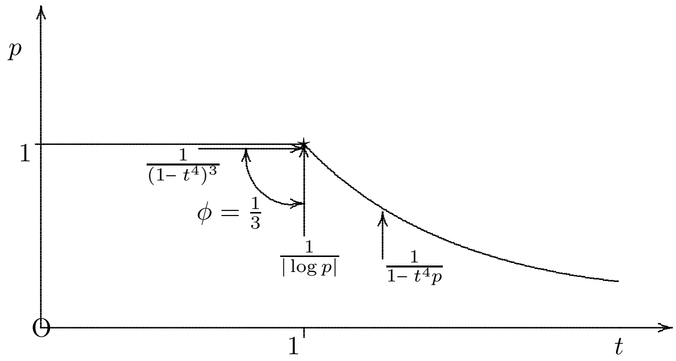


Figure 8. The phase diagram of rectangular vesicles in the tp-ensemble. The critical curve $p(t)$ passes through the tricritical point $p(1) = 1$, and the scaling of the generating function is indicated around this point. The crossover exponent associated with this model has value $1/3$. For values of $t > 1$ the critical curve is given by simple poles in the generating function, and this corresponds to a collapse of the vesicle to a linear sequence of unit cubes. For $t < 1$ the vesicle inflates to a cube. At $t = 1$, the relative scaling associated with p and t indicates that the vesicle similarly has a cubical shape, with perimeter increasing as the $1/3$-power of area.

equal to 1 in each case. The critical surface is defined by three surfaces meeting at a critical point $p = q = t = 1$.

Partial sums in the generating function could be considered to find the phases in this model. Consider partial sums corresponding to inflated cubical vesicles, flat square disc-like vesicles and collapsed linear vesicles. The partial sums of these are

$$V = \sum_{n=1}^{\infty} p^{n^3} q^{6n^2} t^{12n} \tag{62}$$

$$A = \sum_{n=1}^{\infty} p^{n^2} q^{2n^2+4n} t^{8n+4} \tag{63}$$

$$C = \sum_{n=1}^{\infty} p^{n} q^{4n+2} t^{4n+8}. \tag{64}$$

The radii of convergence of these sums indicate that the full generating function has radius of convergence in the qt-plane given by

$$p_c = \min\{1, 1/q^2, 1/(qt)^4\}, \tag{65}$$

since the divergence of one of these sums would imply divergence of the generating function.

The function $F(q,t) = -\log p_c$ is the free energy of the model. The definition of p_c defines the three critical surfaces in the full phase diagram, and this is illustrated in figure 9, which is a projection of the critical surface on the qt-plane.

The critical line in figure 9 given by $q = 1$ separates the critical surfaces $p_c = 1$ and $p_c = 1/q^2$. The critical curve $qt^2 = 1$ separates the critical surfaces $p_c = 1/q^2$ and $p_c = 1/(qt)^4$, the critical curve $qt = 1$, separates the critical surfaces $p_c = 1$ and $p_c = 1/(qt)^4$. For small enough q and t the model is dominated by cubical vesicles; for large q and small enough t, by disc-like vesicles, and for large q and t by collapsed needle-like vesicles. One may refer to these phases as the cubical, the square disc and the needle phases.

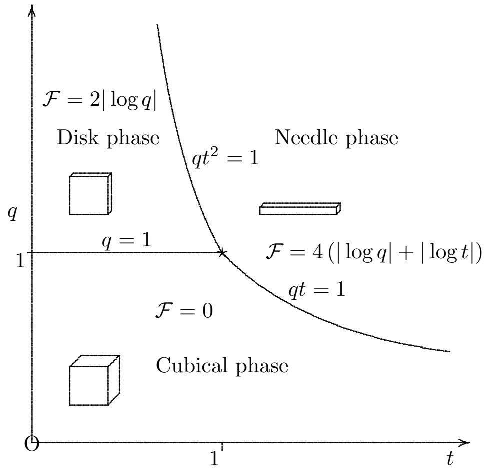


Figure 9. The critical surface of rectangular vesicles projected on the qt-plane. There are three phases separated by critical curves. The free energy $\mathcal{F}(q,t) = -\log p_c$ has a discontinuous first derivative across any one of the three phase boundaries in this diagram, so that the transitions are all first order. These curves of first order transitions meet in a critical point at $q = t = 1$ where $p_c = 1$.

The cubical, square disc and needle phases are separated by lines of first-order transitions in figure 9. The free energy is given by

$$\mathcal{F}(q,t) = -\log p_c = \begin{cases} 0, & \text{in the cubical phase;} \\ 2\log q, & \text{in the square disc phase;} \\ 4(\log q + \log t), & \text{in the needle phase.} \end{cases} \tag{66}$$

Derivatives of $\mathcal{F}(q,t)$ across the phase boundaries show that

$$\frac{\partial \mathcal{F}(q,t)}{\partial \log q} = \begin{cases} 0 \\ 2 \end{cases} \qquad \text{across the boundary } q = 1 \text{ in figure 9.} \tag{67}$$

This jump discontinuity shows that the phase boundary $q = 1$ and $0 < t < 1$ is a coexistence curve of first-order phase transitions separating the cubical and square disc phases.

Similarly, it follows that

$$\frac{\partial \mathcal{F}(q,t)}{\partial \log q} = \begin{cases} 0 \\ 4 \end{cases} \qquad \text{across the boundary } qt = 1 \text{ in figure 9,} \tag{68}$$

and

$$\frac{\partial \mathcal{F}(q,t)}{\partial \log q} = \begin{cases} 2 \\ 4 \end{cases} \qquad \text{across the boundary } qt^2 = 1 \text{ in figure 9.} \tag{69}$$

A derivative to $\log t$ of $\mathcal{F}(q,t)$ can instead be taken to determine the nature of the energy density across the phase boundaries $qt = 1$ and $qt^2 = 1$ in figure 9. Direct computation shows that

$$\frac{\partial \mathcal{F}(q,t)}{\partial \log t} = \begin{cases} 0 \\ 4 \end{cases} \qquad \text{across the boundary } qt = 1 \text{ in figure 9,} \tag{70}$$

but that

$$\frac{\partial \mathcal{F}(q,t)}{\partial \log t} = 0 \qquad \text{across the boundary } qt^2 = 1 \text{ in figure 9.} \tag{71}$$

Thus, there are jump discontinuities in at least one of the first derivatives[2] of $\mathcal{F}(q,t)$ across each of the phase boundaries in figure 9. These phase boundaries are coexistence curves of first-order phase transitions, and they meet in the point $(q,t) = (1,1)$ where the three phases coexist in this model. Aspects of the scaling at the critical point $(q,t) = (1,1)$ have been examined in this paper, and are given by equations (59), (60) and (61).

The free energy $\mathcal{F}(q,t)$ is a linear function of the scaling fields $\log t$ and $\log q$ in each of the three phases in figure 9. Crossing a phase boundary in figure 9 changes $\mathcal{F}(q,t)$ from one linear dependence to another on $\log t$ and $\log q$. The scaling of the free energy with the scaling fields $\log t$ and $\log q$ is also linear on approach of a phase boundary. Such linear scaling of $\mathcal{F}(q,t)$ on approach to the phase boundaries implies that the specific heat exponent associated with these transitions is $\alpha = 1$, as one may see directly from equation (21). This value of α is consistent with first-order phase behaviour across the phase boundaries. However, the hyperscaling relation $2 - \alpha = 1/\phi$ (see equation (22)) breaks down since the crossover exponent associated with anyone of the phase boundaries is not equal to one. The values of the crossover exponents are in each case consistent with the crossover scaling determined for the generating function, as demonstrated in equations (59), (60) and (61).

The phase diagram in figure 9 is somewhat similar to the phase diagrams obtained by studying more general models of random vesicles in the lattice. For example, a model of such three-dimensional vesicles that include fugacities conjugate to area, volume and to curvature (the number of edges where unit squares meet at right angles) has been examined in the literature [11, 22]. This phase diagram is known to include at least three phases, namely a branched polymer phase, an inflated (or cubical) phase and a smooth deflated phase of disc-like to rod-like vesicles. The phase transition to inflated (or cubical) vesicles is again a line of first order transitions, and arguments and results in the literature [22, 23] indicate that $\phi = 2/3$, consistent with the value obtained for inflating rectangular vesicles in three dimensions in this paper.

Our model does not admit a branched polymer phase, since rectangular vesicles would not allow branched conformations. The cubical and square disc phases however, are counterparts to the smooth deflated and cubical phases for crumpling surfaces [11], also observed in other models of lattice surfaces [22, 23]. In other words, although our model is very restricted, it still has a rich phase diagram that incorporates some of the phase behaviour seen in more general models of random surfaces.

Acknowledgment

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Appendix A. Approximating $B(1, q, 1)$

In this appendix we approximate $B(1,q,1)$. The starting point is equation (30), and each of the terms must be approximated. Use the Euler–MacLaurin approximation twice, while

[2] Observe that in only one case do we encounter a continuous first derivative: this occurs across the phase boundary $qt^2 = 1$ separating the disc and needle phases, and in that case the derivative of $\mathcal{F}(q,t)$ to $\log t$ is continuous. This phase boundary is therefore due to the first-order phase behaviour associated with the surface area of the vesicle, which collapses from a square-shaped disc to a needle when the boundary is crossed by increasing q.

keeping track of the error terms introduced:

$$\frac{2}{|\log q^2|}\sum_{k=1}^{\infty}\sum_{m=k+1}^{\infty}\frac{q^{2m(2k+1)}}{mq^{2k^2}}$$
$$= \frac{2}{|\log q^2|}\sum_{k=1}^{\infty}\left[\frac{1}{q^{2k^2}}\int_{k+1}^{\infty}\frac{q^{2x(2k+1)}}{x}\,\mathrm{d}x + \frac{q^{2(k^2+3k+1)}}{2(k+1)} + R_2\right]$$
$$= \frac{2}{|\log q^2|}\sum_{k=1}^{\infty}\left[\frac{1}{q^{2k^2}}\int_{1}^{\infty}\frac{q^{2x(2k^2+3k+1)}}{x}\,\mathrm{d}x + \frac{q^{2(2k^2+3k+1)}}{2(k+1)} + R_2\right]$$
$$= \frac{2}{|\log q^2|}\sum_{k=1}^{\infty}\left[\frac{1}{q^{2k^2}}\int_{1}^{\infty}\frac{q^{2x(2k^2+3k+1)}}{x}\,\mathrm{d}x\right] + P_1 + \frac{2}{|\log q^2|}\sum_{k=1}^{\infty}R_2. \qquad (A.1)$$

The expressions P_1 and R_2 are bounded as follows:

$$P_1 = \frac{2}{|\log q^2|}\sum_{k=1}^{\infty}\frac{q^{2(2k^2+3k+1)}}{2(k+1)} \qquad (A.2)$$

$$|R_2| \leqslant \frac{B_2}{2q^{2k^2}}\left[\frac{|\log q|(4k+2)q^{2k^2+6k+2}}{k+1} + \frac{q^{2k^2+6k+2}}{(k+1)^2}\right]. \qquad (A.3)$$

Approximating the sum over k as well produces

$$\frac{2}{|\log q^2|}\sum_{k=1}^{\infty}\sum_{m=k+1}^{\infty}\frac{q^{2m(2k+1)}}{mq^{2k^2}} = \frac{2}{|\log q^2|}\int_{1}^{\infty}\left[\int_{1}^{\infty}\frac{q^{2x(2y^2+3y+1)-2y^2}}{x}\,\mathrm{d}x\right]\mathrm{d}y + P_1 + P_2$$
$$+ \frac{2}{|\log q^2|}\sum_{k=1}^{\infty}R_2 + R_3, \qquad (A.4)$$

where

$$|R_3| \leqslant \frac{B_2}{2}\int_{1}^{\infty}\frac{q^{12x-2}(14x-4)}{x}\,\mathrm{d}x, \qquad (A.5)$$

and

$$P_2 = \frac{1}{q^2|\log q^2|}\int_{1}^{\infty}\frac{q^{12x}}{x}\,\mathrm{d}x. \qquad (A.6)$$

It remains to evaluate the iterated integral, and then to compute bounds on P_1, P_2, $\sum_{k=1}^{\infty} R_2$ and R_3.

The iterated integral cannot be evaluated in closed form, and so bounds for it must be found. Recall that $0 \leqslant q < 1$, and that the variables x and y are both greater than or equal to 1. Hence

$$q^{12xy^2} \leqslant q^{2x(2y^2+3y+1)-2y^2} \leqslant q^{2xy^2}. \qquad (A.7)$$

In other words, bounds can be found by evaluating integrals of the form

$$\int_{1}^{\infty}\left[\int_{1}^{\infty}\frac{q^{\alpha xy^2}}{x}\,\mathrm{d}x\right]\mathrm{d}y, \qquad (A.8)$$

where $\alpha = 2$ or $\alpha = 12$. Since $|q| < 1$ one may use Fubini's theorem to interchange the order of integration. In that case,

$$\int_{1}^{\infty}\left[\int_{1}^{\infty}\frac{q^{\alpha xy^2}}{x}\,\mathrm{d}y\right]\mathrm{d}x = \sqrt{\frac{\pi}{2\alpha|\log q^2|}}\int_{1}^{\infty}\left[\frac{1-\mathrm{erf}(\sqrt{\alpha x|\log q^2|/2})}{\sqrt{x^3}}\right]\mathrm{d}x. \qquad (A.9)$$

For each value of q there exists an $\alpha_q \in [1, 6]$ such that the iterated integral is equal to the above. Thus, there exists a bounded function α_q, such that $1 \leqslant \alpha_q \leqslant 6$ and

$$\int_1^\infty \left[\int_1^\infty \frac{q^{2x(2y^2+3y+1)-2y^2}}{x}\,\mathrm{d}x\right]\mathrm{d}y = \sqrt{\frac{\pi}{4\alpha_q|\log q^2|}}\int_1^\infty \frac{1-\operatorname{erf}\left(\sqrt{\alpha_q x|\log q^2|}\right)}{\sqrt{x^3}}\,\mathrm{d}x. \tag{A.10}$$

Maple 9 evaluates the integral over the error function as follows:

$$\sqrt{\frac{\pi}{4\alpha_q|\log q^2|}}\int_1^\infty \frac{1-\operatorname{erf}\left(\sqrt{\alpha_q x|\log q^2|}\right)}{\sqrt{x^3}}\,\mathrm{d}x = \frac{1}{\sqrt{\alpha_q|\log q^2|}}\left[\sqrt{\pi} - \sqrt{\alpha_q|\log q^2|}\mathrm{Ei}(1, \alpha_q|\log q^2|) - \sqrt{\pi}\operatorname{erf}\left(\sqrt{\alpha_q|\log q^2|}\right)\right], \tag{A.11}$$

where Ei is an elliptic integral. This may be simplified to the infinite series solution

$$\sqrt{\frac{\pi}{4\alpha_q|\log q^2|}}\int_1^\infty \frac{1-\operatorname{erf}\left(\sqrt{\alpha_q x|\log q^2|}\right)}{\sqrt{x^3}}\,\mathrm{d}x = \sqrt{\frac{\pi}{\alpha_q|\log q^2|}} + \gamma + \log(\alpha_q|\log q^2|) + 2\sum_{n=1}^\infty \frac{(-1)^n(\alpha_q|\log q^2|)^{n-1/2}}{2nn!} - 2\sum_{n=1}^\infty \frac{(-1)^n(\alpha_q|\log q^2|)^n}{(2n+1)n!}. \tag{A.12}$$

It remains now to bound the error terms P_1 in equation (A.2), the sum over R_2 in equations (A.1) and (A.3), the term R_3 in equation (A.5). Then bounds are also needed on the unevaluated terms in equation (30). A bound on R_1 is computed in lemma 3.3.

Consider first P_1 in equation (A.2). Observe that the summand $q^{2(2k^2+3k+1)}/2(k+1)$ decreases with increasing k, and that $q^{2(2k^2+3k+1)} \leqslant q^{4k^2}$. Hence, the summation can be bound from above by an integral if $k \to k-1$:

$$|P_1| \leqslant \frac{2}{|\log q^2|}\int_1^\infty \frac{q^{4x^2}}{2x}\,\mathrm{d}x = \frac{1}{2|\log q^2|}\mathrm{Ei}(1, 2|\log q^2|). \tag{A.13}$$

P_2 can be bound similarly:

$$|P_2| \leqslant \frac{1}{q^2|\log q^2|}\int_1^\infty \frac{q^{12x}}{x}\,\mathrm{d}x = \frac{1}{q^2|\log q^2|}\mathrm{Ei}(1, 6|\log q^2|). \tag{A.14}$$

Next the summation over the bound R_2 should be bounded. Consider the fact that $(4k+2)/(k+1) \leqslant 4$ for all $k \geqslant 1$ in equation (A.3) to observe that

$$\frac{2}{|\log q^2|}\sum_{k=1}^\infty |R_2| \leqslant \frac{B_2}{|\log q^2|}\sum_{k=1}^\infty \left[|\log q^2|q^{6k+2} + \frac{q^{6k+2}}{(k+1)^2}\right]. \tag{A.15}$$

One may now similarly observe that with increasing k, the summand above is decreasing, so by letting $k \to k-1$, one may bound the summation by an integral:

$$\frac{2}{|\log q^2|}\sum_{k=1}^\infty |R_2| \leqslant \frac{B_2}{|\log q^2|}\left[\frac{5q^2}{3} + \frac{3}{q^4}|\log q^2|\mathrm{Ei}(1, 3|\log q^2|)\right]. \tag{A.16}$$

Next, R_3 in equation (A.5) can be bound by evaluating the integral. Maple 9 gives

$$|R_3| \leqslant \frac{B_2}{|\log q^2|}\left[\frac{7q^{10}}{6} + \frac{2|\log q^2|}{q^2}\mathrm{Ei}(1, 6|\log q^2|)\right]. \qquad \text{(A.17)}$$

It only remains to bound the two remaining series in equation (30). Consider then

$$\sum_{k=1}^{\infty}\frac{q^{2(k^2+3k+1)}}{1-q^{4k+2}} + \sum_{k=1}^{\infty}\frac{q^{2k(k+2)}}{1-q^{4k}} \leqslant 2\sum_{k=1}^{\infty}\frac{q^{2k^2}}{1-q^{4k}} \leqslant 2\int_1^{\infty}\frac{q^{2x^2}}{1-q^{4x}}\,\mathrm{d}x \leqslant 2\int_1^{\infty}\frac{q^{2x}}{1-q^{4x}}\,\mathrm{d}x$$
$$= \frac{\log(1+q^2) - \log(1-q^2)}{|\log q^2|}, \qquad \text{(A.18)}$$

where the series can be bounded by the integral since the integrand is monotone decreasing in k for any fixed $q \in (0, 1)$.

Collect all the bounds together with the approximation of the double summation above. The elliptical integrals $\mathrm{Ei}(1, \beta|\log q^2|)$ (where $\beta > 0$) diverge as $q \to 1^-$, but this divergence is very weak. In fact, observe that

$$\lim_{q\to 1^-}[|\log q|^{\delta}\mathrm{Ei}(1, \beta|\log q^2|)] = 0 \qquad \text{(A.19)}$$

for any $\delta > 0$. Thus, if γ is Euler's constant, then there is a function $1 \leqslant \alpha_q \leqslant 6$ such that

$$B(1, q, 1) = \sqrt{\frac{\pi}{\alpha_q|\log q^2|^3}} + \frac{2\gamma}{|\log q^2|} + \frac{2\log(\alpha_q|\log q^2|)}{|\log q^2|}$$
$$+ \frac{4}{|\log q^2|}\sum_{k=1}^{\infty}\frac{(-1)^n}{2n\,n!}(\alpha_q|\log q^2|)^{n-1/2}$$
$$- \frac{4}{|\log q^2|}\sum_{k=1}^{\infty}\frac{(-1)^n}{(2n+1)n!}(\alpha_q|\log q^2|)^n + R_q \qquad \text{(A.20)}$$

where the remainder term R_q is bounded by

$$|R_q| \leqslant \frac{5q^3B_2}{3|\log q^2|} + \frac{7q^{10}B_2}{6|\log q^2|} + \frac{1}{|\log q^2|}\log\left(\frac{1+q^2}{1-q^2}\right) + \frac{1}{2|\log q^2|}\mathrm{Ei}(1, 2|\log q^2|)$$
$$+ \frac{6B_2}{2q^4}\mathrm{Ei}(1, 3|\log q^2|) + \frac{4B_2}{2q^2}\mathrm{Ei}(1, 6|\log q^2|). \qquad \text{(A.21)}$$

By equation (A.19) there exists for every $0 < q_0 < 1$ a constant $C > 0$ such that for every $\epsilon > 0$ the remainder is bounded by

$$|R_q| \leqslant \frac{C}{|\log q^2|^{1+\epsilon}}, \qquad \text{for every} \quad q \in [q_0, 1) \quad \text{and all} \quad \epsilon > 0. \qquad \text{(A.22)}$$

Together with equation (A.20), this proves theorem 3.4.

Appendix B. Approximating $B(1, 1, p)$

In equation (40) the Euler–MacLaurin theorem produces an approximation for $B(1, 1, p)$. It remains to consider both the series and the remainder term R_1.

Consider first the bound on R_1. Observe that the summand is monotonic decreasing for any fixed p and increasing $k \geqslant 1$. Hence, the summation can be bound by an integral over $k \geqslant 1$, the result being that

$$|R_1| \leqslant B_2|\log p|\int_1^{\infty}\frac{xp^{x^2}}{(1-p^{x^2})^2}\,\mathrm{d}x. \qquad \text{(B.1)}$$

This integral can be directly evaluated to give

$$|R_1| \leqslant \frac{B_2 p}{2(1-p)}. \tag{B.2}$$

Consider now the series approximation to $B(1, 1, p)$ in equation (40). The Euler–MacLaurin formula approximates the series as an integral as follows

$$\sum_{k=1}^{\infty} \frac{|\log(1-p^{k^2})|}{k} = \int_1^{\infty} \frac{|\log(1-p^{x^2})|}{x}\,\mathrm{d}x + \frac{1}{2}|\log(1-p)| + R_2 \tag{B.3}$$

where the remainder term R_2 is bounded by

$$|R_2| \leqslant \frac{B_2}{2}\left(|\log(1-p)| + \frac{2p|\log p|}{1-p}\right). \tag{B.4}$$

It only remains to evaluate the integral in equation (B.3). Substitute $p^{k^2} = \mathrm{e}^{-x}$ in the integral and cut the resulting integral into an integration over large x, with small contribution, and an integration for x in the vicinity of $|\log p|$, where the contribution is large. This gives

$$\int_{|\log p|}^{\infty} \frac{\log(1-\mathrm{e}^{-x})}{2x}\,\mathrm{d}x = \int_{|\log p|}^{N} \frac{\log(1-\mathrm{e}^{-x})}{2x}\,\mathrm{d}x + \int_{N}^{\infty} \frac{\log(1-\mathrm{e}^{-x})}{2x}\,\mathrm{d}x. \tag{B.5}$$

Since $1 > 1/N$ for larger values of N, the second integral can be bound as follows.

$$\begin{aligned} R_3 &= \left|\int_N^{\infty} \frac{\log(1-\mathrm{e}^{-x})}{2x}\,\mathrm{d}x\right| \\ &\leqslant \left|\int_N^{\infty} \frac{\log(1-\mathrm{e}^{-x})}{2}\,\mathrm{d}x\right| = \frac{\mathcal{L}i_2(1-\mathrm{e}^{-N})}{2} \leqslant \frac{\mathrm{e}^{-N}}{2}. \end{aligned} \tag{B.6}$$

The dilogarithm is defined by $\mathcal{L}i_2(x) = \int_1^x \frac{\log(t)}{1-t}\,\mathrm{d}t$, and it approaches zero as $x \to 1$. The rate of this approach to zero is proportional to $1 - x$.

Lastly, consider the first integral. Expanding the exponential and simplifying shows that it may be written as

$$\int_{|\log p|}^{N} \frac{\log x}{2x}\,\mathrm{d}x + \int_{|\log p|}^{N} \frac{\log\left(1 - \sum_{n\geqslant 2} \frac{(-x)^{n-1}}{n!}\right)}{2x}\,\mathrm{d}x. \tag{B.7}$$

Define

$$R(N) = \int_{|\log p|}^{N} \frac{\log\left(1 - \sum_{n\geqslant 2} \frac{(-x)^{n-1}}{n!}\right)}{2x}\,\mathrm{d}x, \tag{B.8}$$

and consider the integrand

$$-\frac{x}{2} \leqslant \log\left(1 - \sum_{n\geqslant 2} \frac{(-x)^{n-1}}{n!}\right) \leqslant -\frac{x}{2} + \frac{x^2}{6}. \tag{B.9}$$

Thus, $R(N)$ can be bounded by

$$\frac{-1}{2}\left(N - |\log p|\right) \leqslant R(N) \leqslant \frac{-1}{4}\left(N - N^2/6 - |\log p| + \frac{1}{6}|\log p|^2\right). \tag{B.10}$$

The first integral in equation (B.7) can be directly evaluated to give the following appromixation for $B(1, 1, p)$:

$$B(1,1,p) = \frac{|\log(\log p)|^2}{2|\log p|} + \frac{|\log(1-p)|}{|\log p|} - \frac{|\log N|^2}{2|\log p|} + \frac{2}{|\log p|}(R(N) + R_3 + R_2) + R_1, \tag{B.11}$$

for each $N > |\log p|$. As $p \to 1^-$, $|\log p| \to 0^+$. In particular, one may choose $N = 1$ if $e^{-1} < p < 1$. In that case the remainder terms are bounded by

$$|R(1)| \leqslant \frac{1}{4}\left(\frac{5}{6} + |\log p| + \frac{1}{6}|\log p|^2\right), \tag{B.12}$$

$$|R_1| \leqslant \frac{B_2}{2}\frac{p}{1-p}, \tag{B.13}$$

$$|R_2| \leqslant \frac{B_2}{2}\left(|\log(1-p)| + \frac{2p|\log p|}{1-p}\right), \tag{B.14}$$

$$|R_3| \leqslant \frac{e^{-1}}{2}. \tag{B.15}$$

Generally, if $N = 1$ (and $p > e^{-1}$) then the approximation is

$$B(1, 1, p) = \frac{|\log|\log p||^2}{2|\log p|} + \frac{|\log(1-p)|}{|\log p|} + R, \tag{B.16}$$

where a bound on R is obtained by adding together the bounds on $R(1)$, R_1, R_2 and R_3:

$$|R| \leqslant \frac{5}{6|\log p|} + 1 + \frac{1}{6}|\log p| + \frac{e^{-1}}{|\log p|} + \frac{B_2|\log(1-p)|}{|\log p|} + \frac{2B_2 p}{1-p} + \frac{B_2 p}{2(1-p)}. \tag{B.17}$$

The dominant term in the bound on R is the term proportional to $|\log(1-p)|/|\log p|$; this term grows at the same rate as the second term in equation (B.16). One may thus absorb this term into the remainder to obtain theorem 3.6.

Appendix C. Approximating $B(1, q, p)$

The function $B(1, q, p)$ is a triple summation given by

$$B(1, q, p) = \sum_{i,j,k>0} q^{2(ij+jk+ki)} p^{ijk}. \tag{C.1}$$

Clearly, $B(1, q, p) = \infty$ if $q = p = 1$, and so we shall assume that either $p \in [0, 1)$ and that $pq^4 < 1$. We also assume that both q and p are positive.

Lemma 4.1.

$$B(1, q, p) = 2\sum_{n,k=1}^{\infty} \frac{q^{2k^2+2kn+2n+4k} p^{k^2+nk}}{1 - p^{k^2+nk} q^{2n+4k}} + \frac{H(p, q)}{1 - pq^4}$$

where $H(p, q)$ is a function bounded in every subset of the pq-plane where $q \leqslant q_0$, $p \leqslant 1$ and $pq^4 \leqslant 1$, for any fixed $q_0 > 0$.

Proof. Perform the sum over k in equation (C.1) and observe that

$$\begin{aligned} \sum_{i,j,k>0}^{\infty} q^{2(ij+jk+ki)} p^{ijk} &= \sum_{i,j>0}^{\infty} \frac{q^{2ij+2i+2j} p^{ij}}{1 - p^{ij} q^{2(i+j)}} \\ &= 2\sum_{n,k>0}^{\infty} \frac{q^{2k^2+2kn+2n+4k} p^{k^2+kn}}{1 - p^{k^2+kn} q^{2n+4k}} + \sum_{k=1}^{\infty} \frac{q^{2k^2+4k} p^{k^2}}{1 - p^{k^2} q^{4k}}. \end{aligned} \tag{C.2}$$

Consider the last term above. Surely

$$\sum_{k=1}^{\infty} \frac{q^{2k^2+4k} p^{k^2}}{1 - p^{k^2} q^{4k}} \geqslant \frac{pq^6}{1 - pq^4} \tag{C.3}$$

for all $p < 1$ and $pq^4 < 1$. On the other, upper bounds can be determined as well. If $q \leqslant 1$ and $p < 1$, then

$$\sum_{k=1}^{\infty} \frac{q^{2k^2+4k} p^{k^2}}{1 - p^{k^2} q^{4k}} \leqslant \frac{1}{1 - pq^4} \sum_{k=1}^{\infty} (pq^2)^{k^2} \leqslant \frac{\sqrt{\pi}\left(1 - \mathrm{erf}\left(\sqrt{|\log(pq^2)|}\right)\right)}{2(1 - pq^4)\sqrt{|\log(pq^2)|}} \tag{C.4}$$

and since $1 - \mathrm{erf}(x) \leqslant \mathrm{e}^{-x^2}/(\sqrt{\pi}x)$ for $x > 0$, this shows that

$$\sum_{k=1}^{\infty} \frac{q^{2k^2+4k} p^{k^2}}{1 - p^{k^2} q^{4k}} \leqslant \frac{pq^2}{2(1 - pq^4)|\log(pq^2)|}.$$

On the other hand, if $q > 1$ and $pq^4 < 1$, then

$$\begin{aligned}\sum_{k=1}^{\infty} \frac{q^{2k^2+4k} p^{k^2}}{1 - p^{k^2} q^{4k}} &\leqslant \frac{1}{1 - pq^4} \sum_{k=1}^{\infty} (pq^2)^{k^2} q^{4k} \leqslant \frac{q^{12}}{1 - pq^4} \sum_{k=1}^{\infty} (pq^3)^{k^2} \\ &\leqslant \frac{\sqrt{\pi} q^{12}\left(1 - \mathrm{erf}\left(\sqrt{|\log(pq^3)|}\right)\right)}{2(1 - pq^4)\sqrt{|\log(pq^3)|}} \\ &\leqslant \frac{pq^{15}}{2(1 - pq^4)|\log(pq^3)|}.\end{aligned}$$

In other words, for $p < 1$ and $pq^4 < 1$ there is a function $H(p, q)$ such that

$$\sum_{k=1}^{\infty} \frac{q^{2k^2+4k} p^{k^2}}{1 - p^{k^2} q^{4k}} = \frac{H(p, q)}{1 - pq^4} \tag{C.5}$$

where

$$q^6 \leqslant H(p, q) \leqslant \max\{pq^2/2|\log(pq^2)|, pq^{15}/2|\log(pq^3)|\}.$$

□

Lemma 4.2. *Suppose that* $0 < p < 1$ *and* $pq^4 < 1$.

$$2 \sum_{n,k=1}^{\infty} \frac{q^{2k^2+2kn+2n+4k} p^{k^2+kn}}{1 - p^{k^2+nk} q^{2n+4k}} = 2 \sum_{k>0}^{\infty} \int_1^{\infty} \frac{q^{2k^2+2kx+2x+4k} p^{k^2+kx}}{1 - p^{k^2+kx} q^{2x+4k}} \,\mathrm{d}x + R$$

and there exists a finite numbers C *and* C' *such that*

$$|R| \leqslant \frac{C'}{|\log(pq^2)|(1 - pq^3)} \left(|\log pq^4| + \frac{|\log(pq^2)|}{1 - pq^3} \right) + \frac{C}{(1 - pq^3)\sqrt{|\log(pq^2)|}}.$$

Proof. Approximate the sum over n by the Euler–MacLaurin formula. This gives the approximation above, and the remainder terms are

$$R = \sum_{k>0}^{\infty} \frac{q^{2k^2+6k+2} p^{k^2+k}}{1 - p^{k^2+k} q^{4k+2}} + \sum_{k>0}^{\infty} R(k) \tag{C.6}$$

where

$$|R(k)| \leqslant \frac{B_2 k q^{2k^2+6k+2} p^{k^2+k}}{1 - p^{k^2+k} q^{2+4k}} \left[|\log pq^4| + \left[\frac{|\log p| + |\log q^2|/k}{1 - p^{k^2+k} q^{2+4k}} \right] \right]. \tag{C.7}$$

Since $0 < p < 1$ and $pq^4 < 1$, it follows that if $q \geqslant 1$, then $pq^2 \leqslant pq^4 < 1$, and otherwise, if $q < 1$, then $pq^2 < 1$. Thus, $pq^2 < 1$ and while $k \geqslant 1$, the denominator above is minimized if $k = 1$. This shows that

$$|R(k)| \leqslant \frac{B_2 k q^{2k^2+6k+2} p^{k^2+k}}{1 - p^2q^6} \left[|\log pq^4| + \left[\frac{|\log p| + |\log q^2|}{1 - p^2q^6} \right] \right]$$

$$= \frac{B_2 k q^{2k^2+6k+2} p^{k^2+k}}{1 - p^2q^6} \left[|\log pq^4| + \left[\frac{|\log(pq^2)|}{1 - p^2q^6} \right] \right]. \tag{C.8}$$

It only remains to bound the sum over $k \geqslant 1$ of the above: note that

$$\sum_{k=1}^{\infty} k q^{2k^2+6k+2} p^{k^2+k} \leqslant C \int_1^{\infty} x q^{2x^2+6x+2} p^{x^2+x} \, \mathrm{d}x$$

$$\leqslant C \int_1^{\infty} x q^{2x^2} p^{x^2} \, \mathrm{d}x$$

$$= \frac{Cpq^2}{2|\log(pq^2)|} \tag{C.9}$$

where C is a finite constant. Taking the above and noting that $pq^2 < 1$ shows that there is a constant C' such that

$$\sum_{k=1}^{\infty} |R(k)| \leqslant \frac{C/2}{|\log(pq^2)|(1 - pq^3)} \left(|\log pq^4| + \frac{|\log(pq^2)|}{1 - pq^3} \right). \tag{C.10}$$

Similar to equation (C.9), one may bound

$$\sum_{k=1}^{\infty} \frac{q^{2k^2+6k+2} p^{k^2+k}}{1 - p^{k(k+1)} q^{4k+2}} \leqslant \sum_{k=1}^{\infty} \frac{(pq^2)^{2k^2}}{1 - p^2q^6}$$

$$\leqslant \frac{C}{(1 - pq^3)\sqrt{|\log(pq^2)|}} \tag{C.11}$$

where $C \leqslant \sqrt{\pi/8}$ is a constant independent of q and p. Taking together equations (C.10) and the last equation then proves the lemma. □

The results in lemmas 4.1 and 4.2 are taken together in theorem 4.3.

Theorem 4.3. *Suppose that* $0 < p \leqslant 1$ *and that* $0 < pq^4 < 1$. *Then the function* $B(1, q, p)$ *can be approximated by*

$$B(1, q, p) = 2 \sum_{k=1}^{\infty} (pq^2)^{k^2} q^{4k} \int_1^{\infty} \frac{(pq^2)^{kx} q^{2x}}{1 - p^{k^2+kx} q^{2(x+2k)}} \, \mathrm{d}x + \frac{H(p, q)}{1 - pq^4} + R$$

where $H(p, q)$ *is a function bounded in every subset of the* pq*-plane with* $q < q_0$, $p < 1$ *and* $pq^4 \leqslant 1$, *for any fixed* $q_0 > 0$, *and where* R *is a remainder term bounded by*

$$|R| \leqslant \frac{C_1 |\log pq^4|}{(1 - pq^3)|\log(pq^2)|} + \frac{C_2}{(1 - pq^3)^2} + \frac{C_3}{(1 - pq^3)\sqrt{|\log(pq^2)|}},$$

for some constants C_1, C_2 *and* C_3. *In other words,* R *is bounded by a constant in the region defined by* $0 \leqslant q \leqslant q_0$ *and* $pq^4 \leqslant 1$.

Lemma 4.4. *One may approximate*

$$\sum_{k=1}^{\infty}(pq^2)^{k^2}q^{4k}\int_1^\infty \frac{(pq^2)^{kx}q^{2x}}{1-p^{k^2+kx}q^{2(x+2k)}}\,\mathrm{d}x$$
$$=\int_1^\infty\left[\int_1^\infty \frac{(pq^2)^{(y+1)(y+x+1)}q^{2(2y+x+2)}}{1-p^{(y+1)(y+x+1)}q^{2(2y+x+2)}}\,\mathrm{d}x\right]\mathrm{d}y+\frac{H'(p,q)}{|\log(pq^4)|}+R$$

where $H'(p,q)$ is a function bounded in any subset of the pq-plane such that $0\leqslant p\leqslant 1$ and $0\leqslant pq^4\leqslant 1$ for all finite q_0 such that $q\leqslant q_0$. The remainder term R is bounded by

$$|R|\leqslant\frac{p^6q^{20}}{4(1-p^6q^{10})|\log(pq^3)|}+\frac{B_2}{2}\left[\frac{p^8q^{20}}{2(1-p^6q^{10})|\log(pq^3)|}(3|\log(pq^2)|\right.$$
$$+|\log(pq^2)|/(2|\log(pq^3)|)+2|\log(pq^4)|)$$
$$\left.+\frac{p^{12}q^{30}}{16(1-p^6q^{10})^2|\log(pq^2)|^2}(|\log p|+12|\log p||\log(pq^2)|+8|\log(pq^2)|^2)\right].$$

Thus, R is bounded by a constant in any subset of the first quadrant in the pq-plane defined by fixed $1\leqslant q_0<\infty$, $pq^4<1$ and $0\leqslant q\leqslant q_0$. In other words, the approximation is uniform in any such region.

Proof. Divide the series into the term with $k=1$, and the series with $k\geqslant 2$. This shows that

$$\sum_{k=1}^{\infty}(pq^2)^{k^2}q^{4k}\int_1^\infty \frac{(pq^2)^{kx}q^{2x}}{1-p^{k^2+kx}q^{2x+4k}}\,\mathrm{d}x=pq^6\int_1^\infty\frac{(pq^4)^x}{1-p^{x+1}q^{2x+4}}\,\mathrm{d}x$$
$$+\sum_{k=1}^{\infty}(pq^2)^{k^2}(pq^4)^{2k+1}\int_1^\infty\frac{(pq^2)^{kx}(pq^4)^x}{1-(pq^4)p^{k^2+kx}(pq^2)^{x+2k}}\,\mathrm{d}x.$$

One may bound

$$\frac{p^2q^{10}}{|\log(pq^4)|}\leqslant pq^6\int_1^\infty\frac{(pq^4)^x}{1-p^{x+1}q^{2x+4}}\,\mathrm{d}x\leqslant\frac{p^2q^{10}}{(1-p^2q^6)|\log(pq^4)|}.$$

Clearly, $H'(p,q)$ is a function bounded by p^2q^{10} and $p^2q^{10}/(1-p^2q^6)$, and has the desired properties for $0\leqslant p\leqslant 1$ and $pq^4\leqslant 1$. □

Apply the Euler–MacLaurin formula to the series over k to obtain the integral approximation to the series. The remainder terms are

$$\frac{p^4q^{14}}{2}\int_1^\infty\frac{(p^2q^6)^x}{1-(p^4q^8)(p^2q^2)^x}\,\mathrm{d}x+R_1, \qquad (C.12)$$

where R_1 is bounded by

$$|R_1|\leqslant\frac{B_2}{2}\left[p^4q^{14}|\log(pq^2)|\int_1^\infty\frac{(x+2)(p^2q^6)^x}{1-(p^4q^8)(p^2q^2)^x}\,\mathrm{d}x\right.$$
$$+2p^4q^{14}|\log(pq^4)|\int_1^\infty\frac{(p^2q^6)^x}{1-(p^4q^8)(p^2q^2)^x}\,\mathrm{d}x$$
$$+p^8q^{22}|\log p|\int_1^\infty\frac{(x+2)(p^4q^8)^x}{(1-(p^4q^8)(p^2q^2)^x)^2}\,\mathrm{d}x$$
$$\left.+2p^8q^{22}|\log(pq^2)|\int_1^\infty\frac{(p^4q^8)^x}{(1-(p^4q^8)(p^2q^2)^x)^2}\,\mathrm{d}x\right]. \qquad (C.13)$$

Consider first the integral in equation (C.12). Since $pq^4 \leqslant 1$ and $p \leqslant 1$ in the first quadrant of the pq-plane, it is the case that

$$\frac{p^4q^{14}}{2}\int_1^\infty \frac{(p^2q^6)^x}{1-(p^4q^8)(p^2q^2)^x}\,\mathrm{d}x \leqslant \frac{p^4q^{14}}{2(1-p^6q^{10})}\int_1^\infty (p^2q^6)^x\,\mathrm{d}x = \frac{p^6q^{20}}{4(1-p^6q^{10})|\log(pq^3)|}. \tag{C.14}$$

The bounds on the remainder R_1 can then be simplified to

$$|R_1| \leqslant \frac{B_2}{2}\left[\frac{p^8q^{20}}{2(1-p^6q^{10})|\log(pq^3)|}(3|\log(pq^2)| + |\log(pq^2)|/(2|\log(pq^3)|) + 2|\log(pq^4)|) + \frac{p^{12}q^{30}}{16(1-p^6q^{10})^2|\log(pq^2)|^2}(|\log p| + 12|\log p||\log(pq^2)| + 8|\log(pq^2)|^2)\right].$$

Theorem 4.5. *Let $q_0 > 0$ be a finite fixed constant, and let A be the compact region defined by $pq^4 \leqslant 1$ and $p \leqslant 1$ in the first quadrant in the pq-plane. Then the function $B(1, p, q)$ is approximated in A by*

$$B(1,q,p) = 2\int_1^\infty\int_1^\infty \frac{(pq^2)^{(y+1)(y+x+1)}q^{2(2y+x+2)}}{1-p^{(y+1)(y+x+1)}q^{2(2y+x+2)}}\,\mathrm{d}x\,\mathrm{d}y + \frac{H(p,q)}{1-pq^4} + \frac{H'(p,q)}{|\log(pq^4)|} + R$$

where $H(p, q)$ and $H'(p, q)$ are functions bounded in A and the remainder term R is bounded by the sum of the terms bounding the remainders in lemmas 4.3 amd 4.4, and thus by a constant in the region A.

This result can be understood as follows: the numerator in the integrand, $(pq^2)^{(y+1)(y+x+1)}q^{4y+2x+4}$ generates rectangular vesicles of thickness one, and dimensions generated by $(y+1)\times(y+x+1)$. The denominator, when expanded, adds layers of the same dimension to these slabs. Observe that vesicles of square shape have not been counted—their contributions were bound in equation (C.5).

Appendix D. Approximating $B(t, q, 1)$

$B(t, q, 1)$ is a triple summatrion given by

$$B(t,q,1) = \sum_{i,j,k>0} t^{4(i+j+k)}q^{2(ij+jk+ki)} = 2t^4\sum_{n=1}^\infty\sum_{k=1}^\infty \frac{(t^4q^2)^{n+2k}q^{2nk+2k^2}}{1-t^4q^{2n+4k}} + t^4\sum_{n=1}^\infty \frac{(t^4q^2)^{2n}q^{2n^2}}{1-t^4q^{4n}}. \tag{D.1}$$

First approximate $B(t, q, 1)$ using the Euler–MacLaurin formula.

Lemma 4.6. *Suppose that $0 \leqslant q \leqslant 1$ and that $0 \leqslant tq \leqslant 1$. Then for any finite and fixed t_0 and (q, t) such that $0 \leqslant t \leqslant t_0$,*

$$2t^4\sum_{n=1}^\infty\sum_{k=1}^\infty \frac{(t^4q^2)^{n+2k}q^{2nk+2k^2}}{1-t^4q^{2n+4k}} = 2t^4\sum_{k=1}^\infty\int_1^\infty \frac{(t^4q^2)^{x+2k}q^{2xk+2k^2}}{1-t^4q^{2x+4k}}\,\mathrm{d}x + \frac{L_0(t,q)|\log tq|}{(1-tq)^2}$$

where $|L_0(t, q)|$ is uniformly bounded by a constant for every (q, t) such that $t \leqslant t_0$.

Proof. Use the Euler–MacLaurin formula to approximate the summation over n. The remainder terms are

$$\frac{1}{2}\sum_{k=1}^{\infty}\frac{(t^4q^2)^{1+2k}q^{2k+2k^2}}{1-t^4q^{2+4k}} + \frac{B_2}{2}\sum_{k=1}^{\infty}\left[\frac{2(t^4q^2)^{1+2k}q^{2k+2k^2}[(|\log t^2q|+k|\log q|)(1-t^4q^{2+4k})+t^4q^{2+4k}|\log q|]}{(1-t^4q^{2+4k})^2}\right].$$

Consider bounds on each of these terms. Since $|q|<1$, and $|tq|<1$,

$$\sum_{k=1}^{\infty}\frac{(t^4q^2)^{1+2k}q^{2k+2k^2}}{1-t^4q^{2+4k}} \leqslant \frac{t^4q^2}{1-t^4q^6}\sum_{k=1}^{\infty}(t^4q^2)^{2k}q^{2k+2k^2} \leqslant \frac{t^{12}q^{10}}{(1-t^4q^6)(1-t^8q^8)}.$$

Secondly, noting again that $|q|<1$ and $|tq|<1$,

$$\begin{aligned}
&\frac{B_2}{2}\sum_{k=1}^{\infty}\left[\frac{2(t^4q^2)^{1+2k}q^{2k+2k^2}[(|\log t^2q|+k|\log q|)(1-t^4q^{2+4k})+t^4q^{2+4k}|\log q|]}{(1-t^4q^{2+4k})^2}\right]\\
&\quad\leqslant \frac{B_2t^4q^2}{(1-t^4q^6)^2}\sum_{k=1}^{\infty}t^{8k}q^{6k+2k^2}[(|\log t^2q|+k|\log q|)(1-t^4q^{2+4k})+|\log q|]\\
&\quad\leqslant \frac{B_2t^4q^2}{(1-t^4q^6)^2}\sum_{k=1}^{\infty}t^{8k}q^{8k}\left[|\log t^2q|+(k+1)|\log q|\right]\\
&\quad\leqslant \frac{B_2t^{12}q^{10}(2-t^8q^8)}{4(1-t^4q^6)^2}\left[\frac{|\log t^8q^8|}{(1-t^8q^8)^2}\right].
\end{aligned}$$

Examine these bounds to obtain the desired result. This completes the proof. □

Lemma 4.7. *Suppose that* $0\leqslant q\leqslant 1$ *and that* $0\leqslant tq\leqslant 1$. *Then for any finite and fixed* t_0 *and* (q,t) *such that* $0\leqslant t\leqslant t_0$ *there is a function* $L_1(t,q)$ *bounded by a constant such that*

$$2t^4\sum_{k=1}^{\infty}\int_1^{\infty}\frac{(t^4q^2)^{x+2k}q^{2xk+2k^2}}{1-t^4q^{2x+4k}}\,\mathrm{d}x = 2t^4\int_1^{\infty}\int_1^{\infty}\frac{(t^4q^2)^{x+2y}q^{2xy+2y^2}}{1-t^4q^{2x+4y}}\,\mathrm{d}x\,\mathrm{d}y + \frac{L_1(t,q)}{|\log tq|}.$$

Proof. Apply the Euler–MacLaurin formula again to obtain the double integral. The remainder terms are

$$\frac{1}{2}\int_1^{\infty}\frac{(t^4q^2)^{x+2}q^{2x+2}}{1-t^4q^{2x+4}}\,\mathrm{d}x + \frac{B_2}{2}\int_1^{\infty}\frac{2(tq)^{4x+2}q^{2x+2}}{(1-t^4q^{2x+4})^2}[(2|\log t^2q| + (x+2)|\log q|)(1-t^4q^{2x+4})+2|\log q|t^4q^{2x+4}]\,\mathrm{d}x.$$

The first term can be bounded immediately (using $|tq|<1$) by

$$\frac{1}{2}\int_1^{\infty}\frac{(t^4q^2)^{x+2}q^{2x+2}}{1-t^4q^{2x+4}}\,\mathrm{d}x \leqslant \frac{1}{2}\int_1^{\infty}\frac{t^8q^6(t^4q^4)^x}{1-t^4q^6}\,\mathrm{d}x \leqslant \frac{t^{12}q^{10}}{(1-t^4q^6)|\log t^8q^8|}.$$

Next, consider the second remainder term. Assuming that $|tq|<1$ and $|q|<1$ gives the following:

$$\begin{aligned}
&\frac{B_2}{2}\int_1^{\infty}\frac{2(tq)^{4x+2}}{(1-t^4q^{2x+4})^2}[(2|\log t^2q|+(x+2)|\log q|)(1-t^4q^{2x+4})+2|\log q|]\,\mathrm{d}x\\
&\quad\leqslant \frac{B_2}{2}\int_1^{\infty}\frac{2(tq)^{4x+2}}{(1-t^4q^6)^2}[2|\log t^2q|+(x+4)|\log q|]\,\mathrm{d}x
\end{aligned}$$

$$\leqslant \frac{B_2}{2}\int_1^\infty \frac{(x+4)(tq)^{4x+2}}{(1-t^4q^6)^2}|\log q^4t^4|\,\mathrm{d}x$$
$$\leqslant \frac{B_2}{2}\frac{t^6q^6}{(1-t^4q^6)^2}\left[\frac{1+5|\log t^4q^4|}{|\log t^4q^4|}\right].$$

Examining these bounds gives the required bound on $L_1(t,q)$. □

Lemmas 4.7 and 4.8 together give the following theorem:

Theorem 4.8. *Suppose that* $t_0 > 1$ *is a finite constant and that for all* $0 < t < t_0$, $0 \leqslant q \leqslant 1$ *and* $0 \leqslant tq \leqslant 1$. *Then there exists bounded functions* $L_0(t,q)$, $L_1(t,q)$ *and* $L_2(t,q)$ *such that*

$$B(t,q,1) = 2t^4\int_1^\infty\int_1^\infty \frac{(t^4q^2)^{x+2y}q^{2xy+2y^2}}{1-t^4q^{2x+4y}}\,\mathrm{d}x\,\mathrm{d}y + \frac{L_0(t,q)|\log tq|}{(1-tq)^2} + \frac{L_1(t,q)}{|\log tq|} + \frac{L_2(t,q)}{1-tq}.$$

Proof. It only remains to bound the last term in equation (D.1). Observe that $2n^2 > 4n$ for all $n > 1$, thus

$$t^4\sum_{n=1}^\infty \frac{(t^4q^2)^{2n}q^{2n^2}}{1-t^4q^{4n}} \leqslant t^4\left[\frac{t^8q^6}{1-t^4q^4} + \sum_{n=2}^\infty \frac{(t^8q^8)^n}{1-t^4q^8}\right].$$

The last term grows slower than $t^{16}q^{16}/(1-t^4q^8)(1-t^8q^8)$. In other words, this term grows similar to the remainder terms in lemmas 4.6 and 4.7. Collect all these results to define $L_2(t,q)$ and to prove the theorem. □

Appendix E. Approximating $B(t, 1, p)$

$B(t,1,p)$ is a triple summation

$$B(t,1,p) = \sum_{i,j,k>0} t^{4(i+j+k)}p^{ijk} = t^4\sum_{i,j>0}\frac{t^{4(i+j)}p^{ij}}{1-t^4p^{ij}}$$
$$= 2t^4\sum_{n=1}^\infty\sum_{k=1}^\infty \frac{t^{4(n+2k)}p^{k(n+k)}}{1-t^4p^{k(n+k)}} + t^4\sum_{n=1}^\infty\frac{t^{8n}p^{n^2}}{1-t^4p^{n^2}}. \qquad \text{(E.1)}$$

Consider the double sum, and approximate it as follows:

Lemma 4.9. *Suppose that* $0 \leqslant p \leqslant 1$ *and that* $0 \leqslant t^4p < 1$. *Then for any finite and fixed* t_0 *and* (t,p) *such that* $0 \leqslant t \leqslant t_0$,

$$t^4\sum_{n=1}^\infty\sum_{k=1}^\infty \frac{t^{4(n+2k)}p^{k(n+k)}}{1-t^4p^{k(n+k)}} = 2t^4\sum_{n=1}^\infty\int_1^\infty \frac{t^{4(n+2x)}p^{xn+x^2}}{1-t^4p^{xn+x^2}}\,\mathrm{d}x + \frac{K_0(t,p)|\log(t^4p)|}{(1-t^4p)^2},$$

where $|K_0(t,p)|$ *is uniformly bounded for every* (t,p) *such that* $t \leqslant t_0$.

Proof. Use the Euler–MacLaurin formula to approximate the summation over k by an integral. The resulting approximation is as claimed, while the remainder terms are

$$t^4\sum_{n=1}^\infty \frac{t^{4n+8}p^{n+1}}{1-t^4p^{n+1}}$$
$$+ B_2t^4\sum_{n=1}^\infty \frac{t^{4n+8}p^{n+1}(8|\log t| + (n+2)|\log p|)(1-t^4p^{n+1}) + (n+2)t^4p^{n+1}|\log p|}{(1-t^4p^{n+1})^2}.$$

The first term can be bounded by

$$\frac{t^4}{1-t^4p^2}\sum_{n=1}^{\infty} t^{4n+8}p^{n+1} = \frac{t^{16}p^2}{(1-t^4p^2)(1-t^4p)}.$$

The second term can be simplified and bound from above by

$$\begin{aligned}\frac{B_2t^4}{(1-t^4p^2)^2}&\sum_{n=1}^{\infty} t^{4n+8}p^{n+1}[2|\log t^4| + 2(n+2)|\log p|]\\ &\leqslant \frac{2B_2t^4}{(1-t^4p^2)^2}\sum_{n=1}^{\infty}(n+2)t^{4n+8}p^{n+1}|\log t^4p|\\ &= \frac{2B_2t^{16}p^2(3-2t^4p)|\log t^4p|}{(1-t^4p^2)^2(1-t^4p)^2}.\end{aligned}$$

Putting these bounds together implies the existence of $K_0(t, p)$, uniformly bounded for every (t, p) such that $t \leqslant t_0$. □

One may now approximate the second summation in lemma 4.9 by an integral.

Theorem 4.10. *Suppose that* $0 \leqslant p \leqslant 1$ *and that* $0 \leqslant t^4p < 1$*, and let* $t_0 < \infty$ *be a finite positive number. Then*

$$2t^4\sum_{n=1}^{\infty}\int_1^{\infty}\frac{t^{4(n+2x)}p^{xn+x^2}}{1-t^4p^{xn+x^2}}\,\mathrm{d}x = 2t^4\int_1^{\infty}\int_1^{\infty}\frac{t^{4(y+2x)}p^{xy+x^2}}{1-t^4p^{xy+x^2}}\,\mathrm{d}x\,\mathrm{d}y + \frac{K_1(t,p)}{|\log(t^4p)|},$$

where $|K_1(t, p)|$ *is uniformly bounded for every* (t, p) *such that* $0 < t \leqslant t_0$.

Proof. Approximate the summation by an integral to obtain the result. The Euler–MacLaurin formula gives the remainder terms (where the factor $2t^4$ was left away)

$$\begin{aligned}\frac{1}{2}&\int_1^{\infty}\frac{t^{4(1+2x)}p^{x+x^2}}{1-t^4p^{x+x^2}}\,\mathrm{d}x\\ &+\frac{B_2}{2}\int_1^{\infty}\left[\frac{t^{4+8x}p^{x+x^2}(|\log t^2| + x|\log p|)\left(1-t^4p^{x+x^2}\right) + (x+2)t^4p^{x+x^2}|\log p|}{\left(1-t^4p^{x+x^2}\right)^2}\right]\mathrm{d}x.\end{aligned}$$

The first term can be bounded as follows:

$$\frac{1}{2}\int_1^{\infty}\frac{t^{4(1+2x)}p^{x+x^2}}{1-t^4p^{x+x^2}} \leqslant \frac{t^4}{2(1-t^4p^2)}\int_1^{\infty}(t^8p^2)^x\,\mathrm{d}x = \frac{t^{12}p^2}{4(1-t^4p^2)|\log(t^4p)|}.$$

The second term can be bounded by using the fact that $0 \leqslant p \leqslant 1$ and $t^4p \leqslant 1$. This shows that an upper bound is

$$\begin{aligned}\frac{1}{(1-t^4p^2)^2}&\int_1^{\infty}(t^8p^2)^x(|\log t^4| + 4x|\log p|)\,\mathrm{d}x\\ &\leqslant \frac{4}{(1-t^4p^2)^2}\int_1^{\infty}x(t^8p^2)^x|\log(t^4p)|\,\mathrm{d}x\\ &= \frac{2t^8p^2(1+2|\log(t^4p)|)}{(1-t^4p^2)^2|\log(t^4p)|}.\end{aligned}$$

Together, these bounds on the remainder terms prove the existence of $K_1(t, p)$ as claimed. □

Taken together, these lemmas give the following approximation for $B(t, 1, p)$:

Theorem 4.11. *Suppose that $t_0 > 1$ is a finite constant and that for all $0 < t < t_0$, $0 \leqslant p \leqslant 1$ and $0 \leqslant t^4 p \leqslant 1$. Then there exists bounded functions $K_0(t,p)$, $K_1(t,p)$ and $K_3(t,p)$ such that*

$$B(t,1,p) = 2t^4 \int_1^\infty \int_1^\infty \frac{t^{4(y+2x)} p^{xy+x^2}}{1 - t^4 p^{xy+x^2}} \,\mathrm{d}x\,\mathrm{d}y + \frac{K_0(t,p)|\log(t^4 p)|}{(1-t^4 p)^2} + \frac{K_1(t,p)}{|\log(t^4 p)|} + \frac{K_2(t,p)}{1-t^4 p}.$$

Proof. It only remains to bound the last term in equation (E.1). Consider then that

$$\sum_{n=1}^\infty \frac{t^{8n} p^{n^2}}{1 - t^4 p^{n^2}} \leqslant \frac{t^8 p}{1-t^4 p} + \sum_{n=2}^\infty \frac{(t^8 p^2)^n}{1 - t^4 p^{n^2}} \leqslant \frac{t^8 p}{1-t^4 p} + \frac{t^{16} p^4}{2(1-t^4 p^4)|\log(t^4 p)|},$$

this result proves the existence of $K_2(t,p)$. □

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