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Inflating square and rectangular lattice vesicles

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Abstract
In this paper, two simple models of lattice vesicles in two and in three dimensions are examined. Lattice vesicles have a rich mathematical nature, and the combinatorial and scaling properties of square and rectangular lattice vesicle models are investigated and then generalized to three dimensions. The phase diagram of the vesicles also includes a multicritical point, and scaling of the generating functions of these models are studied to test the models for tricritical scaling behaviour. In the models of square vesicles in the square lattice, and cubical vesicles in the cubic lattice, the tricritical scaling forms are explicitly confirmed. However, rectangular vesicles in the square lattice, and rectangular box vesicles in the cubic lattice, appear not to conform to the expected tricritical scaling forms.

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1. Introduction

Models of lattice *vesicles* (sometimes called *polyominoes*) in the two-dimensional square lattice have received considerable attention in the literature [3–5]. The statistical mechanics of these models is particularly interesting since the phase diagram may include multicritical points. Many of these models are also 'exactly solvable' in the sense that the generating function can be determined in closed form. The mathematical description of these models is rich, drawing on combinatorics, real and complex analysis, and asymptotic analysis to examine scaling behaviour around multicritical points.

In this paper, I consider two simple models of lattice vesicles in two dimensions and then generalize them to their three-dimensional counterparts. I test the scaling assumptions in the models in this paper, and find that, while a model of two-dimensional squares and three-dimensional cubes exhibits the expected scaling behaviour, their generalization to models of rectangular and rectangular box vesicles in three dimensions are apparently incomplete.

Consider a model of lattice vesicles composed of n unit squares and m perimeter edges. The most fundamental quantity in the model is $c_n(m)$, which is the number of vesicles of perimeter m edges and area (or size) n unit squares. The generating function is a two-variable function

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

In many directed models $G(t,q)$ can be determined either in closed form, or as an infinite series or as an infinite product. For example, the well-known generating function of a partition model of lattice vesicles is given by [24]

$$P(t,q) = \sum_{n=1}^{\infty}\left[\sum_{m=1}^{\infty} p_{n,m} t^m\right] q^m = \sum_{n=1}^{\infty} \frac{t^{4n} q^{n^2}}{\prod_{i=1}^{n}(1-t^2 q^{i+1})^2}. \tag{2}$$

In this model, $p_{n,m}$ is the number of partitions of n into a partition polygon with total perimeter length m.

Partitions have been studied widely in the mathematical literature, see for example [8, 10, 16, 19]. Other directed models of lattice vesicles, related to partitions, such as stack polygons [19, 27], staircase polygons [4, 6, 25], and other partially or fully directed models of lattice vesicles (including convex, column-convex and histogram polygons) have also received considerable attention in the literature, see for example [1, 11, 12, 18, 21] and numerous other references.

Tricritical scaling theory [5, 13] indicates that the generic generating function $G(t,q)$ should exhibit certain scaling behaviour in its asymptotic regime. In particular, there are scaling fields g and s such that[1]

$$G(t,q) \sim A(t,q) + g^{2-\alpha_t}\mathcal{H}(g^{-\phi}s) \tag{3}$$

in its asymptotic regime (as both $g \to 0^+$ and $s \to 0^+$), where $A(t,q)$ is an analytic background term. The scaling fields g and s are related to the generating variables q and t, and α_t and ϕ are *critical exponents* that characterize a phase transition in the model. The *crossover exponent* ϕ describes the 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 $G(t,q) \sim A(t,q) + g^{2-\alpha_t}$, and the singular behaviour in $G(t,q)$ at the critical point is described by the exponent $2-\alpha_t$.

By slightly rearranging the terms in equation (3)), it follows that

$$G(t,q) \sim R(t,q) + s^{2-\alpha_u}\mathcal{H}'(g^{-\phi}s) \tag{4}$$

where $\mathcal{H}'(x) = x^{-(2-\alpha_u)}\mathcal{H}(x)$ is still a function of the combined variable $g^{\phi}s$. The exponent α_u describes scaling along the s-axis. It is related to ϕ and α_t by the identity

$$\frac{2-\alpha_t}{2-\alpha_u} = \phi \tag{5}$$

and this can be demonstrated by noting that

$$g^{2-\alpha_t}\mathcal{H}(g^{-\phi}s) = t^{2-\alpha_u}[g^{-\phi}s]^{-(2-\alpha_u)}\mathcal{H}(g^{-\phi}s) = s^{2-\alpha_u}\mathcal{H}'(g^{-\phi}s). \tag{6}$$

[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 $|t - t_c|$.

The relation in equation (5) joins the scaling in the generating function as the critical point is approached into one scaling form describing scaling along both the g and s axes.

The most important thermodynamic quantity in the description of lattice models of vesicles is the limiting free energy $\mathcal{F}(t)$. It may be determined from the generating function by first defining a *partition function* $Z_n(t)$ by

$$G(t,q) = \sum_{n>0} Z_n(t) q^n \tag{7}$$

where $Z_n(t) = \sum_{m>0} c_n(m) t^m$. The *critical curve* $q_c(t)$ is the radius of convergence of $G(t,q)$, given by

$$q_c(t) = \lim_{n\to\infty} [Z_n(t)]^{-1/n}. \tag{8}$$

Existence of this limit demonstrates the existence of a thermodynamic limit in the model, and the phases are separated by non-analyticities in the critical curve $q_c(t)$. The limiting free energy is defined by

$$\mathcal{F}_p(t) = \lim_{n\to\infty} \frac{1}{n} \log Z_n(t) = -\log q_c(t). \tag{9}$$

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:

$$\mathcal{F}_p(t) \sim C_0 |t - t_c|^{2-\alpha} + \text{analytic terms} \qquad \text{as} \quad t \to t_c^+. \tag{10}$$

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 (density) $\mathcal{F}_p(t)$ 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

$$2 - \alpha = 1/\phi \tag{11}$$

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.

It is known that partition polygons do not conform to tricritical scaling in equations (3) and (4). In particular, the critical curve for partition polygons in the perimeter–area ensemble can be read from equation (2), and the limiting free energy is

$$\mathcal{F}_P(t) = \begin{cases} 0 & \text{if} \quad t \leqslant 1 \\ 2\log t & \text{if} \quad t > 1. \end{cases} \tag{12}$$

The critical point is located at $t_c = 1$, and since $-\log t \approx (1-t) = s$ for $t \to 1^+$, this shows that $2 - \alpha = 1$. However, the scaling form in equation (3) does not quite apply: putting $q = 1$ in $P(q,t)$ shows that $P(1,t) = (1-t^2)/(1-2t^2)$. Observe that $P(1,t)$ diverges as $2t^2 \to 1^-$, away from the critical point at $t = 1$. Moreover, as $q \to 1^-$ in $P(q,1)$, an essential singularity is approached, and there is no power law description of the scaling near the critical point. Instead, it appears that $P(1,t) \sim |\sqrt{2^{-1}} - t)|^{-1} \neq s^{-1} = |1-t|^{-1}$, but $t_c \neq \sqrt{2^{-1}}$. This appears contrary to the expected scaling forms proposed by tricritical scaling, and further study of this model may be necessary.

In this paper, I consider models even simpler than partition polygons, and I examine the feasibility of the scaling forms in equations (3) and (4). This approach was used for a variety of models in the literature, and perhaps the best known verification is for staircase polygons in [17]. Models of lattice columns, lattice squares and rectangles have also been considered [18, 19]. Scaling functions for a variety of these models have also been investigated, starting with the important work of Prellberg on staircase polygons [17], and resulting in a number of results for lattice polygon models [18, 20, 22]. In at least one case considerable progress was made for the full model of undirected lattice polygons [23]. I restrict the investigation to lattice squares and rectangles in this paper, and expand them to their three-dimensional counterparts. Examination of these models indicates that square and cubical vesicles conform to the expected scaling forms, and partial results can be obtained in the case of rectangular and rectangular box vesicles. The generating function $S(t, q)$ of square lattice vesicles in the perimeter–area ensemble, and $T(1, q, p)$ of cubical vesicles in the area–volume ensemble are shown to be

$$S(t,q) = \frac{1}{2} + \frac{\sqrt{\pi}}{2|\log q|^{1/2}} \mathcal{G}\left(\frac{2|\log t|}{\sqrt{|\log q|}}\right) + R_1 \qquad (13)$$

$$T(1,q,p) = \frac{1}{2} + \frac{1}{|\log q|^{1/3}} \mathcal{F}\left(\frac{32\log^3 q}{\log^2 p}\right) + R_1 \qquad (14)$$

where $\mathcal{G}(x) = \mathrm{e}^{x^2}(1 - \mathrm{erf}(x))$, and $\mathcal{F}(x)$ is a certain sum of hypergeometric functions multiplied by a power of x.[2] The error terms R_1 can in both cases be bounded to give uniform approximations to $S(t, q)$ and $T(1, q, p)$, see equation (39) and theorems 2.4 and 2.8.

In the case of rectangular vesicles in two dimensions, the generating function can be shown to be approximated by a Lerch-Phi function (see equation (74)):

$$R(t,q) = \frac{t^2}{|\log q|}\left[\frac{|\log q|}{|\log t^2|} - \text{Lerch-Phi}\left(t^2 q, 1, \frac{|\log t^2|}{|\log q|}\right)\right] + R_1. \qquad (15)$$

The error term R_1 can be bounded, but it turns out that $(1 - t^2 q)^2 R(t, q)$ is uniformly approximated. If $t = 1$, then

$$R(1,q) = \frac{\log(1-q)}{\log q} + \frac{q}{2(1-q)} - \frac{B_q q \log q}{(1-q)^2} \qquad (16)$$

and in this case, one may show that the function $|B_q| \leqslant B_2$, where B_2 is the second Bernoulli number, see corollary 3.2. One may therefore guess that $2 - \alpha_t = -1$ in this model, and the appearance of the ratio $|\log q|/|\log t^2|$ in $R(t, q)$ suggest that $\phi = 1$. Since $R(t, 1) = t^4/(1 - t^2)^2$, it appears that the value -2 be assigned to $2 - \alpha_u$; this would be inconsistent with equation (5). On the other hand, the generating function has a simple pole along the curve $t^2 q = 1$ (see equation (66)), and if $q = 1 - \epsilon < 1$ and $t^2 \to q^{-1}$, then one may assign $2 - \alpha_u = -1$, for all small values of $\epsilon > 0$. This would be consistent with equation (5).

Finally, only partial results can be obtained for rectangular box vesicles in three dimensions. In particular, I prove that

$$B(1,q,1) = \frac{\sqrt{\pi}}{\sqrt{|\log q^2|}} \int_1^\infty \frac{\exp(-|\log q^2|(y(y+4)/4))}{1-\exp(-y|\log q^2|)} \,\mathrm{erfi}\left(y\sqrt{|\log q^2|}/2\right) \mathrm{d}y + \frac{B_q}{\sqrt{1-q^2}} \qquad (17)$$

$$B(1,1,p) = \frac{1}{|\log p|} \int_0^p \frac{\log(1-y)}{\log y} \frac{\mathrm{d}y}{y} + \frac{R_p}{1-p} \qquad (18)$$

[2] In all these expressions, I assume that the generating variables are chosen within the radius of convergence of the generating functions.

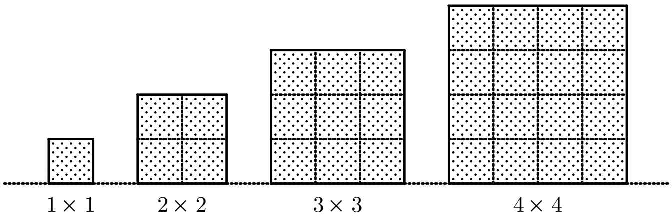

Figure 1. Squares in the square lattice. There is exactly one square each of size $n \times n$ and they are generated by $S(t, q)$ in equation (19).

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) (see theorems 3.6 and 3.8). The integrals in these expressions are divergent; in the first case apparently proportional to $|\log q|^{-1}$ and in the second case slower than any inverse power of $|\log p|$. In other words, one may attempt to assign values to the critical exponents, and it appears that $2 - \alpha_u = -3/2$ while $2 - \alpha_t = -1$. An approximation to $B(1, q, p)$ (equation (107)) suggests that $\phi = 2/3$, and this turns out to be consistent with the values for $2 - \alpha_t$ and $2 - \alpha_u$ as suggested by equation (5). The description of this model is still incomplete.

2. Square and cubical lattice vesicles

It is well known that the generating function of lattice squares can be expressed in terms of q-deformations of factorials and of the exponential. These are related to θ-functions [20], exposing a rich mathematical structure that underlies this simple model. Much less is known about *lattice cubes*, the three-dimensional version of lattice squares, or even higher dimensional versions of the model.

2.1. Square vesicles

Consider lattice vesicles of areas $1^2, 2^2, 3^3, \ldots$, as in figure 1. The generating function in a perimeter–area ensemble is

$$S(t, q) = \sum_{n=0}^{\infty} t^{4n} q^{n^2} \tag{19}$$

where q generates area in unit squares and t generates perimeter edges.

$S(t, q)$ also may be expressed as a nested product

$$S(t, q) = 1 + t^4 q(1 + t^4 q^3(1 + t^4 q^5(1 + t^4 q^7(1 + \cdots)))) \tag{20}$$

and it satisfies a functional recurrence

$$S(t, q) = 1 + [t^4 q] S(t\sqrt{q}, q). \tag{21}$$

$S(t, q)$ is convergent for all $|q| < 1$, and divergent if $|q| > 1$. If $q = 1$, then $S(t, 1) = 1/(1 - t^4)$, so that $S(t, 1)$ is convergent if $t < 1$, and there is a simple pole in the t-plane on the positive real axis at $t = 1$. This point may be considered a critical point, and comparison with equation (4) shows that $2 - \alpha_u = -1$ where the scaling field $s = 1 - t$ was identified.

If $t = 1$ and $q < 1$, then $S(1,q) = \sum_{n=0}^{\infty} q^{n^2}$ and the radius of convergence is $|q| = 1$ in the q-plane. In this instance $S(1,q)$ is related to Ramanujan's two-variable θ-function defined by

$$\Theta(p,q) = \sum_{n=-\infty}^{\infty} p^{\binom{n+1}{2}} q^{\binom{n}{2}} = (-p;\, pq)_\infty(-q;\, pq)_\infty(pq;\, pq)_\infty \tag{22}$$

where $(t;q)_N = \prod_{i=1}^{N}(1 - tq^{i-1})$ is the q-Pochhammer symbol, and $(q;q)_n$ is the q-analogue of the factorial, where

$$(t;q)_\infty^{-1} = \sum_{n=0}^{\infty} \frac{t^n}{(q;q)_n} \tag{23}$$

is the q-analogue of the exponential. The Jacobi triple product identity then shows that

$$\Theta(q,q) = -1 + 2\sum_{n=0}^{\infty} q^{n^2} = (-q;q^2)_\infty(-q;q^2)_\infty(q^2;q^2)_\infty. \tag{24}$$

Thus, $S(1,q)$ may be evaluated in terms of the q-exponential,

$$S(1,q) = \tfrac{1}{2}(1 + (-q;q^2)_\infty(-q;q^2)_\infty(q^2;q^2)_\infty). \tag{25}$$

The θ-function $\Theta(q,q) = \phi(q)$ is also known as Ramanujan's one-variable ϕ-function. Several expressions are known for $\phi(q)$; in particular,

$$\begin{aligned}\phi(q) &= \sqrt{1 + 4\left(\frac{q}{1-q} - \frac{q^3}{1-q^3} + \frac{q^5}{1-q^5} - \frac{q^7}{1-q^7} + \cdots\right)} \\ &= \sqrt{\sqrt{1 + 8\left(\frac{q}{1-q} + \frac{2q^2}{1+q^2} + \frac{3q^3}{1-q^3} + \frac{4q^4}{1+q^4} + \cdots\right)}}.\end{aligned} \tag{26}$$

The singularities in $\phi(q)$ along the curves $1 - q^{2n+1} = 0$ accumulate on $q = 1$ in the q-plane; thus $\phi(q)$ has an essential singularity at $q = 1$ [26]. Ramanujan's one-variable ϕ-function has also been evaluated exactly at some special values of q:

$$\phi(\mathrm{e}^{-\sqrt{2}\pi}) = \frac{\Gamma\left(\frac{9}{8}\right)}{\Gamma\left(\frac{5}{4}\right)}\sqrt{\frac{\Gamma\left(\frac{1}{4}\right)}{\sqrt{\sqrt{2}\pi}}} \qquad \phi(\mathrm{e}^{-\pi}) = \frac{\sqrt{\sqrt{\pi}}}{\Gamma\left(\frac{3}{4}\right)} \qquad \phi'(-\mathrm{e}^{-\sqrt{3}\pi}) = (4\sqrt{3} - 7)^{1/8} \tag{27}$$

see for example [2].

Observe that the derivative of $S(t,q)$ to $\log q$ is $\sum_{n=0}^{\infty} n^2 t^{4n} q^{n^2}$, and this is convergent for all $|q| < 1$, and for $|t| < 1$ whenever $|q| = 1$. In other words, the (left) derivative of $S(t,q)$ to q is finite along the line $q = 1$ if $t < 1$ in the tq-plane. Since $S(t,q)$ is infinite if $q > 1$, this proves (together with equation (26)) that $S(t,q)$ has an essential singularity along the line $q = 1, t \leqslant 1$ in the tq-plane.

For other values of t, it can be verified that

$$S(t,q) + S(1/t,q) = 1 + \sum_{n=-\infty}^{\infty} t^{4n} q^{n^2} = 1 + (-qt;q^2)_\infty(-q/t;q^2)_\infty(q^2;q^2)_\infty. \tag{28}$$

This is convergent for all values of $q < 1$, as noted above. If $q = 1$ and $t > 1$, then $S(t,q)$ is divergent. The q-exponentials in equation (28) are explicitly equal to

$$(-qt;q^2)_\infty(-q/t;q^2)_\infty(q^2;q^2)_\infty = \prod_{i=1}^{\infty}((1 + q^{2i+1}t)(1 + q^{2i+1}/t)(1 - q^{2i})) \tag{29}$$

and by taking logarithms and noting that $(1+q^{2i+1}t)(1+q^{2i+1}/t) \geqslant (1+2q^{2i+1})$ for all $t \geqslant 0$, while applying the bound $\log(1+x) \geqslant x - x^2/2$, the lower bound

$$\begin{aligned}\log((-qt;q^2)_\infty(-q/t;q^2)_\infty(q^2;q^2)_\infty) &\geqslant \sum_{i=1}^{\infty}\log((1+2q^{2i+1})(1-q^{2i}))\\ &\geqslant \sum_{i=1}^{\infty}\log(1+2q^{2i+1}-q^{2i}-2q^{4i+1})\\ &\geqslant \frac{(2+\cdots-4q^{21}+3q^{22})q^2}{2(1-q^{12})(1+q^2+q^4+q^6+q^8)(1+q^4)} \qquad (30)\end{aligned}$$

is obtained. An upper bound on equation (29) can be found by taking logarithms and then using the inequality $x \geqslant \log(1+x)$. This shows that

$$\begin{aligned}\log((-qt;q^2)_\infty(-q/t;q^2)_\infty(q^2;q^2)_\infty) &\leqslant \sum_{i=1}^{\infty}(\log(1+q^{2i+1}t)+\log(1+q^{2i+1}/t))\\ &\leqslant \frac{q(t+1/t)}{1-q^2}. \qquad (31)\end{aligned}$$

Thus, taking the factor $(1-q^2)$ from $(1-q^{12})$ in equation (30), and considering the last equation, it follows from equation (28) that $\log(S(t,q)+S(1/t,q)-1) \sim (1-q^2)^{-1}$ as $q \nearrow 1^-$. Since $S(1/t,q)$ is finite for $t>1$ (and $q \leqslant 1$), the result is that $S(t,q) \sim \mathrm{e}^{O(1/(1-q^2))}$ along the line $q=1$ with $t \geqslant 1$.

If it is noted that $-\log q^2 \approx 1-q^2$ as $q \to 1^-$, then one might propose that $\log(S(t,q)+S(1/t,q)-1) \sim O(1/|\log q^2|)$. This result can be made more precise by using known asymptotics for the q-exponential [15], see also Prellberg [17].

Lemma 2.1 (Moak 1984 [15])**.** *Suppose that* $0<q<1$ *and define* $r=\mathrm{e}^{-4\pi^2/|\log q|}$*. Then*

$$(q;q)_\infty = (r/q)^{1/24}\sum_{n=-\infty}^{\infty}[r^{n(6n+1)}-r^{(3n+1)(2n+1)}]\sqrt{\frac{2\pi}{|\log q|}}.$$

Taking logarithms gives the following asymptotic formula:

$$\begin{aligned}\log(q;q)_\infty &= \frac{-\pi^2}{6|\log q|}+\frac{1}{2}\log\left[\frac{2\pi}{|\log q|}\right]+O(|\log q|)\\ &\approx \frac{-\pi^2}{6|\log q|}+\frac{1}{2}\log\left[\frac{2\pi}{1-q}\right]+O(|\log q|).\end{aligned}$$

A proof of lemma 2.1 can be found in [17]. A uniform asymptotic approximation to $(t;q)_\infty$ is given in lemma 2.2, see [17].

Lemma 2.2 (Prellberg 1994 [17])**.** *For complex t such that* $|arg(1-t)|<\pi$ *and* $q \in (0,1)$*,*

$$\log(t;q)_\infty = \frac{\mathcal{L}i_2(t)}{\log q}+\frac{1}{2}\log(1-t)+R_1$$

where $\mathcal{L}i_2(t)=\sum_{n>0}[t^n/n^2]$ *is the dilogarithm. Moreover,* $R_1 = O(|\log q|)$*, and so* R_1 *approaches zero uniformly as* $q \nearrow 1^-$ *for any t in a compact domain with* $|arg(1-t)|<\pi$*.*

If $t=1$, then lemmas 2.1 and 2.2 can be used to determine an asymptotic approximation to $S(1,q)$. The starting point is equation (25); where $0<q<1$. The factor $(-q;q^2)_\infty$ can

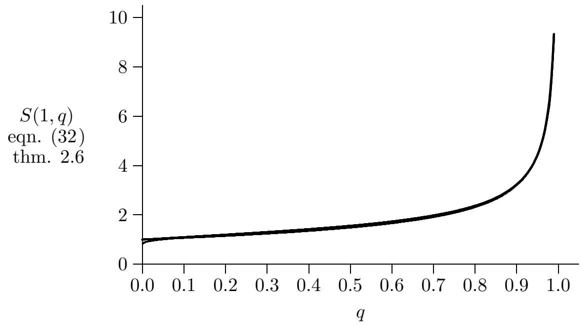

Figure 2. A plot of $S(1, q)$ against its approximations in equations (32) and in theorem 2.6.

be approximated using lemma 2.2, while $(q^2, q^2)_\infty$ can be approximated accurately by taking only the $n = 0$ term in the series in lemma 2.1. Putting this together shows that

$$S(1, q) \approx \frac{1}{2} + \frac{1+q}{2q^{1/12}}\sqrt{\frac{2\pi}{|\log q^2|}}\exp(-(\pi^2/6 + 2\mathcal{L}i_2(-q))/|\log q^2|). \tag{32}$$

This approximation is particularly good as $q \to 1^-$. For example, $S(1, 0.99) = 9.3400\ldots$, while the approximation gives $9.3253\cdots$.

In figure 2 both $S(1, q)$ and its approximation in equation (32) are plotted against q. The approximation is remarkably good over the entire range of q away from $q = 0$. In this graph the approximation $S(1, q) = 1/2 + \sqrt{\pi}|\log q|^{-1/2}/2$ was also plotted—this will be obtained by applying the Euler–MacLaurin formula to $S(1, q)$ in section 1.2.

The dilogarithm above also satisfies the following equality for negative argument[3]:

$$\mathcal{L}i_2(-q) = -\tfrac{1}{2}(\log q)^2 - \frac{\pi^2}{6} - \mathcal{L}i_2(-1/q). \tag{33}$$

The series expansion for $\mathcal{L}i_2(-1/q)$ is uniformly convergent for all $|q| \geqslant 1$ and equation (33) gives a slightly different approximation for $S(1, q)$:

$$S(1, q) \approx \frac{1}{2} + \frac{1+q}{2q^{7/12}}\sqrt{\frac{2\pi}{|\log q^2|}}\exp((\pi^2/6 + 2\mathcal{L}i_2(-1/q))/|\log q^2|). \tag{34}$$

Comparison with equation (3) shows that one might expect $2 - \alpha_t = -1/2$. If the relation in equation (5) applies in this model, then this would indicate that $\phi = 1/2$; it was already indicated that $2 - \alpha_u = -1$, following equation (21).

To determine asymptotics for $S(t, q)$ as $q \to 1^-$ and $t > 1$, consider equation (28). Assume that $qt > 1$ (with t fixed), and note that $S(1/t, q) \nearrow t^4/(t^4 - 1) = 1 + O(t^{-4})$ as

[3] To see this, note that $\mathcal{L}i_2(s)$ satisfies the following equalities:

$$\mathcal{L}i_2(-s) - \mathcal{L}i_2(1-s) + \frac{1}{2}\mathcal{L}i_2(1-s^2) = -\frac{\pi^2}{12} - (\log s)(\log(1+s))$$

$$\mathcal{L}i_2(s) + \mathcal{L}i_2(1-s) = \frac{\pi^2}{6} - (\log s)(\log(1-s))$$

$$\mathcal{L}i_2(1-s) + \mathcal{L}i_2(1-1/s) = -\frac{1}{2}(\log s)^2$$

$$\mathcal{L}i_2(s) + \mathcal{L}i_2(-s) = \frac{1}{2}\mathcal{L}i_2(s^2).$$

Apply these to $\mathcal{L}i_2(-s)$ to prove the identity. Alternatively, the identity can also be found using Maple V [14].

$q \nearrow 1^-$. Approximate the q-Pochhammer symbols $(-tq; q)_\infty$ and $(q^2; q^2)_\infty$ by lemmas 2.1 and 2.2, and use equation (33) to see that

$$S(t,q) \approx \sqrt{\frac{2\pi(1+qt^4)(1+q/t^4)}{|\log q^2|}} \exp((\pi^2/6 + \mathcal{L}i_2(-qt^4) + \mathcal{L}i_2(-q/t^4))/\log q^2) + 1 + O(t^{-4}). \qquad (35)$$

Since $q \to 1^-$, one may replace $|\log q^2|$ by $1 - q^2$, and this shows that $S(t,q) \sim \exp(\pi^2/6(1-q^2) + O(\log q))/\sqrt{1-q^2}$, as claimed in the paragraph before lemma 2.1.

The radius of convergence of $S(t,q)$ is the line $q = 1$ in the tq-plane. Along the line segment $q = 1$ and $0 \leqslant t < 1$ the generating function $S(t,q)$ is finite, with finite left derivative to q. For $q < 1$ and $t > 1$ the singular behaviour of $S(t,q)$ is given by equation (35), and as $q \nearrow 1^-$, $S(t,q) \to \infty$. In this model these are essential singularities, but their characters are qualitatively different from those on the critical curve with $t < 1$. At $t = 1$ the behaviour is given by equation (32), and for $t > 1$, equation (35) gives an approximate asymptotic formula. Taken together, we find that

$$S(t,q) \underset{q\to 1^-}{\approx} \begin{cases} \dfrac{1}{1-t^4} & \text{if } \ 0 \leqslant t < 1 \\ \dfrac{1}{2} + \dfrac{1+q}{2q^{1/12}}\sqrt{\dfrac{2\pi}{|\log q^2|}}\,\mathrm{e}^{H(q)} & \text{if } \ t = 1 \\ \sqrt{\dfrac{2\pi(1+qt^4)(1+q/t^4)}{|\log q^2|}}\,\mathrm{e}^{L(t,q)} & \text{if } \ t > 1. \end{cases} \qquad (36)$$

where

$$\begin{aligned} H(q) &= -(\pi^2/6 + 2\mathcal{L}i_2(-q))/|\log q^2| \\ L(t,q) &= -(\pi^2/6 + \mathcal{L}i_2(-qt^4) + \mathcal{L}i_2(-q/t^4))/|\log q^2|. \end{aligned} \qquad (37)$$

Observe that $\lim_{q\to 1^-} H(q) = -\log 2$, while $L(t,q)$ approaches ∞ as $q \to 1^-$. Moreover, one may use Maple V [14] to develop asymptotics for $L(t,q)$ as $q \to 1^-$ and $t \to 1^-$. It follows that

$$L(t,q) = \frac{4|\log t|^2}{|\log q|} - \log 2 - 4|\log t|^2 + O(\log^3 t) + O(\log q). \qquad (38)$$

In other words,

$$S(t,q) \sim \frac{1}{\sqrt{|\log q|}} \mathcal{G}_0\left(\frac{2|\log t|}{\sqrt{|\log q|}}\right) \qquad (39)$$

for some function $\mathcal{G}_0$, and if we define the scaling fields $s = |\log t|$ and $g = |\log q|$, then

$$S(t,q) \sim \frac{1}{\sqrt{g}} \mathcal{G}_0\left(\frac{s}{\sqrt{g}}\right). \qquad (40)$$

Comparison with equation (3) shows that $2 - \alpha_t = -1/2$ and $\phi = 1/2$. Comparing this instead to equation (4) shows that $2 - \alpha_u = -1$, and this demonstrates that in this model, the relationship in equation (5) is respected. The diagram in figure 3 illustrates the different phases in this model.

The line $q = 1$ is a phase boundary in the phase diagram (qt-plane) separating a phase of small squares as $q < 1$ from a phase of squares of unbounded size if $q > 1$. The only interesting phase behaviour occurs along the phase boundary. If $t < 1$, then the generating function $S(t,1) < \infty$, and if $t \geqslant 1$, then $S(t,1) = \infty$. The entire phase boundary is an

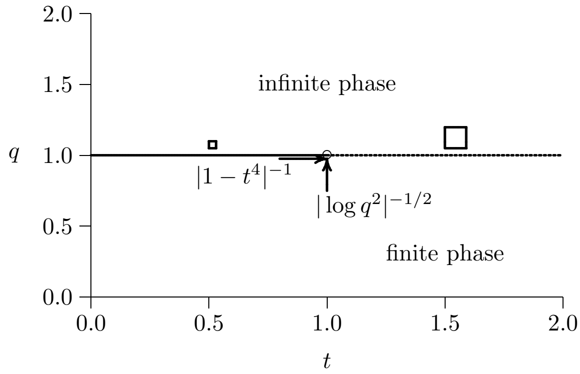

Figure 3. The phase diagram of inflating lattice squares. A phase boundary $q = 1$ separates a phase of finite squares from a phase of infinite (inflated) squares. The phase boundary is a line of essential singularities in the generating function. There is scaling around the point at $(t, q) = (1, 1)$, consistent with tricritical scaling theory. For values of $t < 1$ the transition at $q = 1$ is through a finite generating function where squares of arbitrary large size make a negligible contribution. For values of $t > 1$ the transition at $q = 1$ has a generating function divergent due to contributions of squares of arbitrary large size.

essential singularity in $S(t, q)$, consistent with a first-order transition in the model, separating finite from infinite squares. In the usual (canonical) picture, the free energy density in this model is $\mathcal{F}(t) = -\log q_c(t) = 0$, so that the model is not interesting from a statistical mechanics point of view.

2.2. Cubical vesicles

The simplest three-dimensional model of a vesicle in the cubic lattice would be a cube composed of unit cubes. The generating function of this model in the perimeter–area–volume ensemble is given by

$$T(t, q, p) = 1 + t^{12}q^6p + t^{24}q^{24}p^8 + \cdots = \sum_{n=0}^{\infty} t^{12n}q^{6n^2}p^{n^3}. \tag{41}$$

The generating variable t generates perimeter edges in the surface of the cube where adjacent unit squares meet at right angles, and q generates the surface area of the cube, while p generates volume. It follows that

$$T(t, q, p) = 1 + t^{12}q^6pT\left(tq\sqrt{\sqrt{p}}, q\sqrt{p}, p\right). \tag{42}$$

The generating function $T(t^{1/3}, q^{1/6}, 1) = S(t, q)$ was considered in section 2.1; thus cubical vesicles in the perimeter–area ensemble are equivalent to square vesicles in the perimeter–area ensemble. Observe that

$$T(t, 1, 1) = \frac{1}{1 - t^{12}} \tag{43}$$

and from equation (25) it follows

$$T(1, q, 1) = \tfrac{1}{2}(1 + (-q^6, q^{12})^2_\infty(q^{12}, q^{12})_\infty). \tag{44}$$

In addition, if $|q| < 1$ then $T(t, q, 1)$ is convergent, and there is an essential singularity at $q = 1$. The phase diagram is given in figure 3, and the scaling around the critical point at

$t = q = 1$ is also the same as given there. Scaling exponents in this ensemble are also identical to these for square vesicles, with $\phi = 1/2$, and $2 - \alpha_t = -1/2$ while $2 - \alpha_u = -1$.

The situation becomes more complicated if $p \neq 1$. $T(t, q, p)$ is convergent for all $|p| < 1$, and divergent if $p > 1$. This generating function is also interesting if $p = 1$, as shown above. Since the asymptotics for $T(t, 1, 1)$ and $T(1, q, 1)$ are given in equation (36), $T(1, 1, p)$ should be considered next. The rich set of mathematical results that produced expressions for $S(t, q)$ are not available in this model. Instead, the Euler–MacLaurin formula [9] can be used.

Theorem 2.3 (Euler–MacLaurin)**.** *Suppose that f is $2m$ times continuously differentiable in the interval $[0, N] : (f \in C^{2m}[0, N])$. Then*

$$\sum_{n=0}^{N} f(n) = \int_0^N f(x)\,\mathrm{d}x + \frac{f(0) + f(N)}{2} + \sum_{n=1}^{m-1} \frac{B_{2n}}{(2n)!}(f^{(2n-1)}(N) - f^{(2n-1)}(0)) + R_m$$

where the remainder term is

$$R_m = \int_0^N \left[\frac{B_{2m} - B_{2m}(x - \lfloor x \rfloor)}{(2m)!}\right] f^{(2m)}(x)\,\mathrm{d}x.$$

$B_n(x)$ is the nth *Bernoulli polynomial, and $B_n = B_n(0)$ are Bernoulli numbers. In particular, $B_2 = 1/6$.*

First apply this formula to $S(t^3, q^6) = T(t, q, 1)$ to reproduce the asymptotics of $S(t, q)$ derived in the previous section. In particular, observe that

$$T(t^3, q^6) = \sum_{n=0}^{\infty} t^{12n} q^{6n^2} = \int_0^{\infty} t^{12x} q^{6x^2}\,\mathrm{d}x + \frac{1}{2} + R_1. \tag{45}$$

The integral is related to a complementary error function, and the error term R_1 can be bound as follows:

$$\begin{aligned} |R_1| &= \left| \int_1^{\infty} \frac{1}{2}[B_2 - B_2(x - \lfloor x \rfloor)] \left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} t^{12x} q^{6x^2}\right] \mathrm{d}x \right| \leqslant \left| \frac{1}{2} B_2 \int_1^{\infty} \left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} t^{12x} q^{6x^2}\right] \mathrm{d}x \right| \\ &\leqslant 6 B_2 t^{12} q^6 (|\log t| + |\log q|). \end{aligned} \tag{46}$$

The integral in equation (45) can now be evaluated so that a uniform approximation for $T(t, q, 1)$, for $q \in [q_0, 1]$ and $t \in [t_0, 1]$ is obtained, where q_0 and t_0 are arbitrary but fixed in $(0, 1)$:

$$T(t, q, 1) = \frac{1}{2} + \sqrt{\frac{\pi}{24|\log q|}}\, \mathrm{e}^{\frac{6|\log^2 t|}{|\log q|}} \left(1 - \mathrm{erf}\left(\frac{-\sqrt{6}|\log t|}{\sqrt{|\log q|}}\right)\right) + R_1. \tag{47}$$

Defining $\mathcal{G}(x) = \mathrm{e}^{x^2}(1 - \mathrm{erf}(x))$ then shows that

$$T(t, q, 1) = \frac{1}{2} + \sqrt{\frac{\pi}{24|\log q|}}\, \mathcal{G}\left(\frac{\sqrt{6}|\log t|}{\sqrt{|\log q|}}\right) + R_1. \tag{48}$$

Define the scaling fields $s = |\log t|$ and $x = |\log q|$, where $0 < q < 1$ and $0 < t \leqslant 1$, and the result is the following theorem.

Theorem 2.4. *Let $s = |\log t|$ and $x = |\log q|$. The generating function $T(t, q, 1)$ of cubical vesicles, and the generating function $S(t, q)$ of square vesicles, where $S(t^3, q^6) = T(t, q, 1)$, is given by*

$$T(t, q, 1) = \frac{1}{2} + \sqrt{\frac{\pi}{24x}}\,\mathcal{G}\left(\frac{\sqrt{6}s}{\sqrt{x}}\right) + R_1$$
$$= \frac{1}{2} + \frac{\sqrt{\pi}}{12s}\left[\frac{\sqrt{6}s}{\sqrt{x}}\right]\mathcal{G}\left(\frac{\sqrt{6}s}{\sqrt{x}}\right) + R_1.$$

The error term is bound by

$$|R_1| \leqslant 6B_2 t^{12} q^6 (|\log t| + |\log q|)$$

and $\mathcal{G}(z) = \mathrm{e}^{z^2}(1 - \mathrm{erf}(z))$. This recovers the scaling in equation (40). Moreover, R_1 is uniformly bounded in any rectangle $[q_0, 1] \times [t_0, 1]$ for t_0 and q_0 in $(0, 1)$, and so the approximation is uniform in this closed rectangle.

Consider next the application of the Euler–MacLaurin formula to $T(1, 1, p)$. The result is that

$$T(1, 1, p) = \int_0^\infty p^{x^3}\,\mathrm{d}x + \frac{1}{2} + R_1 \tag{49}$$

where

$$|R_1| = \frac{1}{2}\left|\int_0^\infty (B_2 - B_2(x - \lfloor x \rfloor))\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}p^{x^3}\right)\mathrm{d}x\right|$$
$$\leqslant \frac{B_2}{2}\left|\int_0^\infty \frac{\mathrm{d}^2}{\mathrm{d}x^2}p^{x^3}\,\mathrm{d}x\right| = \frac{B_2}{3}\left(\frac{18}{e}\right)^{2/3}|\log p|^{1/3}.$$

Evaluating the integral in equation (49) produces the approximation in the next theorem.

Theorem 2.5. *The generating function $T(1, 1, p)$ is approximated by*

$$T(1, 1, p) = \frac{1}{2} + \frac{2\sqrt{3}\pi}{9\Gamma(2/3)}|\log p|^{-1/3} + R_1$$

where $|R_1| \leqslant [B_2/3](18/\mathrm{e})^{2/3}|\log p|^{1/3}$. The bound on R_1 shows that this approximation is uniform in any closed interval $[p_0, 1]$, where p_0 is arbitrary and fixed in $(0, 1)$.

The approximation in theorem 2.5 is very accurate for $p \in (0, 1)$; in figure 4 the curve $T(1, 1, p)$ and its approximation in theorem 2.5 are plotted. This approximation is also different from that obtained in the two-dimensional model of squares in equation (32). In this model the q-exponential factors were approximated using lemmas 2.1 and 2.2. In the above, only the Euler–MacLaurin formula was used. This approximation converges uniformly with increasing m in theorem 2.3 on a compact interval in $(0, 1)$.

One may similarly use theorem 2.3 to approximate the generating function $S(1, q^6) = T(1, q, 1)$ of two-dimensional squares.

Theorem 2.6. *The generating function $S(1, q)$ of lattice squares is approximated by*

$$S(1, q) = \frac{1}{2} + \frac{\sqrt{\pi}}{2}|\log q|^{-1/2} + R_1$$

where $|R_1| \leqslant B_2\,\mathrm{e}^{-1/2}\sqrt{2|\log q|}$. This bound shows that the approximation is uniform on any closed interval $[q_0, 1]$ where q_0 is fixed and arbitrary in $(0, 1)$.

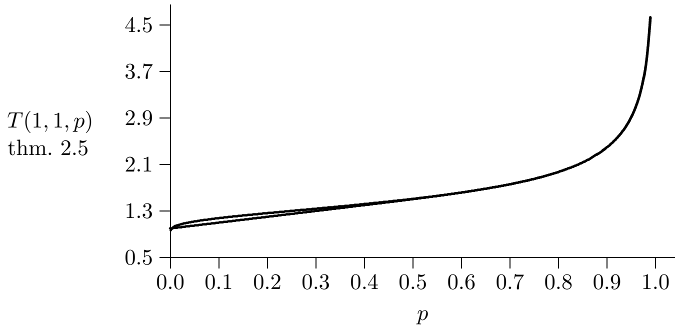

Figure 4. Plots of $T(1, 1, p)$ and its approximation in theorem 2.5.

The approximation in theorem 2.6 is also plotted in figure 2, in addition to $S(1, q)$ and its approximation in equation (32). Theorem 2.6 can also be derived from equation (32) by noting that $\lim_{q\to 1^-}[(\pi^2/6+2\mathcal{L}i_2(-q))/\log q^2] = -\log 2$. Approximating $q = 1-\epsilon$ (while noting that $(1+q) = 2-\epsilon$ and $q^{1/12} \approx 1-\epsilon/12$) then gives theorem 2.6. The approximation in theorem 2.6 now gives the following corollary.

Corollary 2.7. *The generating function* $T(1, q, 1)$ *is approximated by*

$$T(1, q, 1) = S(1, q^6) = \frac{1}{2} + \frac{\sqrt{\pi}}{2}|6\log q|^{-1/2} + R_1$$

where $|R_1| \leqslant B_2\,\mathrm{e}^{-1/2}\sqrt{12|\log q|}$. *This bound shows that the approximation is uniform on any closed interval* $[q_0, 1]$ *where* q_0 *is arbitrary and fixed in* $(0, 1)$.

Determining the full behaviour of $T(t, q, p)$ is more difficult; so consider first the case that $t = 1$. Maple V [14] shows that for $0 < q$ and for $0 < p < 1$,

$$\begin{aligned}\int_0^\infty p^{x^3} q^{6x^2}\,\mathrm{d}x &= \frac{2\sqrt{3}\pi}{9\Gamma(2/3)|\log p|^{1/3}} F_{1,1}\left(\left[\frac{1}{6}\right], \left[\frac{1}{3}\right]; \frac{32\sigma_q|\log^3 q|}{|\log^2 p|}\right) \\ &\quad - \frac{\sigma_q|\log q|}{3|\log p|} F_{2,2}\left(\left[\frac{1}{2}, 1\right], \left[\frac{2}{3}, \frac{4}{3}\right]; \frac{32\sigma_q|\log^3 q|}{|\log^2 p|}\right) \\ &\quad + \frac{\Gamma(2/3)|\log^2 q|}{9|\log p|^{5/3}} F_{1,1}\left(\left[\frac{5}{6}\right], \left[\frac{5}{3}\right]; \frac{32\sigma_q|\log^3 q|}{|\log^2 p|}\right)\end{aligned}$$

where the $F_{a,b}(\cdot)$ are hypergeometric functions, and where

$$\sigma_q = \begin{cases} 1 & \text{if} \quad q \geqslant 1 \\ -1 & \text{if} \quad 0 < q < 1. \end{cases}$$

Taking $q \to 1^-$ reduces the integral to theorem 2.5. In that case the first term is the only surviving contribution. One may also observe that

$$\begin{aligned}\sqrt{|\log q|}\int_0^\infty p^{x^3} q^{6x^2}\,\mathrm{d}x = \Bigg[&\frac{2\sqrt{3}\pi}{9\Gamma(2/3)32^{1/6}}\left(\frac{32|\log^3 q|}{|\log^2 p|}\right)^{1/6} F_{1,1}\left(\left[\frac{1}{6}\right], \left[\frac{1}{3}\right]; \frac{32\sigma_q|\log^3 q|}{|\log^2 p|}\right) \\ &- \frac{\sigma_q}{3\sqrt{32}}\left(\frac{32|\log^3 q|}{|\log^2 p|}\right)^{1/2} F_{2,2}\left(\left[\frac{1}{2}, 1\right], \left[\frac{2}{3}, \frac{4}{3}\right]; \frac{32\sigma_q|\log^3 q|}{|\log^2 p|}\right)\end{aligned}$$

$$
+\frac{\Gamma(2/3)}{9.32^{5/6}}\left(\frac{32|\log^3 q|}{|\log^2 p|}\right)^{5/6} F_{1,1}\left(\left[\frac{5}{6}\right],\left[\frac{5}{3}\right];\frac{32\sigma_q|\log^3 q|}{|\log^2 p|}\right)\Bigg]
$$

$$
= \mathcal{F}\left(\frac{32\sigma_q|\log^3 q|}{|\log^2 p|}\right) \tag{50}
$$

where

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

$$
\left. + \frac{\Gamma(2/3)|x/32|^{5/6}}{9} F_{1,1}\left(\left[\frac{5}{6}\right],\left[\frac{5}{3}\right];x\right)\right]. \tag{51}
$$

With these results, it follows by theorem 2.3 that

$$
\begin{aligned}
T(1,q,p) &= \frac{1}{2} + |\log q|^{-1/2}\mathcal{F}\left(\frac{32\log^3 q}{\log^2 p}\right) + R_1 \\
&= \frac{1}{2} + |\log p|^{-1/3}\left[\frac{|\log^2 p|}{|\log^3 q|}\right]^{1/6}\mathcal{F}\left(\frac{32\log^3 q}{\log^2 p}\right) + R_1 \\
&= \frac{1}{2} + |\log p|^{-1/3}\mathcal{H}\left(\frac{32\log^3 q}{\log^2 p}\right) + R_1
\end{aligned} \tag{52}
$$

where $\mathcal{H}(x) = |x|^{1/6}\mathcal{F}(x)$.

Theorem 2.8. *The generating function $T(1,q,p)$ is approximated by*

$$
\begin{aligned}
T(1,q,p) &= \frac{1}{2} + |\log q|^{-1/2}\mathcal{F}\left(\frac{32\log^3 q}{\log^2 p}\right) + R_1 \\
&= \frac{1}{2} + |\log p|^{-1/3}\left[\frac{|\log^2 p|}{|\log^3 q|}\right]^{1/6}\mathcal{F}(32\log^3 q/\log^2 p) + R_1 \\
&= \frac{1}{2} + |\log p|^{-1/3}\mathcal{H}\left(\frac{32\log^3 q}{\log^2 p}\right) + R_1
\end{aligned}
$$

where $\mathcal{F}(x)$ is given by equation (51) and $\mathcal{H}(x) = |x|^{1/6}\mathcal{F}(x)$. The error term is bounded by

$$
|R_1| \leqslant \frac{B_2}{2}\sum_i \sqrt{6r_i|\log p| + 2|\log q|}\, p^{r_i^3} q^{r_i^2}
$$

where the summation is over the non-negative roots $\{r_i\}$ of the equation

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

The bound is uniform for (p,q) in the rectangle $[p_0,1]\times[q_0,1]$ where p_0 and q_0 are arbitrary and fixed in $(0,1)$.

Proof. It only remains to bound the remainder term. Using Maple [14], the remainder term can be bound by

$$
|R_1| \leqslant \frac{B_2}{2}\left|\int_0^\infty \frac{\mathrm{d}^2}{\mathrm{d}x^2} p^{x^3} q^{6x^2}\,\mathrm{d}x\right| \leqslant \frac{B_2}{2}\sum_i \left|6r_i^2\log p + 4r_i\log q\right| p^{r_i^3} q^{r_i^2}
$$

where the summation is over the non-negative roots $\{r_i\}$ of

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

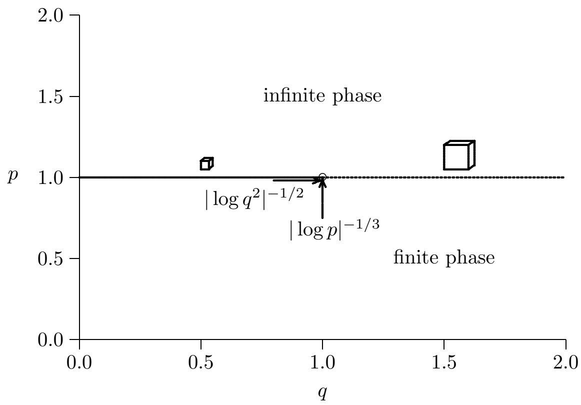

Figure 5. The phase diagram of cubical vesicles in the area–volume plane. There is a critical point at $p = q = 1$, and the divergences in the generating function $T(1, q, p)$ on approaching to this point are indicated in two directions. Asymptotically, $T(1, q, p)$ is a function of the ratio $32\log^3 q/\log^2 p$, see equation (52), and this proves that the crossover exponent in this model is $\phi = 2/3$. For $q < 1$ the transition at $p = 1$ has a finite generating function; the contribution from cubes of arbitrary large size is negligible. If $q > 1$, then the generating function at the transition $p = 1$ is divergent and is dominated by the contributions of vesicles of unbounded size.

The result then follows. If $p \to 1^-$ in theorem 2.8, then $r \to 1/\sqrt{|\log q^2|}$ is the only root. In this case $|R_1| \leqslant B_2\sqrt{|\log q^2|}/\sqrt{4e}$. Thus, the bound is uniform for (p, q) in the rectangle $[p_0, 1] \times [q_0, 1]$ for $0 < p_0 < 1$ and $0 < q_0 < 1$. □

The phase diagram for $T(1, q, p)$ is plotted in figure 5. This diagram is similar to figure 3, except that the behaviour of $T(1, q, p)$ is different along the critical curve $p = 1$. The point $q = p = 1$ is a multicritical point, and theorems 2.5 and 2.7 show that $T(1, q, 1) \sim |\log q^2|^{-1/2}$ as $q \to 1^-$ and $T(1, 1, p) \sim |\log p|^{-1/3}$ as $p \to 1^-$. Defining the scaling fields $s = |\log q^2|$ and $g = |\log p|$ then gives

$$T(1, q, p) = \frac{1}{2} + \frac{1}{\sqrt{s}}\mathcal{F}\left(\frac{32\sigma_q s^3}{g^2}\right). \tag{53}$$

Thus, one may identify $2-\alpha_u = -1/2, \phi = 2/3$ and $2-\alpha_t = -1/3$. Equation (5) is satisfied, and the scaling is completely consistent with equations (3) and (4).

The behaviour of $T(t, q, p)$ can now be estimated by noting that

$$\begin{aligned}\sum_{n=0}^{\infty} t^{12n} q^{6n^2} p^{n^3} &= q^{-6A^2} p^{-2A^3} \sum_{n=0}^{\infty} \left(t^{12} q^{12A} p^{3A^2}\right)^n (q^6 p^{3A})^{(n-A)^2} p^{(n-A)^3} \\ &= q^{-6A^2} p^{-2A^3} \sum_{n=0}^{\infty} T^n Q^{6(n-A)^2} P^{(n-A)^3}\end{aligned}$$

where $Q^6 = q^6 p^{3A}$ and $P = p$, while $T = t^{12} q^{12A} p^{3A^2}$. If one chooses

$$A = -2\frac{|\log q|}{|\log p|} \pm 2\sqrt{\left(\frac{|\log q|}{|\log p|}\right)^2 - \frac{|\log t|}{|\log p|}} \tag{54}$$

then $T = 1$, and it follows that

$$\sum_{n=0}^{\infty} t^{12n} q^{6n^2} p^{n^3} = q^{-6A^2} p^{-2A^3} \sum_{n=0}^{\infty} Q^{6(n-A)^2} P^{(n-A)^3}. \tag{55}$$

This may be approximated similarly to $T(1, q, p)$ above, and the result includes again functions of the ratio $\log^3 q/\log^2 p$. For example, note that $q^{A^2} \sim \log^3 q/\log^2 p$ and $p^{A^3} \sim \log^3 q/\log^2 p$ if $t = 1$. The activity t only appears under the square root in the ratio $\log t/\log p$, and surface effects dominate the effects of the corners and edges of the cubes.

If the terms with $n < A$ in equation (55) are ignored, then

$$\log Q = \pm 6 \log q \sqrt{1 - \frac{|\log t||\log p|}{|\log^2 q|}} \tag{56}$$

and

$$\begin{aligned} q^{-6A^2} p^{-2A^3} &= \exp\left(16\sigma_q \left(\frac{|\log^3 q|}{|\log^2 p|}\right)\left(\left(1 - \frac{|\log t||\log p|}{|\log^2 q|}\right)^{3/2} \right.\right. \\ &\quad \left.\left. + \left(1 - \sqrt{1 - \frac{|\log t||\log p|}{|\log^2 q|}}\right)\right)\right) \\ &\approx \exp\left(16\sigma_q \left(\frac{|\log^3 q|}{|\log^2 p|}\right)\left(\sqrt{1 - \frac{|\log t||\log p|}{|\log^2 q|}}^{\,3} + \sqrt{1 - \frac{|\log t||\log p|}{|\log^2 q|}}\right)\right) \end{aligned} \tag{57}$$

then substitution of Q and P in equation (52) will give an approximate asymptotic expansion for $T(t, q, p)$. Of particular interest is the observation that the combination $|\log q|\sqrt{1 - |\log t||\log p|/|\log^2 q|}$ occurs; this suggests that the natural scaling axes in this model are $|\log p|$ and $|\log q|\sqrt{1 - |\log t||\log p|/|\log^2 q|}$. The natural plane for analysing the model is the $Q - p$ plane, and the generating function has critical behaviour around the point $Q = p = 1$. The crossover exponent is still 2/3 in this model, since the ratio $\log^3 Q/\log^2 p$ is obtained in the generating function.

3. Rectangular and rectangular box vesicles

The limiting free energies of square and cubical vesicles do not have a non-analytic point corresponding to critical points separating two phases in those models. In particular, in each case $\mathcal{F}(t) = -\log q_c(t) = 0$, or $\mathcal{F}(t, q) = -\log p_c(t, q) = 0$, where $q_c(t)$ is the radius of convergence of $S(t, q)$ and $p_c(t, q)$ is the radius of convergence of $B(t, q, p)$. Nevertheless, underlying these models are rich mathematical structures of combinatorial identities and functions, and there is a connection to the expected standard scaling forms based on tricritical scaling theory. It is interesting to observe that in these very simple models of square and cubical vesicles, there is behaviour akin to a phase change. Putting $q = 1$ in $S(t, q)$ and then increasing t takes the model at $t_c = 1$ from a phase where the generating function is dominated by vesicles of finite area (when $t < t_c$), to a phase where vesicles of unbounded area dominate the generating function (when $t > t_c$). Technically, these changes scale in the classical fashion around the critical point $(q_c, t_c) = (1, 1)$ in the qt-plane, but there is no interesting thermodynamic change at this point.

Perhaps the simplest model of vesicles that exhibit a deflated–inflated thermodynamic phase change is a model of rectangular vesicles in the square lattice. The three-dimensional counterparts of rectangular vesicles are rectangular box vesicles. These models are considerably more complex than square and box vesicles, and only partial results below are obtained. In this section, I consider these models in turn.

3.1. Rectangular vesicles

Consider rectangular vesicles in the square lattice. The area–perimeter generating function is given by

$$R(t,q) = \sum_{i>0,j>0} t^{2(i+j)} q^{ij} = \sum_{n\geqslant 1} \frac{t^{2(n+1)} q^n}{1-t^2q^n} \tag{58}$$

where as before, q generates area, and t perimeter. There are simple poles in $R(t,q)$ along curves $1-t^2q^n = 0$ for $n = 1, 2, \ldots$. These poles accumulate on the line $q = 1$ in the tq-plane; and so $q = 1$ is an essential singularity in $R(t,q)$ for all $t > 0$. The radius of convergence of $R(t,q)$ is

$$q_c(t) = \begin{cases} 1 & \text{if} \quad t \leqslant 1 \\ 1/t^2 & \text{if} \quad t > 1. \end{cases} \tag{59}$$

The limiting free energy in this model is given by

$$\mathcal{F}(s) = \begin{cases} 0 & \text{if} \quad t \leqslant 1 \\ 2\log t & \text{if} \quad t > 1. \end{cases} \tag{60}$$

There is a non-analyticity in $\mathcal{F}(t)$ at $t = 1$, and this is a tricritical point in the phase diagram, corresponding to a transition of deflated rectangles for $t > 1$ to a phase of inflated rectangles (on average almost square) for $t < 1$.

One may distinguish between horizontal and vertical edges in this model. Suppose that horizontal edges are generated by u and vertical edges by v, and that the generating function is $R(u,v,q)$. Then

$$R(u,v,q) = \sum_{i=1}^{\infty} \frac{u^i v q^i}{1-vq^i}. \tag{61}$$

Thus, the generating function $R(u,v,q)$ satisfies the recurrence

$$R(u,v,q) = \frac{uvq}{1-vq} + uR(u,vq,q). \tag{62}$$

This recurrence becomes invalid if one puts $u = v = t$, but it can be used to study the properties of the generating function [18].

The generating function $R(t,q)$ is finite if $q = 1$ and $t < 1$. In this case

$$R(t,1) = \frac{t^4}{(1-t^2)^2}. \tag{63}$$

Thus, $R(t,q) \to t^4/(1-t^2)^2$ if $t < 1$ and $q \to 1^-$. If $t > 1$, assume that $t^2q < 1$ so that $1 > 1 - t^2q^n > 0$ for all $n \geqslant 1$. Hence

$$R(t,q) = \frac{t^4 q}{1-t^2q} + \sum_{n=2}^{\infty} \left[\frac{1-t^2q}{1-t^2q^n}\right] t^{2(n-1)} q^{n-1} \tag{64}$$

and observe that

$$\left| \sum_{n=2}^{\infty} \left[\frac{1-t^2q}{1-t^2q^n}\right] t^{2(n-1)} q^{n-1} \right| \leqslant (1-t^2q) \sum_{n=2}^{\infty} (t^2q)^{n-1} = t^2q. \tag{65}$$

In other words,

$$R(t,q) = \frac{t^4 q}{1-t^2q} + O(t^2q) \qquad \text{if} \quad t > 1 \quad \text{and} \quad t^2q \to 1^-. \tag{66}$$

This exposes a curve of simple poles along $t^2q = 1$ in the tq-plane; since these poles are due to rectangles of minimal area and maximal perimeter, this divergence is due to rectangles composed of a single row of unit squares.

In the event that $t = 1$, the asymptotics are more complicated. Every term in $R(1, q)$ becomes singular as $q \to 1^-$. Observe that $R(1, q) = \sum_{n>0}[q^n/(1 - q^n)] = \left[\sum_{n>0} \frac{q^n}{(1-q^n)/(1-q)}\right]/(1 - q)$ and $\lim_{q\to 1^-} [(1 - q^n)/(1 - q)] = n$. Thus, one might quess that $R(1, q) \sim [\log(1 - q)]/(1 - q)$ as $q \to 1^-$. The Euler–MacLaurin theorem can be used to find a better asymptotic expression, see [17] for similar results.

Theorem 3.1 [19]. *$R(1, q)$ has asymptotic expansion*

$$R(1,q) = \frac{\log(1-q)}{\log q} + \frac{q}{2(1-q)} + \sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!}[\log q]^{2n-1}\left[\left(q\frac{\mathrm{d}}{\mathrm{d}q}\right)^{2n-1} \frac{q}{1-q}\right].$$

Proof. Apply the Euler–MacLaurin formula to $R(1, q) = \sum_{m>0}\left[\frac{q^m}{1-q^m}\right] = \sum_{m=0}^{\infty} f(m)$, where $f(m) = \frac{q^{m+1}}{1-q^{m+1}}$. Put $u = q^{m+1}$ and observe that

$$f^{(n)}(m) = \left(\frac{\mathrm{d}}{\mathrm{d}m}\right)^n f(m) = (\log q)^n \left[\left(u\frac{\mathrm{d}}{\mathrm{d}u}\right)^n \frac{u}{1-u}\right]\Bigg|_{u=q^{m+1}}.$$

Moreover, $f^{(n)}(\infty) = 0$ and

$$f^{(n)}(0) = (\log q)^n \left(q\frac{\mathrm{d}}{\mathrm{d}q}\right)^n \frac{q}{1-q}.$$

Thus,

$$\sum_{n=1}^{\infty} \frac{q^n}{1-q^n} = \int_1^{\infty} \frac{q^x}{1-q^x}\,\mathrm{d}x + \left[\frac{q}{2(1-q)}\right] - \sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!}(\log q)^{2n-1}\left[\left(q\frac{\mathrm{d}}{\mathrm{d}q}\right)^{2n-1} \frac{q}{1-q}\right].$$

Finally, observe that

$$\int_1^{\infty}\left[\frac{q^x}{1-q^x}\right]\mathrm{d}x = \frac{1}{\log q}\int_q^0 \frac{\mathrm{d}u}{1-u} = \frac{\log(1-q)}{\log q}. \tag{67}$$

This proves the theorem. □

Truncating the series in theorem 3.1 gives the following approximation:

Corollary 3.2. *One may approximate $R(1, q)$ by*

$$R(1,q) = \frac{\log(1-q)}{\log q} + \frac{q}{2(1-q)} - \frac{B_q q \log q}{(1-q)^2}$$

where B_q is a function bounded by $|B_q| \leqslant B_2$.

Proof. Use theorem 3.1, and bound R_m in theorem 2.3: substitute $u = q^x$ below,

$$\begin{aligned}
|R_m| &= \left|\int_1^{\infty} \frac{B_{2m} - B_{2m}(x - \lfloor x\rfloor)}{(2m)!} f^{(2m)}(x)\,\mathrm{d}x\right| \\
&\leqslant \frac{B_{2m}}{(2m)!}|\log q|^{2m-1}\int_0^q \left|\left(u\frac{\mathrm{d}}{\mathrm{d}u}\right)^{2m}\left[\frac{u}{1-u}\right]\right|\mathrm{d}u \\
&= \frac{B_{2m}}{(2m)!}|\log q|^{2m-1}\int_0^q \left|\frac{\mathrm{d}}{\mathrm{d}u}\left(\left(u\frac{\mathrm{d}}{\mathrm{d}u}\right)^{2m-1}\left[\frac{u}{1-u}\right]\right)\right|\mathrm{d}u \\
&= \frac{B_{2m}}{(2m)!}|\log q|^{2m-1}\left(u\frac{\mathrm{d}}{\mathrm{d}u}\right)^{2m-1}\left[\frac{u}{1-u}\right]\Bigg|_0^q.
\end{aligned}$$

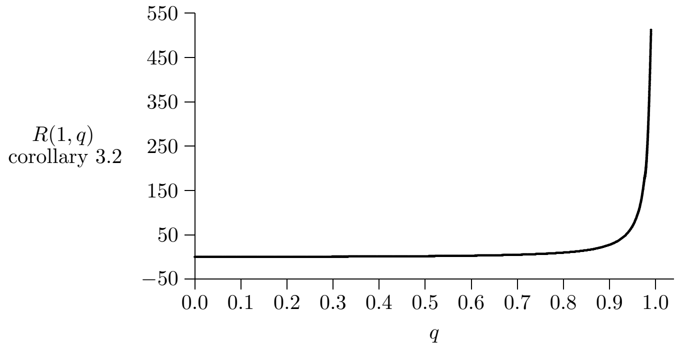

Figure 6. $R(1, q)$ and its approximation in corollary 3.2 plotted against q. The two curves collapse to one on this scale. The approximation is not uniform in [0, 1], but the error is bounded as in equation (69).

The derivatives $\left(u\frac{\mathrm{d}}{\mathrm{d}u}\right)^{2m-1}\left[\frac{u}{1-u}\right]$ can be shown to equal $\frac{u}{(1-u)^{2m}}P_{2m-2}(u)$ where $P_n(u)$ is a polynomial in u with positive coefficients and degree n with $P_n(0) = 1$ and $P_n(1) = (n+1)!$. Taking $q \to 1^-$ in the above increases the bound on $|R_m|$. Hence

$$|R_m| \leqslant \frac{B_{2m}}{m}\left(\frac{q}{1-q}\right)\left[\frac{\log q}{1-q}\right]^{2m-1}.$$

Finally, use equation (67) and put $m = 1$ in theorem 2.3. □

The approximation is accurate over almost the entire range $q \in [0, 1]$. Figure 6 is a plot of $R(1, q)$ and its approximation in corollary 3.2 against q, and on that scale the two curves are collapsed into a single curve. For example $R(1, 0.99) = 515.393\,3977\ldots$ while the approximation gives $515.392\,84\ldots$. One may also check that $R(1, 0.999) = 7480.777\ldots$ and $R(1, 0.9999) = 97\,870.41\ldots$ while the approximation gives $7480.9722\ldots$ and $97\,870.35\ldots$, respectively. The bound on R_m in corollary 3.2 increases as $1/(1-q)$ as $q \to 1^-$, so that the approximation is not uniform in [0, 1]. Instead,

$$(1-q)R(1, q) = \frac{(1-q)\log(1-q)}{\log q} + \frac{q}{2} + (1-q)R_1 \tag{68}$$

where

$$|(1-q)R_1| \leqslant \left|\frac{B_2 q \log q}{1-q}\right| \leqslant B_2 = \frac{1}{6} \qquad \forall q \in [0, 1]. \tag{69}$$

Since the ratio $|\log q|/(1-q)$ approaches 1 as $q \to 1^-$, this shows that a uniform approximation can be obtained for $(1-q)R(1, q)$ or for $|\log q|R(1, q)$.

Theorem 3.3. *The function* $(1-q)R(1, q)$ *is uniformly approximated by* $q/2 + (1-q)\log(1-q)/\log q$ *where* $q \in [q_0, 1]$, *and where* q_0 *is arbitrary and fixed in* $(0, 1)$.

In the general case, the Euler–MacLaurin formula may be used to approximate $R(t, q)$: within its radius of convergence,

$$R(t, q) = \sum_{n=1}^{\infty} \frac{t^2(t^2q)^n}{1-t^2q^n} = \int_1^{\infty} \frac{t^2(t^2q)^x}{1-t^2q^x}\,\mathrm{d}x + \frac{t^4 q}{2(1-t^2q)} + R_1 \tag{70}$$

where

$$|R_1| \leqslant \frac{B_2}{2}\left(\frac{t^2 q|\log t^2|}{1-t^2q} + \frac{|\log q|}{(1-t^2q)^2}\right). \tag{71}$$

Evaluation of the integral proceeds by changing variables $t^2q^x \to t^2qz$, in which case it follows that

$$R(t,q) = \frac{t^4q}{|\log q|}\int_0^1 \frac{z^{\frac{|\log t^2|}{|\log q|}}}{1-t^2qz}\,\mathrm{d}z + \frac{t^4q}{2(1-t^2q)} + R_1. \tag{72}$$

The integral can be evaluated using Maple V [14] and is a Lerch-Phi function:

$$R(t,q) = \frac{t^2}{|\log q|}\left[\frac{|\log q|}{|\log t^2|} - \text{Lerch-Phi}\left(t^2q, 1, \frac{|\log t^2|}{|\log q|}\right)\right] + \frac{t^4q}{2(1-t^2q)} + R_1 \tag{73}$$

where the Lerch-Phi function has the infinite series definition

$$\text{Lerch-Phi}(z,a,v) = \sum_{n=0}^{\infty} \frac{z^n}{(v+n)^a}. \tag{74}$$

There are singularities in the Lerch-Phi function if $z = 1$ and $a = 0$ or $a = 1$. In the situation here, $a = 1$, and Lerch-Phi $(t^2q, 1, |\log t^2|/|\log q|)$ is singular when $t^2q = 1$. Observe that this is a simple pole in $R(t,q)$; this is directly seen from equation (70). I take these results together in the following theorem.

Theorem 3.4. *The generating function $R(t,q)$ is approximated by*

$$R(t,q) = \frac{t^2}{|\log q|}\left[\frac{|\log q|}{|\log t^2|} - \text{Lerch-Phi}\left(t^2q, 1, \frac{|\log t^2|}{|\log q|}\right)\right] + R_1$$

where the remainder term R_1 is bounded by

$$|R_1| \leqslant \frac{t^4q}{2(1-t^2q)}(1 + B_2|\log t^2|) + \frac{B_2}{2}\frac{|\log q|}{(1-t^2q)^2}.$$

In other words, for every $t \geqslant 0$ and for every $q_0 \in (0,1)$, the function $(1-t^2q)^2R(t,q)$ is uniformly approximated for points (t,q) with $q_0 < q < q_c(t)$, and $q_c(t)$ is the critical curve defined in equation (59).

In figure 7 the phase diagram for this model is presented. The inflation–deflation transition occurs at the point $(q_c, t_c) = (1, 1)$, and the scaling of the generating function around this point is indicated. From equation (63) it appears that -2 be assigned to the exponent $2 - \alpha_u$. However, equation (66) indicates that for all $q = 1 - \epsilon$, where ϵ is small, there is a simple pole as t^2 approaches the critical curve. This is even the case if $\epsilon \to 0^+$, and the assignment $2 - \alpha_u = -1$ can be made (as illustrated in figure 7). Note that if $t = 1$, then $R(1,q) = \log(1-q)/\log(q) + \cdots$ as in corollary 3.2. Since $(1-q)^A\log(1-q) \to 0$ as $q \to 1^-$ for any $A > 0$, one may argue that $2 - \alpha_t = -1$ in this model. This would imply that the crossover exponent is $\phi = 1$ (from equation (5)).

Equations (72) and (73) show the scaling fields are $s = |\log t^2|$ and $g = |\log q|$. These fields appear consistently in the ratio $s/g = |\log t^2|/|\log q|$ in $R(t,q)$ in equation (73), suggesting that $\phi = 1$. If one should assign -2 to the exponent $2 - \alpha_u$ as suggested above, then this model would not conform to the assumed scaling forms as set out in the introduction. Thus, it appears that the correct value is $2 - \alpha_u = -1$ in which case equation (5) is satisfied. Lastly, note that the scaling of $R(1,q) \approx \log(1-q)/\log(q)$ is not a pure power law as one would obtain by putting $t = 0$ in equation (3).

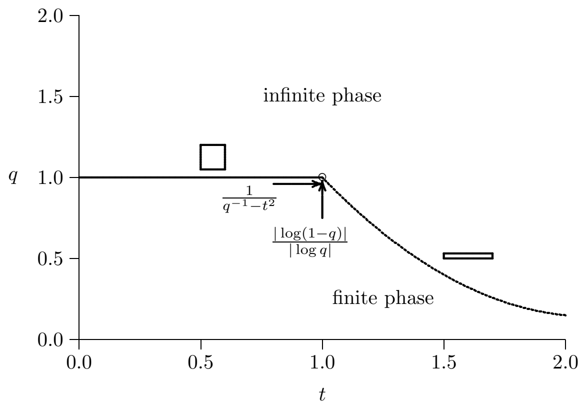

Figure 7. The phase diagram of rectangular vesicles in an area–perimeter ensemble. The generating function is $R(t, q)$ (where t generates perimeter edges, and q generates area). The generating function is approximated in equation (72). The behaviour of $R(t, q)$ is indicated as the critical point at (1, 1) is approached from two directions. The critical curve consists of essential singularities along $q = 1$ and $0 < t \leqslant 1$, and poles along $t^2 q = 1$. The essential singularities are due to terms corresponding the rectangles inflated to maximum area (these are square shaped). The poles are due to the rectangles consisting of a single row of unit squares, or maximal perimeter and minimum area. Along the line $q = 1$, the generating function is given by $t^4/(1-t^2)^2$, but for all $q < 1$, $R(t, q) \sim (q^{-1} - t^2)^{-1}$ as $t^2 \nearrow q^{-1}$.

3.2. Rectangular box vesicles

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

$$B(t, q, p) = \sum_{i,j,k>0} t^{4(i+j+k)} q^{2(ij+jk+ki)} p^{ijk}. \tag{75}$$

Consider first this model if $p = 1$. Then

$$B(t, q, 1) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{t^4 (t^4 q^2)^{i+j} q^{2ij}}{1 - t^4 q^{2i+2j}}. \tag{76}$$

If $i + j = n$ is substituted, then

$$B(t, q, 1) = \sum_{n=2}^{\infty} \frac{t^4 (t^4 q^2)^n}{1 - t^4 q^{2n}} \sum_{m=1}^{n-1} q^{2(n-m)m}. \tag{77}$$

The contribution from the terms $q^{2(n-m)m}$ is at most n if $|q| \leqslant 1$, and there are singularities along the curves $1 - t^4 q^{2n} = 0$, for $n = 1, 2, \ldots$. These singularities accumulate on the curve $q = 1$, which is an essential singularity in $B(t, q, 1)$. The radius of convergence of $B(t, q, 1)$ is given by $q = t^{-2}$ if $t \geqslant 1$; these are simple poles in the generating function. Thus, the radius of convergence in this model is the same as for rectangular vesicles (see equation (59)).

The sum over $q^{2(n-m)m}$ in equation (77) can be approximated by an integral. Applying the Euler–MacLaurin formula shows that

$$\sum_{m=0}^{n} (q^2)^{m(n-m)} = \int_0^n (q^2)^{x(n-x)}\, \mathrm{d}x + 1 + R_1 \tag{78}$$

where $|R_1| \leqslant B_2 n |\log q^2|$, since $|q| \leqslant 1$. Subtracting the first and last terms from the sum, and evaluating the integral gives an error function,

$$\sum_{m=1}^{n-1} (q^2)^{m(n-m)} = \frac{\sqrt{\pi}}{\sqrt{\log q^2}} q^{n^2/2} \operatorname{erf}\big(n\sqrt{\log q^2}/2\big) - 1 + R_1. \tag{79}$$

Since $\log q^2 < 0$ for $q \in (0, 1)$, the argument of the error function is imaginary. It is convenient to introduce the imaginary error function [7] by $\operatorname{erf}(\mathrm{i}x) = \mathrm{i}\operatorname{erfi}(x)$, and it follows that

$$\sum_{m=1}^{n-1} (q^2)^{m(n-m)} = \frac{\sqrt{\pi}}{\sqrt{|\log q^2|}} q^{n^2/2} \operatorname{erfi}\big(n\sqrt{|\log q^2|}/2\big) - 1 + R_1. \tag{80}$$

Thus, the generating function $B(t, q, 1)$ is a series over imaginary error functions:

$$B(t, q, 1) = t^4 \sum_{n=2}^{\infty} \frac{(t^4 q^2)^n}{1 - t^4 q^{2n}} \left[\frac{\sqrt{\pi} q^{n^2/2}}{\sqrt{|\log q^2|}} \operatorname{erfi}\big(n\sqrt{|\log q^2|}/2\big) - 1 + R_1 \right]. \tag{81}$$

At this point it becomes increasingly difficult to continue approximating $B(t, q, 1)$ without giving up some rigour. One may wish to approximate the above series by an integral, using the Euler–MacLaurin formula, and then bound the error. If the error term is ignored, then

$$B(t, q, 1) \approx \frac{t^4 \sqrt{\pi}}{|\log q^2|^2} \int_0^1 \frac{x^{\frac{|\log t^4|}{|\log q^2|} + \frac{|\log^2 x|}{4|\log q^2|}}}{1 - t^4 x} \left[\operatorname{erfi}\left(\frac{|\log x|}{2\sqrt{|\log q^2|}} \right) - 1 + R_1 \right] \mathrm{d}x \tag{82}$$

where $|R_1| \leqslant B_2 n |\log q^2|$. Note the appearance of the ratio $|\log t^4|/|\log q^2|$ in the integrand. The crossover exponent between the scaling fields $|\log t|$ and $|\log q|$ appears to be $\phi = 1$, this value was also obtained in the model of rectangular vesicles.

If $q = 1$, then $B(t, 1, 1) = t^{12}/(1 - t^4)^3$. This suggests assigning the value -3 to the exponent $2 - \alpha_u$, but caution is needed, as was observed in the model of rectangles; this value may be inconsistent with a tricritical description of this model. To determine $2 - \alpha_t$ requires the analysis of $B(1, q, 1)$. Put $t = 1$ in equation (77). Then

$$B(1, q, 1) = \sum_{n=2}^{\infty} \frac{q^{2n}}{1 - q^{2n}} \sum_{m=1}^{n-1} q^{2(n-m)m}. \tag{83}$$

The summation over $q^{2(n-m)m}$ can be approximated by using the result in equation (80). This shows that

$$B(1, q, 1) = \frac{\sqrt{\pi}}{\sqrt{|\log q^2|}} \sum_{n=2}^{\infty} \frac{q^{2n+n^2/2}}{1 - q^{2n}} \operatorname{erfi}\big(n\sqrt{|\log q^2|}/2\big) + \sum_{n=2}^{\infty} \frac{q^{2n+n^2/2}(R_1 - 1)}{1 - q^{2n}}. \tag{84}$$

Recall that $|R_1| \leqslant B_2 n |\log q^2|$ whenever $n \geqslant 2$.

Consider first the final term in equation (84) and use the Euler–MacLaurin formula to approximate it. Since n will be summed to infinity, and since $|q| < 1$, note that $|R_1 - 1| \leqslant |B_2 n |\log q^2| - 1| \leqslant 2 B_2 n |\log q^2|$, whenever n is large enough (but still finite). Hence, there is a constant C such that

$$\left| \sum_{n=2}^{\infty} \frac{q^{2n+n^2/2}(R_1 - 1)}{1 - q^{2n}} \right| \leqslant C |\log q^2| \left| \sum_{n=2}^{\infty} \frac{n q^{2n+n^2/2}}{1 - q^{2n}} \right|. \tag{85}$$

Proceed now by approximating the series by an integral. The remainder term in the Euler–MacLaurin formula can be bound as follows:

$$\begin{aligned}|R_1| &\leqslant \frac{B_2}{2}\int_1^\infty \left|\frac{\mathrm{d}^2}{\mathrm{d}x^2}\frac{xq^{2x+x^2/2}}{1-q^{2x}}\right|\mathrm{d}x \\ &= \frac{B_2}{2}\left|\frac{q^{5/2}(1-q^2+(3-q^2)\log q)}{(1-q^2)^2}\right| \\ &\leqslant \frac{B_2}{2}\left[\frac{1}{1-q^2}+\frac{|\log q^2|(3-q^2)}{2(1-q^2)^2}\right]. \end{aligned} \tag{86}$$

This is a bound on the error term in an Euler–MacLaurin approximation to the series in equation (85). Next, approximate the series itself. Since the series is but one term in equation (84), an upper bound on it would be sufficient. Note therefore that $|nq^{n^2/2}| \leqslant 1/\sqrt{(\mathrm{e}/2)|\log q^2|}$ and use this below:

$$\int_2^\infty \frac{xq^{2x+x^2/2}}{1-q^{2x}}\,\mathrm{d}x \leqslant \frac{1}{\sqrt{(\mathrm{e}/2)|\log q^2|}}\int_1^\infty \frac{q^{2x}}{1-q^{2x}}\,\mathrm{d}x = \frac{|\log(1-q^2)|}{\sqrt{\mathrm{e}/2}|\log q^2|^{3/2}}. \tag{87}$$

Taken together, the last result and the bound in equation (85) together with the results in equations (86) and (87) show that

$$\begin{aligned}\left|\sum_{n=2}^\infty \frac{q^{2n+n^2/2}(R_1-1)}{1-q^{2n}}\right| &\leqslant C|\log q^2|\left[\frac{|\log(1-q^2)|}{\sqrt{(\mathrm{e}/2)}|\log q^2|^{3/2}}\right. \\ &\quad \left.+\frac{B_2}{2}\left[\frac{1}{1-q^2}+\frac{|\log q^2|(3-q^2)}{2(1-q^2)^2}\right]\right]. \end{aligned} \tag{88}$$

As $q \to 1^-$, the ratio $|\log q^2|/(1-q^2)$ approaches 1. Hence, we obtain the following lemma:

Lemma 3.5. *Let $q_0 \in (0,1)$. Then there exists a constant C_0 such that*

$$\left|\sum_{n=2}^\infty \frac{q^{2n+n^2/2}(R_1-1)}{1-q^{2n}}\right| \leqslant \frac{C_0|\log(1-q^2)|}{\sqrt{|\log q^2|}} \tag{89}$$

for all $q \in [q_0, 1)$.

Returning to equation (84), all that remains is to approximate the series in the first term by an integral, using again the Euler–MacLaurin formula. This gives

$$\begin{aligned}B(1,q,1) &= \frac{\sqrt{\pi}}{\sqrt{|\log q^2|}}\int_1^\infty \frac{\exp(-|\log q^2|(y(y+4)/4))}{1-\exp(-y|\log q^2|)}\,\mathrm{erfi}\big(y\sqrt{|\log q^2|}/2\big)\,\mathrm{d}y \\ &\quad + F_q + \sum_{n=2}^\infty \frac{q^{2n+n^2/2}(R_1-1)}{1-q^{2n}} \end{aligned} \tag{90}$$

where F_q can be shown to be bound by

$$\frac{|F_q|}{[B_2/4]} \leqslant \left|\mathrm{erfi}\big(\sqrt{|\log q^2|}/2\big)\right| + \left|\frac{1}{\sqrt{\pi}\sqrt{|\log q^2|}}\right| + \left|\frac{\mathrm{erfi}\big(\sqrt{|\log q^2|}/2\big)}{1-q^2}\right|. \tag{91}$$

It is the case that

$$\lim_{q\to 1^-}\left[\frac{\mathrm{erfi}\big(\sqrt{|\log q^2|}/2\big)}{\sqrt{1-q^2}}\right] = \frac{1}{\sqrt{\pi}}. \tag{92}$$

This shows that the error bound on F_q is of order $O\big(1/\sqrt{1-q^2}\big)$ as $q \to 1^-$. Therefore, taking the bounds on the error terms together in lemma 3.5 and in equation (92), the following theorem can be proved:

Theorem 3.6. *For q in $[q_0, 1)$, and $q_0 < 1$ close enough to 1, there exist a function B_q and a constant C such that $|B_q| < C$, while*

$$B(1, q, 1) = \frac{\sqrt{\pi}}{\sqrt{|\log q^2|}} \int_1^\infty \frac{\exp(-|\log q^2|(y(y+4)/4))}{1-\exp(-y|\log q^2|)} \operatorname{erfi}\big(y\sqrt{|\log q^2|}/2\big)\,\mathrm{d}y + \frac{B_q}{\sqrt{1-q^2}}.$$

Thus, $\sqrt{1-q^2}B(1, q, 1)$ is uniformly approximated by the integral in $[q_0, 1]$.

Numerical estimates of the integral show that it is convergent if $q < 1$, but it diverges as $q \to 1^-$. On the other hand, using the numerical procedures in Maple it appears that for $Y > 1$ and $0 < Z < 1$,

$$\begin{aligned}
&\lim_{q\to 1^-} |\log q^2|^Y \int_1^\infty \frac{\exp(-|\log q^2|(y(y+4)/4))\operatorname{erfi}\big(y\sqrt{|\log q^2|}/2\big)}{1-\exp(-y|\log q^2|)}\,\mathrm{d}y = 0 \\
&\lim_{q\to 1^-} |\log q^2|^Z \int_1^\infty \frac{\exp(-|\log q^2|(y(y+4)/4))\operatorname{erfi}\big(y\sqrt{|\log q^2|}/2\big)}{1-\exp(-y|\log q^2|)}\,\mathrm{d}y = \infty.
\end{aligned} \tag{93}$$

One may take this together in the following conjecture.

Conjecture 3.7. *Suppose that $q_0 \in (0, 1)$. If q_0 is close enough to 1, then there exist constants $C, c_1 > 0$ and $c_2 > 0$, and a function $L(q)$, such that*

$$B(1, q, 1) = \frac{L(q)}{\sqrt{|\log q^2|^3}} + \frac{B_q}{\sqrt{1-q^2}}$$

where B_q is a function such that $\left|B_q\right| \leqslant C$, and there exist constants c_1 and c_2 such that

$$c_1|\log q^2|^Z \leqslant L(q) \leqslant c_2|\log q^2|^{-Z}$$

for any fixed $Z > 0$ and $q \to 1^-$ and close enough to 1.

The scaling in conjecture 3.7 suggests that $2-\alpha_t = -3/2$, in the tq-plane. This scaling is indicated in figure 8. Equation (82) suggests that $\phi = 1$ in this model, not unexpected, since it also has that value for rectangular vesicles considered in the previous section. The argument following equation (82) seems to indicate that $2-\alpha_u = -3$ in this model, while equation (5) would then imply that $2-\alpha_u = -3/2$. This apparent inconsistency could be resolved if one performs the asymptotic analysis of $B(t, q, 1)$ for $q = 1-\epsilon$, and so these results should be considered incomplete.

Consider now this model in the qp-plane. Summing over k in equation (75) and putting $t = 1$ give

$$B(1, q, p) = \sum_{i,j\geqslant 1} \frac{q^{2ij+2i+2j}p^{ij}}{1-q^{2(i+j)}p^{ij}} \tag{94}$$

and note that this is convergent if (q, p) is in the region with $p \leqslant 1$ and $q^2p \leqslant 1$, except at the point $(q, p) = (1, 1)$. For all other values of q and p, this is divergent. The radius of convergence is

$$p_c(q) = \begin{cases} 1 & \text{if} \quad q \leqslant 1 \\ 0 & \text{if} \quad q > 1. \end{cases} \tag{95}$$

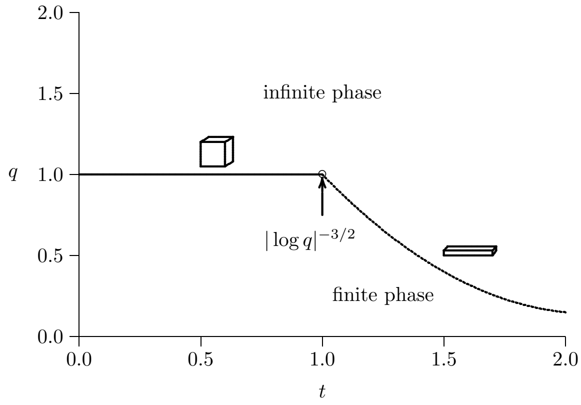

Figure 8. The phase diagram of rectangular box vesicles in an area–perimeter ensemble. The generating function $B(t, q, 1)$ is approximated in equation (82). Scaling around the critical point at $(t, q) = (1, 1)$ is indicated from two directions. The critical curve consists of essential singularities along $q = 1$ and $0 < t \leqslant 1$, and poles along $t^2 q = 1$. Along the essential singularities with $t < 1$ are $q = 1$ the generating function is dominated by rectangular box vesicles of maximal area and minimal perimeter—these are cubical vesicles. Along the curve of poles, the vesicles have minimal area and maximal perimeter, those are vesicles composed of a single row of unit cubes.

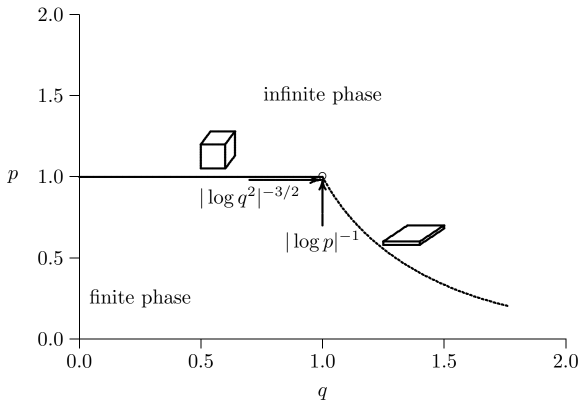

Figure 9. The phase diagram of rectangular box vesicles in a volume–area ensemble. Scaling around the critical point at $(t, q) = (1, 1)$ is indicated from two directions. The critical curve consists of essential singularities along $q^2 p = 1$ and $p < 1$, and along $p = 1$ and $q < 1$. Along the critical curve $p = 1$ the vesicles have maximal volume and minimal area; they are cubical. Along the critical curve $q^2 p = 1$ the vesicles have minimal volume and maximal area; they are disc shaped. The behaviour $|\log q^2|^{-3/2}$ along the critical line $p = 1$ is as in lemma 3.7.

It can be verified that if $pq^2 > 1$ then equation (94) has divergent subsequences. For example, if $i = 1$ and $q^2 p > 1$, then the sequence $\sum_{j=1}^{\infty} \frac{(q^4 p)^j q^2}{1-q^{2(1+j)} p^j}$ is divergent. This subsequence is a sequence of vesicles of dimensions $1 \times j \times k$; they have a rectangular disc shape. The phase diagram of this ensemble is given in figure 9.

To determine the approach of $B(1, q, p)$ to the point $(1, 1)$, observe that the generating function $B(1, q, 1)$ was already considered above, and that it is approximated in theorem 3.6.

Consider $B(1, 1, p)$ next. Then

$$B(1,1,p) = \sum_{i,j,k\geqslant 1} p^{ijk} = \sum_{i,j\geqslant 1} \frac{p^{ij}}{1-p^{ij}} \tag{96}$$

and the summation over j can be approximated using the Euler–MacLaurin formula (theorem 2.3):

$$B(1,1,p) = \sum_{i=1}^{\infty} \left[\frac{\log(1-p^i)}{\log p^i} + \frac{p^i}{2(1-p^i)} + R(i) \right] \tag{97}$$

where the remainder term is bounded for each $0 < p < 1$ by

$$|R(i)| \leqslant \frac{B_2}{2} \frac{p^i |\log p^i|}{(1-p^i)^2}. \tag{98}$$

$B(1, 1, p)$ in equation (97) may again be approximated by an integral. In the first place, note that by corollary 3.2

$$\sum_{i=1}^{\infty} \frac{p^i}{2(1-p^i)} = \frac{\log(1-p)}{2\log p} + \frac{p}{4(1-p)} + F_p \tag{99}$$

where F_p is a remainder term bounded by

$$|F_p| \leqslant \frac{B_2}{2} \frac{p|\log p|}{(1-p)^2}. \tag{100}$$

Secondly,

$$\sum_{i=1}^{\infty} \frac{\log(1-p^i)}{\log p^i} = \frac{1}{|\log p|} \int_0^p \frac{\log(1-y)}{\log y} \frac{\mathrm{d}y}{y} + \frac{\log(1-p)}{2\log p} + S_p \tag{101}$$

where S_p is a second remainder term. It is bounded by

$$|S_p| \leqslant \frac{B_2}{2} \frac{|(1-p)|\log(1-p)| - p|\log p||}{(1-p)|\log p|}. \tag{102}$$

This shows that

$$B(1,1,p) = \frac{1}{|\log p|} \int_0^p \frac{\log(1-y)}{\log y} \frac{\mathrm{d}y}{y} + \frac{\log(1-p)}{\log p} + \frac{p}{4(1-p)} + \sum_{i=1}^{\infty} R(i) + F_p + S_p. \tag{103}$$

It only remains to bound the sum over $|R(i)|$. Maple [14] shows that

$$\sum_{i=1}^{\infty} |R(i)| \leqslant \frac{B_2}{2} \frac{(1-p)|\log(1-p)| + p|\log p|}{(1-p)|\log p|}. \tag{104}$$

Clearly, $|S_p| \leqslant \sum_{i=1}^{\infty} |R(i)|$. Therefore, the remainder in equation (103) can be bound by

$$\left| \sum_{i=1}^{\infty} R(i) + F_p + S_p \right| \leqslant \frac{B_2((1-p)|\log(1-p)| + p|\log p|)}{(1-p)|\log p|} + \frac{B_2}{2} \frac{p|\log p|}{(1-p)^2}. \tag{105}$$

Thus, the approximation to $B(1, 1, p)$ in equation (103) is not uniform. However, since $|\log p|/(1-p)$ approaches 1 as $p \to 1^-$, it appears that $(1-p)B(1, 1, p)$ can be uniformly bounded.

Theorem 3.8. *Let $p_0 \in (0, 1)$. There exists a constant K such that*

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

where $|R_p| \leqslant K$ if $p \in [p_0, 1)$.

The integral in theorem 3.8 diverges as $p \to 1^-$, but further investigation using Maple [14] shows that

$$\begin{aligned} &\lim_{p\to 1^-} |\log p|^Z \int_0^p \frac{\log(1-y)}{\log(y)}\frac{\mathrm{d}y}{y} = 0 \\ &\lim_{p\to 1^-} |\log|\log p\|^Z \int_0^p \frac{\log(1-y)}{\log(y)}\frac{\mathrm{d}y}{y} = \infty \end{aligned} \tag{106}$$

for every $Z > 0$. The integral diverges slower than any positive power of $1/|\log p|$, and faster than any positive power of $1/|\log|\log p\|$. This may be taken together in a lemma.

Lemma 3.9. *Let $p_0 \in (0, 1)$. If p_0 is close enough to 1, then there exist constants K, and $C_1 > 0$ and $C_2 > 0$, and a function $H(p)$, such that*

$$B(1,1,p) = \frac{H(p)}{|\log p|} + \frac{R_p}{1-p}$$

where $|R_p| < K$ and

$$C_1|\log|\log p\|^{-Z} \leqslant H(p) \leqslant C_2|\log p|^{-Z}$$

for every $Z > 0$ and $q \to 1^-$ and close enough to 1.

Thus, one might conclude that $B(1, 1, p) \sim H(p)/|\log p|$, where $H(p)$ diverges slower than $1/|\log p|^Z$ as $p \to 1^-$, for any $Z > 0$. Thus, it is now possible to assign values to the exponents $2 - \alpha_t$ and $2 - \alpha_u$. Conjecture 3.7 indicates that $2 - \alpha_u = -3/2$, see figure 9. Lemma 3.9 shows that $2 - \alpha_t = -1$.

It remains to approximate the full generating function $B(1, q, p)$. In this case, I abandon all rigour, and only focus on using integrals to approximate the double summation in equation (94). A tremendous amount of computer algebra shows that

$$B(1,q,p) \approx \frac{1}{|\log p|}\,\mathrm{e}^{-2\frac{|\log q^2|^3}{|\log p|^2}} \int_{|\log pq^2|}^{\infty} \frac{1}{s}\exp(K(s) + sA(A-1))\text{Lerch-Phi}(\mathrm{e}^{s(A-1)}, 1, A)\,\mathrm{d}s \tag{107}$$

where

$$A = \frac{\log q^2}{\log p} + \frac{(\log q^2)^2}{\log p} \qquad K(s) = s\left(\frac{\log q^2}{\log p}\right)^2 + \frac{1}{s}\left(\frac{(\log q^2)^2}{\log p}\right)^2.$$

Since $|\log pq^2| \to 0^+$ as both $p \to 1^-$ and $q \to 1^-$ the integral will be over the interval $[0, \infty)$ as the critical point is approached. Observe the appearance of ratios $|\log q^2|/|\log p|$, $|\log q^2|^2/|\log p|$, $|\log q^2|^3/|\log p|^2$ in this expression, suggesting a range of crossover scaling between the scaling fields $s = |\log q^2|$ and $g = |\log p|$. Most notably, approaching the scaling limit along curves with $|\log q^2|/|\log p| = 1$, or $|\log q^2|^2/|\log p| = 1$, or $|\log q^2|^3/|\log p|^2 = 1$ may suggest different scaling behaviour, unless it can be demonstrated that one of these behaviours dominates the others in the limit. In only one case do we observe that the exponential factor in equation (107) is a constant, and that would indicate that $\phi = 2/3$. This would be consistent with the result in conjecture 3.7 and lemma 3.9.

Table 1. Tricritical scaling exponents in vesicles.

Generating function	$2-\alpha_u$	$2-\alpha_t$	ϕ
$S(t,q)$	-1	$-1/2$	$1/2$
$T(t,q,1)$	-1	$-1/2$	$1/2$
$T(1,q,p)$	$-1/2$	$-1/3$	$2/3$
$R(t,q)$	-1	-1	1
$B(t,q,1)$	-3?	$-3/2$	1
$B(1,q,p)$	$-3/2$	-1	$2/3$

4. Conclusions

In this paper, I have examined the simplest models of vesicles in the two-dimensional square and the three-dimensional cubic lattice. The intent is to examine the scaling of these models close to a tricritical point in their phase diagrams, and the asymptotics of the generating functions had to be determined to expose the scaling behaviour.

For square vesicles in the square lattice the scaling is exposed in particular in equation (39), in theorem 2.4, and in figure 3. The tricritical point at $(t,q)=(1,1)$ splits the critical curve $q_c(t)=1$ into two parts. If $t<1$, then the transition between the finite and infinite phases in figure 3 is through an essential singularity at $q=1$, and the generating function here is dominated by squares of finite area (since $S(t,1)<\infty$ if $t<1$, and squares with arbitrary large area contribute only a finite value to the generating function). On the other hand, if $t>1$, then theorem 2.4 indicates that $S(t,q)$ diverges as $q\to 1^-$, and on the critical curve $S(t,1)$ is infinite, and dominated by squares of arbitrary (large) size. The scaling exponents in this model can be directly determined from the scaling formulae in theorem 2.4, and $\phi=1/2$ while $2-\alpha_t=-1/2$ and $2-\alpha_u=-1$. This model exhibits tricritical scaling consistent with equation (5), and the scaling of the generating function has been verified as in equations (3) and (4). The results are listed in table 1, and the model of cubical vesicles in the perimeter–area ensemble with the generating function $T(t,q,1)$ has the same scaling exponents.

Similarly, I was able to verify the scaling in a model of cubical vesicles in the area–volume ensemble in three dimensions with the generating function $T(1,q,p)$. In particular, equations (3) and (4) are verified by theorem 2.8. The scaling exponents can be determined: $\phi=2/3$ while $2-\alpha_t=-1/3$ and $2-\alpha_u=-1/2$. This model also exhibits the scaling relation in equation (5). The scaling function is related to hypergeometric functions in equation (51), and although the rich combinatorial structure evident in the model of squares is not explicit in this model, it could nevertheless be present, and is apparently undiscovered. These models can be generalized easily to higher dimensions, and while those are considerably more complicated, it appears that one may conjecture

$$\phi=\frac{d-1}{d}\qquad \text{for hypercubical vesicles in } d \text{ dimensions}$$

in a d-dimensional hypervolume and $(d-1)$-dimensional hypersurface area ensemble. In this model, one may expect that $2-\alpha_t=-1/d$ while $2-\alpha_u=-1/(d-1)$, and in that case equation (5) gives the desired value for ϕ.

Rectangular and rectangular box vesicles are considerably more complicated models than square and cubical vesicles. Asymptotics for the generating function $R(t,q)$ are given in corollary 3.2 and in theorem 3.3, as well as in theorem 3.4. I argue that these results indicate that $\phi=1$ in this model if one considers the ratio of scaling fields in theorem 3.4; and in that case one would have $2 - \alpha_t = -1$. However, an examination of $R(t, q)$ where $q = 1 - \epsilon$ suggests that $2 - \alpha_u = -1$, and this provides a consistent value for the scaling exponents to exhibit the scaling relation in equation (5).

Rectangular box vesicles in three dimensions give a phase diagram as presented in figures 8 and 9. In the perimeter–area ensemble the proposed crossover exponent appears to be $\phi = 1$, as in the two-dimensional version with the generating function $R(t, q)$. However, while the increase in dimension has preserved the value of ϕ in the scaling of the generating function $B(t, q, 1)$, apparently the values of $2 - \alpha_t$ and $2 - \alpha_u$ have changed. Conjecture 3.7 strongly suggests that $2-\alpha_t = -3/2$ in this ensemble. The fact that $B(t, 1, 1) = t^{12}/(1-t^4)^3$ suggests that $2-\alpha_u = -3$, but this value would be inconsistent with the scaling relation in equation (5). One may have to consider $B(t, 1 - \epsilon, 1)$ for small $\epsilon > 0$ to extract this exponent.

In the area–volume–perimeter ensemble, the asymptotic form for $B(1, q, 1)$ is proposed in theorem 3.6 and conjecture 3.7. These suggest that $2 - \alpha_u = -3/2$. $B(1, 1, p)$ was considered in lemma 3.9 and one may assign $2 - \alpha_t = -1$. The (non-exact) proposed scaling of $B(1, q, p)$ in equation (107) is not inconsistent with $\phi = 2/3$. This would indicate that $2 - \alpha_t = -1$, consistent with the indications in lemma 3.9. There are also several ratios involving the scaling fields $|\log q^2|$ and $|\log p|$ in equation (107), and it may be that there are several different scaling regimes around the tricritical point. The description of this model is therefore still incomplete, and it deserves further attention. We are now examining this model numerically.

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