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Layering in the Ising Model

Kenneth S. Alexander · François Dunlop · Salvador Miracle-Solé

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Abstract We consider the three-dimensional Ising model in a half-space with a boundary field (no bulk field). We compute the low-temperature expansion of layering transition lines.

Keywords Ising model · Layering transitions · Low-temperature expansion

1 Introduction and Results

We consider the Ising model in the half-space $Z_+^3 \subset Z^3$, with spins $\sigma_i = \pm 1$, $i \in Z_+^3 = \{(i_1, i_2, i_3),\ i_3 \geq 1\}$. The value -1 of the spin is associated with component or species A of a mixture and the value $+1$ is associated with component or species B, while the other half-space $\{i_3 \leq 0\}$ represents a fixed given substrate or wall W, made of a third component or species. The formal Hamiltonian is

$$H^{ABW} = J_{AB} \sum_{\langle i,j \rangle} (1 - \sigma_i \sigma_j) + J_{WA} \sum_{i_3=1} (1 - \sigma_i) + J_{WB} \sum_{i_3=1} (1 + \sigma_i) \tag{1.1}$$

with energy contributions $2J_{AB}$, $2J_{WA}$, $2J_{WB}$ associated respectively to pairs of nearest neighbors AB, WA, WB. In the first sum, $\langle i, j \rangle$ are nearest neighbors in Z_+^3. A wetting

K.S. Alexander
Department of Mathematics KAP 108, University of Southern California, Los Angeles, CA 90089-2532, USA
e-mail: alexandr@usc.edu

F. Dunlop (✉)
Laboratoire de Physique Théorique et Modelisation (CNRS, UMR 8089), Université de Cergy-Pontoise, 95302 Cergy-Pontoise, France
e-mail: Francois.Dunlop@u-cergy.fr

S. Miracle-Solé
Centre de Physique Théorique, CNRS, Case 907, 13288 Marseille cedex 9, France
e-mail: miracle@cpt.univ-mrs.fr

transition may occur when the bulk phase is B (or B-rich) but the wall prefers A: $J_{WA} < J_{WB}$.

At zero temperature, a macroscopic film of A will separate the wall from the bulk phase if $J_{WA} + J_{AB} < J_{WB}$. One says that the wall is "completely wet" by phase A. Raising the temperature will favor the presence of a film, because the AB interface brings entropy. Therefore, at positive temperature, a film of A will always be present if $J_{WA} + J_{AB} \leq J_{WB}$. There is no wetting transition, only complete wetting.

On the other hand, if $J_{WA} + J_{AB} > J_{WB}$, at zero temperature no A is present, and at low temperature the wall will be only partially wet by phase A. The density of B tends exponentially fast to the bulk density of B as a function of the distance to the wall. Raising the temperature now may produce, at some temperature T_W strictly below the critical temperature T_c, a transition from partial to complete wetting: this is the wetting transition predicted by Cahn [5] on the basis of critical exponents, and then confirmed by numerical and real experiments.

The existence of the wetting transition has been proved mathematically in the two-dimensional Ising model [1], but not in the three-dimensional Ising model. Let us simplify the notation to $J = J_{AB}$ and $K = J_{WB} - J_{WA}$, with

$$J > 0, \quad 0 < K < J. \tag{1.2}$$

Let $\tau^{\pm}$ denote the $+/-$ interface tension, defined for the Ising model in the full space Z^3, without wall, with Hamiltonian equal to the first term of (1.1). Fröhlich and Pfister (see formula (2.20) and Fig. 2 in [8]) have proven

$$K < \frac{1}{2}\tau^{\pm} \quad \Longrightarrow \quad \text{Partial wetting.} \tag{1.3}$$

They also prove that complete wetting is equivalent to unicity of the Gibbs state, and give rigorous monotonicity arguments, implying that increasing K for given T leads to a unique wetting transition at some $K = K_W(T) \leq J$. These are non-perturbative results, valid for all temperatures $0 \leq T < T_c$.

We shall consider only low temperatures, and perturbative arguments (not fully mathematically rigorous), indicating that the partial wetting range is slightly wider than (1.3), and includes first order layering transitions, as we now explain. Consider the model in a box $\Lambda \subset Z^3_+$, with bottom layer at $i_3 = 1$, and boundary condition $\bar{\sigma}$ on the other five sides of the box. Let $\Lambda_1 = \Lambda \cap \{i_3 = 1\}$. The Hamiltonian (1.1) may be cast into the equivalent form

$$H_\Lambda(\sigma_\Lambda|\bar{\sigma}) = -2J|\Lambda_1| + J \sum_{\langle i,j\rangle \cap \Lambda \neq \emptyset} (1 - \sigma_i\sigma_j) + K \sum_{i_3=1} (1 + \sigma_i). \tag{1.4}$$

In the first sum, i, j are nearest neighbors in Z^3_+ (so neither i nor j is in the wall), and σ_i or σ_j should be replaced by $\bar{\sigma}_i$ or $\bar{\sigma}_j$ wherever $i \notin \Lambda$ or $j \notin \Lambda$. In the second sum, $i \in \Lambda$. The constant term in front is a convenient normalization. Boundary condition n, with $n = 0, 1, 2, \ldots,$ is associated with the configuration n in Z^3_+, given by

$$\bar{\sigma}_i = -1 \quad \text{if } i_3 \leq n, \qquad \bar{\sigma}_i = +1 \quad \text{if } i_3 > n. \tag{1.5}$$

A possible scenario for the wetting transition is as follows (see Fig. 1): Let $0 < K < J$ with $J - K$ small. At $T = 0$ we have configuration 0, and for small T, we are close to configuration 0, call it state 0: in the thermodynamic limit, the probability that at a given i the

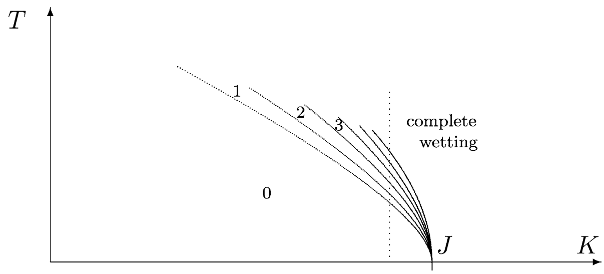

Fig. 1 Layering transition lines near $T = 0$. *Dotted line* shows a path from partial to complete wetting

spin σ_i differs from $\bar{\sigma}_i$, defined by (1.5) with $n = 0$, is small. State n is defined similarly from configuration n, for any n. As the temperature is raised, a first order transition will occur, from state 0 to state 1, then as the temperature is raised further, from state 1 to state 2, and so on. The level of the stable state n goes to infinity as the temperature approaches the wetting transition temperature, which in this case, $J - K$ small, is expected to be strictly below the roughening temperature. This scenario, with a sequence of first order layering transitions leading to the wetting transition, is part of the general picture which emerged based upon various physical heuristics and Monte-Carlo simulations (see [4, 12] and references therein.)

Let $t = e^{-4\beta J} \ll 1$ and $u = 2\beta(J - K) = \mathcal{O}(t^2)$. Note that each factor of t corresponds to two plaquettes of the interface. Based on the low temperature expansion as a formal series, we conjecture the following approximation to the coexistence (first order transition) lines starting from $(t = 0, u = 0)$:

Conjecture 1

$$\begin{aligned}
0/1: &\quad u = -\ln(1-t^2) + t^3 + \mathcal{O}(t^4)\\
1/2: &\quad u = -\ln(1-t^2) - t^3 + 5t^4 + \mathcal{O}(t^5)\\
2/3: &\quad u = -\ln(1-t^2) - t^3 + 4t^4 - 4t^5 + \mathcal{O}(t^6)\\
3/4: &\quad u = -\ln(1-t^2) - t^3 + 4t^4 - 6t^5 + \frac{51}{2}t^6 + \mathcal{O}(t^7)\\
4/5: &\quad u = -\ln(1-t^2) - t^3 + 4t^4 - 6t^5 + \frac{47}{2}t^6 - 51t^7 + \mathcal{O}(t^8)\\
5/6: &\quad u = -\ln(1-t^2) - t^3 + 4t^4 - 6t^5 + \frac{47}{2}t^6 - 53t^7 + 162t^8 + \mathcal{O}(t^9)\\
6/7: &\quad u = -\ln(1-t^2) - t^3 + 4t^4 - 6t^5 + \frac{47}{2}t^6 - 53t^7 + 160t^8\\
&\qquad + (B_9 + 2)t^9 + \mathcal{O}(t^{10})\\
7/8: &\quad u = -\ln(1-t^2) - t^3 + 4t^4 - 6t^5 + \frac{47}{2}t^6 - 53t^7 + 160t^8\\
&\qquad + B_9 t^9 + \mathcal{O}(t^{10}).
\end{aligned} \tag{1.6}$$

Here B_9 is a constant which we do not calculate, but we show it is the same for all interface heights $n \geq 6$. The analogous statement applies to the calculated coefficients as well, for example, the coefficient of t^4 is 4 for all $n \geq 2$. This is a result of the cancellation of all terms proportional to n, n^2, etc. in the low temperature expansion of the increment of surface *free energy from* n *to* $n+1$, *up to the given orders in* t. *We are unable to determine a systematic way in which this cancellation occurs, but we anticipate its validity for all orders in* t. *The consequence is that each successive transition line requires one more order in* t *to discern it. The phases* 0, 1, 2, 3, 4, 5, 6, 7 *are predicted to be stable between the respective transition lines. In particular phase* 0 *should be stable for* $u > t^2 + t^3 + \mathcal{O}(t^4)$. *For comparison,* (1.3) *gives partial wetting for* $u > 2t^2 + 4t^3 + \mathcal{O}(t^4)$. *Basuev* [3] *has given such equations for coexistence of the phases* 0, 1, 2 *with* 1, 2, 3 *respectively.*

Naturally, more is known in the SOS approximation, and in that context full mathematical rigor is possible, see [2, 6]. The low-temperature expansions of the Ising model and the corresponding SOS model agree only up to and including order t^2, which is of little help for (1.6). Order t^3 corresponds to a domino excitation of the interface, same in Ising and SOS, but also to a unit cube bubble, present only in the Ising model.

The stability range of phase n appears to be of width approximately $2t^{n+2}$ in the variable u. This is the same for Ising and SOS, and is the result of a double leg interface excitation reaching the wall (see Fig. 8). The $n/n+1$ coexistence lines are expected to converge as $n \to \infty$ to a part of the wetting transition line. Therefore the low-temperature expansions of all the $n/n+1$ coexistence lines would give the low-temperature expansion of the wetting transition line.

The low-temperature expansion is defined in Sect. 2. The derivation of the 2/3, 3/4, 4/5, 5/6, 6/7, 7/8 transition lines is given in Sect. 3, based partly on a recursion which is explained and illustrated in Sect. 5. Diagrams for the 7/8 transition line are postponed to Sect. 6. The derivation of the 0/1 and 1/2 transition lines is given in Sect. 4.

2 Low Temperature Expansion

Let us consider a finite volume $\Lambda = \Lambda_1 \times \{1, \dots, N\}$ as in (1.4), where the limit $N \nearrow \infty$ will be taken before $\Lambda_1 \nearrow Z^2$. Consider boundary condition n, with $n \geq 1$ for definiteness. The ground state is (1.5), with a flat interface at height $n + \frac{1}{2}$, denoted I_n. At positive temperature, bubbles and interface excitations will appear. If state n is stable, or if the statistical ensemble is restricted by a condition forbidding large-diameter fluctuations, the gas of bubbles and interface excitations should be diluted, and the corresponding dilute gas expansion is expected to give exact asymptotics for low temperatures. As we are only concerned here with calculating the first few terms of this expansion, and not with establishing its convergence, we will not make a precise definition of a restricted ensemble. But the principle is illustrated in the SOS approximation studied in [2], where for a given ground state interface height $n + \frac{1}{2}$, the restriction is that excitations from this height must have diameter bounded by a value of order n. Whatever reasonable restriction is used, in a restricted ensemble the surface free energy density (times β), which we denote f_n, will depend on the height n, and one expects that the value of n minimizing this free energy will be the equilibrium interface height in the full ensemble, with a transition from n to $n+1$ occurring where $f_n - f_{n+1} = 0$. More precisely, the restricted partition function is

$$Z_n^\Lambda = \sum_{\sigma_\Lambda}{}' e^{-\beta H_\Lambda(\sigma_\Lambda | n)}, \tag{2.1}$$

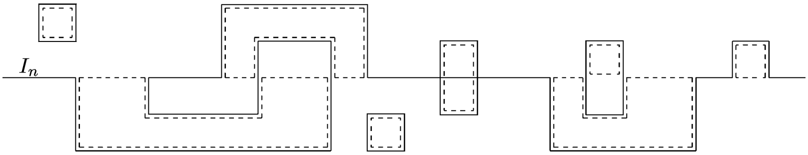

Fig. 2 Bubbles and interface excitations (*closed dashed contours*), with *solid lines* showing boundaries between + and − spins, shown in the 2d analog of our 3d context. The 1×2 contour at the center is a bubble, not an interface excitation

where $\beta = 1/kT$ is the inverse temperature and the $'$ indicates that summation is over a restricted ensemble corresponding to state n, and then

$$f_n - f_{n+1} = \lim_{\Lambda_1 \nearrow Z^2} -\frac{1}{|\Lambda_1|} \lim_{N \nearrow \infty} \log \frac{Z_n^\Lambda}{Z_{n+1}^\Lambda}. \tag{2.2}$$

We are going to compute the leading terms up to some order for $f_n - f_{n+1}$, so as to obtain (1.6). These leading terms should not depend on the particular restricted ensemble chosen.

Bubbles and interface excitations will be called contours, or also polymers, and will be denoted γ. More precisely, contours are defined as boundaries of maximal connected sets of points in $\mathbb{Z}^3$ where the spin differs from its ground state value in the corresponding restricted ensemble. Here a set of points is called *connected* if any two points can be connected by a path of nearest neighbor bonds in the set, and the *boundary* of a set A of points is the set of those plaquettes which separate a point in A from a point not in A. Thus a contour need not be a connected set of plaquettes. Interface excitations are contours distinguished by the property of sharing at least one plaquette with I_n; bubbles are those contours which do not share such a plaquette. This means that a bubble crossing I_n without such sharing of a plaquette is not an interface excitation.

The low-temperature polymer expansion starts with

$$Z_n^\Lambda = e^{u|\Lambda_1|\delta(n)} \sum_{\{\gamma\}} \prod_\gamma \varphi(\gamma) \tag{2.3}$$

where $\{\gamma\}$ is a compatible family of contours, and $\varphi(\gamma)$ is the weight of a contour,

$$\varphi(\gamma) = t^{\frac{1}{2}|\gamma| - |\gamma \cap I_n|} e^{u|\gamma \cap \{z = \frac{1}{2}\}|} \tag{2.4}$$

where $|\cdot|$ is the number of plaquettes in γ or in $\gamma \cap I_n$ or in $\gamma \cap \{z = \frac{1}{2}\}$. A family is compatible if any pair of contours in the family is compatible. Two contours are compatible if their interiors are disjoint and they share no plaquette. In view of (2.4), we will henceforth represent an interface excitation with plaquettes in I_n removed (see Figs. 3–8 below), but when deciding compatibility, it must be remembered that these plaquettes do belong to the interface excitation, as in Fig. 2.

Since the interaction between contours is a two-body interaction—compatibility between any two polymers is not affected by the presence of other polymers—the general theory of polymer expansion (see e.g. [9–11]) gives, from (2.3),

$$\log(Z_n^\Lambda) = \sum_\omega \varphi^T(\omega) \tag{2.5}$$

where ω is a cluster or family of contours, with contour γ repeated n_γ times, and

$$\varphi^T(\omega) = \prod_{\gamma\in\omega}\left(\frac{1}{n_\gamma!}\varphi(\gamma)^{n_\gamma}\right)\sum_G(-1)^l \tag{2.6}$$

where the sum over G is over connected graphs on the cluster, and l is the number of edges in G. An edge may exist between γ and γ' if and only if γ and γ' are incompatible.

For the expansion of $\tau^\pm$, interface excitations were expanded in terms of walls and ceilings by Dobrushin [7], who proved convergence of the resulting expansion. For the SOS approximation of the present wetting model, a two-scale convergent expansion was used in [2]. Here we consider only the finite volume expansion and the formal infinite volume series, which is why our derivation of (1.6) is not fully rigorous.

All the clusters in (2.5) lie within Λ. For a cluster which contains an interface excitation, we write $\omega\in I_n$. For a cluster of bubbles only, compatible (i.e. not sharing a plaquette) with I_n, we write $\omega\sim I_n$. For a cluster which reaches the bottom $\{i_3=1/2\}$, we write $\omega\in W$, otherwise $\omega\approx W$. We write W_N for the top boundary $\{i_3=N+\frac{1}{2}\}$ of Λ. All clusters $\omega\subset\Lambda$ are compatible with the top boundary; we write $\omega\approx W_N$. Then

$$\begin{aligned}\log(Z_n^\Lambda) &= \sum_{\substack{\omega\in I_n,W\\ \omega\approx W_N}}\varphi^T(\omega) + \sum_{\substack{\omega\in I_n,\\ \omega\approx W,W_N}}\varphi^T(\omega) + \sum_{\substack{\omega\in W,\\ \omega\sim I_n,\omega\approx W_N}}\varphi^T(\omega) + \sum_{\substack{\omega\approx W,W_N\\ \omega\sim I_n}}\varphi^T(\omega)\\ &= \sum_{\substack{\omega\in I_n,W\\ \omega\approx W_N}}\varphi^T(\omega) + \sum_{\substack{\omega\in I_n,\\ \omega\approx W,W_N}}\varphi_0^T(\omega) + \sum_{\substack{\omega\in W,\\ \omega\sim I_n,\omega\approx W_N}}\varphi_1^T(\omega) + \sum_{\substack{\omega\approx W,W_N\\ \omega\sim I_n}}\varphi_2^T(\omega)\end{aligned} \tag{2.7}$$

where

$$\varphi_0(\gamma) = t^{\frac{1}{2}|\gamma|-|\gamma\cap I_n|},\qquad \varphi_1(\gamma) = t^{\frac{1}{2}|\gamma|}e^{u|\gamma\cap\{z=\frac{1}{2}\}|},\qquad \varphi_2(\gamma) = t^{\frac{1}{2}|\gamma|}. \tag{2.8}$$

The first term in (2.7) depends explicitly upon n. The sums consist of clusters $\omega\subset\Lambda$, but in order to extract the n-dependent part of the following three terms, it is convenient to relax this condition into $\omega\cap\Lambda\neq\emptyset$, allowing "boundary-overlapping" clusters which overlap W or W_N. In this context the notations $\omega\approx W,\omega\in W$ and $W\approx W_N$ apply only to clusters which do not overlap W and W_N respectively. Then applying inclusion-exclusion to the summation conditions, the last three sums in (2.7) become

$$\begin{aligned}\sum_{\substack{\omega\in I_n,\\ \omega\approx W,W_N}}\varphi^T(\omega) &= \sum_{\omega\in I_n}\varphi_0^T(\omega) - \sum_{\substack{\omega\in I_n,\\ \omega\not\approx W}}\varphi_0^T(\omega) - \sum_{\substack{\omega\in I_n,\\ \omega\not\approx W_N}}\varphi_0^T(\omega) + \sum_{\substack{\omega\in I_n,\\ \omega\not\approx W,W_N}}\varphi_0^T(\omega),\\ \sum_{\substack{\omega\in W,\\ \omega\sim I_n,\omega\approx W_N}}\varphi^T(\omega) &= \sum_{\omega\in W}\varphi_1^T(\omega) - \sum_{\substack{\omega\in W,\\ \omega\not\sim I_n}}\varphi_1^T(\omega) - \sum_{\substack{\omega\in W,\\ \omega\not\approx W_N}}\varphi_1^T(\omega) + \sum_{\substack{\omega\in W,\\ \omega\not\sim I_n,\omega\not\approx W_N}}\varphi_1^T(\omega),\\ \sum_{\substack{\omega\approx W,W_N,\\ \omega\sim I_n}}\varphi^T(\omega) &= \sum_{\omega\cap\Lambda\neq\emptyset}\varphi_2^T(\omega) - \sum_{\omega\not\sim I_n}\varphi_2^T(\omega) - \sum_{\omega\not\approx W}\varphi_2^T(\omega) - \sum_{\omega\not\approx W_N}\varphi_2^T(\omega)\\ &\quad + \sum_{\substack{\omega\not\sim I_n,\\ \omega\not\approx W}}\varphi_2^T(\omega) + \sum_{\substack{\omega\not\sim I_n,\\ W\not\approx W_N}}\varphi_2^T(\omega) + \sum_{\omega\not\approx W,W_N}\varphi_2^T(\omega)\\ &\quad - \sum_{\substack{\omega\not\approx W,W_N\\ \omega\not\sim I_n}}\varphi_2^T(\omega).\end{aligned} \tag{2.9}$$

Note that the sums from (2.7), on the left side in (2.9), are not affected by the relaxation from $\omega \subset \Lambda$ to $\omega \cap \Lambda \neq \emptyset$. Terms with $\omega \not\sim I_n, \omega \not\approx W_N$ or $\omega \not\approx W, W_N$ or $\omega \not\approx W, W_N, \omega \not\sim I_n$ are negligible in the limit $N \nearrow \infty$ and will be omitted in the sequel. This is the meaning of $\simeq$ instead of $=$ below. Apart from these negligible terms, only one sum on the right side each of the three equalities in (2.9) actually depends upon n. Therefore

$$\log(Z_n^\Lambda) \simeq \sum_{\omega \in I_n, W} \varphi^T(\omega) - \sum_{\substack{\omega \in I_n, \\ \omega \not\approx W}} \varphi_0^T(\omega) - \sum_{\substack{\omega \in W, \\ \omega \not\sim I_n}} \varphi_1^T(\omega) + \sum_{\substack{\omega \not\sim I_n, \\ \omega \not\approx W}} \varphi_2^T(\omega) + \text{indep. of } n. \tag{2.10}$$

In order to compare Z_n^Λ and Z_{n+1}^Λ using translation invariance, the wall W will be denoted W_0, and W_{-1} will denote a wall translated vertically by -1. The following is immediate from (2.10).

Proposition 1 *For $n \geq 1$, starting from a box $\Lambda = \Lambda_1 \times \{1, \ldots, N\}$,*

$$\begin{aligned}\lim_{N \nearrow \infty} \log(Z_n^\Lambda / Z_{n+1}^\Lambda) &= \sum_{\omega \in I_n, W} \varphi^T(\omega) - \sum_{\substack{\omega \in I_n, \\ \omega \not\approx W_0 \\ \omega \approx W_{-1}}} \varphi_0^T(\omega) - \sum_{\omega \in I_{n+1}, W} \varphi^T(\omega) \\ &\quad - \Bigg(\sum_{\substack{\omega \in W, \\ \omega \not\sim I_n \\ \omega \sim I_{n+1}}} \varphi_1^T(\omega) - \sum_{\substack{\omega \in W, \\ \omega \not\sim I_{n+1} \\ \omega \sim I_n}} \varphi_1^T(\omega) \Bigg) \\ &\quad + \Bigg(\sum_{\substack{\omega \not\approx W, \\ \omega \not\sim I_n}} \varphi_2^T(\omega) - \sum_{\substack{\omega \not\approx W, \\ \omega \not\sim I_{n+1}}} \varphi_2^T(\omega) \Bigg).\end{aligned} \tag{2.11}$$

The limit $\Lambda_1 \nearrow Z^2$ raises non-trivial mathematical questions not addressed here. We shall assume that the limit exists and is given by a low-temperature expansion, yielding power series in t which agree to the order required with those given by the formal low-temperature expansion. From here onwards, we shall consider only surface free energy densities in the thermodynamic limit as in (2.2). Anticipating a leading term t^{2n}, (2.11) leads to

$$t^{-2n}(f_{n+1} - f_n) = A_n(u) - A_n(0) - t^2 A_{n+1}(u) - B_n(u) + B_n^\infty(0) \tag{2.12}$$

where each of the five terms is defined by the corresponding term in (2.11). We can simplify $B_n^\infty(0)$ as follows. The terms in $B_n^\infty(0)$ correspond to clusters of bubbles only, and the set of such clusters may be divided into equivalence classes consisting of clusters which are vertical translates of one another. Within each equivalence class there is a unique special bubble ω satisfying $\omega \in W$. For a given equivalence class, the number of terms from that class in the first sum in $B_n^\infty(0)$ is the number of heights $k \geq n$ for which the special bubble has a horizontal plaquette at height $k + \frac{1}{2}$, and similarly for the second sum, but with heights $k \geq n + 1$. Hence the net number of terms in $B_n^\infty(0)$ from the equivalence class, counted with $+/-$ sign, is 1 if the special bubble ω has a horizontal plaquette at height $n + \frac{1}{2}$ (that is, if $\omega \not\succ I_n$), and 0 otherwise. It follows that

$$t^{2n} B_n^{\infty}(0) = \sum_{\substack{\omega \in W \\ \omega \not\succ I_n}} \varphi_2^T(\omega) = t^{2n} \sum_{m=0}^{\infty} t^{2m} B_{n+m}(0). \tag{2.13}$$

Since

$$t^{2n} B_n(u) = \sum_{\substack{\omega \in W, \\ \omega \not\succ I_n}} \varphi_1^T(\omega) - \sum_{\substack{\omega \in W, \\ \omega \not\succ I_{n+1}}} \varphi_1^T(\omega),$$

and since $\varphi_1^T = \varphi_2^T$ for $u = 0$, we have $B_n^{\infty}(0) = B_n(0) + t^2 B_{n+1}^{\infty}(0)$ so that

$$t^{-2n}(f_{n+1} - f_n) = A_n(u) - A_n(0) - t^2 A_{n+1}(u) - \big(B_n(u) - B_n(0) - t^2 B_{n+1}^{\infty}(0)\big). \tag{2.14}$$

3 Stability Regions of Phases 3, 4, 5, 6, 7

Conjecture 1 for the 2/3, 3/4, 4/5, 5/6, 6/7, 7/8 transition lines follows from the following more precise statement:

Conjecture 2 *For sufficiently small t, and*

$$u = -\ln(1 - t^2) + b_3 t^3 + \cdots + b_8 t^8 + b_9 t^9 + \mathcal{O}(t^{10}) \tag{3.1}$$

the following is expected:

- *If $b_3 > -1$, or $b_3 = -1$, $b_4 > 4$, then*

$$f_{n+1} - f_n > 0, \quad n \geq 2, \tag{3.2}$$

  and phase 2 is stable relative to phases $3, 4, \ldots$.
- *If $b_3 = -1$, $b_4 = 4$, and $-6 < b_5 < -4$, then*

$$\begin{aligned} t^{-4}(f_3 - f_2) &\simeq (b_5 + 4)t^5 < 0, \\ t^{-2n}(f_{n+1} - f_n) &\simeq (b_5 + 6)t^5 > 0, \quad n \geq 3, \end{aligned} \tag{3.3}$$

  and phase 3 is stable relative to phase 2 and to phases $4, 5, \ldots$.
- *If $b_3 = -1$, $b_4 = 4$, $b_5 = -6$, and $\frac{47}{2} < b_6 < \frac{51}{2}$, then*

$$\begin{aligned} t^{-4}(f_3 - f_2) &\simeq -2t^5 < 0, \\ t^{-6}(f_4 - f_3) &\simeq \left(b_6 - \frac{51}{2}\right)t^6 < 0, \\ t^{-2n}(f_{n+1} - f_n) &\simeq \left(b_6 - \frac{47}{2}\right)t^6 > 0, \quad n \geq 4, \end{aligned} \tag{3.4}$$

  and phase 4 is stable relative to phases 2, 3 and to phases $5, 6, \ldots$.

- *If* $b_3 = -1$, $b_4 = 4$, $b_5 = -6$, $b_6 = \frac{47}{2}$, *and* $-53 < b_7 < -51$, *then*

$$\begin{aligned} t^{-2n}(f_{n+1} - f_n) &\simeq -2t^{n+3} < 0, \quad 2 \le n \le 3, \\ t^{-8}(f_5 - f_4) &\simeq (b_7 + 51)t^7 < 0, \\ t^{-2n}(f_{n+1} - f_n) &\simeq (b_7 + 53)t^7 > 0, \quad n \ge 5, \end{aligned} \tag{3.5}$$

  and phase 5 *is stable relative to phases* 2, 3, 4 *and to phases* 6, 7, ….
- *If* $b_3 = -1$, $b_4 = 4$, $b_5 = -6$, $b_6 = \frac{47}{2}$, $b_7 = -53$, *and* $160 < b_8 < 162$, *then*

$$\begin{aligned} t^{-2n}(f_{n+1} - f_n) &\simeq -2t^{n+3} < 0, \quad 2 \le n \le 4, \\ t^{-10}(f_6 - f_5) &\simeq (b_8 - 162)t^8 < 0, \\ t^{-2n}(f_{n+1} - f_n) &\simeq (b_8 - 160)t^8 > 0, \quad n \ge 6, \end{aligned} \tag{3.6}$$

  and phase 6 *is stable relative to phases* 2, 3, 4, 5 *and to phases* 7, 8, ….
- *There exists* B_9 *as follows. If* $b_3 = -1$, $b_4 = 4$, $b_5 = -6$, $b_6 = \frac{47}{2}$, $b_7 = -53$, $b_8 = 160$ *and* $B_9 < b_9 < B_9 + 2$, *then*

$$\begin{aligned} t^{-2n}(f_{n+1} - f_n) &\simeq -2t^{n+3} < 0, \quad 2 \le n \le 5, \\ t^{-10}(f_7 - f_6) &\simeq (b_9 - B_9 - 2)t^9 < 0, \\ t^{-2n}(f_{n+1} - f_n) &\simeq (b_9 - B_9)t^9 > 0, \quad n \ge 7, \end{aligned} \tag{3.7}$$

  and phase 7 *is stable relative to phases* 2, 3, 4, 5, 6 *and to phases* 8, 9, ….

In order to derive Conjecture 2, we first write the u dependence in (2.12), (2.13) and (2.14) as

$$A_n(u) = e^u P_n + e^{2u} Q_n + e^{3u} R_n + e^{4u} S_n + e^{5u} T_n + e^{6u} U_n + \cdots, \tag{3.8}$$

$$B_n(u) = e^u \tilde{P}_n + e^{2u} \tilde{Q}_n + e^{3u} \tilde{R}_n + e^{4u} \tilde{S}_n + e^{5u} \tilde{T}_n + e^{6u} \tilde{U}_n + \cdots. \tag{3.9}$$

For $n \ge 3$ we have $P_n = \mathcal{O}(1)$ corresponding to interface fluctuations placing a single plaquette on the wall, and similarly $Q_n = \mathcal{O}(t^2)$, $R_n = \mathcal{O}(t^4)$, $S_n = \mathcal{O}(t^5)$, $T_n = \mathcal{O}(t^7)$, $U_n = \mathcal{O}(t^8)$. Relative to these, $\tilde{P}_n, \tilde{Q}_n, \tilde{R}_n, \tilde{S}_n$ have an extra factor t at leading order. The remainder in (3.8), (3.9) is $\mathcal{O}(t^{10})$. For $n = 2$ we have $P_2 = \mathcal{O}(1)$, $Q_2 = \mathcal{O}(t^2)$, $R_2 = \mathcal{O}(t^4)$, $S_2 = \mathcal{O}(t^4)$, $T_2 = \mathcal{O}(t^6)$, $U_2 = \mathcal{O}(t^6)$, while $\tilde{P}_2, \tilde{Q}_2, \tilde{R}_2, \tilde{S}_2$ are of the same order as for $n \ge 3$. The remainder in (3.8) for $n = 2$ is $\mathcal{O}(t^8)$, but in (3.9) it is still $\mathcal{O}(t^{10})$.

Let $Q_n = Q_n^1 + Q_n^2$ and $R_n = R_n^1 + R_n^2 + R_n^3$, where the upper index 1, 2, 3 is the number of contours (in the cluster) touching the wall, so that $Q_n^1 = \mathcal{O}(t^2)$, $Q_n^2 = \mathcal{O}(t^3)$, etc. We are going to expand (2.12) up to order t^9, requiring A_{n+1} up to order t^7, using the following recursion in n:

$$\begin{aligned}
P_{n+1} &= P_n + 2Q_n + 3R_n + 4S_n + 5T_n + 6U_n - t(P_n + 2Q_n + 3R_n + 4S_n) \\
&\quad + \mathcal{O}(t^7), \\
Q^1_{n+1} &= (4t^2 - 4t^3)P_n + (t + 6t^2 - 7t^3)Q^1_n + (8t^2 - 8t^3)Q^2_n \\
&\quad + 2tR^1_n + 9t^2 R_n + tR^2_n + 4tS_n + \mathcal{O}(t^7), \\
Q^2_{n+1} &= (-5t^3 + 5t^4)P_n + (-10t^3 + 10t^4)Q^1_n + t^2 Q^2_n - 12t^3 Q^2_n + \mathcal{O}(t^7), \\
Q_{n+1} &= (4t^2 - 9t^3 + 5t^4)P_n + (t + 6t^2 - 17t^3 + 10t^4)Q^1_n + (9t^2 - 20t^3)Q^2_n \\
&\quad + 2tR^1_n + 9t^2 R_n + tR^2_n + 4tS_n + \mathcal{O}(t^7), \\
R^1_{n+1} &= (18t^4 - 18t^5)P_n + (6t^3 + 24t^4)Q^1_n + t^2 R_n + 4t^2 S_n + \mathcal{O}(t^7), \\
R^2_{n+1} &= (-48t^5 + 48t^6)P_n - 8t^4 Q^1_n + \mathcal{O}(t^7), \\
R^3_{n+1} &= 31t^6 P_n + \mathcal{O}(t^7), \\
R_{n+1} &= (18t^4 - 66t^5 + 79t^6)P_n + (6t^3 + 16t^4)Q^1_n + t^2 R_n + 4t^2 S_n + \mathcal{O}(t^7), \\
S_{n+1} &= (4t^5 + 60t^6)P_n + 2t^4 Q_n + \mathcal{O}(t^7)
\end{aligned} \tag{3.10}$$

and the same recursion relations for $\tilde{P}_n, \tilde{Q}_n, \tilde{R}_n, \tilde{S}_n$, with an error $\mathcal{O}(t^8)$. The recursion relations (3.10) have been found with the help of diagrams, see Sect. 5.

Solving these recursion relations for formal power series in t requires as input P_n, or $\tilde{P}_n$, for all n, to the required order. Indeed the order obtained in the output P_{n+1} or $\tilde{P}_{n+1}$ is the same as in the input P_n or $\tilde{P}_n$, so that the recursion formula does not help. On the other hand, if the power series expansion for P_n or $\tilde{P}_n$ is obtained by other methods, up to the required order, for all n, then the initial condition, at $n = 2$, given by $Q^1_2 = 4t^2 + 2t^2 + \mathcal{O}(t^3)$, $Q^2_2 = -5t^3 + \mathcal{O}(t^4)$, $R^1_2 = \mathcal{O}(t^4)$, $R^2_2 = \mathcal{O}(t^5)$, $S_2 = \mathcal{O}(t^4)$, or $\tilde{Q}^1_2 = 4t^3 + \mathcal{O}(t^4)$, $\tilde{Q}^2_2 = -5t^4 + \mathcal{O}(t^5)$, $\tilde{R}^1_2 = 18t^5 + \mathcal{O}(t^6)$, together with P_n or $\tilde{P}_n$, will give one more order in t with each recursion step. The recursion equation giving P_{n+1} or $\tilde{P}_{n+1}$ may be checked at the end for consistency. The final result of this for P_n, Q_n, R_n, S_n or $\tilde{P}_n, \tilde{Q}_n, \tilde{R}_n, \tilde{S}_n$ is given as "first excitations":

First Excitations in $A_n(u)$

$$\begin{aligned}
P_n &= 1 - (n-5)t + c_n t^2 - a_n t^3 + d_n t^4 + \mathcal{O}(t^5), \quad n \geq 5, \\
Q^1_n &= 4\big[t^2 - (n-6)t^3 + (c_{n-1} + 7)t^4 - (a_{n-1} + c_{n-1} - c_{n-2} + 6n - 41)t^5 \\
&\quad + (d_{n-1} + a_{n-1} - a_{n-2} + 5c_{n-2} + c_{n-3} + 2n + C)t^6\big] \\
&\quad + 2t^n + \mathcal{O}(t^7), \quad n \geq 6, \\
Q^2_n &= -5t^3 + 5(n-5)t^4 - (5c_n + C)t^5 + \mathcal{O}(t^6), \quad n \geq 3, \\
R^1_n &= 18t^4 - (18n - 114)t^5 + (18c_n - 24n + C)t^6 + \mathcal{O}(t^7), \quad n \geq 4, \\
R^2_n &= -48t^5 + (48n + C)t^6 + \mathcal{O}(t^7), \quad n \geq 3, \\
S_n &= 4t^5 - (4n + C)t^6 + \mathcal{O}(t^7), \quad n \geq 3, \\
T_n &= Ct^7 + \mathcal{O}(t^8), \quad n \geq 3,
\end{aligned} \tag{3.11}$$

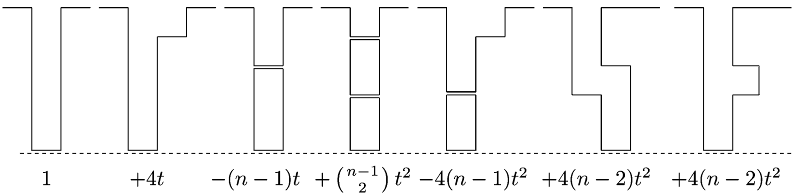

Fig. 3 P_n: constant and t-terms, and t^2-terms which depend on n. The 4th diagram, for example, shows a cluster consisting of an interface excitation and two bubbles

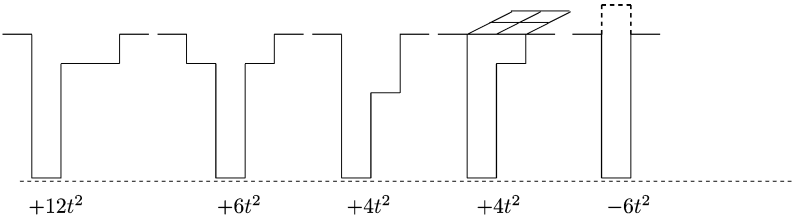

Fig. 4 P_n: t^2-terms independent of n. The 5th diagram shows a cluster consisting of 2 contours: a downward leg (*solid line*) and a unit upward excitation (*dashed line*)

with

$$c_n = \binom{n-1}{2} + 4(n-2) + 16, \tag{3.12}$$

$$a_n = \binom{n-1}{3} + 12\binom{n-1}{2} - 10n - 48, \tag{3.13}$$

$$d_n = \binom{n-1}{4} + 20\binom{n-1}{3} + 32\binom{n-1}{2} + 54n + C. \tag{3.14}$$

In (3.11) and in what follows, C is a generic constant, not depending on n and different at different appearances, which we do not calculate or use. The expansion for P_n is valid for $n = 3$ with two orders less (that is, $\mathcal{O}(t^3)$ instead of $\mathcal{O}(t^5)$), and for $n = 2$ with three orders less, and for $n = 1$ with four orders less. It is obtained by listing diagrams—see below. The results for $Q_n^1, \ldots, S_n$ in (3.11) follow from the result for P_n using (3.10). One can start the induction from $n = 1$ with (3.10) adjusted for $n = 1$, or from $n = 2$ with $Q_2^1 = 4t^2 + 2t^2 + \mathcal{O}(t^3)$, $Q_2^2 = -5t^3 + \mathcal{O}(t^4)$, $R_2^1 = \mathcal{O}(t^4)$, $R_2^2 = \mathcal{O}(t^5)$, $S_2 = \mathcal{O}(t^4)$. The expansion for Q_n^1 is valid for $n = 4$ with one order less, and for $n = 3$ with two orders less, and for $n = 2$ with three orders less. The expansion for R_n^1 is valid for $n = 3$ with one order less.

The result for P_n is displayed in Figs. 3–7. The dashed line at the bottom of each diagram represents the wall, and the horizontal lines at the top represent portions of the interface I_n. All diagrams should be understood in three dimensions. The depth is one in the third dimension, with certain exceptions: (i) In the 4th diagram in Figs. 4 and 6 the depth is two in the top layer, as shown. (ii) In diagrams like the first two in Fig. 4, the three cubes in the top layer are not required to be collinear. (iii) In diagrams like the first and third in Fig. 7, in which the vertical column is shifted or appended-to at multiple locations, the directions of these shifts and appendages need not all be the same.

Formula (3.12) for c_n was obtained using Figs. 3 and 4 with (2.6). The factor 6 for the last diagram in Fig. 4 is: one incompatible unit cube upward interface excitation, as drawn,

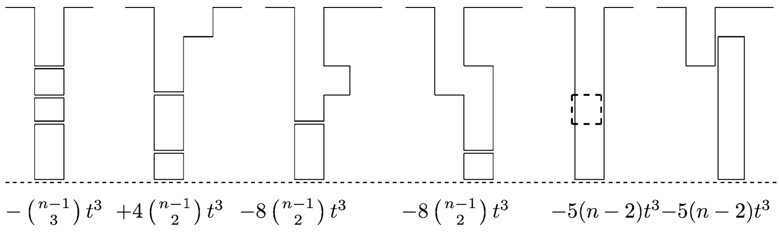

Fig. 5 P_n: t^3-terms, cubic, quadratic, linear (continued on next two figures) in n. The 5th diagram shows a cluster consisting of 2 contours: a downward leg (*solid line*) and a unit bubble (*dashed line*)

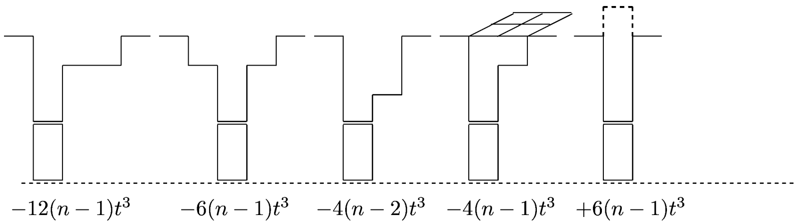

Fig. 6 P_n: t^3-terms, analog of t^2 terms on Fig. 4

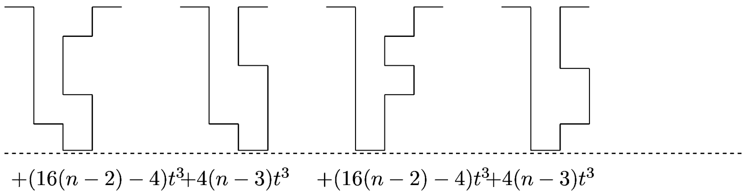

Fig. 7 P_n: t^3-terms, linear in n (continued from previous figures)

or any of five incompatible unit cube downward interface excitations. Formula (3.13) for a_n was obtained using Figs. 5, 6, 7 with (2.6). The factor $5(n-2)$ for the next-to-last diagram in Fig. 5 is: one incompatible unit cube bubble in the interface leg at height $2, \dots, n-1$, as drawn, and four incompatible unit cube bubbles adjacent to the leg at height $2, \dots, n-1$, and similarly for the last diagram in Fig. 5. Formula (3.14) was obtained using the diagrams in Figs. 14 and 15.

The leading terms up to t^3 and the double leg in Q_n are shown in Fig. 8.

Formulas (3.12) and (3.13) for c_n and a_n are consistent with the recursion relations, notably the equation giving P_{n+1} not used so far, implying

$$\begin{aligned} c_{n+1} &= c_n + n + 3, \\ a_{n+1} &= a_n + c_n + 8n - 30. \end{aligned} \tag{3.15}$$

For later purposes we note that

$$\begin{aligned} a_n - a_{n-1} &= \frac{1}{2}(n-1)(n-2) + 11n - 32, \\ a_n - a_{n-1} + 2c_n - 4c_{n-1} + c_{n-2} &= 9n - 35. \end{aligned} \tag{3.16}$$

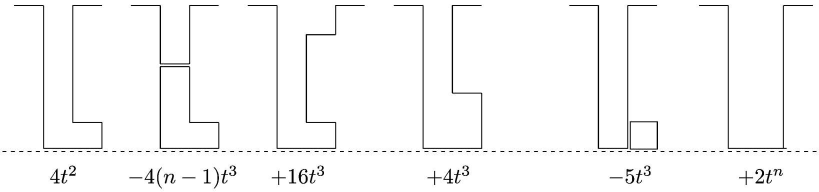

Fig. 8 $Q_n = Q_n^1 + Q_n^2$: up to order t^3, and double leg

Putting together (3.8), (3.10) and assuming $u = \mathcal{O}(t^2)$ gives for $n \geq 3$

$$\begin{aligned}
&A_n(u) - A_n(0) - t^2 A_{n+1}(u) \\
&\quad = (e^u - 1 - e^u t^2 + e^u t^3 - 4e^{2u} t^4 + 9e^{2u} t^5 \\
&\qquad - 5e^{2u} t^6 - 18e^{3u} t^6 + 66e^{3u} t^7 - 4e^{4u} t^7 - 139t^8 + Ct^9) P_n \\
&\qquad + (e^{2u} - 1 - 2e^u t^2 + 2e^u t^3) Q_n + (-e^{2u}(t^3 + 6t^4) + 11t^5 - 28t^6 + Ct^7) Q_n^1 \\
&\qquad + (-9t^4 + 20t^5 + Ct^6) Q_n^2 + (e^{3u} - 1 - 3e^u t^2 + 3e^u t^3) R_n \\
&\qquad - (2t^3 + 10t^4 + Ct^5) R_n^1 - (t^3 + Ct^4) R_n^2 \\
&\qquad + (e^{4u} - 1 - 4e^u t^2 + 4e^u t^3 + Ct^4) S_n - (4t^3 + Ct^4) S_n \\
&\qquad + (e^{5u} - 1 - 5e^u t^2) T_n + \mathcal{O}(t^{10}).
\end{aligned} \tag{3.17}$$

Contributions from U_n have been absorbed into $\mathcal{O}(t^{10})$, thanks to $u = \mathcal{O}(t^2)$. For $n = 2$, (3.17) is valid up to order t^6, with an error $\mathcal{O}(t^7)$. By (3.11), in each of the expansions P_n, Q_n^1, Q_n^2, etc., n-dependent terms only appear at one or more orders less in t than the largest-order term, and when (3.17) is multiplied out, the unspecified constants C only appear at order t^9 or less. Therefore the constants C appear in n-dependent terms only at order t^{10} or less, so that, while the constants C are relevant to the value of B_9 in (1.6), they are not relevant to establishing that B_9 is n-independent. The constants C thus play the role of placeholders, permitting the $\mathcal{O}(t^{10})$ error term which allows analysis of the dependence of B_9 on n.

First Excitations in $B_n(u)$

$$\begin{aligned}
\tilde{P}_n &= t - (n-1)t^2 + \tilde{c}_n t^3 - \tilde{a}_n t^4 + \tilde{d}_n t^5 + \mathcal{O}(t^6), \quad n \geq 4, \\
\tilde{Q}_n^1 &= 4\big[t^3 - (n-2)t^4 + (\tilde{c}_{n-1} + 7)t^5 + (-\tilde{a}_{n-1} - \tilde{c}_{n-1} + \tilde{c}_{n-2} - 6n + 17)t^6\big] \\
&\qquad + 2t^{n+2} + \mathcal{O}(t^7), \quad n \geq 4, \\
\tilde{Q}_n^2 &= -5t^4 + 5(n-1)t^5 + \mathcal{O}(t^6), \quad n \geq 2, \\
\tilde{R}_n^1 &= 18t^5 - (18n - 42)t^6 + \mathcal{O}(t^7), \quad n \geq, 2 \\
\tilde{R}_n^2 &= -48t^6 + \mathcal{O}(t^7), \quad n \geq 2,
\end{aligned} \tag{3.18}$$

with

$$\tilde{c}_n = \binom{n-1}{2} + 8n - 13, \tag{3.19}$$

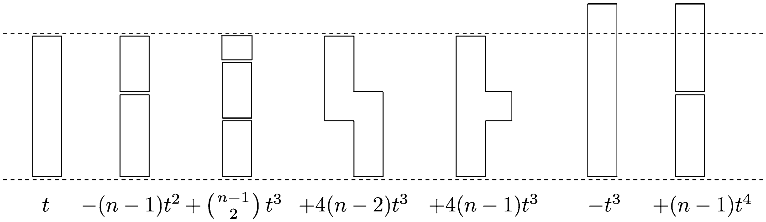

Fig. 9 $\tilde{P}_n$: t^3-terms, and t^4-term incompatible with I_{n+1}

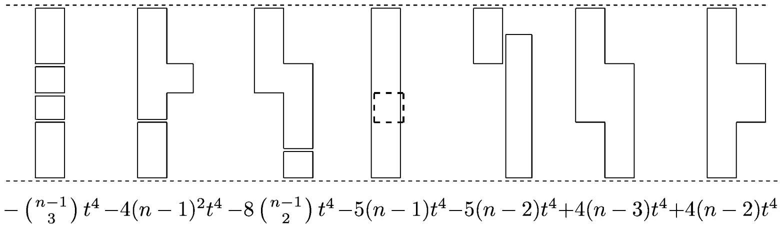

Fig. 10 $\tilde{P}_n$: t^4-terms, other than Fig. 9

$$\tilde{a}_n = \binom{n-1}{3} + 16\binom{n-1}{2} + 5n + 2, \tag{3.20}$$

$$\tilde{d}_n = \binom{n-1}{4} + 24\binom{n-1}{3} + 79\binom{n-1}{2} - 31n + 75. \tag{3.21}$$

The expansion for $\tilde{P}_n$ is valid for $n = 3$ with one order less, and for $n = 2$ with two orders less, and for $n = 1$ with three orders less. The expansion for $\tilde{Q}_n$ is valid for $n = 3$ with one order less, and for $n = 2$ with two orders less. Formula (3.19) was obtained using Fig. 9. The last two diagrams in Fig. 9 belong to the second term inside the parentheses, 4th term in (2.11), defining $\tilde{P}_n$. Formula (3.20) was obtained using the last diagram in Fig. 9 and all diagrams in Fig. 10. Formula (3.21) was obtained using the diagrams in Fig. 16. The lower and upper dashed lines in Figs. 9 and 10 represent the wall and the interface I_n, respectively.

These $\tilde{c}_n$ and $\tilde{a}_n$ are consistent with the recursion relations, which imply

$$\begin{aligned} \tilde{c}_{n+1} &= \tilde{c}_n + n + 7, \\ \tilde{a}_{n+1} &= \tilde{a}_n + \tilde{c}_n + 8n + 2. \end{aligned} \tag{3.22}$$

Then

$$\begin{aligned} \tilde{c}_n - \tilde{c}_{n-1} &= n + 6, \\ \tilde{a}_{n+2} - \tilde{a}_n &= (n-1)(n-2) + 33n - 7, \end{aligned} \tag{3.23}$$

and from this we obtain

$$\tilde{a}_{n+2} - \tilde{a}_n + 2\tilde{c}_n - 4\tilde{c}_{n-1} = 21n + 43. \tag{3.24}$$

Putting together (3.9) and the analog of (3.10) for $\tilde{P}_n$, $\tilde{Q}_n$, etc., and assuming $u = \mathcal{O}(t^2)$, gives for $n \geq 2$

$$\begin{aligned}
&B_n(u) - B_n(0) - t^2 B_{n+1}(0) \\
&\quad = (e^u - 1 - t^2 + t^3 - 4t^4 + 9t^5 - 23t^6 + 62t^7 - 139t^8)\tilde{P}_n \\
&\qquad + (e^{2u} - 1 - 2t^2 + 2t^3)\tilde{Q}_n + (-t^3 - 6t^4 + 11t^5 - 28t^6)\tilde{Q}_n^1 \\
&\qquad - (9t^4 - 20t^5)\tilde{Q}_n^2 + (e^{3u} - 1 - 3t^2 + 3t^3)\tilde{R}_n - (2t^3 + 10t^4)\tilde{R}_n^1 \\
&\qquad - t^3 \tilde{R}_n^2 + \mathcal{O}(t^{10}),
\end{aligned} \tag{3.25}$$

while from (3.9) and (3.18),

$$\begin{aligned}
t^4 B_{n+2}(0) &= t^5 - (n+1)t^6 + (\tilde{c}_{n+2} + 4)t^7 - (\tilde{a}_{n+2} + 4n + 5)t^8 \\
&\qquad + (\tilde{d}_{n+2} + 4\tilde{c}_{n+1} + 5n + 41)t^9 + \mathcal{O}(t^{10}),
\end{aligned} \tag{3.26}$$

$$t^6 B_{n+3}(0) = t^7 - (n+2)t^8 + (\tilde{c}_{n+3} + 4)t^9 + \mathcal{O}(t^{10}), \tag{3.27}$$

$$t^8 B_{n+4}(0) = t^9 + \mathcal{O}(t^{10}). \tag{3.28}$$

We now insert the series expansion of u in powers of t, (3.1),

$$\begin{aligned}
u &= -\ln(1 - t^2) + b_3 t^3 + \cdots + b_8 t^8 + b_9 t^9 + \mathcal{O}(t^{10}) \\
&= t^2 + b_3 t^3 + \left(b_4 + \frac{1}{2}\right)t^4 + b_5 t^5 + \left(b_6 + \frac{1}{3}\right)t^6 + b_7 t^7 \\
&\qquad + \left(b_8 + \frac{1}{4}\right)t^8 + b_9 t^9 + \mathcal{O}(t^{10}).
\end{aligned} \tag{3.29}$$

For such u, with $b_3 = -1$ and $b_4 = 4$ where b_3 and b_4 don't appear explicitly,

$$\begin{aligned}
e^u(1 - t^2) - 1 + e^u t^3 &= (b_3 + 1)t^3 + b_4 t^4 + (b_5 + 1)t^5 + \mathcal{O}(t^6) \\
&= 4t^4 + (b_5 + 1)t^5 + \left(b_6 - \frac{1}{2}\right)t^6 + (b_7 + 1)t^7 \\
&\qquad + (b_8 + 7)t^8 + (b_9 + C)t^9 + \mathcal{O}(t^{10}), \\
e^{2u} - 1 - 2e^u(t^2 - t^3) &= 2(b_3 + 1)t^3 + (2b_4 + 1)t^4 + \mathcal{O}(t^5) \\
&= 9t^4 + 2b_5 t^5 + (2b_6 + 10)t^6 + \mathcal{O}(t^7), \\
e^{3u} - 1 - 3e^u(t^2 - t^3) &= 3(b_3 + 1)t^3 + 3(b_4 + 1)t^4 + \mathcal{O}(t^5), \\
e^{4u} - 1 - 4e^u(t^2 - t^3) &= 4(b_3 + 1)t^3 + (4b_4 + 18)t^4 + \mathcal{O}(t^5)
\end{aligned} \tag{3.30}$$

and

$$\begin{aligned} e^u - 1 - t^2 + t^3 &= (b_3+1)t^3 + (b_4+1)t^4 + \mathcal{O}(t^5) \\ &= 5t^4 + (b_5-1)t^5 + \left(b_6 + \frac{11}{2}\right)t^6 + (b_7+b_5-5)t^7 \\ &\quad + \left(-b_5 + b_6 + b_8 + \frac{27}{2}\right)t^8 + \mathcal{O}(t^9), \end{aligned} \tag{3.31}$$

$$\begin{aligned} e^{2u} - 1 - 2t^2 + 2t^3 &= 2(b_3+1)t^3 + (2b_4+3)t^4 + \mathcal{O}(t^5) \\ &= 11t^4 + (2b_5-4)t^5 + (2b_6+22)t^6 + \mathcal{O}(t^7), \\ e^{3u} - 1 - 3t^2 + 3t^3 &= 18t^4 + \mathcal{O}(t^5). \end{aligned}$$

Then for $n \geq 2$, from (3.17), (3.30), (3.11),

$$\begin{aligned} &A_n(u) - A_n(0) - t^2 A_{n+1}(u) \\ &\quad = \left[(b_3+1)t^3 + (b_4-4)t^4\right]P_n + \mathcal{O}(t^5) \\ &\quad = (b_3+1)t^3 + \left[b_4 - 4 - (b_3+1)(n-5)\right]t^4 + \mathcal{O}(t^5), \end{aligned} \tag{3.32}$$

while from (3.25), (3.26), (3.31), (3.18),

$$\begin{aligned} B_n(u) - \sum_{m=0}^{\infty} t^{2m} B_{n+m}(0) &= \left[(b_3+1)t^3 + (b_4-3)t^4\right]\tilde{P}_n - t^5 + \mathcal{O}(t^6) \\ &= (b_3+1)t^4 + \left[b_4 - 4 - (b_3+1)(n-1)\right]t^5 + \mathcal{O}(t^6), \end{aligned} \tag{3.33}$$

giving

$$t^{-2n}(f_{n+1} - f_n) = (b_3+1)t^3 + \left[b_4 - 4 - (b_3+1)(n-4)\right]t^4 + \mathcal{O}(t^5). \tag{3.34}$$

If $b_3 = -1$, then from (3.17), (3.30), (3.11), still for $n \geq 2$,

$$\begin{aligned} &A_n(u) - A_n(0) - t^2 A_{n+1}(u) \\ &\quad = \left[(b_4-4)t^4 + (b_5+10)t^5\right]P_n - t^3 Q_n + \mathcal{O}(t^6) \\ &\quad = (b_4-4)t^4 + \left[b_5 + 6 - (b_4-4)(n-5)\right]t^5 - 2t^{n+3} + \mathcal{O}(t^6), \end{aligned} \tag{3.35}$$

giving

$$t^{-2n}(f_{n+1} - f_n) = (b_4-4)t^4 + \left[b_5 + 6 - (b_4-4)(n-4)\right]t^5 - 2t^{n+3} + \mathcal{O}(t^6). \tag{3.36}$$

If $b_4 = 4$, then from (3.17), (3.30), (3.11), now for $n \geq 3$,

$$\begin{aligned} &A_n(u) - A_n(0) - t^2 A_{n+1}(u) \\ &\quad = \left[(b_5+10)t^5 + \left(b_6 - \frac{1}{2} - 31\right)t^6\right]P_n + 9t^4 Q_n - (t^3 + 6t^4)Q_n^1 + \mathcal{O}(t^7) \\ &\quad = (b_5+6)t^5 + \left[b_6 - \frac{47}{2} - (b_5+6)(n-5)\right]t^6 - 2t^{n+3} + \mathcal{O}(t^7) \end{aligned} \tag{3.37}$$

while from (3.25), (3.31), (3.18),

$$B_n(u) - \sum_{m=0}^{\infty} t^{2m} B_{n+m}(0) = \left[t^4 + (b_5+8)t^5\right]\tilde{P}_n - t^3\tilde{Q}_n - t^5 + (n+1)t^6 + \mathcal{O}(t^7)$$
$$= (b_5+6)t^6 + \mathcal{O}(t^7) \tag{3.38}$$

giving

$$t^{-2n}(f_{n+1} - f_n) = (b_5+6)t^5 + \left[b_6 - \frac{47}{2} - (b_5+6)(n-4)\right]t^6 - 2t^{n+3} + \mathcal{O}(t^7). \tag{3.39}$$

If $b_5 = -6$, then from (3.17), (3.30), (3.11), now for $n \geq 4$,

$$\begin{aligned}
&A_n(u) - A_n(0) - t^2 A_{n+1}(u) \\
&\quad = \left[4t^5 + \left(b_6 - \frac{1}{2} - 31\right)t^6 + (b_7+89)t^7\right]P_n + [9t^4 - 12t^5]Q_n \\
&\qquad - (t^3 + 6t^4 - 9t^5)Q_n^1 - 9t^4 Q_n^2 - 2t^3 R_n^1 + \mathcal{O}(t^8) \\
&\quad = \left(b_6 - \frac{47}{2}\right)t^6 + \left[b_7 + 4(c_n - c_{n-1} - 3n) - \left(b_6 - \frac{65}{2}\right)(n-5) + 85\right]t^7 \\
&\qquad - 2t^{n+3} + \mathcal{O}(t^8) \\
&\quad = \left(b_6 - \frac{47}{2}\right)t^6 + \left[b_7 + 53 - \left(b_6 - \frac{47}{2}\right)(n-5)\right]t^7 - 2t^{n+3} + \mathcal{O}(t^8),
\end{aligned} \tag{3.40}$$

while from (3.25), (3.31), (3.18),

$$\begin{aligned}
&B_n(u) - B_n(0) - t^2 B_{n+1}(0) \\
&\quad = \left[t^4 + 2t^5 + \left(b_6 - \frac{35}{2}\right)t^6 + (b_7+51)t^7\right]\tilde{P}_n + (11t^4 - 16t^5)\tilde{Q}_n \\
&\qquad + (-t^3 - 6t^4 + 11t^5)\tilde{Q}_n^1 - 9t^4\tilde{Q}_n^2 - 2t^3\tilde{R}_n + \mathcal{O}(t^9) \\
&\quad = t^5 - (n+1)t^6 + \left[\tilde{c}_n + 2n + b_6 - \frac{7}{2}\right]t^7 \\
&\qquad + \left[b_7 - \tilde{a}_n + 2\tilde{c}_n - 4\tilde{c}_{n-1} - \left(b_6 + \frac{5}{2}\right)n + b_6 - \frac{41}{2}\right]t^8 + \mathcal{O}(t^9)
\end{aligned} \tag{3.41}$$

so that, with (3.26), (3.27), (3.24),

$$\begin{aligned}
&B_n(u) - \sum_{m=0}^{\infty} t^{2m} B_{n+m}(0) \\
&\quad = \left(b_6 - \frac{47}{2}\right)t^7 + \left[b_7 + b_6 + \tilde{a}_{n+2} - \tilde{a}_n + 2\tilde{c}_n - 4\tilde{c}_{n-1} - \left(b_6 - \frac{5}{2}\right)n - \frac{27}{2}\right]t^8 \\
&\qquad + \mathcal{O}(t^9) \\
&\quad = \left(b_6 - \frac{47}{2}\right)t^7 + \left[b_7 + 53 - \left(b_6 - \frac{47}{2}\right)(n-1)\right]t^8 + \mathcal{O}(t^9),
\end{aligned} \tag{3.42}$$

giving

$$t^{-2n}(f_{n+1}-f_n)=\left(b_6-\frac{47}{2}\right)t^6 + \left(b_7+53-\left(b_6-\frac{47}{2}\right)(n-4)\right)t^7-2t^{n+3}+\mathcal{O}(t^8). \quad (3.43)$$

If $b_6=\frac{47}{2}$, then from (3.17), (3.30), (3.11), now for $n\geq 5$,

$$\begin{aligned}
&A_n(u)-A_n(0)-t^2A_{n+1}(u)\\
&\quad=\big[4t^5-8t^6+(b_7+89)t^7+(b_8-258)t^8\big]P_n\\
&\qquad+(-t^3+3t^4-3t^5+19t^6)Q_n^1\\
&\qquad+8t^5Q_n^2+(-2t^3+5t^4)R_n^1-t^3R_n^2-4t^3S_n+\mathcal{O}(t^9)\\
&\quad=(b_7+53)t^7+\big[b_8-4(a_n-a_{n-1}+2c_n-4c_{n-1}+c_{n-2})\\
&\qquad-(b_7+53)(n-5)+36n-300\big]t^8-2t^{n+3}+\mathcal{O}(t^9)\\
&\quad=(b_7+53)t^7+\big[b_8-160-(b_7+53)(n-5)\big]t^8-2t^{n+3}+\mathcal{O}(t^9),
\end{aligned} \quad (3.44)$$

while (3.42) becomes

$$B_n(u)-\sum_{m=0}^{\infty}t^{2m}B_{n+m}(0)=(b_7+53)t^8+\mathcal{O}(t^9) \quad (3.45)$$

giving

$$\begin{aligned}
&t^{-2n}(f_{n+1}-f_n)\\
&\quad=(b_7+53)t^7+\big[b_8-160-(b_7+53)(n-4)\big]t^8-2t^{n+3}+\mathcal{O}(t^9).
\end{aligned} \quad (3.46)$$

Finally, if $b_7=-53$ then

$$\begin{aligned}
&A_n(u)-A_n(0)-t^2A_{n+1}(u)\\
&\quad=\big[4t^5-8t^6+36t^7+(b_8-258)t^8+(b_9+C)t^9\big]P_n\\
&\qquad+(-t^3+3t^4-3t^5+19t^6+Ct^7)Q_n^1+(8t^5+Ct^6)Q_n^2\\
&\qquad+(-2t^3+5t^4+Ct^5)R_n^1-(t^3+Ct^4)R_n^2-(4t^3+Ct^4)S_n+\mathcal{O}(t^9)\\
&\quad=(b_8-160)t^8+\big[b_9+4(d_n-d_{n-1})+8a_n-12a_{n-1}\\
&\qquad-4(a_{n-1}-a_{n-2})\\
&\qquad-24c_{n-1}-8c_{n-2}-4c_{n-3}-92n+C\big]t^9-2t^{n+3}+\mathcal{O}(t^{10})\\
&\quad=(b_8-160)t^8+\big[b_9-C-(b_8-160)(n-5)\big]t^9-2t^{n+3}+\mathcal{O}(t^{10}),
\end{aligned} \quad (3.47)$$

while from (3.25)–(3.28), (3.31), (3.45),

$$\begin{aligned}
&B_n(u) - \sum_{m=0}^{\infty} t^{2m} B_{n+m}(0) \\
&\quad = \big[t^4 + 2t^5 + 6t^6 - 2t^7 + (b_8 - 96)t^8\big]\tilde{P}_n + (11t^4 - 16t^5 + 69t^6)\tilde{Q}_n \\
&\qquad + (-t^3 - 6t^4 + 11t^5 - 28t^6)\tilde{Q}_n^1 - (9t^4 - 20t^5)\tilde{Q}_n^2 + (-2t^3 + 8t^4)\tilde{R}_n^1 \\
&\qquad - t^3 \tilde{R}_n^2 + \mathcal{O}(t^{10}) \\
&\quad = \big[b_8 + \tilde{d}_n - \tilde{d}_{n+2} - 2\tilde{a}_n + 4\tilde{a}_{n-1} - \tilde{c}_{n+3} - 4\tilde{c}_{n+1} + 6\tilde{c}_n + 20\tilde{c}_{n-1} - 4\tilde{c}_{n-2} \\
&\qquad + 87n + 130\big]t^9 + \mathcal{O}(t^{10}) \\
&\quad = (b_8 - 26)t^9 + \mathcal{O}(t^{10}),
\end{aligned} \tag{3.48}$$

giving

$$\begin{aligned}
t^{-2n}(f_{n+1} - f_n) = (b_8 - 160)t^8 + \big[b_9 - C - (b_8 - 160)(n-4)\big]t^8 \\
- 2t^{n+3} + \mathcal{O}(t^9).
\end{aligned} \tag{3.49}$$

Now, collecting (3.34), (3.36), (3.39), (3.43), (3.46), (3.49) gives (3.2)–(3.7) in Conjecture 2.

4 Phases 0, 1, 2

For $n = 0$, (2.3) takes the form

$$Z_0^\Lambda = e^{u|\Lambda_1|} \sum_{\{\gamma\}} \prod_{\gamma} \psi(\gamma) \tag{4.1}$$

with

$$\psi(\gamma) = t^{\frac{1}{2}|\gamma| - |\gamma \cap I_n|} e^{-u|\gamma \cap \{z = \frac{1}{2}\}|} \tag{4.2}$$

so that

$$\begin{aligned}
\log(Z_0^\Lambda) &= u|\Lambda_1| + \sum_{\omega} \psi^T(\omega) \\
&= u|\Lambda_1| + \sum_{\substack{\omega \in W \\ \omega \approx W_N}} \psi^T(\omega) + \sum_{\omega \approx W, W_N} \varphi_2^T(\omega)
\end{aligned} \tag{4.3}$$

while

$$\begin{aligned}
\log(Z_1^\Lambda) &= \sum_{\substack{\omega \in I_1 \\ \omega \approx W_N}} \varphi^T(\omega) + \sum_{\substack{\omega \sim I_1, \omega \in W \\ \omega \approx W_N}} \varphi^T(\omega) + \sum_{\substack{\omega \sim I_1 \\ \omega \approx W, W_N}} \varphi^T(\omega) \\
&= \sum_{\substack{\omega \in I_1 \\ \omega \approx W_N}} \varphi^T(\omega) + \sum_{\substack{\omega \sim I_1, \omega \in W \\ \omega \approx W_N}} \varphi_1^T(\omega) + \sum_{\substack{\omega \sim I_1 \\ \omega \approx W, W_N}} \varphi_2^T(\omega).
\end{aligned} \tag{4.4}$$

Therefore

$$\begin{aligned}
&\lim_{N\nearrow\infty} \log(Z_0^\Lambda/Z_1^\Lambda)\\
&\quad = u|\Lambda_1| + \sum_{\omega\in W}\psi^T(\omega) - \sum_{\omega\in I_1}\varphi^T(\omega) + \sum_{\substack{\omega\approx W\\ \omega\not\sim I_1}}\varphi_2^T(\omega) - \sum_{\substack{\omega\in W\\ \omega\sim I_1}}\varphi_1^T(\omega),
\end{aligned}\tag{4.5}$$

giving

$$\begin{aligned}
f_1 - f_0 &= u + (e^{-u}t^2 + 2e^{-2u}t^3) - (t^2 + e^u t^2 + 2t^3 + 2e^{2u}t^3) + t^3 + \mathcal{O}(t^4)\\
&= (b_3 - 1)t^3 + \mathcal{O}(t^4).
\end{aligned}\tag{4.6}$$

For $n = 1$, in order to use (2.12), we need $A_1(u)$, $A_2(u)$, $B_1(u)$, $B_2(0)$. The expansion

$$t^2 A_1(u) = e^u t^2 + 2e^{2u}t^3 + 6e^{3u}t^4 + e^{4u}t^4 - e^u t^4 - \frac{1}{2}e^{2u}t^4 - 2e^{2u}t^4 + \mathcal{O}(t^5)\tag{4.7}$$

gives

$$\begin{aligned}
t^2\big(A_1(u) - A_1(0)\big) &= (e^u - 1)t^2 + 2(e^{2u} - 1)t^3 + 6(e^{3u} - 1)t^4 + (e^{4u} - 1)t^4\\
&\quad - (e^u - 1)t^4 - \frac{1}{2}(e^{2u} - 1)t^4 - 2(e^{2u} - 1)t^4 + \mathcal{O}(t^7)\\
&= t^4 + (b_3 + 4)t^5 + (b_4 + 4b_3 + 17)t^6 + \mathcal{O}(t^7).
\end{aligned}\tag{4.8}$$

We then compute $A_2(u)$ using P_2, Q_2:

$$\begin{aligned}
P_2 &= (1 + 4t - t - 4t^2) + (12t^2 + 6t^2 + 4t^2 - 6t^2) + \mathcal{O}(t^3)\\
&= 1 + 3t + 12t^2 + \mathcal{O}(t^3)
\end{aligned}\tag{4.9}$$

where the first parenthesis is adapted from Fig. 3 and the second from Fig. 4. Also, adapted from Fig. 8,

$$\begin{aligned}
Q_2 &= 4t^2 - 4t^3 + 12t^3 - 5t^3 + 2t^2 + 12t^3 + \mathcal{O}(t^4)\\
&= 6t^2 + 15t^3 + \mathcal{O}(t^4)
\end{aligned}\tag{4.10}$$

giving

$$\begin{aligned}
t^4 A_2(u) &= e^u t^4(1 + 3t + 12t^2) + 6e^{2u}t^6 + \mathcal{O}(t^7)\\
&= t^4 + 3t^5 + 19t^6 + \mathcal{O}(t^7)
\end{aligned}\tag{4.11}$$

and

$$t^2 A_1(u) - t^2 A_1(0) - t^4 A_2(u) = (b_3 + 1)t^5 + (b_4 + 4b_3 - 2)t^6 + \mathcal{O}(t^7).\tag{4.12}$$

Then

$$t^2 B_1(u) = e^u t^3 + 2e^{2u}t^5 - e^u t^5 + \mathcal{O}(t^7),\tag{4.13}$$

$$t^4 B_2(0) = t^5 + \mathcal{O}(t^7),\tag{4.14}$$

$$t^2 B_1(u) - t^2 B_1(0) - t^4 B_2(0) = b_3 t^6 + \mathcal{O}(t^7) \tag{4.15}$$

so that finally

$$f_2 - f_1 = (b_3 + 1)t^5 + (b_4 + 3b_3 - 2)t^6 + \mathcal{O}(t^7), \tag{4.16}$$

which completes the derivation of (1.6).

5 Recursion Diagrams, $n \geq 3$

For the recursion relations (3.10) relating n to $n+1$, we consider ways in which a cluster $\omega \in I_n, W$ can be extended to produce a new $\omega' \in I_{n+1}, W$. One choice is that one or more

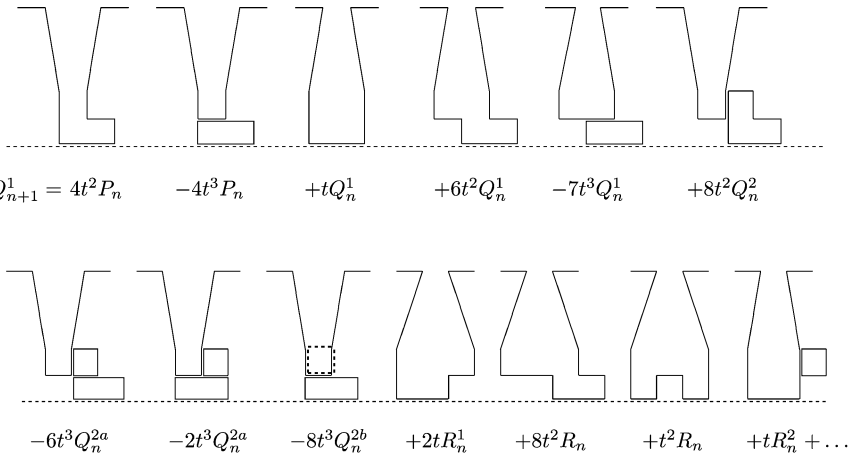

Fig. 11 Recursion for Q^1_{n+1}

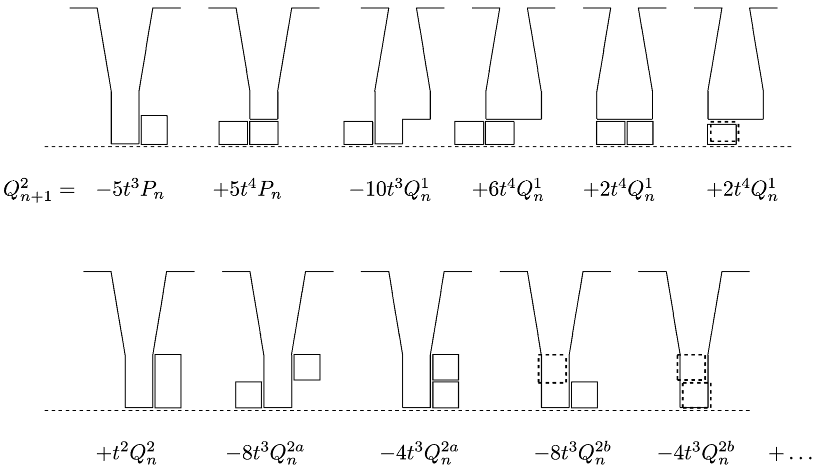

Fig. 12 Recursion for Q^2_{n+1}

contours in ω may be extended without adding contours or changing incompatibility relations within ω. Then the combinatoric factor in (2.6) is unchanged, only the $\varphi(\gamma)$ for the extended contours change, and it remains to find a geometric factor, the number of ways to extend the contour, or the number of diagrams of a given type.

Next, one may have $\omega' = \omega \cup \{\gamma'\}$ with the new contour incompatible with only one contour from ω. Then (2.6) gives $\varphi^T(\omega') = -\varphi(\gamma')\varphi^T(\omega)$, with $\varphi^T(\omega)$ taking into account possible contour extensions as in the first case.

Next, one may have $\omega' = \omega \cup \{\gamma'\}$ with the new contour incompatible with two contours γ_1, γ_2 from ω. At the order considered here, one may assume that $\gamma_1 \not\sim \gamma_2$ and that $\omega = \{\gamma_1, \gamma_2\}$ or $\omega = \{\gamma_0, \gamma_1, \gamma_2\}$. Then (2.6) gives

$$\varphi^T(\omega') = -2\varphi(\gamma')\varphi^T(\omega), \tag{5.1}$$

with $\varphi^T(\omega)$ taking into account possible contour extensions as in the first case. Formula (5.1) affects the coefficients in the 2nd and 3rd diagrams in the 2nd line of Fig. 11, and in the 3rd and 5th diagrams in the 2nd line of Fig. 12.

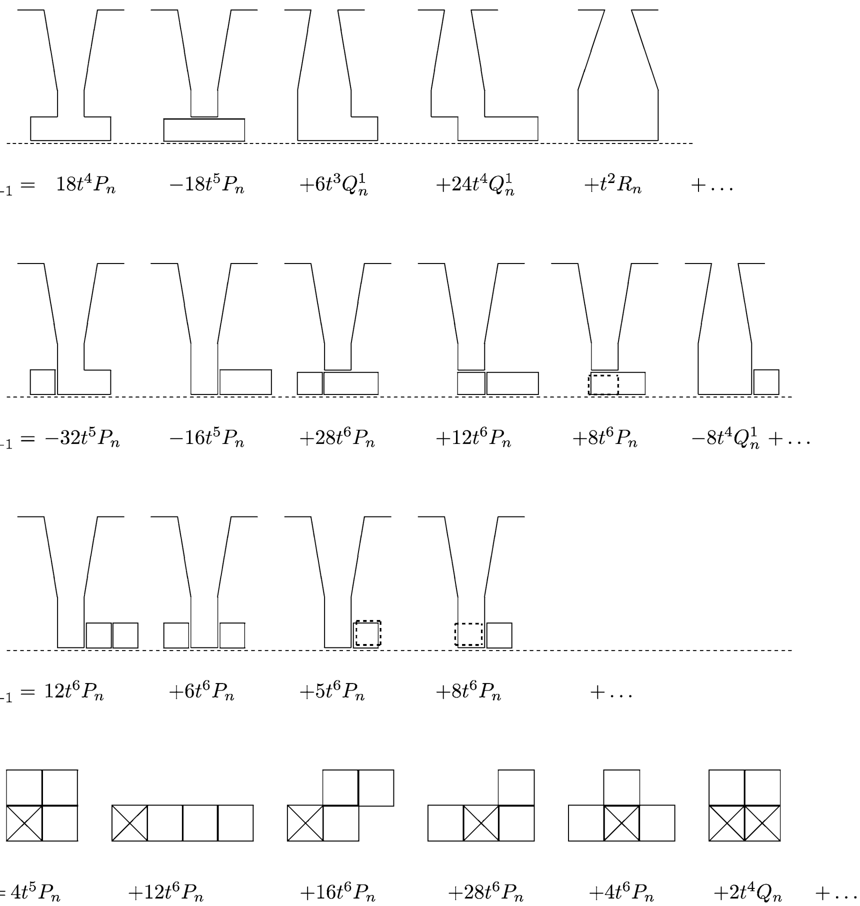

Fig. 13 Recursions for R^1_{n+1}, R^2_{n+1}, R^3_{n+1} and S_{n+1}. For S_{n+1}, the diagrams show a top view of the bottom layer, with $\times$ representing the location of a cube in the next layer up

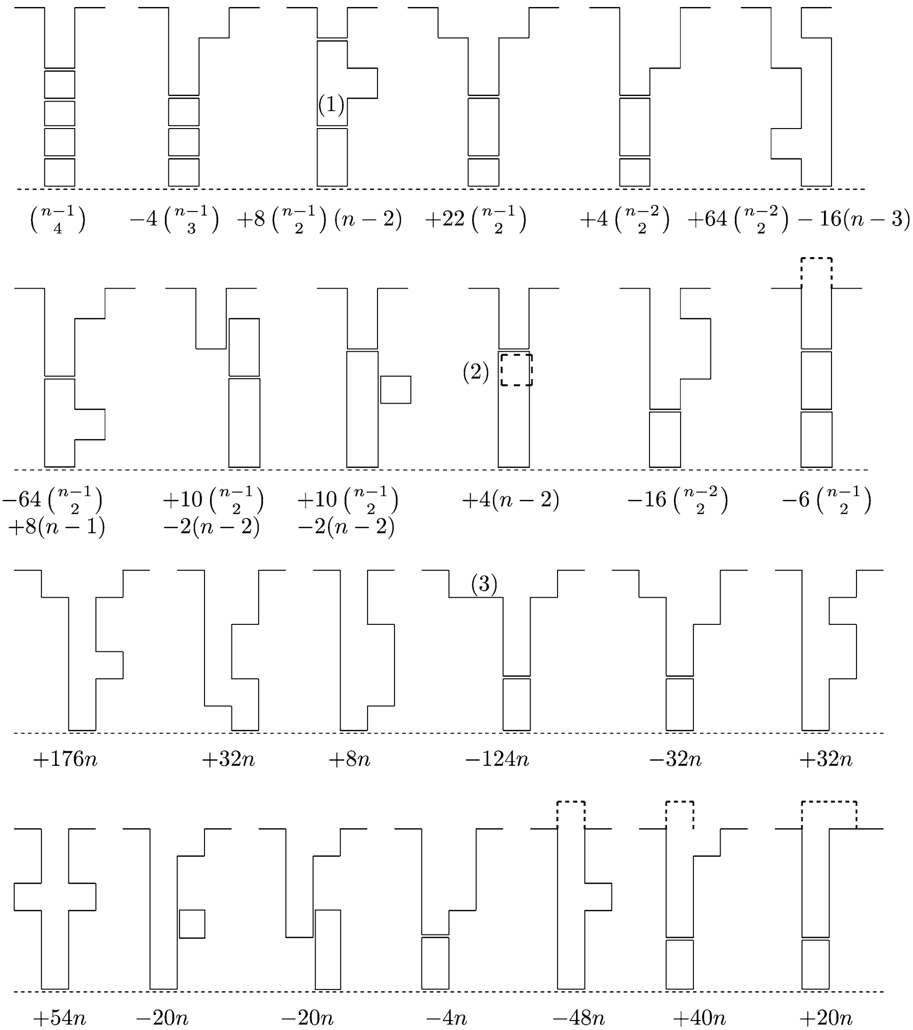

Fig. 14 P_n: t^4 terms dependent on n. Continuation downward from levels containing two cubes, as in configuration (1), may be from below either cube. Configurations (2) in which all three contours share a plaquette are excluded from the preceding two diagrams. For (3) see Fig. 15

The diagrams in Figs. 11 and 12 are idealized. The important feature in each is the bottom two layers; the rest is meant to be generic. Each diagram represents a layer added below the bottom of a height-n cluster, to create a height-$(n+1)$ cluster. The horizontal lines at the top represent pieces of I_{n+1}.

In Figs. 11 and 12, we have split Q_n^2 into Q_n^{2a} and Q_n^{2b}, the former corresponding to clusters in which the two cubes in the lowest level have disjoint interiors, and the latter corresponding to clusters in which these interiors are the same. Since the total contribution in each figure from Q_n^{2a} is the same as that from Q_n^{2b}, the split does not appear in (3.10).

Next, one may have $\omega' = \omega \cup \{\gamma_1', \gamma_2'\}$ with each of γ_1', γ_2' incompatible with at most one contour in ω. If $\gamma_2' \nsim \gamma_1' \nsim \omega$ and $\gamma_2' \sim \omega$, or $\gamma_2' \nsim \omega \nsim \gamma_1'$ and $\gamma_2' \sim \gamma_1'$, then (2.6) gives $\varphi^T(\omega') = \varphi(\gamma_1')\varphi(\gamma_2')\varphi^T(\omega)$, with $\varphi^T(\omega)$ taking into account possible contour extensions as

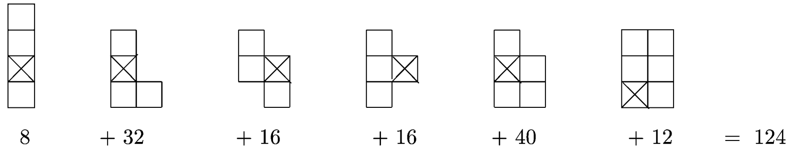

Fig. 15 Terms contributing to (3) in Fig. 14. Top view of the top layer is shown; $\times$ represents a possible location of the column below

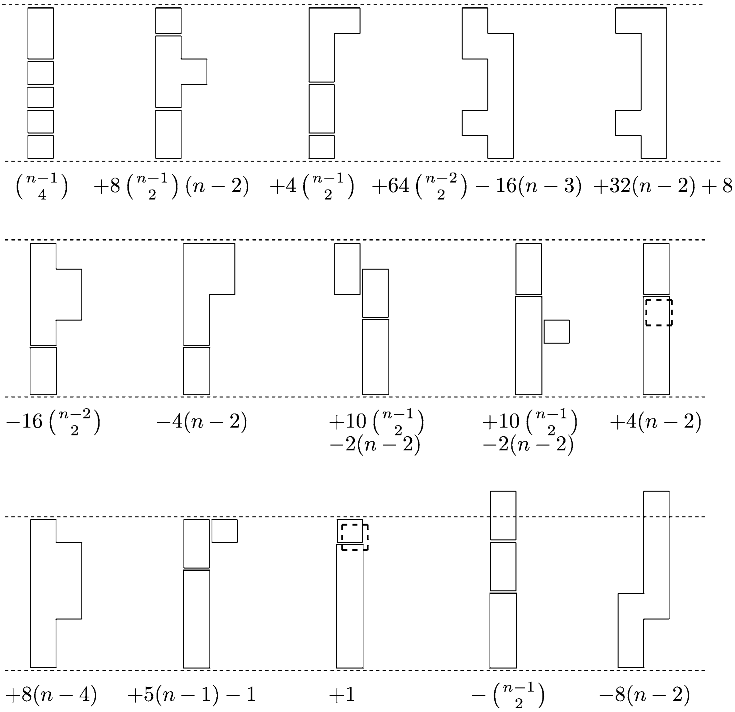

Fig. 16 $\tilde{P}_n$: t^5 terms dependent on n

in the first case. If $\gamma_2' \not\sim \gamma_1' \not\sim \omega \not\sim \gamma_2'$ and $\gamma_2' \neq \gamma_1'$, and γ_1' and γ_2' are incompatible with the same contour in ω, then (2.6) gives

$$\varphi^T(\omega') = 2\varphi(\gamma_1')\varphi(\gamma_2')\varphi^T(\omega), \tag{5.2}$$

with $\varphi^T(\omega)$ taking into account possible contour extensions as in the first case. Formula (5.2) occurs in the 5th diagram in the 1st line for Q_{n+1}^2 and in the 5th diagram for R_{n+1}^2 and in the last diagram for R_{n+1}^3. If $\gamma_2' = \gamma_1'$, then $\varphi^T(\omega') = \varphi(\gamma_1')\varphi(\gamma_2')\varphi^T(\omega)$, with $\varphi^T(\omega)$ taking into account possible contour extensions as in the first case.

Factors larger than the ± 2 in (5.1) and (5.2) are possible for extensions ω'. At the given orders, though, such factors do not appear in our formulas for $\varphi^T(\omega')$ or contribute to the recursion formulas (3.10), because the added contours, γ', or γ_1' and γ_2', do not create new cycles in the incompatibility graph other than possibly cycles of length 3, namely $\gamma' \not\sim \gamma_1 \not\sim \gamma_2 \not\sim \gamma'$ or $\gamma_1' \not\sim \gamma \not\sim \gamma_2' \not\sim \gamma_1'$.

6 Diagrams for the 7/8 Transition Line

See Figs. 14, 15 and 16.

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