

AN ALGORITHM FOR HIGH-ORDER STRONG-COUPPLING EXPANSIONS: The mass gap in 3d pure Z_2 lattice gauge theory ^{*}

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An efficient description of all clusters contributing to the strong coupling expansion of the mass gap in three-dimensional pure Z_2 lattice gauge theory is presented. This description is correct to all orders in the strong coupling expansion and is chosen in such a way that it remains valid in four dimensions for gauge group Z_2 . Relying on this description an algorithm has been constructed which generates and processes all the contributing graphs to the exact strong coupling expansion of the mass gap in the three-dimensional model in a fully automatic fashion. A major component of this algorithm can also be used to generate exact strong coupling expansions for the free energy $\log Z$. The algorithm is correct to any order; thus the order of these expansions is only limited by the available computing power. The presentation of the algorithm is such that it can serve as a guideline for the construction of a generalized one which would also generate exact strong coupling expansions for the masses of low-lying excited states of four-dimensional pure Yang-Mills theories.

1. Introduction

In the last years, in the framework of euclidean lattice gauge theory [1], several attempts have been made to compute the mass spectrum of pure gauge theories with abelian and nonabelian gauge groups in a reliable fashion. So far, however, neither within an analytic calculation of the mass levels by means of strong coupling expansions [2–4] nor in a numerical evaluation of the theory in a finite volume with the help of the Monte Carlo method (for a review see [5]), has this goal been achieved. In both cases, in order to obtain predictions for the physical masses, the

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cutoff(s) finally must be removed, i.e. if a denotes the lattice spacing, the continuum limit $a \rightarrow 0$ has to be performed and in addition, in case of a calculation in a finite volume V , the limit $V \rightarrow \infty$ has to be taken.

In the analytic approach, although the calculation is already performed in the infinite volume limit, the removal of the UV cutoff provided by the lattice regularization causes problems to the mass estimates calculated in the strong coupling regime because in general it must be assumed that the region of convergence of the strong coupling expansion does not extend to the physical region, $a \rightarrow 0$. Consequently, an essential ingredient in the calculation of physical masses starting from strong coupling expansions are series extrapolation techniques, such as for example Padé approximants, possibly in combination with series reexpansions. However, although their computation already has been very tedious, the currently available strong coupling expansions are much too short to apply extrapolation techniques unambiguously.

The Monte Carlo simulation in general suffers from both the UV lattice cutoff and the IR cutoff due to the finite size of the system. Up to the present, these systematic errors cannot be disentangled in a clear-cut way from the statistical errors inherent in the Monte Carlo method. Furthermore, an extra difficulty which arises in mass calculations stems from the fact that the mass is determined from the asymptotic decay of the connected (2-point) correlation function; however, the states generated by the operators currently in use have insufficient projection on the lowest mass eigenstate (whose mass is to be calculated) in any sector of states selected by the $J^{P(C)}$ transformation properties of the operators. Therefore at short distances the signal is still not dominated by the contribution from this lowest mass eigenstate and for large distances, the signal gets lost in the noise. The general belief is that improvement of the current status of mass calculations in the pure gauge sector by means of the Monte Carlo method will crucially depend on first of all the construction of low-dimensional operators generating states which have improved projection properties and secondly on the development of new calculational techniques and *not only* on the available computing power [6]. Given this context, a more ambitious investigation of analytic methods is motivated quite naturally.

There are in principle two possibilities to pursue: first of all one can try to extend the existing strong coupling expansions substantially such that series extrapolation techniques work more reliable. Secondly, being more sophisticated, one may try to construct effective large-distance actions by means of block-spin transformations which already in the strong coupling region will simulate continuum behaviour. However, exact block-spin transformations generate all kinds of complicated, nonlocal interactions which render the strong coupling expansion much more complicated. Consequently, in order to keep the calculation tractable, approximate block-spin transformations must be used and series extrapolation techniques cannot in general be avoided. As already mentioned above, these techniques only work reliably if many coefficients in the strong coupling expansion are available.

We conclude from the discussion above that the logical first step in a systematic investigation of analytic methods is the development of a tool which is capable of generating exact high-order strong coupling expansions.

It is the purpose of this article to report on the elaboration of such a device: We first present an efficient description of all clusters which contribute to the strong coupling expansion of the mass gap in three-dimensional pure Z_2 lattice gauge theory. Secondly, making use of this description, we describe the main components of an algorithm which can in principle generate exact strong coupling expansions of any order of the mass gap in the above model. Because this model is dual to the three-dimensional Ising model, the algorithm may be used to evaluate extended low-temperature expansions of the inverse correlation length of the latter model which by direct methods are very hard to get. This then again allows the determination of the critical temperature and the critical exponent ν' [7].

However, despite of the immediate physical relevance of this algorithm, we mainly consider this article as an introduction to algorithms which may be constructed for more general cases. In particular, the present algorithm could become a major building-block of a generalized one, being capable of generating also exact high-order strong coupling expansions for the masses of low-lying states of four-dimensional pure Yang-Mills theories.

Furthermore, along the lines described in this article similar algorithms could also be constructed for two other approaches: in the first one, partially summed strong coupling series would be computed where the partial summation is motivated by the requirements of the continuum [8] (for an elaboration of this idea and its application to the calculation of the free energy and string tension of the three-dimensional Z_2 lattice gauge theory see [9]). In the second approach, one would treat the full problem in a semianalytic calculation. This means, one would try to relate the beginning problem by exact analytic expansion techniques to a collection of problems which are not directly calculable by analytic methods, but which can be treated easily to *high precision* by Monte Carlo simulations. This semianalytic method would be useful in all cases where the full problem does not admit a reasonable complete analytic treatment. It seems possible that this approach might become a new and powerful field in which the potential of both methods, strong coupling expansion and Monte Carlo calculation, could be combined.

Finally, a major component of the algorithm which we shall describe in this article can be used to generate also exact high-order strong coupling expansions for the free energy $\log Z$.

The organization of this paper is as follows: Sect. 2 defines the model; sect. 3 defines the mass gap and sect. 4 discusses in detail the cluster expansion of the connected correlation function Γ . The determination of the strong coupling expansion of the mass gap from the cluster expansion of Γ is treated in sect. 5. Sect. 6 describes the distinct steps of the algorithm and its implementation on a computer. Finally, the two appendices A and B provide some basic definitions in mathematical

graph theory needed in this article and some factorization property of the usual combinatorial coefficients $\hat{a}(C_D)$, respectively.

2. The model

We consider pure Z_2 euclidean lattice gauge theory in three dimensions on a simple cubic lattice Λ with lattice spacing a . The dynamics of this model is specified by the action

$$S := \sum_{p \in \Lambda} S_p = \beta \sum_{p \in \Lambda} \chi(U_p), \tag{2.1}$$

which is the simple Wilson action. The sum runs over all unoriented plaquettes p of Λ . U_p is the product of the group-valued gauge fields attached to the links in the boundary of p . χ is the character of the nontrivial irreducible representation of Z_2 and the coupling parameter β is related to the bare coupling constant g_0 of the theory by

$$\beta = \frac{2}{g_0^2} a^{-1}. \tag{2.2}$$

3. The mass gap

The mass gap m is defined to be the lowest mass in the mass spectrum of the theory, i.e. m is the mass of the lowest mass eigenstate in the $J^P = 0^+$ sector. Consequently, m governs the asymptotic behaviour of the connected correlation function Γ : Let x_3 and t with $x_3 = ta$ denote the dimensionful and dimensionless time coordinate, respectively; for any two local lattice operators Θ_1, Θ_2 which create states out of the vacuum $|0\rangle$ which have nonzero projection on the eigenstate with mass m and zero momentum, we have

$$\begin{aligned} \Gamma(t) &:= \langle 0 | \Theta_1(t) \Theta_2(0) | 0 \rangle - \langle 0 | \Theta_1(t) | 0 \rangle \langle 0 | \Theta_2(0) | 0 \rangle \\ &\xrightarrow[t \rightarrow \infty]{} \text{const.} \times \exp(-mat). \end{aligned} \tag{3.1}$$

Using (3.1), the mass gap in lattice units can be obtained from Γ :

$$ma = - \lim_{t \rightarrow \infty} \frac{1}{t} \log \Gamma(t). \tag{3.2}$$

We now describe how the lattice operators Θ_1 and Θ_2 can be constructed. In order to make an optimal projection on the $J^P = 0^+$ sector, we choose Θ_1 and Θ_2 as space-like loops* transforming trivially under the symmetry group of the spatial

* For completeness, we note that a space-like loop is as usual a loop in a (hyper-) plane $t = \text{const}$: see also definition 4.6.

sublattice Λ_s . Adopting the simplest choice, in three dimensions Θ_1 and Θ_2 are just space-like plaquette operators $\chi(U_{p_1})$ and $\chi(U_{p_2})$. Furthermore, in order to project out the zero momentum part, we sum separately over all possible positions of p_1 and p_2 in the time-slices defined by the time coordinates of p_1 and p_2 respectively. Consequently, $\Theta_{1,2}$ can be written as

$$\Theta_{1,2}(t) = \frac{1}{\sqrt{N_s}} \sum_{(x_1, x_2) \in \Lambda_s} \chi(U_{(x_1, x_2); ta}), \tag{3.3}$$

where the sum runs over unoriented plaquettes only, Λ_s is the two-dimensional spatial sublattice and N_s is the number of sites of Λ_s .

4. The cluster expansion of the connected correlation function Γ

4.1. SOME PREPARATORY NOTATION

In order to provide the necessary formalism which will become important for the future construction of generalized algorithms, this subsection is held completely general.

Definition 4.1. A graph \mathcal{G} is a map which assigns an irreducible representation r_p of the gauge group G to every plaquette $p \in \Lambda$. We write $p \in |\mathcal{G}| \subset \Lambda \Leftrightarrow r_p \neq 0$. $|\mathcal{G}|$ is called the support of the graph \mathcal{G} and $r = 0$ denotes the trivial representation of G .

In general, depending on how many nontrivial irreducible representations G has, there may exist several graphs $\mathcal{G}, \mathcal{G}', \dots$ which all have the same support $|\mathcal{G}| = |\mathcal{G}'| = \dots = \mathcal{P}$. These graphs can be distinguished from each other by the distribution of the irreducible representations $r_p \neq 0$ over the plaquettes $p \in \mathcal{P}$. For example, for gauge group $G = Z_2$, to every support $|\mathcal{G}|$ we have exactly one graph \mathcal{G} .

We next define the contribution of a graph.

Definition 4.2. Let \mathcal{G} be a graph with support $|\mathcal{G}| \subset \Lambda$. The contribution or activity $\phi(\mathcal{G})$ of the graph \mathcal{G} is defined as

$$\phi(\mathcal{G}) := \int_G \prod_{b \in \Lambda} dU_b \prod_{p \in |\mathcal{G}|} d_{r_p} a_{r_p}(\beta) \chi_{r_p}(U_p), \tag{4.1}$$

or symbolically

$$\phi(\mathcal{G}) := \int_G \mathcal{G}. \tag{4.2}$$

dU is the invariant normalized Haar measure on the group manifold, d_{r_p} is the

dimension of the irreducible representation r_p assigned to the plaquette p , χ_{r_p} is the character in the irreducible representation r_p and $a_{r_p}(\beta)$ is the usual expansion coefficient [10]

$$a_{r_p}(\beta) := d_{r_p}^{-1} \frac{c_{r_p}(\beta)}{c_0(\beta)}, \tag{4.3}$$

where $c_{r_p}(\beta)$ and $c_0(\beta)$ are the character expansion coefficients for the irreducible r_p and trivial representation respectively of the single plaquette Boltzmann weight e^{S_p} : if r denotes any irreducible representation of the gauge group, we have

$$c_r(\beta) = \int_G dU_p \chi_r(U_p^{-1}) e^{S_p}. \tag{4.4}$$

As an immediate consequence of the orthogonality relation of the group characters,

$$\int_G dU \chi_r(UV) \chi_s(U^{-1}W) = \frac{\delta_{rs}}{d_s} \chi_s(VW), \quad U, V, W \in G, \tag{4.5}$$

a graph \mathcal{G} has only nonvanishing activity, if its support is a closed surface on the lattice which for gauge groups other than Z_2 may have branch-lines.

We now introduce the concept of connectedness which will play a central role in the subsequent discussion.

Definition 4.3. Let $\mathcal{P} \subset \Lambda$ be a set of plaquettes. \mathcal{P} is called disconnected \Leftrightarrow there exist disjoint subsets $\mathcal{P}_1, \mathcal{P}_2 \subset \mathcal{P}$, $\mathcal{P}_1 \cap \mathcal{P}_2 = \emptyset$ with $\mathcal{P} = \mathcal{P}_1 + \mathcal{P}_2$ which have the following property: let

$$B(\mathcal{P}_i) := \{ \ell | \ell \in \partial p \text{ for some } p \in \mathcal{P}_i \}, \quad i = 1, 2 \tag{4.6}$$

be the set of all links contained in the boundary of some $p \in \mathcal{P}_i$. Then there exists no loop of links which is contained in $B(\mathcal{P}_1) \cap B(\mathcal{P}_2)$. \mathcal{P} is called connected, if it is not disconnected.

It is clear that successive application of this definition to an arbitrary set $\mathcal{P} \subset \Lambda$ results in the unique decomposition into pairwise disconnected subsets which themselves are connected.

Graphs which have a connected support are of particular significance in the theory of cluster expansion.

Definition 4.4. Let $\mathcal{P} \subset \Lambda$ be a nonempty connected set of plaquettes. Any graph X with $|X| = \mathcal{P}$ is called a connected graph or polymer.

Definition 4.5. Let X_1, X_2, \dots be pairwise different polymers with supports $|X_1|, |X_2|, \dots \subset \Lambda$. Let $n_1, n_2, \dots \geq 1$. Then the collection

$$C := (X_1^{n_1}, X_2^{n_2}, \dots). \tag{4.7}$$

is called a cluster, if its support $|C| := |X_1| \cup |X_2| \cup \dots$ is connected. n_i is called the multiplicity of the polymer X_i in the cluster C . If C consists of only one polymer with multiplicity one, C is called a 1-polymer or single-polymer cluster. Otherwise C is called a multi-polymer cluster.

We close this subsection by defining some auxiliary notions.

Definition 4.6. Let $\ell \in \Lambda$ be a link and let $s_1, s_2 \in \Lambda$ be two sites which are the end points of ℓ . Then the time t_ℓ of ℓ is defined as

$$t_\ell := a^{-1} \text{ average}(\text{time coordinates of } s_1, s_2), \quad t_\ell \in \mathbb{R}. \tag{4.8}$$

With this notation, ℓ is called space-like, if t_ℓ is integer; otherwise ℓ is called time-like. Analogously, let $p \in \Lambda$ be a plaquette and let $s_1, s_2, s_3, s_4 \in \Lambda$ be four sites which are the corners of p . Then the time t_p of p is defined as

$$t_p := a^{-1} \text{ average}(\text{time coordinates of } s_1, s_2, s_3, s_4), \quad t_p \in \mathbb{R}. \tag{4.9}$$

p is called space-like, if t_p is integer; otherwise p is called time-like. If p is space-like (time-like), then $L = \{\ell_1, \ell_2, \ell_3, \ell_4\} := \partial p$ is called a space-like (time-like) loop and $t_L \equiv t_p$ denotes the (dimensionless) time of L .

4.2. THE CLUSTER EXPANSION

We now restrict mainly again to gauge group Z_2 . As Z_2 has only one nontrivial irreducible representation, to each support there exists exactly one graph. Thus the distinction between a graph and its support could be dropped. However, we shall keep it for the conceptual reason mentioned at the beginning of subsect. 4.1.

As already described in [2], with the simple choice (3.3) for the lattice operators \mathcal{O}_1 and \mathcal{C}_2 , we may obtain a strong coupling cluster expansion of Γ from the cluster expansion of $\log Z$ [10] in the following way:

$$\begin{aligned} \Gamma(t) &= \frac{1}{N_s} \sum_{(x_1, x_2) \in \Lambda_s} \sum_{(y_1, y_2) \in \Lambda_s} \left. \partial_{\beta_1} \partial_{\beta_2} \log Z(\beta, \beta_1, \beta_2) \right|_{\beta_1 = \beta = \beta_2} \\ &= \frac{1}{N_s} \sum_{(x_1, x_2) \in \Lambda_s} \sum_{(y_1, y_2) \in \Lambda_s} \left. \partial_{\beta_1} \partial_{\beta_2} \sum_C a(C)(\phi(C))(\beta, \beta_1, \beta_2) \right|_{\beta_1 = \beta = \beta_2}, \tag{4.10} \end{aligned}$$

where we introduced a plaquette-dependent coupling in the lattice action (2.1) which we choose to be β_1 for all plaquettes p_1 with $\chi(U_{p_1})$ contributing to Θ_1 , β_2 for all plaquettes p_2 with $\chi(U_{p_2})$ contributing to Θ_2 and β elsewhere. The further notation is the following. The third sum extends over all clusters $C = (X_1^{n_1}, X_2^{n_2}, \dots)$, $n_i \geq 1$. $\phi(C)$ is the activity of the (multi-) polymer cluster C which factorizes according to

$$\phi(C) = \prod_i \phi(X_i)^{n_i}. \tag{4.11}$$

For gauge group Z_2 the polymer activities $\phi(X_i)$ are simply given by

$$\phi(X_i) = \int_G \prod_{b \in \Lambda} dU_b \prod_{p \in |X_i|} d_f a_f(\beta) \chi_f(U_p) = u(\beta)^{\|X_i\|}, \tag{4.12}$$

where f denotes the nontrivial irreducible representation of Z_2 with $d_f = 1$, $\|X_i\| > 0$ is the number of plaquettes in the support $|X_i|$ and $u(\beta)$ is the usual strong coupling expansion variable $u(\beta) := a_f(\beta)$ which for gauge group Z_2 is given by

$$u(\beta) = \tanh \beta = \beta + O(\beta^3). \tag{4.13}$$

Finally, the combinatorial coefficients $a(C)$ take into account the multiplicities n_1, n_2, \dots of the polymers X_1, X_2, \dots and how they are connected:

$$\begin{aligned} a(C) &= \left\{ \prod_i n_i! \right\}^{-1} \hat{a}(C) \\ &= \left\{ \prod_i n_i! \right\}^{-1} [X_1, \dots, X_1, X_2, \dots, X_2, \dots], \end{aligned} \tag{4.14}$$

where the cumulant $\hat{a}(C) = [\dots]$ has n_1 arguments X_1 , n_2 arguments X_2, \dots and is defined as follows:

$$\begin{aligned} [Y_1, \dots, Y_N] &:= \sum_{k=1}^N (-1)^{k-1} (k-1)! \\ &\times \sum_{\text{part}(N, k)} \langle Y_{\alpha_1}, \dots, Y_{\omega_1} \rangle \langle Y_{\alpha_2}, \dots, Y_{\omega_2} \rangle \cdots \langle Y_{\alpha_k}, \dots, Y_{\omega_k} \rangle. \end{aligned} \tag{4.15}$$

The second sum runs over all partitions of the N polymers Y_1, Y_2, \dots, Y_N into k sets with no regard to the sequence within the sets or the sequence of the sets themselves; $1 \leq \omega_1, \omega_2, \dots, \omega_k \leq N$. The moments $\langle Y_{\alpha_l}, \dots, Y_{\omega_l} \rangle$, $l = 1, 2, \dots, k$ are defined as

$$\langle Y_{\alpha_l}, \dots, Y_{\omega_l} \rangle := \begin{cases} 1, & \text{if all pairs } (|Y_a|, |Y_b|), |Y_a|, |Y_b| \text{ in } (|Y_{\alpha_l}|, \dots, |Y_{\omega_l}|) \\ & \text{are disconnected otherwise,} \end{cases} \tag{4.16}$$

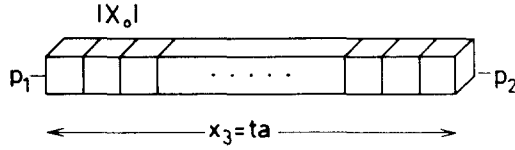


Fig. 1. The leading-order term in the cluster expansion of Γ which is the 1-polymer cluster X_0 illustrated by its support $|X_0| \cdot \chi(U_{p_{1,2}})$ contributing to $\mathfrak{C}_{1,2}$.

with

$$\langle \emptyset \rangle := 0. \tag{4.17}$$

With this definition of the moments, the cumulant (4.15) is zero unless the support of the corresponding cluster is connected. Another interesting property of $\hat{a}(C)$ will be discussed later.

4.2.1. *Leading-order term in the cluster expansion of Γ .* Every cluster contributing to (4.10) must necessarily contain some p_1 and some p_2 in its support which are separated t lattice spacings in time direction; p_1 and p_2 as defined in the context of (4.10). Hence, the leading-order contribution to the cluster expansion of Γ is the 1-polymer cluster X_0 whose support $|X_0|$ is geometrically the closed straight minimal tube connecting p_1 and p_2 (fig. 1) which has activity

$$\phi(X_0) = u(\beta_1)u(\beta_2)u^{4t}, \quad t := t_{p_2} - t_{p_1}, \tag{4.18}$$

which follows immediately from eqs. (4.12).

4.2.2. *Correction terms.* Two basic types of clusters can be distinguished which we call pure tube contributions and geometrical contributions respectively. For later use we keep their definition slightly more general than necessary, in so far as we admit arbitrary time differences between those space-like plaquettes of $|C|$ which have minimal and maximal time of all $p \in |C|$ respectively:

Definition 4.7. Let $C \neq X_0$ be a cluster with support $|C| \subset \Lambda$. Let $p_a, p_b \in |C|$ be two space-like plaquettes with time t_{p_a} and t_{p_b} respectively. Let for all $p \in |C|$ with time t_p be $t_{p_a} \leq t_p \leq t_{p_b}$. C is called a pure tube contribution \Leftrightarrow

- (i) p_a and p_b are not shifted spatially relative to each other.
- (ii) For all $t' = t_{p_a}, t_{p_a} + 1, \dots, t_{p_b}$, $|C|$ has a space-like circumference of four links.

C is called a geometrical contribution $\Leftrightarrow C \neq X_0$ is no pure tube contribution.

For an illustration of definition 4.7 we refer to figs. 2 and 3.

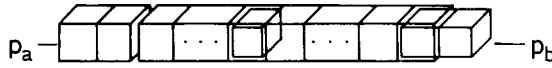


Fig. 2. The support of a cluster which is a pure tube contribution according to definition 4.7. Presented are the three basic types of pure tube contributions.

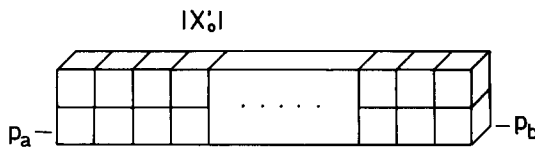
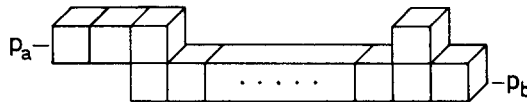
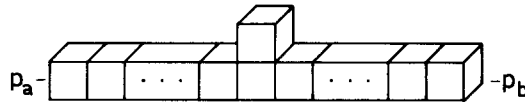


Fig. 3. The supports of three clusters which are geometrical contributions according to definition 4.7. Chosen are the simplest geometrical contribution, a more complicated one and the 1-polymer cluster X'_0 which will be also referred to in the text in subsect. 5.2.1.

5. Determination of the strong coupling expansion of m from the cluster expansion of Γ

5.1. LEADING-ORDER TERM

Using (3.2), the leading-order term $m^{(0)}$ of the mass gap $m := m^{(0)} + \Delta m$ can be immediately determined from (4.18). In lattice units, it reads

$$m^{(0)}a = -4 \log u. \tag{5.1}$$

5.2. CORRECTIONS

As already indicated at the end of sect. 3, the lattice operators $\mathcal{O}_{1,2}$ defined in (3.3) have non-vanishing matrix elements with, in particular, all mass eigenstates which are simultaneously (lattice) spin eigenstates with spin zero. Therefore the cluster expansion of Γ does not exponentiate with a single exponential with the decay constant provided by the mass gap. However, this desired behaviour can be achieved in the following way.

5.2.1. Truncation of the cluster expansion of Γ . We first note that without loss of generality we can always choose $t \gg n$ where n is the desired order of the strong coupling expansion of m . Restricting now to all those clusters C which have

$$\phi(C) < u^{6t} \quad (5.2)$$

complements the projection of $\mathcal{O}_{1,2}$ on the lowest mass eigenstate in the subspace of spin-zero eigenstates. This is the mass gap m :

$$\begin{aligned} \hat{\Gamma}(t) &:= \Gamma(t)|_{\text{cluster expansion, truncated}} \\ &= \text{const.} \times \exp(-mat). \end{aligned} \quad (5.3)$$

The reason why this truncation is necessary is that in the cluster expansion of Γ at order u^{6t} there exists a 1-polymer cluster X'_0 from which the leading term in the strong coupling expansion of the mass m' of the first excited state above the mass gap [11] can be derived. The support of X'_0 is geometrically the double tube, i.e. the support consists of all those plaquettes contained in the surface which is swept over by a space-like, planar 6-link loop when this loop is translated in time direction, starting at p_1 and ending at p_2 closed at each end which two adjacent space-like plaquettes (fig. 3).

Any cluster fulfilling (5.2) can be considered as a local modification of X'_0 ; the set of all these clusters which are constituting the truncated cluster expansion $\hat{\Gamma}$, i.e. the set of all the clusters which are relevant for the expansion of m will be denoted by \mathcal{C} .

5.2.2. Exponentiation of the truncated cluster expansion. Taking the logarithm of the truncated cluster expansion $\hat{\Gamma}$, it can be verified that the contributions to Δm arise from the t -linear term of this expansion. This procedure is in analogy to the case of the string tension [10]. As we shall not perform the proof of this exponentiation, further explanation is necessary, how the t -linear term is to be determined. This will be done in subsect. 5.2.3.

The problem is to generate the relevant set \mathcal{C} of clusters of the truncated cluster expansion $\hat{\Gamma}$ systematically up to the desired order. Aiming at a high-order calculation, though being straightforward, this is expected to be a quite difficult task,

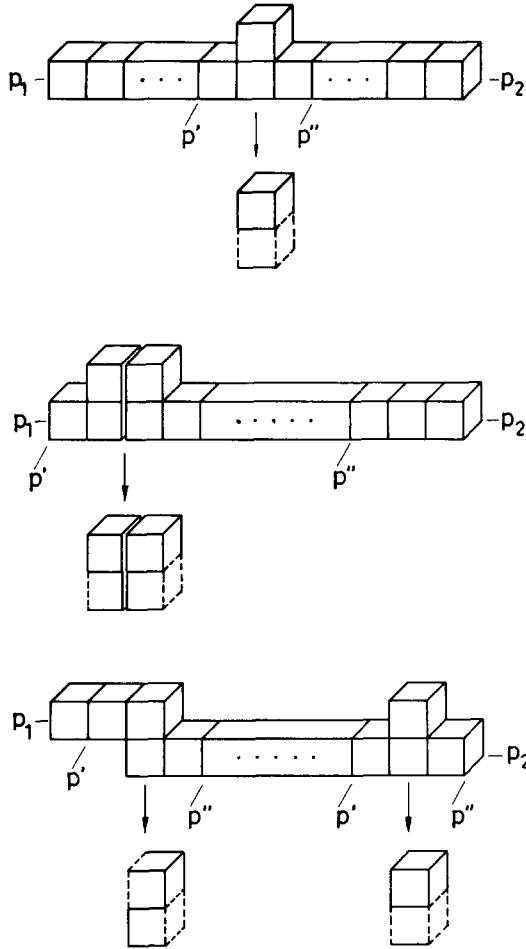


Fig. 4. Three clusters contributing to the truncated cluster expansion \hat{I} and corresponding possible collections of decorations. The illustration is as usual by the corresponding supports. The entrance and exit plaquettes p_{in} and p_{out} of the decorations are indicated by dashed lines.

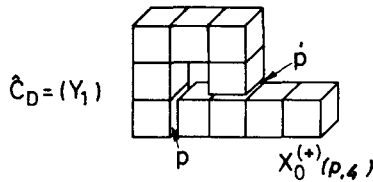


Fig. 5. Checking rule (iii) of definition 5.2 for a p_{out} candidate p of a 1-polymer cluster $\hat{C}_D = (Y_1)$. As $B(\hat{C}_D) \cap B(\chi_0^{(+)}(p, 4)) = \partial p \cup \partial p'$, p is not an admissible p_{out} according to definition 5.2.

with n^-, n^+ restricted by

$$n^- + v + n^+ = t := t_{p_2} - t_{p_1} \quad (5.7)$$

and the volume v of a decoration D is defined as:

Definition 5.3. Let $D = (\hat{C}_D, p_{in}, p_{out})$ be a decoration. The volume v of D is defined as

$$v := t_{p_{out}} - t_{p_{in}}. \quad (5.8)$$

For large t , i.e. neglecting the volume of D , there are essentially t pairs (n^-, n^+) which fulfill (5.7). Hence we obtain the result that a single decoration D collectively describes t clusters of the relevant set of clusters \mathcal{C} . In a sloppy manner of speaking, we shall sometimes say that “a single decoration represents all those clusters $C \in \mathcal{C}$ which transform into each other by translation of this decoration along the tube”. The above discussion analogously generalizes to the case where we have more than one decoration.

Summarizing, we note that mapping clusters to collections of decorations induces a decomposition of the set \mathcal{C} into subsets. It is obvious that this decomposition would imply a considerable simplification of the truncated cluster expansion, if the subsets of \mathcal{C} would be pairwise disjoint, i.e. if the representation of any cluster C by a collection of decorations would be unique. In addition, the cardinality of some subset, that is the number of the clusters represented by some collection of decorations, should be calculable easily from the properties of the representing collection of decorations.

However, this has not been achieved yet. We shall explain this heuristically with the help of fig. 4.

In the first two examples it is clear from the discussion following definition 5.3 that each decoration represents t clusters of \mathcal{C} . However, definition 5.2 does not forbid the possibility to represent each set of clusters by a collection of some other decorations which would extend from p' to p'' as indicated in the figure. Moreover, the second cluster might as well be represented by a collection of two identical decorations of the type given in the first example which touch each other. In this case we would say that the decoration given in the second example is “reducible”.

Closely related is a problem which arises in the third example; as one does not know so far if the two decorations may touch each other or not, the cardinality of the set of clusters represented by the two decorations remains unknown.

Finally, starting from some cluster \hat{C}_D , it is still ambiguous which of the space-like plaquettes of \hat{C}_D may serve as p_{in} and p_{out} . Although in general there will be several

because increasing the order of the calculation, the number of contributing clusters grows exponentially. A lot of these clusters may have a complicated geometry and even their topology may become nontrivial at already rather low order. Consequently, the first step in the generation of \mathcal{C} is the development of an efficient bookkeeping scheme.

We first introduce such a scheme for the subset of clusters which are geometrical contributions according to definition 4.7. Pure tube contributions will be discussed in subsect. 5.2.4.

5.2.3. *Decorations – an efficient bookkeeping device for geometrical contributions.* Before we come to the precise definition of a decoration, we define the important notion of a basic tube part.

Definition 5.1. A basic tube part of length j extending in positive time direction is a polymer $X_0^{(+)}(\mathbf{p}, j)$ with support

$$|X_0^{(+)}(\mathbf{p}, j)| := \begin{cases} \mathfrak{P}^{(+)}(\mathbf{p}, 0), & \text{if } j = 0 \\ \mathfrak{P}^{(+)}(\mathbf{p}, j), & \text{if } j > 0, \end{cases} \quad (5.4)$$

where $\mathfrak{P}^{(+)}(\mathbf{p}, 0) := \{\mathbf{p}\}$ is the set consisting of the single space-like plaquette $\mathbf{p} \in \Lambda$ with time $t_{\mathbf{p}}$ and $\mathfrak{P}^{(+)}(\mathbf{p}, j)$ is the set of all those plaquettes $\mathbf{p}' \in \Lambda$ which are contained in the surface of a closed straight minimal tube of length j beginning at the space-like plaquette \mathbf{p} and extending j lattice spacings in positive time direction where for all $t' = t_{\mathbf{p}}, t_{\mathbf{p}} + 1, \dots, t_{\mathbf{p}} + j$ the tube $\mathfrak{P}^{(+)}(\mathbf{p}, j)$ has a circumference of four links. Correspondingly, a basic tube part of length j extending in negative time direction is a polymer $X_0^{(-)}(\mathbf{p}, j)$ with support

$$|X_0^{(-)}(\mathbf{p}, j)| := \begin{cases} \mathfrak{P}^{(-)}(\mathbf{p}, 0), & \text{if } j = 0 \\ \mathfrak{P}^{(-)}(\mathbf{p}, j), & \text{if } j > 0, \end{cases} \quad (5.5)$$

where $\mathfrak{P}^{(-)}(\mathbf{p}, 0) := \{\mathbf{p}\}$ is the set consisting of the single space-like plaquette $\mathbf{p} \in \Lambda$ with time $t_{\mathbf{p}}$ and $\mathfrak{P}^{(-)}(\mathbf{p}, j)$ is the set of all those plaquettes $\mathbf{p}' \in \Lambda$ which are contained in the surface of a closed straight minimal tube of length j beginning at the space-like plaquette \mathbf{p} and extending j lattice spacings in negative time direction where for all $t' = t_{\mathbf{p}}, t_{\mathbf{p}} - 1, \dots, t_{\mathbf{p}} - j$ the tube $\mathfrak{P}^{(-)}(\mathbf{p}, j)$ has a circumference of four links.

Now, as any cluster $C \in \mathcal{C}$ fulfills (5.2), pictorially its support $|C|$ can be considered as composed of some of the basic tube parts defined above plus some

localized parts which are “thicker” than $|X_0|$. Stated differently, starting at $|C|$ and cutting out all basic tube parts, we end at a collection of certain objects; these objects are the supports of the decorations. Precisely*:

Definition 5.2. Let $\hat{C}_D := (Y_1^{n_1}, Y_2^{n_2}, \dots)$ be a cluster with support $|\hat{C}_D|$. Let \hat{C}_D be a geometrical contribution according to definition 4.7 and let $t_{p_b} - t_{p_a} \ll t$. A decoration is a collection of this cluster together with a choice of two plaquettes $p_{in}, p_{out} \in |\hat{C}_D|$ called entrance- and exit plaquette of D , $D := (\hat{C}_D, p_{in}, p_{out})$ with $|D| := |\hat{C}_D| \setminus \{p_{in}, p_{out}\} \Leftrightarrow p_{in}, p_{out}$ are chosen according to the following rules:

(i) p_{in}, p_{out} are space-like.

(ii) There exists exactly one $Y_m \in \hat{C}_D$ with support $|Y_m|$ and multiplicity $n_m = 1$ such that $p_{in} \in |Y_m|$; correspondingly, there exists exactly one $Y_n \in \hat{C}_D$ not necessarily distinct from Y_m with support $|Y_n|$ and multiplicity $n_n = 1$ such that $p_{out} \in |Y_n|$.

(iii) Consider $\hat{C}'_D := (Y_1^{n_1}, Y_2^{n_2}, \dots, X_0^{(-)}(p_{in}, j))$; according to definition 5.1 we have $|\hat{C}'_D| \cap |X_0^{(-)}(p_{in}, j)| = \{p_{in}\}$ for $j = 0$; then for all $j = 1, 2, \dots$ we demand $B(|\hat{C}'_D|) \cap B(|X_0^{(-)}(p_{in}, j)|) = \partial p_{in}$. Correspondingly for p_{out} ($X_0^{(-)} \rightarrow X_0^{(+)}, p_{in} \rightarrow p_{out}$).

Two decorations $D = (\hat{C}_D, p_{in}, p_{out})$ $D' = (\hat{C}'_D, p'_{in}, p'_{out})$ are identified, if \hat{C}_D, p_{in} and p_{out} translate into \hat{C}'_D, p'_{in} and p'_{out} respectively, i.e. decorations are only defined modulo translations.

Some examples for the illustration of the notion of decorations and basic tube parts are compiled in figs. 4 and 5.

The significance of the concept of a decoration follows from the property that it is defined modulo translations, i.e. a single decoration collectively describes a whole set of clusters of \mathcal{C} . As already indicated above, this set consists of all those clusters which can be obtained by complementing the decoration with suitable basic tube parts $X_0^{(-)}$ and $X_0^{(+)}$. More precisely, let $D = (\hat{C}_D, p_{in}, p_{out})$ with $\hat{C}_D := (Y_1^{n_1}, Y_2^{n_2}, \dots), p_{in} \in |Y_m|, p_{out} \in |Y_n|$; then the supports of the polymers of the cluster $C = (X_1^{n_1}, X_2^{n_2}, \dots) \in \mathcal{C}$ contained in the set of clusters described by D can be represented as follows:

$$|X_i| = |Y_i|, \quad \text{if } i \neq m, n,$$

$$|X_m| = |Y_m| \cup |X_0^{(-)}(p_{in}, n^-)| \setminus \{p_{in}\},$$

$$|X_n| = |Y_n| \cup |X_0^{(+)}(p_{out}, n^+)| \setminus \{p_{out}\}, \quad (5.6)$$

* Unless explicitly stated differently, the convention in the following is that C always denotes a cluster in the truncated cluster expansion \hat{T} , $C \in \mathcal{C}$, whereas \hat{C}_D stands for the cluster associated with some decoration D .

possibilities, this depends on whether or not we consider \hat{C}_D as a representative of a whole set of clusters $\{\hat{C}_D, \hat{C}'_D, \dots\}$ which can be transformed into each other by some symmetry operations (excluding translations in time direction), i.e. rotations around the time axis, reflection at a space-like plane, etc. Although such a grouping might be profitable in a hand calculation, it seems not to be adequate in view of the usage of this description in a fast computer algorithm: it has to be expected that the gain in computer time due to the fact that less terms have to be generated is easily over-compensated by the computer time consumption of the additional piece of algorithm needed to guarantee that these symmetries are respected by the algorithm. Consequently, the idea of considering clusters \hat{C}_D only modulo some symmetry operations will not be discussed in any further detail.

We conclude that so far there still exists some arbitrariness in the precise definitions of an ‘irreducible’ decoration, the determination of p_{in} and p_{out} and the evaluation of the cardinality of the set of clusters C represented by some collection of decorations. As the detailed analysis shows, there does not exist a uniquely fixed set of rules, and we are free to make for our purpose an adequate and convenient choice.

We retain the notion of p_{in} and p_{out} as defined previously. Next we introduce some further notions:

Definition 5.4. Let D be a decoration with support $|D|$ and volume v . Let $\|D\|$ be the number of plaquettes in $|D|$. Then the order $O(D)$ of D is defined as

$$O(D) := \|D\| - 4v. \tag{5.9}$$

Definition 5.5. Let $\hat{C}_D = (Y_1^{n_1}, Y_2^{n_2}, \dots)$ be a cluster with support $|\hat{C}_D|$. Let $B(|Y_i|)$ be the set of all links contained in the boundary of $p \in |Y_i|$, $Y_i \in \hat{C}_D$. A four-link loop L , $L = \{\ell_1, \ell_2, \ell_3, \ell_4\} \subset B(|Y_k|)$, $Y_k \in \hat{C}_D$ is called a bottle-neck of $\hat{C}_D \Leftrightarrow$

- (i) L is space-like.
- (ii) There exists no $p \in |Y_k|$ with $L = \partial p$.
- (iii) $n_k = 1$.
- (iv) L is not contained in any $B(|Y_i|)$ for $i \neq k$.

Let $X := \{x_1, x_2, x_3, x_4\}$ be the vertex set of L . Let $(V, B(|\hat{C}_D|))$ be the vertex-edge graph* associated with $|\hat{C}_D|$ where the vertex set V is the union of all boundary

* For a discussion of vertex-edge graphs and some of their properties which we shall need in the following we refer to appendix A.

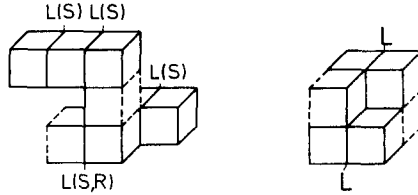


Fig. 6. The supports of two decorations with their entrance and exit plaquettes p_{in} and p_{out} as indicated by the dashed lines and their bottle-necks L . Bottle-necks marked with S are separating bottle-necks. The decorations are reducible at the bottle-necks marked with R.

points of the links of $B(|\hat{C}_D|)$. L is called a separating bottle-neck of $\hat{C}_D \Leftrightarrow X$ is a separating set of $(V, B(|\hat{C}_D|))$.

Pictorially, bottle-necks are four link space-like loops winding around exactly one polymer $Y_k \in \hat{C}_D$ with multiplicity $n_k = 1$. For an illustration of the notion of a bottle-neck see fig. 6.

We finally introduce the notion of an expansion. Roughly speaking, one obtains the expansion D_L of $D = (\hat{C}_D, p_{in}, p_{out})$ at the separating bottle-neck L of \hat{C}_D by decomposing \hat{C}_D at L into two disconnected pieces by removing the vertices of L , shifting these pieces one lattice spacing apart and closing the resulting hole with time-like links such that the resulting object is again connected:

Definition 5.6. Let $D = (\hat{C}_D, p_{in}, p_{out})$ be a decoration, $\hat{C}_D = (Y_1^{n_1}, Y_2^{n_2}, \dots)$ with support $|\hat{C}_D|$. Let $L = \{\ell_1, \ell_2, \ell_3, \ell_4\} \subset B(|Y_k|)$, $Y_k \in \hat{C}_D$ be a separating bottle-neck of \hat{C}_D with time t_L . Let $X := \{x_1, x_2, x_3, x_4\}$ be the vertex set of L . Let $(V, B(|Y_k|))$ be the vertex-edge graph embedded in the lattice associated with $|Y_k|$ where the vertex set V is the union of all boundary points of the links of $B(|Y_k|)$. $D_L := (\hat{C}'_D, p_{in}, p_{out})$ with $\hat{C}'_D = (\hat{Y}_1^{n_1}, \hat{Y}_2^{n_2}, \dots)$ is called the expansion of D at $L \Leftrightarrow$

- (i) $\hat{Y}_i = Y_i$ with support $|\hat{Y}_i| = |Y_i|$ for all those polymers $Y_i \neq Y_k$ for which all $p \in |Y_i|$ have $t_p < t_L$.
- (ii) $\hat{Y}_i = Y_i^{(+)}$ with support $|\hat{Y}_i| = |Y_i|^{(+)}$ for all those polymers $Y_i \neq Y_k$ for which all $p \in |Y_i|$ have $t_p \geq t_L$ where '(+)' indicates translation of $|Y_i|$ by one lattice spacing in positive time direction.
- (iii) \hat{Y}_k is a polymer with support $|\hat{Y}_k|$ defined in the following way: Following from the definition of a separating bottle-neck, the vertex-edge graph $(V, B(|Y_k|)) \setminus X$ decomposes into two parts which are not connected. The part which has $t_v \leq t_\ell$ for all its vertices is called left part, the part which has $t_v \geq t_\ell$ for all its vertices is called right part. Let \hat{L} be a copy of L but shifted one lattice spacing in positive time direction, $t_{\hat{L}} = t_L + 1$ and let $\hat{X} = \{\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4\}$ be the vertex set of \hat{L} . Then the vertex set \hat{V} of the

vertex-edge graph $(\hat{V}, B(|\hat{Y}_k|))$ associated with $|\hat{Y}_k|$ is the union of the vertex set of the left part with X and \hat{X} and the vertex set of the right part translated one lattice spacing in positive time direction; the set $B(|\hat{Y}_k|)$ of edges is the union of the set of edges of the left part with the set of edges of the translated right part and all the edges ℓ incident on X in $(V, B(|Y_k|))$ (translated one lattice spacing in positive time direction, if $t_\ell \geq t_L$) and the edges $\{x_1, \hat{x}_1\}, \{x_2, \hat{x}_2\}, \{x_3, \hat{x}_3\}$ and $\{x_4, \hat{x}_4\}$.

We are now prepared to provide a constructive criterion whether a decoration D is reducible:

Definition 5.7. Let $D = (\hat{C}_D, p_{in}, p_{out})$ be a decoration and let L be a separating bottle-neck of \hat{C}_D . Let D_L be the expansion of D at the separating bottle-neck L . D is reducible at $L \Leftrightarrow O(D_L) = O(D)$.

Now the precise definition of an irreducible decoration reads:

Definition 5.8. Let $D = (\hat{C}_D, p_{in}, p_{out})$ be a decoration as in the previous definition. D is irreducible $\Leftrightarrow D$ is not reducible at any separating bottle-neck L of \hat{C}_D .

Two examples for a reducible and an irreducible decoration respectively are compiled in fig. 6.

These rules are sufficient to provide a uniquely determined map from a cluster $C \in \mathcal{C}$ to a collection of irreducible decorations:

Partition Theorem. Let \mathcal{C} be the set of all clusters C contributing to the truncated cluster expansion \hat{F} as introduced in subsect. 5.2.1. Let \mathfrak{D} be the set of all irreducible decorations D^* . Then there exists a unique map

$$\mathfrak{F}_p: \begin{cases} \mathcal{C} \rightarrow \sum_{l \geq 1} \mathfrak{D}^l = \sum_{l \geq 1} \mathfrak{D} \times \dots \times \mathfrak{D}, \\ C \mapsto (D_1, \dots, D_k) \end{cases} \quad (5.10)$$

from \mathcal{C} into Cartesian products of \mathfrak{D} which maps any cluster $C \in \mathcal{C}$ to an ordered collection of not necessarily distinct decorations. The order of the decorations in the collection reflects the order of the local modifications in C . Furthermore, there exists a decomposition of \mathcal{C} into disjoint subsets, i.e.

$$\mathcal{C} = \mathcal{C}_1 + \mathcal{C}_2 + \dots, \quad (5.11)$$

with $\mathcal{C}_i \cap \mathcal{C}_j = \emptyset$ for all $i \neq j$ such that

$$C \text{ and } C' \text{ belong to the same subset } \mathcal{C}_i \Leftrightarrow \mathfrak{F}_p(C) = \mathfrak{F}_p(C'). \quad (5.12)$$

This means that there is a one-to-one correspondence between subsets \mathcal{C}_i and ordered collections (D_1, \dots, D_k) of irreducible decorations for some fixed k depending on \mathcal{C}_i .

* In the following D always stands for an irreducible decoration.

The proof is sketched as follows: Proving that to any $C \in \mathcal{C}$ the representing collection of irreducible decorations is uniquely determined, we make use of the fact that C itself may be considered as a necessarily reducible decoration D with entrance plaquette $p_{\text{in}} = p_1$ and exit plaquette $p_{\text{out}} = p_2$. Then we start for example at p_1 . It can easily be seen that the successive disintegration of D when proceeding along C in positive time direction is uniquely determined by the above set of definitions. Completely analogous for starting at p_2 .

Conversely, starting from the collection of irreducible decorations obtained above, we recover a cluster C' by connecting neighbouring $p_{\text{in}}, p_{\text{out}}$ plaquettes of neighbouring irreducible decorations with basic tube parts. C' belongs necessarily to the same subset \mathcal{C}_i as C because in definition 5.2 of a decoration, property (iii) imposed on p_{in} and p_{out} plaquettes prevents any irreducible decoration from being converted into another one by adding basic tube parts at p_{in} or p_{out} . ■

At this point, we would like to make several comments. First of all we emphasize that the above description of all the clusters in the truncated cluster expansion \hat{T} in terms of irreducible decorations is correct to all orders in the strong coupling expansion of m . Furthermore, for the definitions we do not make any reference to the geometrical properties of the clusters which eventually may not be fulfilled in more than three dimensions. Consequently, our description remains valid without any changes to mass calculations in four-dimensional pure Z_2 lattice gauge theories. Finally, modifying condition (ii) in definition 5.2 and condition (ii) in definition 5.5 the description becomes valid for arbitrary gauge group. Stated differently, the description presented above is already the major part of a generalized one which may be used for mass calculations in four-dimensional pure Yang-Mills theories.

The problem still to be solved is the evaluation of the cardinality of some given subset of clusters from the properties of the representing collection of irreducible decorations.

We consider a subset $\mathcal{C}_i \subset \mathcal{C}$ of clusters represented by an ordered collection (D_1, \dots, D_k) of decorations with volumes v_1, \dots, v_k . The corresponding cardinality will be denoted by N_k . The demand of reducibility of D_1, \dots, D_k at their p_{in} and p_{out} plaquettes implies in general that the decorations exclude each other from several positions on the tube. More precisely, the requirement of irreducibility imposes lower bounds on the lengths of the various basic tube parts which have to be supplemented such that a cluster $C \in \mathcal{C}_i$ is obtained. We denote the lower bound on the basic tube part between two neighbouring decorations D_i and D_j by v_{ij} and shall call it the exclusion volume of D_i for D_j . Then it follows from the detailed elaboration of the proof of the exponentiation that N_k has to be calculated according to the following rules:

- (i) Each individual decoration contributes a factor t , independent of the volume of the decoration.
- (ii) The numbers of positions, the decorations exclude each other on the tube have to be subtracted; boundary effects have to be omitted.

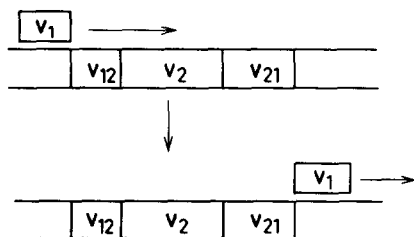


Fig. 7. The determination of the cardinality of a set of clusters represented by two decorations with volumes v_1, v_2 and exclusion volumes v_{12}, v_{21} .

The case $k = 1$ is trivial and was already discussed subsequently to definition 5.2. In the case $k = 2$, the above rules yield

$$N_2(v_1, v_{12}) + N_2(v_2, v_{21}) = t(t - (v_1 + v_{12} + v_2 + v_{21} - 1)) \quad (5.13)$$

(cf. fig. 7) and $N_2(v_1, v_{12})$ can be obtained from (5.13) by symmetric decomposition of the expression on the rhs.

We now return to the general case. As N_k specifies how many clusters of \mathcal{C} are represented by (D_1, \dots, D_k) , N_k is also called the configuration number of (D_1, \dots, D_k) . The t -linear coefficient of N_k is called reduced configuration number N_k^r and is according to subsect. 5.2.2 the weight with which the clusters of the subset \mathcal{C}_i contribute to the strong coupling expansion of m . Hence the contribution $\Delta m(\mathcal{C}_i)$ due to the clusters of the subset \mathcal{C}_i to the strong coupling expansion of m reads in lattice units

$$-\Delta m(\mathcal{C}_i)a = N_k^r(v_a, v_{ab})a(C)\hat{\phi}(C), \quad (5.14)$$

where $\hat{\phi}(C)$ is the relative activity of a generic cluster $C \in \mathcal{C}_i$, defined by

$$\hat{\phi}(C) := \phi(C)\phi(X_0)^{-1}. \quad (5.15)$$

We now express $\Delta m(\mathcal{C}_i)$ in terms of the contributions due to D_1, \dots, D_k . This then allows the convenient computation of (5.14) from the properties of the irreducible decorations alone.

The factorization of the relative activity follows immediately from the properties of irreducible decorations. As at the worst we have $B(|D_i|) \cap B(|D_j|) = L \subset B(|X|)$ (where L is a bottle-neck of a particular polymer X of C) for all $D_i \neq D_j$ in (D_1, \dots, D_k) any cluster $C \in \mathcal{C}_i$ can be integrated out “top down” at each decoration independently and consequently the relative activity $\hat{\phi}(C)$ factorizes according to

$$\hat{\phi}(C) = \prod_{j=1}^k \hat{\phi}(D_j). \quad (5.16)$$

For gauge group Z_2 , $\hat{\phi}(D_j)$ is according to (4.12) and (5.9)

$$\hat{\phi}(D_j) = u(\beta)^{O(D_j)}. \tag{5.17}$$

Now we still have to express $a(C)$ in terms of $a(\hat{C}_{D_1}), \dots, a(\hat{C}_{D_k})$, which amounts to proving that the cumulant $\hat{a}(C)$ factorizes into $\hat{a}(\hat{C}_{D_1}) \dots \hat{a}(\hat{C}_{D_k})$, since the product over the multiplicities factorizes trivially (cf. (4.14)). For the details of the proof see appendix B.

Consequently, the final expression for the contribution due to the subset \mathcal{C}_j of clusters C is in lattice units

$$-\Delta m(\mathcal{C}_j) a = N_k^f(v_a, v_{ab}) \prod_{j=1}^k \left\{ a(\hat{C}_{D_j}) \hat{\phi}(D_j) \right\}. \tag{5.18}$$

Concluding that by now the strong coupling expansion of the mass gap m is mapped to the determination of the set \mathfrak{D} of all irreducible decorations (leaving aside pure tube contributions), we have completed the discussion of geometrical contributions. The reduced configuration numbers $N_k^f(v_a, v_{ab})$ for $k = 2, 3$ and 4 are compiled in table 1.

5.2.4. *Corrections due to pure tube contributions.* All corrections of this type can be studied simultaneously in a tube model [4] where the transfer matrix T for gauge group Z_2 can be calculated exactly. Then the contribution $\Delta m(X_0)$ of all pure tube

TABLE 1
The reduced configuration numbers $N_k^f(v_a, v_{ab})$

$$N_2^f(v_1, v_{12}) = -\frac{1}{2} [2v_1 + 2v_{12} - 1]$$

$$N_3^f(v_1, v_{12}, v_2, v_{23}) = \frac{1}{2} \left[v_1^2 + 2v_1v_2 + 2v_1v_{12} + 2v_1v_{23} - 3v_1 \right. \\ \left. + 2v_2v_{12} + v_{12}^2 + 2v_{12}v_{23} - 3v_{12} + \frac{2}{3} \right]$$

$$N_4^f(v_1, v_{12}, v_2, v_{23}, v_3, v_{34}) = \frac{1}{6} \left[-v_1^3 - 3v_1^2v_2 - 3v_1^2v_3 - 3v_1^2v_{12} - 3v_1^2v_{23} \right. \\ - 3v_1^2v_{34} + 6v_1^2 - 3v_1v_2^2 - 6v_1v_2v_3 \\ - 6v_1v_2v_{12} - 6v_1v_2v_{23} - 6v_1v_2v_{34} + 12v_1v_2 \\ - 6v_1v_3v_{12} - 6v_1v_3v_{23} + 6v_1v_3 - 3v_1v_{12}^2 \\ - 6v_1v_{12}v_{23} - 6v_1v_{12}v_{34} + 12v_1v_{12} - 3v_1v_{23}^2 \\ - 6v_1v_{23}v_{34} + 12v_1v_{23} - 3v_1v_{34}^2 + 12v_1v_{34} \\ - 11v_1 - 3v_2^2v_{12} - 6v_2v_3v_{12} - 3v_2v_{12}^2 \\ - 6v_2v_{12}v_{23} - 6v_2v_{12}v_{34} + 12v_2v_{12} - 6v_3v_{12}v_{23} \\ - v_{12}^3 - 3v_{12}^2v_{23} - 3v_{12}^2v_{34} + 6v_{12}^2 - 3v_{12}v_{23}^2 \\ \left. - 6v_{12}v_{23}v_{34} + 12v_{12}v_{23} + 6v_{12}v_{34} - 11v_{12} + \frac{3}{2} \right]$$

contributions to the mass gap is given in lattice units by

$$-\Delta m(X_0)a = \log \frac{\lambda_2}{\lambda_1}, \tag{5.19}$$

where λ_1 and λ_2 are the largest and next-to-largest eigenvalues of T respectively.

Making use of the results obtained in the tube model, the generalization to the case where we have geometrical and pure tube contributions is straightforward. Employing the factorization of the cumulants (4.15) which will be proven in appendix B, it turns out that the combinatorial coefficients $a(C)$ of the full cluster, i.e. geometrical and pure tube contributions, is just proportional to $a(C_g)$ in which only the geometrical contributions are taken into account. The relative activity factorizes, too, which is of course again due to the properties of irreducible decorations.

With $\mathcal{C}_i, (D_1, \dots, D_k)$ and N_k^r as defined in subsect. 5.2.3, $\Delta m(\mathcal{C}_i, X_0)$ which denotes the contribution to m due to the subset \mathcal{C}_i of clusters C which now carry additional pure tube contributions, can be put into the final form

$$-\Delta m(\mathcal{C}_i, X_0)a = [N_k^r(v_a, v_{ab}) + F_k(v_a, v_{ab})] \prod_{j=1}^k \{a(\hat{C}_{D_j})\hat{\phi}(D_j)\}, \tag{5.20}$$

where all pure tube contributions are respected by F_k . The functions F_k are of the generic type

$$F_k(v_a, v_{ab}) = \sum_{l \geq 2} f_{kl}(v_a, v_{ab})u^l \tag{5.21}$$

and can be found in table 2. They are displayed for $k = 1, k = 2$ and $k = 3$ up to $O(\beta^{12}), O(\beta^8)$ and $O(\beta^4)$ respectively, which is sufficient for a $O(\beta^{16})$ calculation of m . They may be extended to higher order without any fundamental difficulties.

By the functions $F_k(v_a, v_{ab})$ pure tube contributions are completely covered; hence, the further discussion can be restricted to the question, how decorations can be treated any further.

5.2.5. The relationship between the set \mathfrak{D} of all irreducible decorations and the cluster expansion of $\log Z$. The first simplification in the determination of \mathfrak{D} follows from the defining property of a decoration, i.e. that every decoration D is a collection of a cluster \hat{C}_D together with a restricted but in general not uniquely fixed choice of two plaquettes:

Definition 5.9. Let \mathfrak{D} be the set of all irreducible decorations D and let $\hat{\mathcal{C}}$ be the set of all clusters \hat{C}_D , i.e. $\hat{\mathcal{C}}$ also contains those clusters \hat{C}_D which only result in reducible decorations for any choice $p_{in}, p_{out} \in |\hat{C}_D|$. Then for an irreducible decoration $D = (\hat{C}_D, p_{in}, p_{out}), D \in \mathfrak{D}$ with support $|D|$ and entrance and exit plaquettes

TABLE 2
The functions F_1 , F_2 and F_3 as defined in (5.21)

$$F_1(v_a, v_{ab}) = (v_1 + 1)u^2 + \frac{1}{2!}(v_1 + 1)(v_1 + 2)u^4 + \frac{1}{3!}(v_1 + 1) \dots (v_1 + 3)u^6 + 2(v_1 + 2)u^6 + \frac{1}{4!}(v_1 + 1) \dots (v_1 + 4)u^8 + [2(v_1 + 2)(v_1 + 3) - 4(v_1 + 2)]u^8 + \frac{1}{5!}(v_1 + 1) \dots (v_1 + 5)u^{10} + 2(v_1 + 3)u^{10} + [(v_1 + 2) \dots (v_1 + 4) - 4(v_1 + 2)(v_1 + 3) + 2(v_1 + 2)]u^{10} + \frac{1}{6!}(v_1 + 1) \dots (v_1 + 6)u^{12} + \left[\frac{1}{3}(v_1 + 2) \dots (v_1 + 5) - 2(v_1 + 2) \dots (v_1 + 4) + 2(v_1 + 2)(v_1 + 3) \right] u^{12} + [2(v_1 + 3)(v_1 + 4) + 2(v_1 + 2)(v_1 + 5) + 4 - 12(v_1 + 3) - 3(v_1 + 2)] u^{12} + O(\beta^{14})$$

$$F_2(v_a, v_{ab}) \quad \left(v := \sum_i v_i \right)$$

$$F_2(v_a, v_{ab}) = [N_2'(v_1, v_{12})(v + 2) - \delta_{v_{12,0}}]u^2 + \frac{1}{2!} [N_2'(v_1, v_{12})(v + 2)(v + 3) - 2\delta_{v_{12,0}}(v + 2)]u^4 + \frac{1}{3!} [N_2'(v_1, v_{12})(v + 2) \dots (v + 4) - 3\delta_{v_{12,0}}(v + 2)(v + 3)]u^6 + 2[N_2'(v_1, v_{12})(v + 4) - 3\delta_{v_{12,0}} - \delta_{v_{12,1}}]u^6 + \frac{1}{4!} [N_2'(v_1, v_{12})(v + 2) \dots (v + 5) - 4\delta_{v_{12,0}}(v + 2) \dots (v + 4)]u^8 + 2[N_2'(v_1, v_{12})(v + 4)^2 - 2\delta_{v_{12,0}}\{(v + 3) + (v + 4)\} - \delta_{v_{12,1}}(v + 4)]u^8 - 4[N_2'(v_1, v_{12})(v + 4) - 3\delta_{v_{12,0}} - \delta_{v_{12,1}}]u^8 + O(\beta^{10})$$

$$F_3(v_a, v_{ab}) \quad \left(v := \sum_i v_i \right)$$

(a) $v_{12} \geq 1, v_{23} \geq 1$.

$$F_3(v_a, v_{ab}) = [N_3'(v_1, v_{12}, v_2, v_{23})(v + 3)]u^2 + \frac{1}{2!} [N_3'(v_1, v_{12}, v_2, v_{23})(v + 3)(v + 4)]u^4 + O(\beta^6)$$

(b) $v_{12} \geq 1, v_{23} = 0$.

$$F_3(v_a, v_{ab}) = [N_3'(v_1, v_{12}, v_2, v_{23} = 1)(v + 3)]u^2 + [N_2'(v_1, v_{12})(v + 2)]u^2 + \frac{1}{2!} [N_3'(v_1, v_{12}, v_2, v_{23} = 1)(v + 3)(v + 4)]u^4 + \frac{1}{2!} [N_2'(v_1, v_{12})(v + 2)(v + 3)]u^4 + O(\beta^6)$$

TABLE 2 (continued)

(c) $v_{12} = 0, v_{23} \geq 1$.

$$\begin{aligned}
 F_3(v_a, v_{ab}) &= [N_3^r(v_1, v_{12} = 1, v_2, v_{23})(v + 3)] u^2 \\
 &\quad + [N_2^r((v_1 + v_2), v_{23})(v + 2)] u^2 \\
 &\quad + \frac{1}{2!} [N_3^r(v_1, v_{12} = 1, v_2, v_{23})(v + 3)(v + 4)] u^4 \\
 &\quad + \frac{1}{2!} [N_2^r((v_1 + v_2), v_{23})(v + 2)(v + 3)] u^4 + O(\beta^6)
 \end{aligned}$$

(d) $v_{12} = 0, v_{23} = 0$.

$$\begin{aligned}
 F_3(v_a, v_{ab}) &= [N_3^r(v_1, v_{12} = 1, v_2, v_{23} = 1)(v + 3)] u^2 \\
 &\quad + [\{N_2^r(v_1, v_{12} = 1) + N_2^r((v_1 + v_2), v_{23} = 1)\}(v + 2)] u^2 \\
 &\quad + [(v + 1)] u^2 \\
 &\quad + \frac{1}{2!} [N_3^r(v_1, v_{12} = 1, v_2, v_{23} = 1)(v + 3)(v + 4)] u^4 \\
 &\quad + \frac{1}{2!} [N_2^r(v_1, v_{12} = 1)(v + 2)(v + 3)] u^4 \\
 &\quad + \frac{1}{2!} [N_2^r((v_1 + v_2), v_{23} = 1)(v + 2)(v + 3)] u^4 \\
 &\quad + \frac{1}{2!} [(v + 1)(v + 2)] u^4 + O(\beta^6)
 \end{aligned}$$

p_{in}, p_{out} the map \mathfrak{F}_Z is defined as

$$\mathfrak{F}_Z: \begin{cases} \mathfrak{D} \rightarrow \hat{\mathcal{C}}, \\ D \mapsto \hat{\mathcal{C}}_D \end{cases} \tag{5.22}$$

where $|\hat{\mathcal{C}}_D| := |D| \cup \{p_{in}, p_{out}\}$ and p_{in}, p_{out} carry the nontrivial irreducible representation of the gauge group Z_2 .

The map \mathfrak{F}_Z is onto because in general there exist several irreducible decorations which are all mapped to the same cluster $\hat{\mathcal{C}}_D$. Consequently, the map \mathfrak{F}_Z induces a decomposition of the set \mathfrak{D} .

Moreover, $\hat{\mathcal{C}}$ is identified with the set of clusters which constitutes the cluster expansion of the free energy $\log Z$. Thus, with the help of the map $\mathfrak{F}_Z \circ \mathfrak{F}_p$, the cluster expansion of $\hat{\Gamma}$ is reduced to the cluster expansion of $\log Z$.

The first step in the cluster expansion of $\log Z$, i.e. in the determination of the set $\hat{\mathcal{C}}$ is the classification of all $\hat{\mathcal{C}} \in \hat{\mathcal{C}}^*$ according to the supports of the included

* As in the following there will be no more reference to the irreducible decoration associated with a cluster $\hat{\mathcal{C}}$, we drop the subscript D in order to avoid clumsy notation.

polymers. This means that we perform the map

$$\mathfrak{S} : \begin{cases} \hat{\mathcal{C}} \rightarrow \mathfrak{S} \\ \hat{\mathcal{C}} = (Y_1^{n_1}, Y_2^{n_2}, \dots) \mapsto S(\hat{\mathcal{C}}) := (|Y_1|^{n_1}, |Y_2|^{n_2}, \dots). \end{cases} \quad (5.23)$$

As the gauge group Z_2 has only one nontrivial irreducible representation, this step is trivial in the case under consideration because the map is one-to-one.

The next step is to characterize each collection $S(\hat{\mathcal{C}})$ of polymer supports of a cluster $\hat{\mathcal{C}}$ with support $|\hat{\mathcal{C}}|$ according to its volume $V_{S(\hat{\mathcal{C}})}$. This amounts to a classification of the elements \mathfrak{S} according to identical volumes. For example, all clusters $\hat{\mathcal{C}}, \hat{\mathcal{C}}', \dots$ which consist of the same choice of polymers but which have different multiplicities $n_1 \neq n_1', \dots, n_2 \neq n_2', \dots$ assigned to them are mapped to different collections $S(\hat{\mathcal{C}}), S(\hat{\mathcal{C}}'), \dots$, but have the same volume V :

Definition 5.10. Let $|\hat{\mathcal{C}}|$ be the support of a cluster $\hat{\mathcal{C}} \in \hat{\mathcal{C}}$ with $S(\hat{\mathcal{C}}) = \mathfrak{S}(\hat{\mathcal{C}})$ and let $\{A_1, A_2, \dots\}$ be the complete set of all subsets of $|\hat{\mathcal{C}}|$ which satisfy

$$\partial A_i = 0, \quad i = 1, 2, \dots, \quad (5.24)$$

where the boundary is to be computed modulo Z_2 and the subsets A_i are considered as chains of plaquettes. (5.24) implies the existence of volumes V_{A_i} with $\partial V_{A_i} = A_i$. Then the volume $V_{S(\hat{\mathcal{C}})}$ of $S(\hat{\mathcal{C}})$ is defined by

$$V_{S(\hat{\mathcal{C}})} = \bigcup_{A_i} V_{A_i}. \quad (5.25)$$

The notion of the volume is illustrated in fig. 8.

Now, as already indicated above, the classification of all $S(\hat{\mathcal{C}})$ according to their volumes induces a decomposition of the set \mathfrak{S} into pairwise disjoint subsets,

$$\mathfrak{S} = \sum_{V \in \mathfrak{V}} \mathfrak{S}_V, \quad \mathfrak{S}_V \cap \mathfrak{S}_{V'} = \emptyset \quad \text{for all } V \neq V', \quad (5.26)$$

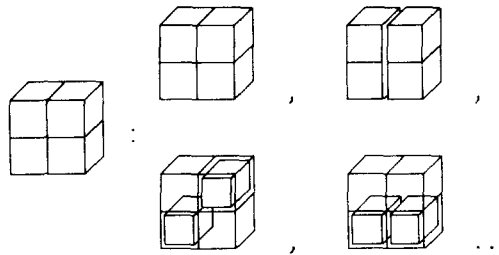


Fig. 8. The supports of four clusters which have the same volume.

where $\mathcal{S}_V \subset \mathcal{S}$ is the set of all $S(\hat{C})$ which have volume V and the sum runs over the set \mathcal{V} of all volumes. Note that each ∂V itself is the support of a 1-polymer cluster $\hat{C} = (Y_V)$ with $S(\hat{C}) = (|Y_V|) = (\partial V)$. Consequently we have $\partial V \in \mathcal{S}_V$ for all V .

We finally discuss how \mathcal{S}_V can be reconstructed from the volume V . This is essentially the reversal of the construction presented in definition 5.10: On the lattice, the volumes have a cell structure, i.e. they may be considered as connected chains

$$V = \sum_k c_k, \quad c_k \neq c_{k'} \Leftrightarrow k \neq k' \tag{5.27}$$

of cubes c_k of the lattice.

Definition 5.11. Let V be a connected chain of cubes on the lattice with volume V . Let $w_1, w_2, \dots \subseteq V$ be connected subchains of V . Then the collections \hat{V} are defined as

$$\hat{V} := (w_1^{n_1}, w_2^{n_2}, \dots), \quad n_i \geq 1, \tag{5.28}$$

where

$$\bigcup_{w_i} w_i = V. \tag{5.29}$$

Using the cell structure, the generation of all non-equivalent collections \hat{V} derived from some connected chain V is not very complicated. Identification of ∂w_i with $|Y_i|$ completes the reconstruction of \mathcal{S}_V .

5.2.6. *The Cluster expansion of $\log Z$ and point configurations on the dual lattice.* The remaining step in the cluster expansion of $\log Z$ and therefore in the truncated cluster expansion of \hat{T} as well as in the strong coupling expansion of the mass gap m is the determination of \mathcal{V} .

The essential trick is the utilization of the duality transformation $*$; in particular, duality maps cubes $c \in \Lambda$ one-to-one to points $a^* \in \Lambda^*$,

$$* : \begin{cases} \Lambda \rightarrow \Lambda^* \\ c \mapsto a^*, \end{cases} \tag{5.30}$$

where the dual lattice Λ^* is isomorphic to Λ because the simple cubic lattice is self-dual [12]. Hence, by duality, the determination of \mathcal{V} is mapped to the easier task of generating a certain set of point configurations on Λ^* .

Next we note that up to volumes which result in corrections to m of $O(\beta^{24})$ and more*, the cubes of all volumes have the additional property of being plaquette-connected:

* The minimal volume of this type is composed of six cubes which are arranged in a completely symmetric way, i.e. any two cubes share one link only.

Definition 5.12. Let V be a chain of cubes on Λ . V is called plaquette-connected (p-connected) \Leftrightarrow there exist no $V_1, V_2 \subset V$ such that $V = V_1 + V_2$ and $V_1 \cap V_2 = \emptyset$ with $\{p|p \in \partial c, \text{ for some } c \in V_1\} \cap \{p|p \in \partial c, \text{ for some } c \in V_2\} = \emptyset$.

Although the generation of the set of all point configurations (including those which are not dual to p-connected chains) causes no fundamental difficulties, we restrict the following discussion to the subset of point configurations which is dual to the set of p-connected chains. From a practical point of view this is a completely irrelevant restriction because a computation of m up to $O(\beta^{24})$ is not feasible at least in the near future due to lack of computer power.

With this limitation in mind, we have

$$\begin{array}{ll}
 c_1, c_2 \in \Lambda & \text{p-connected} \Leftrightarrow c_2 \in \nabla \partial c_1 \\
 \downarrow^* & \downarrow^* \\
 a_1^*, a_2^* \in \Lambda^* & \text{co-p-connected} \Leftrightarrow a_2^* \in \partial \nabla a_1^*,
 \end{array} \tag{5.31}$$

where we identify a_1^* and a_2^* to be link-connected points on Λ^* . Consequently, the duality transformation (5.30) maps p-connected chains V on Λ to link-connected point configurations K on Λ^* .

How should a useful algorithm for the generation of these point configurations look like? First of all, as we expect a very large number of these configurations needed in a high order computation of Δm , the algorithm should be such that each configuration is generated in a unique way because due to computer storage requirements one cannot afford to store the data of all configurations and to scan through this set each time a new configuration is generated in order to avoid double-counting. Secondly, in order to meet the speed requirements, a fast algorithm should be such that in the average only a very small number of operations is needed to generate a new point configuration from the previous one. This can be achieved if the algorithm provides for a tree structure on the set of point configurations. This then would avoid double-counting by construction.

Now we describe such an algorithm in detail. For notational convenience, we agree upon dropping the superscripts $*$ in the following. That we actually deal with the dual lattice and with quantities defined on it is to be understood implicitly. Furthermore, we choose the (dual) lattice to be finite; the following construction can of course also be performed if this restriction is dropped. However, the limitation to a finite lattice allows us to keep the presentation as close to the actual algorithm as possible.

Definition 5.13. Let $\Lambda = L \times L \times L \subset \mathbb{Z}^3$ be a simple cubic lattice with lattice spacing $a = 1$ and linear extent L . A lattice point $s \in \Lambda$ is a triple of integer numbers $s = (n_1, n_2, n_3)$. Without loss of generality we choose the coordinate frame such that

$$s = (n_1, n_2, n_3) \in \Lambda \Leftrightarrow 0 \leq n_i \leq L. \tag{5.32}$$

Then the map

$$\mathcal{L}: \begin{cases} \mathbb{Z}^3 \supset \Lambda \rightarrow \hat{\Lambda} \subset \mathbb{N}_0 \\ s = (n_1, n_2, n_3) \mapsto \hat{s} = n_1 + (L + 1)n_2 + (L + 1)^2 n_3 \end{cases} \quad (5.33)$$

is linear and one-to-one for all $s \in \Lambda$. \mathcal{L} is called linearization of Λ .

Before we give the precise definition of a link-connected point configuration K , we define some elementary geometrical properties of Λ .

Definition 5.14. Two lattice points $a, b \in \Lambda$ are called neighbouring $\Leftrightarrow |\hat{a} - \hat{b}| \in \{1, L + 1, (L + 1)^2\}$.

Next we define an order relation. The canonical ordering of the natural numbers \mathbb{N}_0 induces an ordering of lattice points of Λ by means of the map \mathcal{L} :

Definition 5.15. Let $a, b \in \Lambda$.

- (i) $a > 0 \Leftrightarrow \hat{a} > 0$,
- (ii) $a > b \Leftrightarrow (\hat{a} - \hat{b}) > 0$.

If the statement (ii) is true, we say that a is larger than b with respect to $>$.

Definition 5.16. Let $x_1, x_2, \dots, x_\ell \in \Lambda$.

$$K := \{x_1, x_2, \dots, x_\ell\} \quad (5.34)$$

is called a link-connected point configuration \Leftrightarrow any two points $y, z \in K$ can be connected with a path composed of edges of length 1 which passes only through points which are contained in K .

For notational convenience, a link-connected point configuration is also simply called a connected configuration where this does not lead to any confusion with the notion of connectedness as used in the context of polymers and clusters.

The next step is the construction of a unique numbering scheme for all points of a configuration. To begin with, we define the notion of the generation:

Definition 5.17. Let K be a connected configuration. Let $x, y \in K$. Furthermore, let x_1 be the base point of K , i.e. x_1 is the smallest point in K with respect to $<$.

- (i) The one-element point set $\{x_1\}$ is called 1st generation G_1 (of points of K),

$$G_1 := \{x_1\}. \quad (5.35)$$

- (ii) The 2nd generation G_2 is defined as

$$G_2 := \{y | y \text{ is a neighbour of } x_1\}. \quad (5.36)$$

(iii) The $(n + 1)$ th generation G_{n+1} , $n \geq 1$, is then defined as

$$G_{n+1} := \{ y | y \text{ is a neighbour of some } x \in G_n \wedge y \notin G_k \text{ for any } k \leq n \}. \quad (5.37)$$

Now the actual numbering scheme is established by affixing labels to all points of K :

Definition 5.18. Let K be a connected configuration and let $x \in K$. A label is a map

$$x \mapsto (n_x, m_x), \quad n_x, m_x \in \mathbb{N}. \quad (5.38)$$

n_x is called generation index, m_x is denoted as generation element number.

Definition 5.19. Let K be a connected configuration. A numbering is a map

$$K \mapsto \{ (n, m) \} \quad (5.39)$$

according to the following rules:

- (i) The base point $x_1 \in G_1$ obtains the label $(1, 1)$.
- (ii) All points $y \in G_2$ carry the generation index 2; within G_2 , the generation element numbers m are assigned to successively with respect to the order $<$, i.e. for two points $y, y' \in G_2$ with $y < y'$ which have labels $(2, m_y)$ and $(2, m_{y'})$ respectively, we have $m_y < m_{y'}$.
- (iii) All points of G_{n+1} , $n \geq 1$, carry generation index $n + 1$; within G_{n+1} , we first attach labels to all points neighbouring to $z_{(n,1)} \in G_n$ with respect to $<$; then we label all neighbours of $z_{(n,2)} \in G_n$ with respect to $<$ etc., until G_n is exhausted.

Points which already have been labelled are passed over.

An immediate consequence of this numbering scheme is that to every point $x_{(n,m)} \in K$ of a connected configuration there exists a path of length $n - 1$

$$W_{x_{(n,m)}} = (x_1, x_{(2,\dots)}, \dots, x_{(n-1,\dots)}, x_{(n,m)}) \quad (5.40)$$

which connects $x_{(n,m)}$ with the base point x_1 .

Proposition 5.20. Let K be a connected configuration. Then the numbering (5.39) is uniquely determined. That is, to every point $x_{(n,m)} \in K$, there exists exactly one path of the type (5.40).

This proposition is obvious from the definition of the numbering scheme. Next we define an order relation on the set of points of a connected configuration:

Definition 5.21. Let K be a connected configuration and let $x_{(n_x, m_x)} \in K$, $y_{(n_y, m_y)} \in K$. x is called smaller than y with respect to \triangleleft , $x \triangleleft y \Leftrightarrow$

- (i) $n_x < n_y$, or
- (ii) $m_x < m_y$, if $n_x = n_y$.

x is called larger than y with respect to \triangleright , $x \triangleright y \Leftrightarrow y \triangleleft x$.

Another obvious consequence of the numbering scheme given above is that neighbouring points $x_{(n_x, m_x)}, y_{(n_y, m_y)} \in K$ obey

$$|n_x - n_y| \leq 1. \tag{5.41}$$

Moreover, in the case under consideration, we have

Proposition 5.22. Let K be a connected configuration on a simple cubic lattice. Then for two neighbouring points $x, y \in K$ with generation indices n_x and n_y , we have the strict equality

$$|n_x - n_y| = 1. \tag{5.42}$$

Proof. We assume that $n_x = n = n_y$ and prove that this leads to a contradiction with the lattice geometry.

According to the properties of the numbering scheme, there exist two uniquely determined paths $W_{x_{(n, \dots)}}$ and $W_{y_{(n, \dots)}}$ with $n - 1$ edges each which connect x and y with the base point. Two cases have to be distinguished:

(i) W_x and W_y have no point in common. Consequently, the closed path

$$(x_1, x_{(2, \dots)}, \dots, x_{(n, \dots)}, y_{(n, \dots)}, y_{(n-1, \dots)}, \dots, y_{(2, \dots)}, x_1) \tag{5.43}$$

is nonselfintersecting and has $2n - 1$ edges, which is clearly in contradiction to the geometrical properties of a simple cubic lattice.

(ii) W_x and W_y have one point in common, say the point u . If there exist several points u, u', \dots shared by W_x and W_y , take the largest one with respect to the order \triangleright . If this point carries generation index n' , then the closed path

$$(u_{(n', \dots)}, x_{(n'+1, \dots)}, \dots, x_{(n, \dots)}, y_{(n, \dots)}, y_{(n-1, \dots)}, \dots, y_{(n'+1, \dots)}, u_{(n', \dots)}) \tag{5.44}$$

is nonselfintersecting and has $2(n - n') + 1$ edges, ... ■

For the determination of further properties of the above numbering scheme we define

Definition 5.23. Let $K^{(l+1)}$ be a connected configuration with $l + 1$ points and n generations. Let $x_{l+1} \equiv x_{(n, m)} \in K^{(l+1)}$ where m is maximal, i.e. x_{l+1} is the largest

point of $K^{(l+1)}$ with respect to the order \triangleright . Then a reduction R of $K^{(l+1)}$ is a map

$$R: K^{(l+1)} \mapsto K^{(l)} := K^{(l+1)} \setminus \{x_{l+1}\}. \quad (5.45)$$

Now we have

Proposition 5.24. Let $K^{(l+1)}$ as defined above. Then $K^{(l)} = R[K^{(l+1)}]$ has the properties

- (i) $K^{(l)}$ is connected.
- (ii) $K^{(l)}$ is numbered correctly.

The proof is obvious from the definition of the numbering.

It is clear that successive application of R to a connected configuration $K^{(l+1)}$ defines a uniquely determined chain of maps

$$K^{(l+1)} \mapsto K^{(l)} \mapsto \dots \mapsto K^{(2)} \mapsto K^{(1)}. \quad (5.46)$$

Hence, the reduction R generates a tree structure on the set \mathfrak{K} of connected configurations.

For the construction of a recursive algorithm for the determination of the set $\mathfrak{K}^{(l+1)} := \{K^{(l+1)}\}$ of all connected configurations with $l+1$ points from the set $\mathfrak{K}^{(l)} := \{K^{(l)}\}$ of all l -point configurations the map R has to be inverted:

Definition 5.25. Let $K^{(l)} = \{x_1, x_2, \dots, x_l\}$ be a connected configuration with l points and n generations. An extension of $K^{(l)}$ is a configuration

$$K^{(l+1)} := K^{(l)} \cup \{a\}, \quad a \in \Lambda, \quad (5.47)$$

with the properties

- (i) $a > x_1 \in K^{(l)}$.
- (ii) $K^{(l+1)}$ is connected.
- (iii) $R[K^{(l+1)}] = K^{(l)}$.

We note that the third property means that in $K^{(l+1)}$ the points x_1, x_2, \dots, x_l carry the same labels as they do in $K^{(l)}$.

For the determination of the set

$$\hat{\mathfrak{K}}^{(l+1)}(K^{(l)}) := \{K^{(l+1)} \mid K^{(l+1)} \text{ is extension of } K^{(l)}\}, \quad (5.48)$$

of $l+1$ point configurations $K^{(l+1)}$ which are extensions of some fixed $K^{(l)}$, it is clearly sufficient to determine the members of $\hat{\mathfrak{K}}^{(l+1)}(K^{(l)})$ in fixed order. As the

$\mathfrak{K}^{(l+1)}(K^{(l)})$ provide a decomposition of $\mathfrak{K}^{(l+1)}$,

$$\mathfrak{K}^{(l+1)} = \sum_{K^{(l)} \in \mathfrak{K}^{(l)}} \hat{\mathfrak{K}}^{(l+1)}(K^{(l)}), \tag{5.49}$$

with

$$\hat{\mathfrak{K}}^{(l+1)}(K^{(l)}) \neq \hat{\mathfrak{K}}^{(l+1)}(K^{(l)'}) \text{ for } K^{(l)} \neq K^{(l)'}, \tag{5.50}$$

this determination of all $K^{(l+1)} \in \hat{\mathfrak{K}}^{(l+1)}(K^{(l)})$ in fixed order for some $K^{(l)}$ is also sufficient for the determination of $\mathfrak{K}^{(l+1)}$.

We first note that for a given $K^{(l)}$, not all points $s \in \Lambda$ with $s \notin K^{(l)}$ may be used for an extension of $K^{(l)}$. Hence, for later convenience, we introduce the notion of a free point $a \in \Lambda$ which is chosen such that property (iii) of the definition of an extension,

$$R[K^{(l)} \cup \{a\}] = K^{(l)} \tag{5.51}$$

is fulfilled automatically.

Definition 5.26. Let $K^{(l)}$ be a connected configuration with l points, n generations and base point x_1 . Let $x_l \in G_n$ be the largest point of $K^{(l)}$ with respect to the order \triangleright and a neighbour of $z = z_{(n-1, m)} \in G_{n-1}$. A point $a \in \Lambda$ is called free with respect to $K^{(l)} \Leftrightarrow$

- (i) $a \triangleright x_1 \wedge a \notin K^{(l)}$.
- (ii) a is not neighbouring to any $x \in K^{(l)}$ with $x \triangleleft z$.
- (iii) a is neighbouring to z or any $y \in K^{(l)}$ with $y \triangleright z$; if a is neighbouring to z , then $a \triangleright x_l$.

We now define the sequence of extensions of a connected configuration $K^{(l)}$ which amounts to define an ordering on the set of points which are free with respect to $K^{(l)}$:

Definition 5.27. Let $K^{(l)}$ be as defined above. Let

$$A := \{a_1, a_2, \dots, a_r, b_1, b_2, \dots, b_s, \dots\}, \quad a_i, b_i, \dots \in \Lambda \tag{5.52}$$

be the entire set of points neighbouring $K^{(l)}$ which are free with respect to $K^{(l)}$ where the a_i, b_i, \dots are defined by

- (i) a_1, a_2, \dots, a_r are neighbouring to z with

$$x_l \triangleleft a_1 \triangleleft a_2 \triangleleft \dots \triangleleft a_r. \tag{5.53}$$

- (ii) b_1, b_2, \dots, b_s are neighbouring to z' with

$$\begin{aligned} b_1 \triangleleft b_2 \triangleleft \dots \triangleleft b_s \\ \vdots \end{aligned} \tag{5.54}$$

where z, z', \dots are immediately successive points contained in $K^{(l)}$ such that

$$z \triangleleft z' \triangleleft \dots \quad (5.55)$$

Then the configurations

$$\begin{aligned} & K^{(l)} \cup \{a_1\} \\ & \vdots \\ & K^{(l)} \cup \{a_r\} \\ & K^{(l)} \cup \{b_1\} \\ & \vdots \end{aligned} \quad (5.56)$$

are called 1st extension, ..., r th extension, $(r + 1)$ th extension, ... of $K^{(l)}$.

This ordering on the collection of extensions assigns to every $K^{(l+1)} \in \hat{\mathfrak{K}}^{(l+1)}(K^{(l)})$ an unique sequence

$$K^{(1)} \xrightarrow{\alpha_1 \text{th ext.}} K^{(2)} \xrightarrow{\alpha_2 \text{th ext.}} \dots \xrightarrow{\alpha_l \text{th ext.}} K^{(l+1)}. \quad (5.57)$$

If $K^{(l)}$ runs over the set $\mathfrak{K}^{(l)}$, the property (5.57) extends to all $K^{(l+1)} \in \mathfrak{K}^{(l+1)}$. This then manifests the tree structure on

$$\mathfrak{K} = \sum_{l \geq 1} \mathfrak{K}^{(l)}. \quad (5.58)$$

6. The algorithm and its implementation on a computer

Conceptually, the algorithm which has been developed, exactly performs the graphical expansion in terms of polymers and clusters of the truncated cluster expansion \hat{I} , eq. (5.3). Therefore the distinct steps of the algorithm correspond to subjects 5.2.3 to 5.2.6 (fig. 9). It is widely believed that such an algorithm which for any given order of the calculation generates and processes all the necessary graphs is much more efficient than one which evaluates the strong coupling expansion in a purely algebraic way for a finite system. Hence, relying on graphical techniques, there is some hope to obtain real high order expansions.

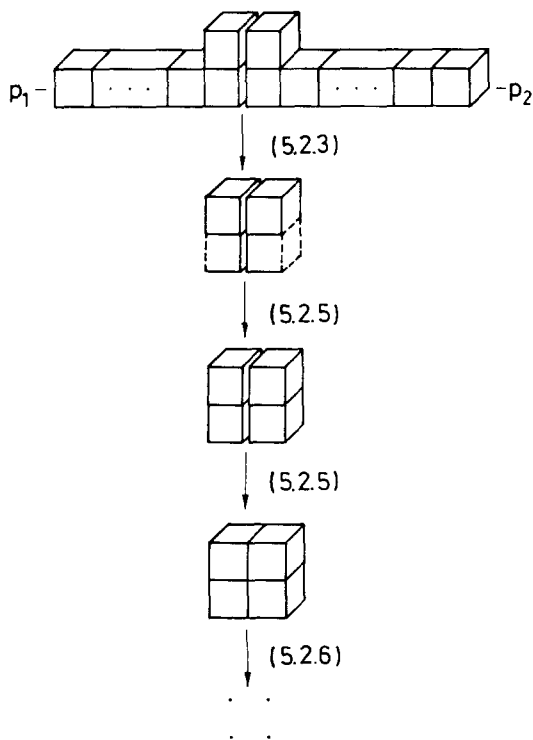


Fig. 9. The distinct steps of the algorithm illustrated with the help of the support of a 2-polymer cluster. The numbers in parentheses refer to the sections where the details of the corresponding step are described.

6.1. SCHEMATICAL FLOW-CHART

Before we discuss some basic principles how the algorithm can be put on the computer, we first give a schematical flow-chart:

- (1) Choose desired maximal order $O(\beta)_{\max}$ of computation; $l \leftarrow 0$.
- ▷ (2) $l \leftarrow l + 1$; generate the set $\mathfrak{K}^{(l)}$ of all link-connected point configurations with l points.
- ▷ (3) Take one $K^{(l)} \in \mathfrak{K}^{(l)}$ and map to the dual volume V .
- ▷ (4) Generate one collection $S(\hat{C}) = (|Y_1|^{n_1}, |Y_2|^{n_2}, \dots)$ of polymer supports which has volume V .
- ▷ (5) Determine one cluster \hat{C} which can be constructed from $S(\hat{C})$.
- ▷ (6) Determine one irreducible decoration D which can be constructed from \hat{C} .
- (7) Compute all contributions to Δm up to $O(\beta)_{\max}$ due to the set of clusters represented by (D) .
- (8) Keep the characteristic data of all those decorations which are needed for the representation of those sets of clusters which are represented by a collection of more than one irreducible decoration and which contribute to Δm up to $O(\beta)_{\max}$.

- (9) Continue at (6) until no more irreducible decoration D can be obtained from the current cluster \hat{C} .
- (10) Continue at (5) until all clusters which can be derived from the current $S(\hat{C})$ have been constructed.
- (11) Continue at (4) until all $S(\hat{C})$ which have the current volume V have been generated.
- (12) Continue at (3) until $\mathfrak{K}^{(l)}$ is exhausted.
- (13) Continue at (2) until all corrections Δm have $O(\beta) > O(\beta)_{\max}$.
- (14) Compute all contributions to Δm up to $O(\beta)_{\max}$ due to those sets of clusters which are represented by (D_1, D_2) ; (D_1, D_2, D_3) ; \dots , according to an analogous scheme.

6.2. IMPLEMENTATION ON A COMPUTER

We first comment on the point configurations on the dual lattice Λ^* . As suggested by (5.33), the (dual) lattice is realized as an one-dimensional array which we call lattice site list. Describing the lattice by an one-dimensional array corresponds to a specific numbering of the lattice sites of Λ^* .

Now for each point configuration we establish an one-dimensional array called point configuration site list which holds the numbers of the lattice sites contained in the point configuration. Hence the point configuration site list operates as an index list to the lattice site list. As we only have to know, whether a site of the lattice is occupied by the point configuration or not, the lattice site list is realized as a logical array. This helps to keep the program small. It also makes possible quick references, whether a site of the lattice is contained in a point configuration or not. Besides the point configuration site list, we set up a label list which contains the set of labels affixed to the points of the point configuration. Finally, in order to speed up the operation of the extension (of a given point configuration to a point configuration with one more point), we mark in the lattice site list all those lattice points as being occupied which are not defined as free with respect to the point configuration under consideration. The corresponding list of lattice sites is called marked lattice points list and is specific for each point configuration.

With this terminology, the recursive generation of the set $\mathfrak{K}^{(l+1)}$ of point configurations with $l+1$ points from the set $\mathfrak{K}^{(l)}$ of point configurations with l points is described as follows:

- ▷ (1) Read the lists representing the next l -point configuration $K^{(l)}$ from the data set containing $\mathfrak{K}^{(l)}$ (i.e. the point configuration site list, the label list and the marked lattice points list).
- (2) With the help of the point configuration site list, mark all points of the configuration as being occupied in the lattice site list; do the same with the help of the marked lattice points list for all lattice points which are not free with respect to the point configuration under consideration.

- ▷ (3) Determine the next extension of $K^{(l)}$; if there exists no next extension, continue at (5).
- (4) Evaluate the appropriately supplemented lists representing the new $l + 1$ point configuration $K^{(l+1)}$ and store on the data set containing the $l + 1$ point configurations generated up to the present; continue at (3).
- ▷ (5) Initialize the lattice site list (mark as being free all lattice sites with the help of the point configuration site list and the marked lattice points list); continue at (1) until $\mathfrak{K}^{(l)}$ is exhausted.

This algorithm needs only a few bytes to store the specific data of each configuration which is absolutely necessary in view of the fact that in high order runs 10^6 and more point configurations have to be tackled and stored in between. In addition, it is very fast; it turns out that the actual time needed for the generation and storage of the point configurations is roughly of the order of one to three percent of the time needed for the whole calculation.

We now turn to the further steps. The lattice Λ needed for explicit coordinate handling is realized as described above for Λ^* . Then a point configuration on Λ^* is mapped point by point to the corresponding cubes on Λ by explicit construction of the corners of each cube. Simultaneously, the corners, the links and the plaquettes of the resulting chain of connected cubes (dual to the point configuration) are subject to canonical numbering. In addition, incidence tables, i.e. link boundary and plaquette boundary tables of the chain of cubes considered as a cell complex are determined and a matrix describing the sense of connectedness of the cubes of the cell complex is established. Finally, marking one lattice action as time direction enables one to distinguish between time-like and space-like oriented plaquettes.

This information is enough to perform all the remaining steps like construction of the volume V , generation of \mathfrak{S}_V , determination of p_{in} and p_{out} etc. However, in the actual algorithm, in the course of the processing of a single configuration, additional lists and tables are established with the help of the basic information described above. They are merely rearrangements of this information according to different aspects. Although in principle being completely redundant, they help to speed up the processing considerably.

We close this section by noting that the set of programs has been written in Fortran. From a conceptual point of view, this is clearly not the optimal choice. However, the Fortran compilers currently available, in particular the Fortran HXE compiler, generate a very efficient and fast code. This has been checked by direct Assembler programming of some CPU time controlling parts of the algorithm. The gain in execution speed was only of the order of a few percent.

6.3. TESTING THE ALGORITHM

The test of the algorithm has been carried through in several steps.

First of all, some subtle parts of the program have been programmed twice independently, as for example the generation of all link-connected point configura-

tions \mathfrak{H}_i , the determination of the set \mathfrak{S}_V of all $S(\hat{C})$ which have volume V and the determination of all p_{in} and p_{out} of a given cluster \hat{C} . We then made sure that the results produced by the program are invariant under the exchange of one or several of these parts.

Next we checked the logic of the set of programs developed very carefully. In particular, we independently tested that component of the algorithm which is sufficient for the computation of the cluster expansion of the free energy $\log Z$ by reproducing a nontrivial part of the series presented in ref. [13]. It turns out that this part of the algorithm is very fast, i.e. roughly 250 configurations can be generated and processed each second on an IBM 3081-K. Therefore it seems feasible to enlarge the $O(\beta^{40})$ series given in [13] with the help of our algorithm.

The last check was dedicated to the whole set of programs. We recovered the $O(\beta^{10})$ series for the mass gap of Tarko and Fisher [14] on the first attempt without any difficulties. The CPU-time needed for this calculation corresponds roughly to 12 s on an IBM 3081-K.

We finally comment on the consistency checks which have been performed in production runs. To begin with, aiming at a certain order n , we generated the corresponding strong coupling expansion step by step: we first performed an order-4 run. Then we calculated up to order 6 and checked that the result of the order-4 run was reproduced. We repeated this procedure until the desired order was obtained. The other check made use of the fact that in an order n calculation (n even), contributions arise only from decorations which are deduced from point configurations which have $n-2$ points or less. In particular, the contributions derived from $n-3$ and $n-2$ point configurations are known: they are $+16u^n$ and $-8u^n$ respectively (for example, the only contributing decorations which can be deduced from $n-2$ point configurations each have a support which is a double tube of length $\frac{1}{2}(n-2)$). We carefully checked that these contributions were generated at each step mentioned above.

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Appendix A

SOME BASIC DEFINITIONS IN MATHEMATICAL GRAPH THEORY

We recollect some basic definitions of mathematical graph theory necessary for the discussion in sect. 5 and appendix B.

The graphs which will be considered here are the usual graphs defined in mathematical graph theory, i.e. graphs consisting of vertices and edges. In particular

they should not be confused with graphs in the spirit of definition 4.1. In order to distinguish this different kind of graphs to be introduced here, we shall denote them explicitly as vertex-edge graphs. We shall always implicitly assume that these vertex-edge graphs are finite. This is no restriction for our purpose but it helps to keep the discussion simple. Furthermore, we shall not distinguish between vertex-edge graphs and their embedding in some lattice structure.

Definition A.1. A vertex-edge graph is a pair $\mathcal{G} = (V, E)$ consisting of a set V and a set E of two-element subsets of V . The elements of V are called vertices, the elements of E are the edges of the graph \mathcal{G} .

Definition A.2. Let $\mathcal{G} = (V, E)$ and $\mathcal{G}' = (V', E')$ be two vertex-edge graphs. \mathcal{G}' is called a sub-vertex-edge graph of \mathcal{G} , if $V' \subseteq V$ and $E' \subseteq E$.

Definition A.3. Let $\mathcal{G} = (V, E)$ be a vertex-edge graph. A finite sequence $W := (x_1, \dots, x_n)$ in V is a path from x_1 to x_n in \mathcal{G} , if for $1 \leq i \leq n-1$ we always have $\{x_i, x_{i+1}\} \in E$. The number $n-1$ which is the number of edges of W is called the length of the path.

Definition A.4. Let $\mathcal{G} = (V, E)$ be a vertex-edge graph. The distance $d(x, y)$ between $x \in V$ and $y \in V$ in \mathcal{G} is defined by

$$d(x, y) := \inf\{\text{length of } W \mid W \text{ is a path } W = (x, \dots, y) \text{ in } \mathcal{G}\}. \quad (\text{A.1})$$

If there exists some path $W = (x, \dots, y)$ in \mathcal{G} , we write $d(x, y) < \infty$, otherwise we write $d(x, y) = \infty$.

Definition A.5. Let $\mathcal{G} = (V, E)$ be a vertex-edge graph. \mathcal{G} is called connected, if $d(x, y) < \infty$ for all $x, y \in V$.

Definition A.6. Let $\mathcal{G} = (V, E)$ be a connected vertex-edge graph. Let $X \subset V$ and let $\mathcal{G}' := \mathcal{G} \setminus X$ be the vertex-edge graph obtained from \mathcal{G} by removing all vertices in X from V and removing all edges which are incident on the vertices in X from E . If \mathcal{G}' is not connected, then X is called separating set of vertices of the graph \mathcal{G} . If the separating set of vertices consists only of one element $x \in V$, then x is called articulation point or cut vertex of \mathcal{G} . The number of connectedness of \mathcal{G} is defined by

$$\kappa(\mathcal{G}) = \inf\{\text{card } X \mid X \text{ is separating set of } \mathcal{G}\}. \quad (\text{A.2})$$

\mathcal{G} is called n -times connected, if $\kappa(\mathcal{G}) = n$. In particular, if $\kappa(\mathcal{G}) = 1$, \mathcal{G} is called simply connected.

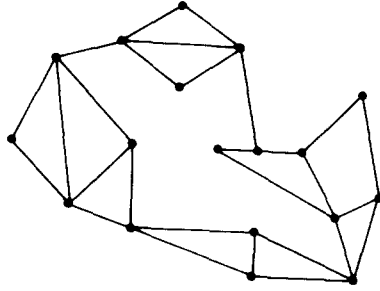


Fig. 10. A graph $\mathcal{G}(C)$ which has no articulation points.

Appendix B

PROOF OF THE FACTORIZATION OF $\hat{a}(C)$

The proof makes use of a convenient representation of the cumulant $\hat{a}(C)$ which is proven in ref. [15].

The notation is as follows: Let $C = (X_1^{n_1}, X_2^{n_2}, \dots)$ be a (connected) cluster. We draw a vertex for every polymer in C ; if two polymer supports $|X|, |X'| \in C$ are connected in the sense of connectedness as following from definition 4.3, we connect the corresponding vertices by an edge. Then the sense of connectedness of C is represented by a (vertex-edge) graph $\mathcal{G}(C)^*$ (fig. 10) in the sense of definition A.1 and we have according to ref. [15]

$$\hat{a}(C) = \sum_{\mathcal{G}' \subset \mathcal{G}} (-1)^{l(\mathcal{G}')}. \quad (\text{B.1})$$

The sum runs over all connected partial graphs \mathcal{G}' of \mathcal{G} , i.e. all connected subgraphs which have the same vertex set as \mathcal{G} and $l(\mathcal{G}')$ is the number of edges contained in \mathcal{G}' . \mathcal{G} is the usual intersection graph of a set system where the vertex set V is the set of polymer supports of the cluster C .

We now restrict to the relevant case $C \in \mathcal{C}$. Then $\mathcal{G}(C)$ is always of the type as indicated in fig. 11. There exist articulation points or cut vertices, the deletion of which (and all their incident edges) produces a graph which is not connected. The subgraphs which are obtained by disintegration of \mathcal{G} at its articulation points are called stars \mathcal{S} (fig. 11) and \mathcal{G} is called simply connected.

An important property of a simply connected graph \mathcal{G} is that each connected partial graph \mathcal{G}' of \mathcal{G} is composed of connected partial graphs \mathcal{G}'_i which lie in the stars \mathcal{S}_i of \mathcal{G} ,

$$\mathcal{G}' = (\mathcal{G}'_1, \mathcal{G}'_2, \dots). \quad (\text{B.2})$$

* In the following we shall only use vertex-edge graphs; for notational convenience, they will be simply denoted by graphs.

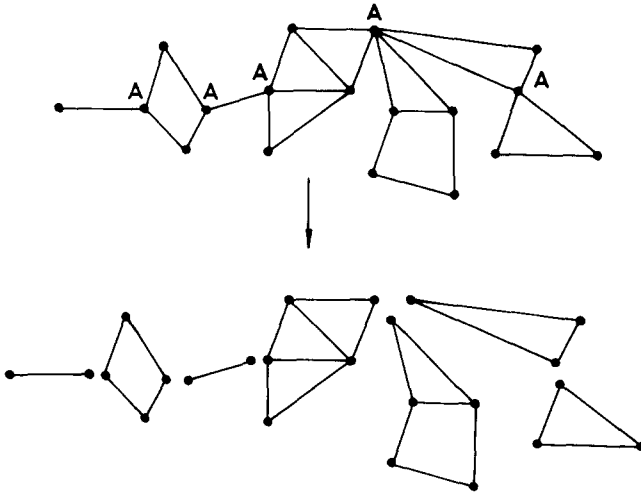


Fig. 11. A graph $\mathcal{G}(C)$ with its articulation points indicated by "A". The stars of $\mathcal{G}(C)$ are indicated in the second line.

Clearly, if $\mathcal{G}' \subset \mathcal{G}$ is a connected partial graph of \mathcal{G} , \mathcal{G}'_i must be a connected partial graph of \mathcal{S}_i for all i because \mathcal{G} is simply connected and consequently there exists no possibility of connecting two eventually disconnected vertices within some star \mathcal{S}_i by a path of edges leaving \mathcal{S}_i .

Conversely, if \mathcal{G}'_i is a connected partial graph of \mathcal{S}_i , $i = 1, 2, \dots$, then $\mathcal{G}' = (\mathcal{G}'_1, \mathcal{G}'_2, \dots)$ is a partial graph of \mathcal{G} and is connected.

Hence, we obtain from (B.1)

$$\begin{aligned}
 \hat{a}(C) &= \sum_{(\mathcal{G}'_1, \mathcal{G}'_2, \dots) \subset \mathcal{G}} (-1)^{l(\mathcal{G}')} \\
 &= \sum_{\mathcal{G}'_1 \subset \mathcal{S}_1} \sum_{\mathcal{G}'_2 \subset \mathcal{S}_2} \dots (-1)^{l(\mathcal{G}'_1) + l(\mathcal{G}'_2) + \dots} \\
 &= \sum_{\mathcal{G}'_1 \subset \mathcal{S}_1} (-1)^{l(\mathcal{G}'_1)} \sum_{\mathcal{G}'_2 \subset \mathcal{S}_2} (-1)^{l(\mathcal{G}'_2)} \dots \\
 &= \hat{a}(\mathcal{S}_1) \cdot \hat{a}(\mathcal{S}_2) \dots,
 \end{aligned} \tag{B.3}$$

which is the factorization of the cumulants claimed in subsect. 5.2.3. ■

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