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Central limit theorems, Lee–Yang zeros, and graph-counting polynomials

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A B S T R A C T

We consider the asymptotic normalcy of families of random variables X which count the number of occupied sites in some large set. If $P(z) = \sum_{j=0}^{N} p_j z^j$ is the generating function associated to the random sets (i.e., there are p_j choices of random sets with j occupied sites), we will consider the probability measures $\mathrm{Prob}(X = m) = p_m z^m / P(z)$, for z real positive. We give sufficient criteria, involving the location of the zeros of $P(z)$, for these families to satisfy a central limit theorem (CLT) and even a local CLT (LCLT); the theorems hold in the sense of estimates valid for large N (we assume that $\mathrm{Var}(X)$ is large when N is). For example, if all the zeros lie in the closed left half plane then X is asymptotically normal, and when the zeros satisfy some additional conditions then X satisfies an LCLT. We apply these results to cases in which X counts the number of edges in the (random) set of "occupied" edges in a graph, with constraints on the number of occupied edges attached to a given vertex. Our results also apply to systems of interacting particles, with X counting the number of particles in a box Λ whose size $|\Lambda|$ approaches infinity; $P(z)$

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is then the grand canonical partition function and its zeros are the Lee–Yang zeros.

1. Introduction

In this note we investigate the asymptotic normalcy of the number X of elements in a random set M when the expected size of M is very large. We shall be concerned in particular with the case in which M is a random set of edges, called *occupied edges*, in some large graph G, under certain rules which constrain the admissible configurations of occupied edges. Our analysis is however not restricted to such examples; in particular, it includes many cases of interest in statistical mechanics, for which X is the number of occupied sites in some region $\Lambda \subset \mathbb{Z}^d$ (or the number of particles in $\Lambda \subset \mathbb{R}^d$).

The probability that $X = m$ is written as

$$\mathrm{Prob}\{X = m\} := \frac{p_m z_0^m}{P(z_0)}, \tag{1.1}$$

where

$$P(z) := \sum_{m=0}^{N} p_m z^m \tag{1.2}$$

is a polynomial of degree N and z_0 is a strictly positive parameter; we will often take $z_0 = 1$. The coefficient p_m will be, in the graph counting case, the number of admissible configurations of occupied edges of size m. By convention we take $p_m = 0$ if $m > N$ or $m < 0$. In some cases we will consider P as the fundamental object of study and will then write X_P and N_P for X and N.

A simple example is that in which a configuration is admissible if the number of occupied edges attached to each vertex v, $d_M(v)$, is zero or one. In this case the polynomial $P(z)$ coincides with one of several definitions of the *matching polynomial* of the graph, properties of which have been studied extensively in the graph theory literature. In particular, a local central limit theorem (see below) for X has been proved in the case $z_0 = 1$ [15]. Our primary examples in this paper will be *graph-counting polynomials*, which arise when the restriction $d_M(v) \in \{0, 1\}$ discussed above is generalized to $d_M(v) \in C(v)$ for some set $C(v)$; we will obtain a local central limit theorem for X when $C(v) = \{0, 1, 2\}$ for all v.

The above examples are also natural objects of study in equilibrium statistical mechanics; there one refers to the case with $d_M(v) \in \{0, 1\}$ as a system of *monomers* and *dimers*, and to that with $d_M(v) \in \{0, 1, 2\}$ as a system of monomers and *unbranched polymers*. In this setting one thinks of the edges belonging to M as occupied by particles, and the parameter z_0 is then the *fugacity* of these particles. The restriction $d_M(v) \in C(v)$ with $C(v) = \{0, 1, \dots, c_v\}$ corresponds to *hard core* interactions between the particles, and is a special or limiting case of a more general model for which a configuration M is assigned a Gibbs weight $w_M := e^{-\beta U(M)}$, with $U(M)$ the *interaction energy* of M and β the inverse of the temperature, and $p_m := \sum_{\{M \mid |M|=m\}} w_M$. p_m is then called the *canonical partition function* for m particles and $P(z)$ the *grand canonical partition function* of the system.

In this statistical mechanics setting the graph G is usually a subset of a regular lattice. For example, the vertices may be the sites of the lattice $\mathbb{Z}^d$ which belong to some cubical box $B = \{1, \dots, L\}^d \subset \mathbb{Z}^d$, with edges, usually called bonds, joining nearest-neighbor sites; one also considers such a box with periodic boundary conditions, in which an additional bond joins any pair of sites whose coordinate vectors differ in only one component, in which the values for the two sites are 1 and L. Such a box contains $|B|$ vertices and $\sim d|B|$ edges. The particles are most often thought of as occupying the sites of the lattice, that is, the vertices of the graph, but for our examples they occupy the bonds, as noted above. For the monomer–dimer problem on such a box B one would have $N \sim |B|/2$. Considering potentials U for the periodic box which are translation invariant and sufficiently regular we are then in the usual situation for equilibrium statistical mechanics, see e.g. [32,13].

In the statistical mechanics setting there are many cases in which one can prove that $E[X] \sim c_1 N$ and $\mathrm{Var}(X) \sim c_2 N$ for some $c_1, c_2 > 0$ and that X satisfies a central limit theorem (CLT), that is, that

$$\mathrm{Prob}\big\{X \leq E[X] + x\sqrt{\mathrm{Var}(X)}\,\big\} \sim G(x) \tag{1.3}$$

when $N \to \infty$, where $G(x)$ is the cumulative distribution function of the standard normal random variable. A discussion of different proofs is given in [13, p. 469]; most of these make use of the approximate independence of distant regions of $\mathbb{Z}^d$ to write X as a sum of many approximately independent variables, and do not extend directly to general graphs without any spatial structure. See also [7] for a broad review of proof methods in the context of combinatorial enumeration. Here, inspired by a proof due to Iagolnitzer and Souillard [19] in a statistical mechanics context, we prove a CLT that requires only that for large N there be no zeros of $P(z)$ in some disc of uniform size around z_0, and that $\mathrm{Var}(X)$ grow faster than $N^{2/3}$ as $N \to \infty$. We describe the method in Section 2 and in Section 6 verify the variance condition, and thus obtain a CLT, for the random variables associated with a certain class of graph-counting polynomials; in Section 7 we discuss applications to statistical mechanical systems. We note here and will show later that when the zeros of $P(z)$ lie in the left half plane it is sufficient for the CLT that $\mathrm{Var}(X) \to \infty$ as $N \to \infty$.

Once one has a CLT for X, in the usual sense (1.3) of convergence of distributions, one would like also a *local* CLT (LCLT), that is, one would like to show that for large N,

$$\operatorname{Prob}\{X=m\} \sim \frac{1}{\sqrt{2\pi \operatorname{Var}(X)}} e^{-(m-E[X])^2/2\operatorname{Var}(X)}. \tag{1.4}$$

If (1.4) holds for m belonging to some set S of integers then one speaks of an LCLT *on* S, but in the cases we will consider we will prove an LCLT on all of $\mathbb{Z}$. In the statistical mechanics setting such a result was established for certain systems in [9]; see also [8,13]. An LCLT for dimers on general graphs was given by Godsil [15], with a very different proof. Earlier Heilmann and Lieb [18] proved that all the zeros of the attendant matching polynomial $P(z)$, whose coefficients p_m enumerate incomplete matchings (monomer–dimer configurations) by the number m of edges (dimers), lie on the negative real axis. Harper [17] was the first to recognize—in a particular case of Stirling numbers—that such a property of a generating function $P(z)$ meant that the distribution of the attendant random variable is one of a sum of independent, $(0,1)$-valued, random variables; it instantly opened the door for his proof of asymptotic normality of those numbers. Godsil used Heilmann–Lieb's result and Harper's method to prove a CLT for $\{p_m\}$, under a constraint on the ground graph guaranteeing that the variance tends to infinity. Significantly, since Heilmann–Lieb's result and Menon's theorem [26] implied log-concavity of $\{p_m\}$, Godsil was able to prove the stronger LCLT by using the quantified version of Bender's LCLT for log-concave distributions [3] due to Canfield [6]. We refer the reader to Kahn [20] for several necessary and sufficient conditions under which the variance of the random matching size tends to infinity, and to Pitman [28] for a broad range survey of the probabilistic bounds when the generating function has real roots only.

Years later Ruelle [33] found that the polynomial $P(z)$ whose coefficients enumerate the *unbranched* subgraphs (2-matchings) of a general graph G has roots in the left half of the z-plane, but not necessarily on the negative real line. This result followed from a general localization theorem based on a classic Grace's Theorem, the notion of Asano contraction and the Asano–Ruelle Lemma. (Later Wagner [37] proved counterparts of Ruelle's results for a more general case of subgraphs with *weighted* edges by using the Grace–Szegö–Walsh Coincidence Theorem.) Our key observation is that here again the related random variable X is, in distribution, a sum of independent random variables, this time each having a 3-element range $\{0,1,2\}$. Since the range remains bounded, a CLT for unbranched polymers follows whenever $\operatorname{Var}(X)$ goes to infinity with the degree of P. However, only when the roots are within a certain wedge enclosing the negative real axis can we prove log-concavity of the distribution of X. Still we are able to prove an LCLT, with an explicit error term, under certain mild conditions on G.

We now summarize briefly some of our results. Assuming that the mean $E[X]$ and variance $\operatorname{Var}(X)$ go to infinity as $N \to \infty$, then:

1. For all $z_0 > 0$ the random variable X satisfies an LCLT, with additive error $O(1/\operatorname{Var}(X))$, when all roots ζ of P lie in a wedge of opening angle 2α, $\alpha < \pi/2$, centered on the negative real axis. For example, if $z_0 = 1$ then the error is at most $25/(\pi \operatorname{Var}(X))$ when $\operatorname{Var}(X)$ is large enough so that

$$\frac{\operatorname{Var}(X)}{\log^3 \operatorname{Var}(X)} \geq \frac{2^5\pi^6}{3^3}(1+\sec\alpha)^3;$$

the inequality is satisfied if $\operatorname{Var}(X) > 5.5\times 10^7$ for $\alpha = 0$ and if $\operatorname{Var}(X) > 2.2\times 10^8$ for $\alpha = 2\pi/3$. (We single out $2\pi/3$ since for $\alpha < 2\pi/3$ the distribution of X is provably log-concave, an extension of the classic result for the case of negative roots.)

2. For all $z_0 > 0$ the random variable X satisfies a CLT, with additive error $O(1/\sqrt{\operatorname{Var}(X)})$, when all roots ζ satisfy $\operatorname{Re}\zeta \leq 0$.
3. The random variable X satisfies a CLT if there are no zeros of P in a disc of radius $\delta > 0$ around z_0 and $\operatorname{Var}(X)$ grows faster than $N^{2/3}$; the additive error is then $O(N^{1/3}/\operatorname{Var}(X)^{1/2})$. This extends and makes completely rigorous results of [19].
4. Finally, certain of the above conditions are satisfied by many graph-counting polynomials and statistical mechanical systems—for example, unbranched polymers—and we give an explicit LCLT or CLT in some of these cases.

The result mentioned in 1 above has also been used in [12] to establish an LCLT for determinantal point processes.

We should mention here the papers by Borcea and Brändén [4,5]. Though disjoint in content from the present paper, they contain an elegant characterization of linear operators on multivariate polynomials that preserve the property of non-vanishing on a prescribed open circular domain, which is the paradigm at the core of [28]. In a broader context our paper is not far from the field of algebraic combinatorics; see, for instance, Bender [3], Canfield [6] and Flajolet and Soria [11]. A key difference is that while we deal with spanning subgraphs of general graphs, the setup in these papers is based on the notion of a component structure having lots of symmetry, with the focus on deriving asymptotic distributions from the analytical properties of a single generating function, whose coefficients enumerate the components by their sizes.

The outline of the rest of the paper is as follows. In Section 2 we apply the method of [19] to derive a CLT for the random variable X from rather weak hypotheses on the location of the zeros of $P(z)$, and in Section 3 we obtain an LCLT under the stronger hypothesis that the zeros lie in the left half plane. In Section 4 we describe more precisely the class of graph-counting polynomials and what can be said about the location of their zeros. In Section 5 we obtain central limit theorems and, in some cases, local central limit theorems for graph-counting polynomials from the results of Section 3, and in Section 6 obtain, from the results of Section 2, central limit theorems for further graph-counting examples. In Section 7 we discuss briefly the applications to statistical mechanics. Throughout our discussions we will, rather than considering sequences of polynomials, say that a family $\mathcal{P}$ of polynomials, of unbounded degrees, satisfies a CLT or an LCLT when one can give estimates for the errors in the approximations (1.3) and (1.4), respectively, which are valid for all polynomials in $\mathcal{P}$ and which vanish as the degree N of the polynomial goes to infinity.

2. A central limit theorem

In this section we first consider a fixed polynomial $P(z) = \sum_{m=0}^{N} p_m z^m$, as in (1.2), and assume throughout that $p_m \geq 0$ and that $p_N > 0$, i.e., that P is in fact of degree N. We fix also a number $z_0 > 0$ (a fugacity, in the language of statistical mechanics) and let X be a random variable with probability distribution given by (1.1). We will let ζ_j, $j = 1, \ldots, N$, denote the roots of P.

Our first result is an estimate corresponding to an (integrated) central limit theorem. To state it we define, for $x \in \mathbb{R}$,

$$F_P(x) := \frac{1}{P(z_0)} \sum_{m \leq E[X] + x\sqrt{\mathrm{Var}(X)}} p_m z_0^m = \mathrm{Prob}\left\{ \frac{X - E[X]}{\sqrt{\mathrm{Var}(X)}} \leq x \right\}, \tag{2.1}$$

$$G(x) := (2\pi)^{-1/2} \int_{-\infty}^{x} e^{-u^2/2}\, du. \tag{2.2}$$

Theorem 2.1. *Suppose that there exists a $\delta > 0$ such that $z_0 \geq \delta$ and $|z_0 - \zeta_j| \geq \delta$ for all j, $j = 1, \ldots, N$. Then there exist constants $N_0, B_1, B_2 > 0$, depending only on δ and z_0, such that for $N \geq N_0$,*

$$\sup_{x \in \mathbb{R}} |F_P(x) - G(x)| \leq \frac{B_1 N}{\mathrm{Var}(X)^{3/2}} + \frac{B_2 N^{1/3}}{\mathrm{Var}(X)^{1/2}}. \tag{2.3}$$

Remark 2.2. We record here some standard results, adopting the notation of Theorem 2.1. For z in the disk $D := \{z \in \mathbb{C} \mid |z - z_0| < \delta\}$ we will fix a canonical branch of $\log P(z)$ by defining

$$\log P(z) := \log p_N + \sum_{j=1}^{N} \log\bigl(z - \zeta_j\bigr), \tag{2.4}$$

with $\log p_N$ real and

$$\log(z - \zeta_j) := \log(z_0 - \zeta_j) + \log \frac{z - \zeta_j}{z_0 - \zeta_j}, \tag{2.5}$$

where

$$\mathrm{Im} \log(z_0 - \zeta_j) \in (-\pi, \pi) \quad \text{and} \quad \mathrm{Im} \log \frac{z - \zeta_j}{z_0 - \zeta_j} \in (-\pi/2, \pi/2). \tag{2.6}$$

In (2.6) the first specification is possible since ζ_j cannot be a positive real number and the second since $\bigl|(z - \zeta_j)/(z_0 - \zeta_j) - 1\bigr| < 1$ for $z \in D$; in particular, $\log(z - \zeta_j)/(z_0 - \zeta_j)$ is analytic for $z \in D$. Moreover, $\log P(z)$ is real for real z, because non-real roots occur in complex conjugate pairs, and furthermore

$$\log P(z) - \log P(z_0) = \sum_{j=1}^{N} \log \frac{z-\zeta_j}{z_0-\zeta_j}, \quad z \in D. \tag{2.7}$$

Then for all z in D,

$$\begin{aligned} z\frac{d}{dz}\log P(z) &= \frac{\sum_m m p_m z^m}{P(z)}, \\ \left(z\frac{d}{dz}\right)^2 \log P(z) &= \frac{\sum_m m^2 p_m z^m}{P(z)} - \left(\frac{\sum_m m p_m z^m}{P(z)}\right)^2, \end{aligned} \tag{2.8}$$

and so

$$z\frac{d}{dz}\log P(z)\Big|_{z=z_0} = E[X], \quad \left(z\frac{d}{dz}\right)^2 \log P(z)\Big|_{z=z_0} = \mathrm{Var}(X), \tag{2.9}$$

which can be restated as

$$\frac{d}{du}\log P(e^u z_0)\Big|_{u=0} = E[X], \quad \frac{d^2}{du^2}\log P(e^u z_0)\Big|_{u=0} = \mathrm{Var}(X). \tag{2.10}$$

To state the next lemma we observe that there exists an $\epsilon > 0$, depending only on δ and z_0, such that if $|u| \le \epsilon$ then $|e^u z_0 - z_0| \le \min\{\delta/2, |z_0|\}$, so that for $|u| \le \epsilon$ we may define, as in Remark 2.2,

$$\begin{aligned} f(u) := \log E[e^{uX}] &= \log P(e^u z_0) - \log P(z_0) \\ &= \sum_{j=1}^{N} \log \frac{e^u z_0 - \zeta_j}{z_0 - \zeta_j}. \end{aligned} \tag{2.11}$$

Lemma 2.3. *Let δ be as in Theorem 2.1 and let $\epsilon = \epsilon(z_0, \delta)$ be as above. Then for $K = 2\log 2/\epsilon^3$,*

$$f(u) = uE[X] + \frac{u^2}{2}\mathrm{Var}(X) + u^3 R(u), \quad \textit{with} \quad |R(u)| \le NK. \tag{2.12}$$

Proof. Suppose that $|u| \le \epsilon/2$. Then we have, by Cauchy's integral formula and (2.10),

$$\begin{aligned} f(u) &= f(0) + uf'(0) + \frac{u^2}{2}f''(0) + u^3 R(u) \\ &= uE[X] + \frac{u^2}{2}\mathrm{Var}(X) + u^3 R(u), \end{aligned} \tag{2.13}$$

where

$$R(u) := \frac{1}{2\pi i} \oint_{|v|=\epsilon} \frac{f(v)}{v^3(v-u)}\,dv. \tag{2.14}$$

Then from (2.11),

$$|R(u)| \leq \sum_{j=1}^{N} \left| \frac{1}{2\pi i} \oint_{|v|=\epsilon} \log\left(\frac{e^v z_0 - \zeta_j}{z_0 - \zeta_j}\right) \frac{dv}{v^3(v-u)} \right|$$
$$\leq \frac{2}{\epsilon^3} \sum_{j=1}^{N} \sup_{|v|=\epsilon} \left| \log \frac{e^v z_0 - \zeta_j}{z_0 - \zeta_j} \right| < \frac{2}{\epsilon^3} N \log 2. \tag{2.15}$$

Here we have used $|(e^v z_0 - \zeta_j)/(z_0 - \zeta_j)| < (\delta/2)/\delta = 1/2$ for $|v| = \epsilon$ and $|\log(1-t)| \leq -\log(1-|t|)$ for $|t| < 1$; the latter is easily verified for example from the expansion $\log(1-t) = -\sum_{k\geq 1} t^k/k$. □

Proof of Theorem 2.1. The proof follows closely the proof of the Berry–Esseen Theorem given in Feller [10, Section XVI.5] and in particular is based on the "smoothing inequality" [10, Section XVI.4, Lemma 2]. If we specialize to the particular application we need, then the latter implies that for any $T > 0$,

$$\sup_{x\in\mathbb{R}} |F_P(x) - G(x)| \leq \frac{1}{\pi} \int_{-T}^{T} \left| \frac{\psi(t) - e^{-t^2/2}}{t} \right| dt + \frac{24}{\pi\sqrt{2\pi}T}, \tag{2.16}$$

where $\psi(t) = E[e^{itY}]$ is the characteristic function of $Y = (X - E[X])/\sigma$, with $\sigma = \sqrt{\mathrm{Var}(X)}$. We will apply this inequality with $T = \sigma/N^{1/3}$. For $|t| \leq T$, then, $|t/\sigma| \leq N^{-1/3}$, so that for $N \geq N_0 := 8/\epsilon^3$ we have $t/\sigma \leq \epsilon/2$ and, from Lemma 2.3,

$$\psi(t) = e^{-itE[X]/\sigma} e^{f(it/\sigma)} = e^{-t^2/2 - it^3 R(it/\sigma)/\sigma^3}, \tag{2.17}$$

with $|R(it/\sigma)| \leq NK$ and hence $|it^3 R(it/\sigma)/\sigma^3| \leq K$. Now let $K_* = \max_{|u|\leq K} |(e^{iu} - 1)/u|$, so that

$$|e^{-it^3 R(it/\sigma)/\sigma^3} - 1| \leq |t/\sigma|^3 NKK_* \quad \text{for } N \geq 8/\epsilon^3 \text{ and } t \leq T. \tag{2.18}$$

Then

$$\int_{-T}^{T} \left| \frac{\psi(t) - e^{-t^2/2}}{t} \right| dt \leq \frac{NKK_*}{\sigma^3} \int_{-T}^{T} t^2 e^{-t^2/2}\, dt$$
$$\leq \frac{NKK_*}{\sigma^3} \int_{-\infty}^{\infty} t^2 e^{-t^2/2}\, dt = \frac{NKK_*\sqrt{2\pi}}{\sigma^3}. \tag{2.19}$$

Inserting this estimate into (2.16) we obtain (2.3) with

$$B_1 := \sqrt{\frac{2}{\pi}}\, KK_*, \qquad B_2 := \frac{24}{\pi\sqrt{2\pi}}. \qquad \square \tag{2.20}$$

In Section 6 we will apply Theorem 2.1 to obtain central limit theorems for families of graph-counting polynomials and for families of polynomials arising from statistical mechanics. To do so we must establish that, for P in the family under consideration, $\mathrm{Var}(X_P)$ grows faster than $N_P^{2/3}$. Our tool for this will be a result due to Ginibre [14], which we recall as Theorem 6.2 below; our next result, which is similar to Theorem 2.1, will be needed in the application of Ginibre's result to graph-counting polynomials.

Proposition 2.4. *Suppose that p_0 and p_1 are nonzero and that c_1 and δ_1 are positive constants such that (i) $p_1 \ge c_1 p_0 N$ and (ii) $|\zeta_j| \ge \delta_1$, $j = 1, \ldots, N$. Then there exists a constant $M > 0$, depending only on c_1, δ_1, and z_0, such that $E[X] \ge MN$.*

Proof. For z real and nonnegative, $\log P(z)$ is well defined by the requirement that it be real; further,

$$E[X] = z\frac{d}{dz}\log P(z)\big|_{z=z_0} \tag{2.21}$$

and

$$z_0\frac{d}{dz_0}E[X] = \mathrm{Var}(X) > 0, \tag{2.22}$$

so that $E[X]$ is an increasing function of z_0. Thus it suffices to verify the conclusion for sufficiently small z_0. Now we allow z to be complex, and for $|z| < \delta_1$ define as in (2.7)

$$g(z) := \log P(z) - \log P(0) = \sum_{j=1}^{N} \log\frac{\zeta_j - z}{\zeta_j}, \tag{2.23}$$

where again $\mathrm{Im}\log((\zeta_j - z)/\zeta_j) \in (-\pi/2, \pi/2)$. Now for $|z| < \delta_1/4$ we have

$$\begin{aligned} zg'(z) &= z\frac{d}{dz}\left(g(0) + zg'(0) + \frac{z^2}{2\pi i}\oint_{|y|=\delta_1/2}\frac{g(y)}{y^2(y-z)}\,dy\right) \\ &= z\frac{p_1}{p_0} + z^2 R_1(z), \end{aligned} \tag{2.24}$$

with

$$R_1(z) := \frac{1}{2\pi i}\oint_{|y|=\delta_1/2}\frac{(2y-z)\,g(y)}{y^2(y-z)^2}\,dy. \tag{2.25}$$

Since for $|y| = \delta_1/2$ and $|z| \le \delta_1/4$ we have $1/|y|^2 = 4/\delta_1^2$, $1/|y-z| \le 4/\delta_1$, $|2y-z| < 5\delta_1/4$, and $|g(y)| \le \log 2$ (see (2.15)), we find that

$$|R_1(z)| \le \frac{40}{\delta_1^2} N \log 2. \tag{2.26}$$

Let $z_* = \min\{\delta_1/4, c_1\delta_1^2/(80\log 2)\}$; then for $0 < z_0 \le z_*$,

$$E[X] = zg'(z)\Big|_{z=z_0} \ge z_0\frac{p_1}{p_0} - \frac{40z_0^2}{\delta_1^2} N \log 2 \ge \frac{z_0 c_1 N}{2}. \tag{2.27}$$

Thus $E[X] \ge MN$ holds with $M = z_0c_1/2$ for $z_0 \le z_*$ and with $M = z_*c_1/2$ otherwise. □

3. Polynomials with zeros in the left half plane

In this section we again consider a polynomial $P(z)$ as in (1.2), and continue to assume that P is of degree N and that all the coefficients p_m are nonnegative. Moreover, we assume that all roots of P lie in the closed left-half plane, and no root is zero, i.e., $p_0 > 0$. For convenience we now write these roots as $-\eta_j$, so that

$$\mathrm{Re}(\eta_j) \ge 0 \ (j = 1, \dots, N), \quad \text{and} \quad P(z) = p_N \prod_{j=1}^{N} (z + \eta_j). \tag{3.1}$$

We will take the fugacity z_0 to be 1, but our results extend easily to any $z_0 > 0$.

3.1. A central limit theorem

Under the assumption (3.1) the derivation of a CLT given in Section 2 can be simplified; moreover, the result is strengthened since we require only that $\mathrm{Var}(X_P) \to \infty$ as $N_P \to \infty$, in contrast to the power growth condition needed to apply Theorem 2.1. The key idea is to write X_P as a sum of independent random variables; the central limit theorem then follows, for example from the Berry–Esseen theorem. In the case in which all the η_j are nonnegative the method goes back to Harper [17].

To decompose X_P as such a sum, we partition $\{1, \dots, N\}$ as $J_1 \cup J_2 \cup J_2'$, where $j \in J_1$ iff η_j is real and $j \in J_2$ (respectively $j \in J_2'$) iff $\mathrm{Im}(\eta_j) > 0$ (respectively $\mathrm{Im}(\eta_j) < 0$); the corresponding factorization of $P(z)$ is

$$P(z) = p_N \prod_{j\in J_1} (z + \eta_j) \prod_{j\in J_2} (z^2 + 2\,\mathrm{Re}(\eta_j)z + |\eta_j|^2). \tag{3.2}$$

We then introduce independent random variables X_j, $j \in J_1 \cup J_2$, where if $j \in J_1$ (respectively $j \in J_2$) then X_j takes values 0 and 1 (respectively 0, 1, and 2). With

$P_j(z) = z + \eta_j$ for $j \in J_1$ and $P_j(z) = z^2 + 2z\,\mathrm{Re}(\eta_j) + |\eta_j|^2$ for $j \in J_2$, the individual distribution of these random variables is

$$\Pr\{X_j = 0\} = \frac{1}{P_j(1)}, \quad \Pr\{X_j = 1\} = \frac{\eta_j}{P_j(1)} \qquad (j \in J_1);$$

$$\left.\begin{array}{c} \Pr\{X_j = 0\} = \dfrac{|\eta_j|^2}{P_j(1)}, \quad \Pr\{X_j = 1\} = \dfrac{2\,\mathrm{Re}(\eta_j)}{P_j(1)}, \\ \Pr\{X_j = 2\} = \dfrac{1}{P_j(1)} \end{array}\right\} \quad (j \in J_2).$$

Then $E[z^{X_j}] = P_j(z)/P_j(1)$ and so

$$E[z^{\sum_{j\in J_1\cup J_2} X_j}] = \prod_{j\in J_1\cup J_2} \frac{P_j(z)}{P_j(1)} = \frac{P(z)}{P(1)} = E[z^{X_P}] \tag{3.3}$$

for all z. Thus X_P and $\sum_{j\in J_1\cup J_2} X_j$ have the same distribution, and we may identify these two random variables.

Theorem 3.1. *Let $\mathcal{P}$ be a family of polynomials as in (1.2), of unbounded degrees, all of which satisfy (3.1). Then for each $P \in \mathcal{P}$,*

$$\sup_{x\in\mathbb{R}} |F_P(x) - G(x)| \le \frac{12}{\sqrt{\mathrm{Var}(X_P)}}. \tag{3.4}$$

Consequently, if $Var(X_P) \to \infty$ as $N_P \to \infty$ in $\mathcal{P}$ then $\mathcal{P}$ satisfies a CLT in the sense described in Section 1.

Proof. From [10, Section XVI.5, Theorem 2] and $|X_j| \le 2$ we have immediately that the left hand side of (3.4) is bounded by

$$\frac{6}{\mathrm{Var}(X)^{3/2}} \sum_{j\in J_1\cup J_2} E\left(\left|X_j - E(X_j)\right|^3\right) \le \frac{12}{\mathrm{Var}(X)^{3/2}} \sum_{j\in J_1\cup J_2} \mathrm{Var}(X_j). \qquad \square \tag{3.5}$$

This theorem calls for explicit bounds for $\mathrm{Var}(X_P)$. From Remark 2.2,

$$\begin{aligned} \mathrm{Var}(X_P) &= \left(z\frac{d}{dz}\right)^2 \left(p_N \prod_{j=1}^{N} (z + \eta_j)\right)\Bigg|_{z=1} \\ &= \sum_{j=1}^{N} \frac{\eta_j}{(1+\eta_j)^2} = \sum_{j=1}^{N} \frac{\mathrm{Re}(\eta_j)(1 + |\eta_j|^2) + 2|\eta_j|^2}{|1+\eta_j|^4}. \end{aligned} \tag{3.6}$$

Then since $|1+\eta_j|^2 = 1 + 2\,\mathrm{Re}(\eta_j) + |\eta_j|^2 \geq 1 + |\eta_j|^2$ and $|\eta_j|/(1+|\eta_j|^2) \leq 1/2$,

$$\mathrm{Var}(X_P) \leq \sum_{j=1}^{N} \left(\frac{\mathrm{Re}(\eta_j)}{1+|\eta_j|^2} + \frac{1}{2} \right) \leq N. \tag{3.7}$$

On the other hand, (3.6) also yields

$$\mathrm{Var}(X_P) \geq W(X_P) := \frac{1}{4} \sum_{j=1}^{N} \frac{\mathrm{Re}(\eta_j)}{1+|\eta_j|^2}. \tag{3.8}$$

In our proof of the general case of the LCLT we will need $\mathrm{Var}(X_P)$ (respectively $W(X_P)$) to bound $\left|E[e^{itX_P}]\right|$ for "small" $|t|$ (respectively for "large" $|t|$). Here is a useful upper bound for $\mathrm{Var}(X_P)$. Introduce $\alpha_P = \max_j |\arg(\eta_j)|$ ($\alpha_P \in [0, \pi/2]$). If $\alpha < \pi/2$, then

$$\mathrm{Var}(X_P) \leq 4(1 + \sec\alpha_P) W(X_P). \tag{3.9}$$

Indeed, denoting $r_j = \mathrm{Re}(\eta_j)$, $\alpha_j = |\arg(\eta_j)|$, we bound the j-th term in (3.6) by

$$\begin{aligned} \frac{r_j}{1 + r_j^2 \sec^2\alpha_j} + \frac{2r_j^2 \sec^2\alpha_j}{(1+r_j^2\sec^2\alpha_j)^2} &\leq \frac{r_j}{1+r_j^2\sec^2\alpha_j} + \frac{2r_j^2\sec^2\alpha_j/(2r_j\sec\alpha_j)}{1+r_j^2\sec^2\alpha_j} \\ &\leq \frac{\mathrm{Re}(\eta_j)}{1+|\eta_j|^2} \cdot (1+\sec\alpha_j), \end{aligned}$$

and (3.9) follows. Thus, as $N_P \to \infty$, $\mathrm{Var}(X_P)$ and $W(X_P)$ are of the same order of magnitude if α_P is bounded away from $\pi/2$.

We will need a lower bound for $W(X_P)$ that can make it easier to prove that $W(X_P)$ diverges. To this end we define, for $P \in \mathcal{P}$,

$$\Delta\ (= \Delta_P) := \min_{1 \leq j \leq N} |\eta_j|^2, \quad f\ (= f_P) := \frac{p_1}{p_0}. \tag{3.10}$$

Let $\theta_j := 1/\eta_j$, $j = 1, \ldots, N$, be the roots of $z^N P(1/z)$. It is easy to establish that

$$f = \frac{p_1}{p_0} = \sum_{j=1}^{N} \theta_j = \sum_{j=1}^{N} \mathrm{Re}(\theta_j). \tag{3.11}$$

Then the inequality

$$\frac{1}{1+|\theta_j|^2} \geq \frac{1}{2} \min_j \min\{1, |\theta_j|^{-2}\}$$

yields

$$4W(X_P) = \sum_j \frac{\mathrm{Re}(\eta_j)}{1+|\eta_j|^2} = \sum_j \frac{\mathrm{Re}(\theta_j)}{1+|\theta_j|^2} = f \sum_j \frac{\mathrm{Re}(\theta_j)}{f} \frac{1}{1+|\theta_j|^2}$$
$$\geq \frac{f}{2} \min\{1, |\theta_j|^{-2}\} = \frac{f}{2} \min\{1, \Delta\}. \tag{3.12}$$

Thus we have proved

Lemma 3.2.

$$\mathrm{Var}(X_P) \geq W(X_P) := \frac{1}{4} \sum_{j=1}^{N} \frac{\mathrm{Re}(\eta_j)}{1+|\eta_j|^2},$$
$$W(X_P) \geq \frac{f}{8} \min\{1, \Delta\},$$

with $\Delta = \Delta_P$ and $f = f_P$ as defined in (3.10).

3.2. A local central limit theorem: log-concavity case

Let us show that the CLT proved in Section 3.1 implies an LCLT when the locations of the roots ζ_j of the polynomials P (see (3.1)) are further confined to a sharp wedge enclosing the negative axis in the complex plane.

Definition 3.3. A sequence a_n, $n \geq 0$, of nonnegative real numbers is *log-concave* if for all $n \geq 1$, $a_n^2 \geq a_{n-1}a_{n+1}$.

In the factorization (3.2) of P the coefficients η_j and 1 of each linear factor, augmented from the right with an infinite tail of zeros, obviously form a log-concave sequence, and so do the coefficients $|\eta_j|^2$, $2\,\mathrm{Re}(\eta_j)$, and 1 of each quadratic factor, provided that

$$4(\mathrm{Re}(\eta_j))^2 \geq |\eta_j|^2 \quad \Leftrightarrow \quad |\arg(\eta_j)| \leq \pi/3. \tag{3.13}$$

In terms of the roots $\zeta_j = -\eta_j$, the last condition is equivalent to

$$|\arg(\zeta_j)| \in [2\pi/3, \pi], \tag{3.14}$$

for all non-zero roots ζ_j. Since the convolution of log-concave sequences is log-concave (Menon [26]), we see that, under the condition (3.13), the coefficients of P are also log-concave. This result appears as a special case in Karlin [21] (Theorem 7.1, p. 415). (See Stanley [36] for a more recent, comprehensive, survey of log-concave sequences.)

We say that a random variable X taking nonnegative integer values is *log-concave distributed* if the sequence $\{\Pr\{X = n\}\}$ is log-concave. Bender [3] discovered that an LCLT holds for a sequence $\{X_n\}$ of log-concave distributed random variables if $\lim_{n\to\infty} \sup_{x\in\mathbb{R}} |F_{X_n}(x) - G(x)| = 0$ (where here $F_X(x)$ corresponds to $F_P(x)$ in (2.1));

remarkably, X_n does not have to be a sum of independent random variables. Later Canfield [6] quantified Bender's theorem. For this he needed a stronger notion of log-concavity.

Definition 3.4. A sequence a_n, $n \geq 0$, of nonnegative real numbers is *properly* log-concave if

(a) there exist integers L and U such that $a_n = 0$ iff $n < L$ or $n > U$ (in the terminology of [36], $\{a_n\}$ has no *internal zeros*);
(b) for all $n \geq 1$, $a_n^2 \geq a_{n-1}a_{n+1}$, with equality iff $a_n = 0$.

Canfield showed that the convolution of properly log-concave sequences is also properly log-concave. Observe that the linear and quadratic factors of our polynomial $P(z)$ are properly log-concave iff $|\arg(\zeta_j)| \in (2\pi/3, \pi]$. Subject to this stronger condition, the coefficients of $P(z)$ form therefore a properly log-concave sequence.

Here is a slightly simplified formulation of Canfield's result.

Theorem 3.5 *(Canfield). Suppose that X has a properly log-concave distribution and that*

$$\sup_{x\in\mathbb{R}} |F_X(x) - G(x)| \leq \frac{K}{\sqrt{\operatorname{Var}(X)}}.$$

If $K > 7$, $K/\operatorname{Var}(X)^{1/2} < 10^{-7}$, $K/\operatorname{Var}(X)^{1/4} < 10^{-2}$, then

$$\sup_m \left| \Pr(X = m) - \frac{1}{\sqrt{2\pi \operatorname{Var}(X)}} \exp\left(-\frac{(m - E[X])^2}{2\operatorname{Var}(X)} \right) \right| \leq \frac{c}{\operatorname{Var}(X)^{3/4}},$$

with $c := 14.5K + 4.87$.

This theorem and Theorem 3.1 imply an LCLT for X_P with the roots ζ_j satisfying the condition $|\arg(\zeta_j)| \in (2\pi/3, \pi]$.

Corollary 3.6. *If the roots ζ_j of $P(z)$ satisfy $|\arg(\zeta_j)| \in (2\pi/3, \pi]$, and $\operatorname{Var}(X_P) > 144 \times 10^7$, then*

$$\sup_m \left| \Pr(X_P = m) - \frac{1}{\sqrt{2\pi \operatorname{Var}(X_P)}} \exp\left(-\frac{(m - E[X_P])^2}{2\operatorname{Var}(X_P)} \right) \right| \leq \frac{180}{\operatorname{Var}(X_P)^{3/4}}.$$

3.3. A local central limit theorem: the general case

While we proved the LCLT for the roots ζ_j in the wedge $|\arg(\zeta_j)| > 2\pi/3$ under a single condition, $\operatorname{Var}(X_P) \to \infty$, we cannot expect this condition to be sufficient in general. A trivial example is $P(z)$ with purely imaginary, non-zero roots, in which case the distribution of X_P is supported by the positive even integers only. We will see shortly, however, that a stronger condition, $f_P \min\{1, \Delta_P\} \to \infty$ fast enough, does the job perfectly.

We first state the fundamental estimate, in terms of the variance $\mathrm{Var}(X_P)$ and its lower bound $W(X_P)$ defined in (3.8).

Theorem 3.7. *Suppose* $\mathrm{Var}(X_P) \ge 1$. *Then setting* $X := X_P$,

$$\sup_m \left| \Pr(X = m) - \frac{1}{\sqrt{2\pi\,\mathrm{Var}(X)}} \exp\left(-\frac{(m - E[X])^2}{2\,\mathrm{Var}(X)}\right) \right| \le \frac{\pi}{4^{2/3}} \frac{\mathrm{Var}(X)^{1/3}}{W(X)} \exp\left(-\frac{4^{1/3}}{\pi^2}\frac{W(X)}{\mathrm{Var}(X)^{2/3}}\right) + \frac{24}{\pi\,\mathrm{Var}(X)}. \tag{3.15}$$

Corollary 3.8. *If*

$$W(X_P) \ge \frac{\pi^2}{3 \cdot 2^{1/3}} \mathrm{Var}(X_P)^{2/3} \log(\mathrm{Var}(X_P)), \tag{3.16}$$

then for $X := X_P$,

$$\sup_m \left| \Pr(X = m) - \frac{1}{\sqrt{2\pi\,\mathrm{Var}(X)}} \exp\left(-\frac{(m - E[X])^2}{2\,\mathrm{Var}(X)}\right) \right| \le \frac{25}{\pi\,\mathrm{Var}(X)}.$$

Remark 3.9. (a) For $|\arg(\zeta_j)| \equiv \pi$, we have $W(X_P) \ge (1/8)\mathrm{Var}(X_P)$, see (3.9). Therefore the condition (3.16) is satisfied for $\mathrm{Var}(X_P) > 5.5 \times 10^7$, the last number being a close upper bound for the larger root of

$$v = \frac{8\,\pi^2}{3 \cdot 2^{1/3}} v^{2/3} \log v.$$

An LCLT with the error term $C/\mathrm{Var}(X)$, C left unspecified, was proved by Platonov [29] back in 1980.

(b) For $|\arg(\zeta_j)| \in (2\pi/3, \pi]$, we have $W(X_P) \ge (1/12)\mathrm{Var}(X_P)$, see (3.9). Therefore the condition (3.16) is satisfied for $\mathrm{Var}(X_P) > 2.2 \times 10^8$, an upper bound for the larger root of

$$v = \frac{12\,\pi^2}{3 \cdot 2^{1/3}} v^{2/3} \log v.$$

The resulting error estimate, $25/(\pi \mathrm{Var}(X_P))$, is noticeably better than the estimate $180/\mathrm{Var}(X_P)^{3/4}$ in Corollary 3.6.

(c) In general, by (3.7) and Lemma 3.2,

$$\mathrm{Var}(X_P) \le N_P, \quad W(X_P) \ge \frac{p_1}{8p_0} \min\{1, \Delta_P\} \quad (\Delta_P := \min_j |\eta_j|^2).$$

So the condition (3.16) is certainly met if

$$\frac{p_1}{p_0}\min\{1,\Delta_P\} \ge \frac{8\pi^2}{3\cdot 2^{1/3}}\, N_P^{2/3}\log N_P. \tag{3.17}$$

For the proof of Theorem 3.7 we introduce the characteristic functions $\phi(t)$ of X and $\phi^*(t)$ of $X^* = X - E[X]$: $\phi(t) := E[e^{itX}]$ and $\phi^*(t) := E[e^{itX^*}] = e^{-itE[X]}\phi(t)$. The next two lemmas give estimates for these functions. In Lemma 3.10 we use crucially the fact that all roots of $P(z)$ lie in the left hand plane; this is also used in the proof of Lemma 3.11, although some version of this result could be obtained as in Section 2, using only the fact that a neighborhood of $z_0 = 1$ is free from zeros of $P(z)$.

Lemma 3.10. *For all* $t \in [-\pi,\pi]$,

$$|\phi(t)| \le \exp\left(-\frac{4t^2}{\pi^2}W(X_P)\right). \tag{3.18}$$

Proof. First of all,

$$\phi(t) = \frac{P(e^{it})}{P(1)} = \prod_j \frac{\eta_j + e^{it}}{\eta_j + 1}. \tag{3.19}$$

So, using $1 + u \le e^u$ for u real, $1 - \cos t = 2\sin^2(t/2) \ge 2t^2/\pi^2$ for $t \in [-\pi,\pi]$, and $|1+\eta_j|^2 \le 2(1+|\eta_j|^2)$,

$$\begin{aligned}
|\phi(t)|^2 &= \prod_j \frac{|\eta_j + e^{it}|^2}{|\eta_j+1|^2} \\
&= \prod_j \left(1 + \frac{2\,\mathrm{Re}\,\eta_j(\cos t - 1) + 2\,\mathrm{Im}\,\eta_j \sin t}{|\eta_j+1|^2}\right) \\
&\le \exp\left(\sum_j \frac{\mathrm{Re}(\eta_j)(\cos t - 1)}{1+|\eta_j|^2}\right) \\
&\le \exp\left(-\frac{2t^2}{\pi^2}\sum_j \frac{\mathrm{Re}(\eta_j)}{1+|\eta_j|^2}\right).
\end{aligned}$$

Invoking the definition of $W(X_P)$ in (3.8) then yields the bound (3.18) immediately. □

Unlike Lemma 3.10, the next claim and its proof are more or less standard; we give the argument to make the presentation more self-contained.

Lemma 3.11. *If* $|t| \le 1$ *then*

$$\phi^*(t) = \exp\left(-\frac{t^2}{2}\operatorname{Var}(X) + D(t)\right) \quad \textit{with} \quad |D(t)| \le 3|t|^3 \operatorname{Var}(X). \tag{3.20}$$

Proof. We write $X = \sum_{j \in J_1 \cup J_2} X_j$ as in Section 3.1. It is easy to check that $\operatorname{Var}(X_j) \le 1$, and $\operatorname{Var}(X_j) = 1$ iff $\Pr(X_j = 0) = \Pr(X_j = 2) = 1/2$. Introducing $X_j^* = X_j - E[X_j]$, $j \in J_1 \cup J_2$, we write

$$\phi^*(t) = \prod_{j \in J_1 \cup J_2} \phi_j^*(t), \quad \phi_j^*(t) := E[e^{itX_j^*}]; \tag{3.21}$$

here, see Feller [10, Section XVI.5],

$$\phi_j^*(t) = 1 - \frac{t^2}{2}\operatorname{Var}(X_j) + R_j(t), \quad |R_j(t)| \le \frac{|t|^3}{6} E\big[|X_j^*|^3\big] \le \frac{|t|^3}{3}\operatorname{Var}(X_j),$$

as $|X_j^*| \le 2$. Denoting $u_j := \frac{t^2}{2}\operatorname{Var}(X_j) - R_j(t)$, and using $\operatorname{Var}(X_j) \le 1$, we see that, for $|t| \le 1$,

$$|u_j| \le \frac{t^2}{2}\operatorname{Var}(X_j) + \frac{|t|^3}{3}\operatorname{Var}(X_j) \le \frac{5}{6} t^2 \operatorname{Var}(X_j) \le \frac{5}{6}.$$

So, using $\log(1-u) = -\sum_{j>0} u^j/j$, we obtain

$$\phi_j^*(t) = \exp\big[\log(1-u_j)\big] = \exp\big[-u_j + S_j(t)\big],$$

where

$$|S_j(t)| \le \sum_{\ell \ge 2} \frac{|u_j|^\ell}{\ell} \le \frac{u_j^2}{2(1-|u_j|)} \le 3u_j^2 \le \frac{25}{12} t^4 \operatorname{Var}(X_j).$$

Therefore

$$\phi_j^*(t) = \exp\left[-\frac{t^2}{2}\operatorname{Var}(X_j) + D_j(t)\right],$$

where

$$\begin{aligned} |D_j(t)| &= |R_j(t) + S_j(t)| \\ &\le \frac{|t|^3}{3}\operatorname{Var}(X_j) + \frac{25t^4}{12}\operatorname{Var}(X_j) \le 3|t|^3 \operatorname{Var}(X_j). \end{aligned}$$

Consequently, for $|t| \le 1$,

$$\phi^*(t) = \prod_j \phi_j^*(t) = \exp\left(-\frac{t^2}{2}\sum_j \mathrm{Var}(X_j) + D(t)\right)$$
$$= \exp\left(-\frac{t^2}{2}\mathrm{Var}(X) + D(t)\right), \tag{3.22}$$

with $D(t) := \sum_j D_j(t)$, and

$$|D(t)| \le \sum_j |D_j(t)| \le 3|t|^3 \,\mathrm{Var}(X). \qquad \square \tag{3.23}$$

Proof of Theorem 3.7. For any $T \in [0,\pi]$ we write

$$\left|\Pr(X=m) - \frac{1}{\sqrt{2\pi\,\mathrm{Var}(X)}}\exp\frac{(m-E[X])^2}{2\,\mathrm{Var}(X)}\right|$$
$$= \left|\frac{1}{2\pi}\int_{-\pi}^{\pi}\phi(t)e^{-itm}\,dt - \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-t^2\,\mathrm{Var}(X)/2}e^{-it(m-E[X])}\,dt\right|$$
$$\le \frac{1}{2\pi}\left|\int_{T\le|t|\le\pi}\phi(t)e^{-itm}\,dt\right|$$
$$+ \frac{1}{2\pi}\left|\int_{|t|\ge T} e^{-t^2\,\mathrm{Var}(X)/2}e^{-it(m-E[X])}\,dt\right|$$
$$+ \frac{1}{2\pi}\int_{|t|\le T}\left|\phi^*(t) - e^{-t^2\,\mathrm{Var}(X)/2}\right|\,dt. \tag{3.24}$$

Let us denote the three terms in the final expression in (3.24) by I_1, I_2, and I_3, respectively. Then from Lemma 3.10 and the inequality

$$\int_{|y|\ge x} e^{-ay^2/2}\,dy \le \frac{2}{ax}e^{-ax^2/2} \tag{3.25}$$

we have, for any $T \in (0,\pi]$,

$$I_1 \le \frac{\pi}{8W(X)T}\exp\left(-\frac{4T^2}{\pi^2}W(X)\right);$$
$$I_2 \le \frac{1}{\pi\,\mathrm{Var}(X)T}\exp\left(-\frac{T^2}{2}\,\mathrm{Var}(X)\right). \tag{3.26}$$

We now turn to I_3. Let us pick $T = (4\,\mathrm{Var}(X))^{-1/3}$; then $T < 1$ since $\mathrm{Var}(X) \geq 1$. Also, for $|t| \leq T$, $|D(t)|$ in Lemma 3.11 is at most $3/4 < 1$. So using that lemma and the inequality

$$|e^x - 1| \leq \frac{|x|}{1-|x|} \quad (|x| < 1),$$

we have that for $|t| \leq T$,

$$\begin{aligned}\left|\phi^*(t) - e^{-t^2\,\mathrm{Var}(X)/2}\right| &\leq e^{-t^2\,\mathrm{Var}(X)/2}\frac{D(t)}{1-|D(t)|}\\ &\leq 24\mathrm{Var}(X)|t|^3 e^{-t^2\,\mathrm{Var}(X)/2}.\end{aligned}$$

Therefore

$$I_3 \leq \frac{12\,\mathrm{Var}(X)}{2\pi}\int_{-\infty}^{\infty}|t|^3 e^{-t^2\mathrm{Var}(X)/2}\,dt = \frac{24}{\pi\,\mathrm{Var}(X)}. \tag{3.27}$$

For this choice of T, the bounds (3.26) become

$$\begin{aligned}I_1 &\leq \frac{\pi 4^{1/3}}{8}\frac{\mathrm{Var}(X)^{1/3}}{W(X)}\exp\left(-\frac{4^{1/3}}{\pi^2}\frac{W(X)}{\mathrm{Var}(X)^{2/3}}\right);\\ I_2 &\leq \frac{4^{1/3}}{\pi}\mathrm{Var}(X)^{-2/3}\exp\left(-\frac{4^{1/3}}{8}\mathrm{Var}(X)^{1/3}\right).\end{aligned} \tag{3.28}$$

We notice that the bound on I_1 exceeds the one on I_2 since $\mathrm{Var}(X) \geq W(X)$ and $\pi^2 > 8$. Adding the bound (3.27) and twice the bound (3.28), we get the bound claimed in Theorem 3.7. □

4. Graph-counting polynomials

Let G be a finite graph with vertex set V and edge set E; each edge $e \in E$ connects distinct vertices $v_1(e)$ and $v_2(e)$ (i.e., G contains no loops) and different edges may connect the same two vertices. We identify the (spanning) subgraphs of G with the subsets $M \subset E$. For $v \in V$ we let d_v be the degree of v in G and $d_M(v)$ be the degree of v in the subgraph M; to avoid trivialities we assume that $d_v > 0$ for all v.

Now suppose that for each $v \in V$ we choose a finite nonempty subset $C(v)$ of non-negative integers and define a set (C) of subgraphs of G, associated with the family $(C(v))_{v\in V}$, by

$$M \in (C) \qquad \Leftrightarrow \qquad d_M(v) \in C(v) \text{ for all } v \in V. \tag{4.1}$$

We assume throughout that $(C) \neq \emptyset$. Then the *graph-counting polynomial* associated with (C) is

$$P_{(C)}(z) = \sum_{M \in (C)} z^{|M|}. \tag{4.2}$$

For example, as discussed in Section 1, if $C(v) = \{0, 1\}$ for each $v \in V$ then (C) corresponds to the set of matchings in G or, in the language of statistical mechanics, to the set of monomer–dimer configurations on G, while if $C(v) = \{0, 1, 2\}$ for all v then (C) is the set of unbranched polymer configurations. If $C(v) = \{0, 2\}$ for all v then the subgraphs in (C) are unions of disjoint circuits.

The proofs of the CLT and LCLT given in later sections depend on information about the locations of the zeros of the polynomials $P_{(C)}$, and this can be obtained from corresponding information for certain subsidiary polynomials associated with the vertices. Given a nonempty finite set C of nonnegative integers and a positive integer d we define

$$p_{C,d}(z) = \sum_{k \in C} \binom{d}{k} z^k; \tag{4.3}$$

we will often write $p_v = p_{C(v),d_v}$. The next two results control respectively the magnitudes and arguments of the roots of $P_{(C)}$ in terms of corresponding information for the roots of the p_v; the proofs rely on known results, some of which are reported in Appendix A.

Theorem 4.1. *Suppose that, for each $v \in V$, there is a constant $r_v > 0$ such that $|\zeta| \geq r_v$ for each root ζ of p_v. Then every root ξ of $P_{(C)}$ satisfies $|\xi| \geq R$, where*

$$R = \min_{e \in E} r_{v_1(e)} r_{v_2(e)}. \tag{4.4}$$

Notice that $p_{C,d}(0) = 0$ if and only if $0 \notin C$, so that the hypotheses of Theorem 4.1 imply that $0 \in C(v)$ for each $v \in V$.

Proof of Theorem 4.1. The proof uses Grace's Theorem, the notion of Asano contraction, and the Asano–Ruelle Lemma; these topics are reviewed in Appendix A. Let $E_v \subset E$ be the set of edges of G incident on the vertex v. To each polynomial p_v there corresponds a unique symmetric multi-affine polynomial q_v in the d_v variables $(z_{v,e})_{e \in E_v}$ such that $q_v(z, \ldots, z) = p_v(z)$. Since $p_v(z) \neq 0$ for $|z| < r_v$, Grace's Theorem implies that $q_v \neq 0$ if $|z_{v,e}| < r_v$, $\forall e \in E_v$. Now we define a multi-affine polynomial

$$Q^{(0)}\big((\mathbf{z}_{v,e})_{v \in V,\, e \in E_v}\big) = \prod_{v \in V} q_v\big((\mathbf{z}_{v,e})_{e \in E_v}\big) \tag{4.5}$$

and generate, by repeated Asano contractions $(z_{v_1(e),e}, z_{v_2(e),e}) \to z_e$, a sequence of polynomials $Q^{(0)}, Q^{(1)}, \ldots, Q^{(|E|)}$, where $Q^{(k)}$ depends on k variables z_e and $(|E| - k)$ pairs of uncontracted variables $z_{e,v_1(e)}$, $z_{e,v_2(e)}$. From the Asano–Ruelle Lemma and an inductive argument, $Q^{(k)}((z_e),(z_{v,e})) \neq 0$ when the variables satisfy $|z_e| < r_{v_1(e)} r_{v_2(e)}$, $|z_{e,v}| < r_v$. In particular, $Q^{(|E|)}((z_e)_{e\in E}) \neq 0$ when $|z_e| < R$ for all $e \in E$. But $P_{(C)}(z) = Q^{(|E|)}(z, z, \ldots, z)$, completing the proof. $\square$

Theorem 4.2. *(a) Suppose that there is an angle $\phi \in [0, \pi/2]$ such that, for each $v \in V$, each nonzero root ζ of p_v satisfies $|\arg(\zeta)| \in [\pi - \phi, \pi]$. Then every nonzero root ξ of $P_{(C)}$ satisfies $|\arg(\xi)| \in [\theta_0, \pi]$, where $\theta_0 = \pi - 2\phi$.*

(b) Suppose that the graph G is bipartite, so that V may be partitioned as $V = V_1 \cup V_2$ with each $e \in E$ satisfying $v_1(e) \in V_1$, $v_2(e) \in V_2$. Suppose further that there are angles $\phi_1, \phi_2 \in [0, \pi/2]$ such that, for each $v \in V_i$, each nonzero root ζ of p_v satisfies $|\arg(\zeta)| \in [\pi - \phi_i, \pi]$ for $i = 1, 2$. Then every nonzero root ξ of $P_{(C)}$ satisfies $|\arg(\xi)| \in [\theta_0, \pi]$, where $\theta_0 = \pi - \phi_1 - \phi_2$.

Proof. We adopt the notations q_v and $Q^{(k)}$ from the proof of Theorem 4.1, and for $\varepsilon > 0$ define also $p_{v,\varepsilon}(z) = p_v(z + \varepsilon)$ and $q_{v,\varepsilon}((z_{v,e})_{e\in E_v}) = q_v((z_{v,e} + \varepsilon)_{e\in E_v})$; then $q_{v,\varepsilon}$ is the unique symmetric multi-affine polynomial such that $q_{v,\varepsilon}(z, \ldots, z) = p_{v,\varepsilon}(z)$. We also define

$$Q_\varepsilon^{(0)}\big((\mathbf{z}_{v,e})_{v\in V,\, e\in E_v}\big) = \prod_{v\in V} q_{v,\varepsilon}\big((\mathbf{z}_{v,e})_{e\in E_v}\big), \tag{4.6}$$

and let $Q_\varepsilon^{(0)}, Q_\varepsilon^{(1)}, \ldots, Q_\varepsilon^{(|E|)}$ be obtained by Asano–Ruelle contractions, as in the proof of Theorem 4.1. Finally, we define P_ε by $P_\varepsilon(z) = Q_\varepsilon^{(|E|)}(z, z, \ldots, z)$.

We assume that $\theta_0 > 0$, since otherwise the conclusion is trivial, and fix θ with $|\theta| < \theta_0$. We claim that if, for each $e \in E$, z_e belongs to the ray $\rho_\theta = \{e^{i\theta} x \mid x > 0\}$, then $Q_\varepsilon^{(|E|)}\big((z_e)_{e\in E}\big) \neq 0$. It follows then that $P_\varepsilon(z) \neq 0$ for $z \in \rho_\theta$, so that P_ε does not vanish on the open set

$$G := \{\, z \in \mathbb{C} \mid z \neq 0,\ |\arg(z)| < \max S \,\}. \tag{4.7}$$

But $\lim_{\varepsilon\to 0} P_\epsilon = P_{(C)}$ uniformly on compacts, and $P_{(C)}$ does not vanish identically since $(C) \neq \emptyset$. So, by an application on G of the theorem of Hurwitz, $P_{(C)}(z) \neq 0$ if $z \in G$. This is the desired conclusion.

We now prove the claim. For each vertex v we define angles ϕ_v and θ_v by $\phi_v = \phi$ for part (a) and $\phi_v = \phi_i$, if $v \in V_i$, for part (b), and then $\theta_v = (\pi/2 - \phi_i)(\theta/\theta_0)$. Clearly $|\theta_v| < \pi/2 - \phi_v$ and $\theta = \theta_{v_1(e)} + \theta_{v_1(e)}$ for each edge e.

Now let $\mathcal{H}$ and $\overline{\mathcal{H}}$ denote respectively the open and closed right half planes, and for $\epsilon > 0$ and $v \in V$ define

$$K_\epsilon(v) = -(\epsilon + e^{i\theta_v}\overline{\mathcal{H}}). \tag{4.8}$$

No root ζ of $p_v(z)$ can belong to $e^{i\theta_v}\mathcal{H}$; for $\zeta = 0$ this is trivial and for $\zeta \neq 0$ follows from $|\arg(\zeta)| \in [\pi - \phi_v, \pi]$ and $|\theta_v| < \pi/2 - \phi_v$. Thus $p_{v,\varepsilon}(z) \neq 0$ if $z + \varepsilon \in e^{i\theta_v}\mathcal{H}$, that is, if $z + \varepsilon \notin -e^{i\theta_v}\overline{\mathcal{H}}$ or equivalently if $z \notin K_\epsilon(v)$. Grace's Theorem then implies that $q_{v,\epsilon}((z_{ve})_{e\in E_v}) \neq 0$ if $z_{v,e} \notin K_\epsilon(v)$ for all $e \in E_v$. Repeatedly using the Asano–Ruelle Lemma, as in the proof of Theorem 4.1, we then conclude that $Q^{(|E|)}\big((z_e)_{e\in E}\big) \neq 0$ if $z_e \notin -K_\epsilon(v_1(e)) \times K_\epsilon(v_2(e))$ for all $e \in E$.

Now, the set $-K_\varepsilon(v_1(e)) \times K_\varepsilon(v_2(e))$ and the ray $\rho_{\theta_{v_1(e)}+\theta_{v_2(e)}} = \rho_\theta$ do not intersect. Otherwise there would exist $(s_1 \geq 0, t_1)$, $(s_2 \geq 0, t_2)$ and $x > 0$ such that

$$-(\varepsilon + e^{i\theta_{v_1(e)}}(s_1 + it_1))(\varepsilon + e^{i\theta_{v_2(e)}}(s_2 + it_2)) = xe^{i(\theta_{v_1(e)}+\theta_{v_2(e)})},$$

or equivalently

$$y_1 y_2 = \rho e^{i\pi}, \quad y_j = e^{-i\theta_{v_j(e)}}\varepsilon + (s_j + it_j), \quad j = 1, 2. \tag{4.9}$$

But $\mathrm{Re}(y_j) \geq 0$, since $s_j \geq 0$ and $|\theta_j| < \pi/2$, and hence $|\arg(y_j)| < \pi/2$; this is inconsistent with the first equation in (4.9). This completes the proof of the claim. □

Remark 4.3. If G is disconnected and has one or more bipartite components then the zero-free region for $P_{(C)}$ obtained by applying Theorem 4.2 to each component, and using the fact that $P_{(C)}$ is the product of the polynomials for the components, may be larger than that obtained by applying the theorem to G as a whole.

5. Local central limit theorems for graph-counting polynomials

In this section we consider various infinite families of graphs, each with an associated assignment $(C(v))_{v\in V}$ of finite sets to vertices; we let $\mathcal{G}$ denote such a family and $\mathcal{P} = \mathcal{P}(\mathcal{G})$ denote the class of associated graph polynomials, which we now denote by P_G. We will measure the size of a graph G by the size of its edge set $E = E(G)$ and let $d_{\max} = d_{\max}(G)$ denote the maximum degree of any vertex of G; for convenience we assume that $d_{\max} \geq 2$ (the case $d_{\max} = 1$ is trivial to analyze).

For simplicity we restrict our attention to the two cases implicit in Theorem 4.2, and thus assume that either (a) there is a fixed angle $\phi \in [0, \pi/2]$ such that for each graph in $G \in \mathcal{G}$ and each $v \in V(G)$, every nonzero root ζ of p_v satisfies $|\arg(\zeta)| \in [\pi - \phi, \pi]$, or (b) each graph in $\mathcal{G}$ is bipartite, with $V(G)$ partitioned as $V_1(G) \cup V_2(G)$, and there are fixed angles $\phi_1, \phi_2 \in [0, \pi/2]$ such that for each G and each $v \in V_i(G)$, $i = 1, 2$, every nonzero root ζ of p_v satisfies $|\arg(\zeta)| \in [\pi - \phi_i, \pi]$. We will give examples in which the results of Section 4 imply that the roots of each $P \in \mathcal{P}$ lie in the left half plane, and then apply the results of Section 3 to obtain a CLT or LCLT for $\mathcal{P}$.

Note that the proofs of CLT and LCLT in Section 3 require two sorts of hypotheses: on the one hand, the roots of the polynomials must lie in the left hand plane, or in some more restricted region; on the other, the variance of the random variable X_P, or more precisely the related quantity $W(X_P)$, must grow sufficiently fast with N_P (see, for example, Remark 3.9). When the graphs in the family under consideration have bounded vertex degree the latter condition is, in our examples, automatically satisfied. For the more general situation with unbounded degrees one must impose conditions on their growth to obtain the result; we will work this out in detail only for some of our examples.

Example 5.1. When $C(v) = C = \{0,1\}$ for each vertex v the admissible edge configurations are matchings or monomer–dimer configurations, as discussed in the introduction. It is well known [18] that in this case all roots of $P(z)$ lie on the negative real axis. This follows also from Theorem 4.2(a); one may take $\phi = 0$ there, using the fact that for any vertex v the vertex polynomial $p_v(z) = 1 + d_v z$ has negative real root $-1/d_v$. To obtain an LCLT from Corollary 3.6 we need to find the quantities Δ and f defined in (3.10). Theorem 4.2 implies that the roots $-\eta_j$ of P_G are negative real numbers satisfying $\eta_j > 1/d_{max}^2$, so that $\Delta = \min_{1\le j\le N} |\eta_j|^2 \ge 1/d_{\max}^4$. Further, $p_0 = 1$ and $p_1 = |E|$, since any subgraph with exactly one edge is admissible, so that $f = p_1/p_0 = |E|$. Then from Lemma 3.2 we have $\mathrm{Var}(X) \ge \frac{|E|}{8\,d_{\max}^4}$. In fact Godsil [16] (Lemma 3.5) had used a powerful result of Heilmann and Lieb [18] to obtain a qualitatively stronger bound $\mathrm{Var}(X_P) \ge \frac{|E(G)|}{(4d_{\max}(G)-3)^2}$. So, using Godsil's bound, an LCLT follows immediately from Corollary 3.8 and Remark 3.9(i), whenever $d_{max}(G)$ grows slower than $|E(G)|^{1/2}$ in the class of graphs $\mathcal{G}$:

Theorem 5.1. *If for each $G \in \mathcal{G}$, $C(v) = \{0,1\}$ for each vertex v, and $|E(G)| \ge 2.2 \times 10^7\, d_{\max}^2(G)$, then*

$$\sup_m \left| \Pr(X_P = m) - \frac{e^{-\frac{(m-E[X_P])^2}{2\,\mathrm{Var}(X_P)}}}{\sqrt{2\pi\,\mathrm{Var}(X_P)}} \right| \le \frac{25\, d_{\max}^2(G)}{\pi|E(G)|}.$$

We note that Godsil [16] used his bound for $\mathrm{Var}(X)$ in conjunction with Canfield's theorem for log-concave distributions to get his LCLT for X_P with the error bound $O\big(d_{\max}^{3/2}/|E|^{3/4}\big)$, weaker than the bound in Theorem 5.1.

Example 5.2. When $C(v) = \{0,1,2\}$ for each vertex v the admissible edge configurations are unbranched subgraphs, as discussed in the introduction. In this case the vertex polynomial is

$$p_v(z) = 1 + d_v z + \frac{d_v(d_v-1)}{2} z^2. \tag{5.1}$$

If $d_v = 1$ then p_v has root $\zeta_v = -1$, while if $d_v \ge 2$ the roots are

$$\zeta_v^{\pm} := \frac{-d_v \pm i\sqrt{d_v^2 - 2d_v}}{d_v(d_v-1)}. \tag{5.2}$$

From $|\zeta_v^\pm|^2 = 2/\bigl(d_v(d_v-1)\bigr)$ we see that each root ζ of p_v satisfies

$$|\zeta|^2 \geq \frac{2}{d_{\max}(d_{\max}-1)}; \tag{5.3}$$

note that when $d_v = 1$ this follows from our convention $d_{\max} \geq 2$. Thus from Theorem 4.1 each root $-\eta_j$ of P_G satisfies

$$|\eta_j| \geq \frac{2}{d_{\max}(d_{\max}-1)}. \tag{5.4}$$

Similarly, each root ζ of p_v satisfies $|\arg(\zeta)| = \pi - \phi_v$ with

$$\phi_v \leq \phi_{\max} := \sin^{-1}\sqrt{\frac{d_{\max}-2}{2(d_{\max}-1)}}; \tag{5.5}$$

when $d_v = 1$ this is trivial and for $d_v \geq 2$ follows immediately from (5.2). Thus Theorem 4.2(a) gives $|\arg(-\eta_j)| \geq \pi - 2\phi_{\max}$. Since

$$\cos(2\phi_{\max}) = 1 - 2\sin^2\phi_{max} = \frac{1}{d_{\max}-1} > 0, \tag{5.6}$$

all the roots $-\eta_j$ lie in the open left-half plane; moreover, from (3.10), (5.4)

$$\Delta = \min_j |\eta_j|^2 \geq \frac{4}{d_{\max}^2(d_{\max}-1)^2}. \tag{5.7}$$

As in Example 5.1, $f = p_1/p_0 = |E|$, so that from Lemma 3.2,

$$\mathrm{Var}(X) \geq \frac{|E|}{2\,d_{\max}^2(d_{\max}-1)^2}. \tag{5.8}$$

An LCLT then follows from Corollary 3.8 and Remark 3.9(iii) when $d_{max}(G)$ grows logarithmically slower than $|E(G)|^{1/12}$ in the class of graphs $\mathcal{G}$ (the precise condition is (5.9)).

Theorem 5.2. *Suppose that for each $G \in \mathcal{G}$ and vertex v of G, $C(v)$ is $\{0,1\}$ or $\{0,1,2\}$. If $|E(G)|$ is large enough so that*

$$|E(G)| \geq \frac{2^{2/3}\pi^2}{3}\, d_{\max}^4(G)\lambda(G)^{2/3}\log\lambda(G)$$
$$\bigl(\lambda(G) := \min\{|E(G)|,\, |V(G)|\}\bigr) \tag{5.9}$$

(for instance, if $|E(G)| \geq 150\, d_{max}^{12}(G) \log^3 |V(G)|$), then

$$\sup_m \left| \Pr(X_P = m) - \frac{e^{-\frac{(m-E[X_p])^2}{2\,\mathrm{Var}(X_P)}}}{\sqrt{2\pi\,\mathrm{Var}(X_P)}} \right| \leq \frac{50\, d_{\max}^4(G)}{\pi |E(G)|}. \tag{5.10}$$

Proof. By Lemma 3.2 and $\mathrm{Var}(X_P) \leq N_P$ (see (3.7)), the condition of Corollary 3.8 is met if

$$\frac{p_1}{p_0} \min\{1, \Delta_P\} \geq \frac{8\pi^2}{3 \cdot 2^{1/3}}\, N_P^{2/3} \log N_P.$$

By $p_1/p_0 = |E(G)|$ and (5.7), this inequality is satisfied if

$$\frac{4|E(G)|}{d_{\max}^4(G)} \geq \frac{8\pi^2}{3 \cdot 2^{1/3}} N_{P_G}^{2/3} \log N_{P_G}. \tag{5.11}$$

Now $N_{P_G} \leq \lambda(G) = \min\{|E(G)|, |V(G)|\}$, since $2N_{P_G} \leq \sum_v c_v \leq 2|V(G)|$. Therefore (5.11) follows from the condition (5.9). Thus when (5.9) is satisfied the condition of Corollary 3.8 holds, and with (5.8) this implies (5.10). □

Remark 5.3. If $d_{\max}(G) \leq 3$ for all $G \in \mathcal{G}$, for example if the graphs in $\mathcal{G}$ are all finite subgraphs of the planar hexagonal lattice, then $\phi_{\max} = \pi/6$ in the above analysis and all roots $-\eta_j$ of P_G satisfy the condition (3.14) that $|\arg(-\eta_j)| \in [2\pi/3, \pi]$. (It follows from (3.13) and (3.14) in Section 3.2 that the distribution $\{\Pr(X = m)\}_{m \geq 0}$ is log-concave.) Then from Corollary 3.8, Remark 3.9(ii), and (5.8) we obtain an LCLT with the error bound $\frac{1800}{\pi|E|}$, provided that $|E| > 1.6 \cdot 10^{10}$.

In the next four examples we consider families of bipartite graphs, assuming, as discussed above, that the vertex set $V(G)$ of each graph G is partitioned as $V(G) = V_1(G) \cup V_2(G)$. We assume that $C_v \equiv C^{(i)}$, $v \in C^{(i)}$, where $C^{(1)}$ may differ from $C^{(2)}$. We also assume that there is a uniform bound on the vertex degrees; specifically, $d_v \leq d_i$ for $v \in V_i(G)$, $i = 1, 2$, $G \in \mathcal{G}$. In some cases this assumption is made for simplicity and one could, in principle, dispense partially or completely with it, but in others it is strictly necessary, at least for our methods.

Example 5.3. Here we take $C_v = \{0, 1\}$ for $v \in V_1(G)$ and, for $v \in V_2(G)$, $C_v = \{0, 1, \ldots, c_2\}$ with c_2 either 2, 3, or 4. For $v \in V_1$, $p_v(z) = 1 + d_v z$ as in Example 5.1, with a single negative real root. Moreover, for $v \in V_2$, each root ζ of $p_v(z)$ satisfies $|\arg(\zeta)| \in [\pi - \phi_v, \pi]$, where $\phi_v \leq \phi_{\max} < \pi/2$ for some angle $\phi_{\max}$ which depends on c_2 and d_2; for $c_2 = 2$ this was shown in Example 5.2 above (with $\phi_{\max} = \pi/4$) and for $c_2 = 3$ or 4 was shown in [23] (see Theorem 5.1 there). Thus taking $\phi_1 = 0$ and $\phi_2 = \phi_{\max}$ in Theorem 4.2(b) we see that the roots $-\eta_j$ of P_G satisfy $|\arg(-\eta_j)| \in [\pi - \phi_{\max}, \pi]$.

On the other hand, each root ζ of any p_v will satisfy $|\zeta| \geq r_0$ for some $r_0 > 0$, so that $\Delta = \min_{1\leq j\leq N} |\eta_j|^2 \geq \Delta_0 > 0$ uniformly for all graphs in $\mathcal{G}$; for notational simplicity we may assume that $\Delta_0 \leq 1$. We still have $f = p_1/p_0 = |E(G)|$, so that $\mathrm{Var}(X_{P_G}) \geq \Delta_0|E|/8$ from Lemma 3.2. Furthermore, by (3.9),

$$\mathrm{Var}(X_{P_G}) \leq (1 + \sec\phi_{\max})W(X_{P_G}),$$

and therefore the condition (3.16) of Corollary 3.8 is satisfied if $\mathrm{Var}(X_{P_G}) \geq v^*$, where v^* is the larger root of

$$v^{1/3} = \frac{\pi^2(1 + \sec\phi_{\max})}{3 \cdot 2^{1/3}} \ln v.$$

So for $\mathrm{Var}(X_{P_G}) \geq v^*$ from Corollary 3.8 we obtain an LCLT in the form

$$\sup_m \left| \Pr(X_P = m) - \frac{e^{-\frac{(m-E[X_P])^2}{2\,\mathrm{Var}(X_P)}}}{\sqrt{2\pi\,\mathrm{Var}(X_P)}} \right| \leq \frac{C}{|E(G)|}, \tag{5.12}$$

with $C = 200/\pi\Delta_0$.

With more precise information on the location of the roots of p_v for $v \in V_2(G)$ one could extend this result to families in which the vertex degrees are not bounded, in the style of Theorem 5.2. For $c_2 = 2$ the necessary information was obtained in the discussion of Example 5.2; for $c_2 = 3, 4$ one would have to determine the locations of roots of cubic and quartic polynomials, respectively.

Example 5.4. Here $C_v = \{0, 1, 2\}$ for $v \in V_1(G)$ and $C_v = \{0, 1, 2, 3\}$ for $v \in V_2(G)$, with d_1 arbitrary and $d_2 \leq 4$ (the cases $C_2 = \{0, \ldots, c_2\}$ with $c_2 = 1$ or 2 are covered by earlier examples). For $v \in V_1(G)$ a root ζ of $p_v(z)$ satisfies $|\arg(\zeta)| < \pi/4$; for $v \in V_2(G)$ all roots of $p_v(z)$ are $\zeta = -1$ when $d_v \leq 3$, while when $d_v = 4$ the roots of $p_v(z) = 1 + 4z + 6z^2 + 4z^3$ are $-1/2$ and $(-1 \pm i)/2$, so that all roots ζ satisfy $|\arg(\zeta)| \leq \pi/4$. Thus from Theorem 4.2(b) the roots $-\eta_j$ of P_G satisfy $|\arg(-\eta_j)| \in [\pi - \phi_{\max}, \pi]$ for some $\phi_{\max} < \pi/2$. As in Example 5.3 we find again $\Delta > \Delta_0$ for some d_1-dependent Δ_0, leading to an LCLT of the form (5.12). Again, one may also find as in Example 5.2 an LCLT for a family of graphs in which $d_1(G)$ can increase with $|E(G)|$.

Example 5.5. This example relies on numerical computations, although one could probably justify these by obtaining rigorous bounds. We take $C_v = \{0, 1, 2\}$ for $v \in V_1(G)$ and, for $v \in V_2(G)$, $C_v = \{0, 1, \ldots, c_2\}$ with c_2 either 3 or 4. The possible values of d_1 and d_2 are shown in Table 1; for example, one may take $d_1 = 3$, $c_2 = 3$, and $d_2 = 5$, 6, or 7. There are a total of five possible examples. Also shown are angles ϕ_1, ϕ_2, obtained by computation with Maple, such that for $v \in V_i$ $(i = 1, 2)$, each root ζ of $p_v(z)$ lies in $[\pi - \phi_i, \pi]$. Since in each case $\phi_1 + \phi_2 < \pi/2$ we obtain an LCLT of the form (5.12) as in the two previous examples.

Table 1
Possible values of d_1 and d_2 with corresponding values of ϕ_1 and ϕ_2.

		$c_2 = 3$		$c_2 = 4$	
d_1	ϕ_1	d_2	ϕ_2	d_2	ϕ_2
3	$0.1666666666\cdots\pi$	5, 6, 7	$0.3276761158\cdots\pi$	5	0.30π
4	$0.1959132762\cdots\pi$	5	$0.2932617986\cdots\pi$		

Example 5.6. In the examples considered above, each C_v has been of the form $\{0, 1, \dots, k\}$ for some k. Now we take $C_v = \{0, 1\}$ for $v \in V_1(G)$, but for $v \in V_2(G)$ take C_v to be either $\{0, 2\}$ or $\{0, 2, 4\}$. To avoid vertices which are effectively disconnected from the rest of the graph we assume that $d_v \geq 2$ for $v \in V_2(G)$, and again assume that $d_v \leq d_i$ for $v \in V_i(G)$, $i = 1, 2$, with d_1 and d_2 fixed. Again $p_v(z)$, $v \in V_1$, has a single negative real root, while for $v \in V_2(G)$, $p_v(z) = \tilde{p}_v(z^2)$, and one finds easily that $\tilde{p}(w)$, which is either linear or quadratic, has only negative real roots, so that p_v has purely imaginary roots. Thus taking $\phi_1 = 0$ and $\phi_2 = \pi/2$ in Theorem 4.2(b) we see that the roots $-\eta_j$ of P_G satisfy $\mathrm{Re}(-\eta_j) \leq 0$, so that a CLT will follow from Theorem 3.1 once we verify that $\mathrm{Var}(X_P) \to \infty$ as $N_P \to \infty$ in the family $\mathcal{P}$ under consideration.

Since in this case the roots $-\eta_j$ of P may lie on the imaginary axis, the estimates that we have been using for the variance, which begin with (3.8), are no longer effective. On the other hand, from (3.6) we have

$$\mathrm{Var}(X_P) \geq \frac{1}{2} \sum_{j=1}^{N_P} \frac{|\eta_j|^2}{(1 + |\eta_j|^2)^2} \geq \frac{N_P}{2} \min_j \{|\eta_j|^2, |\eta_j|^{-2}\}. \tag{5.13}$$

Since d_1 and d_2 are fixed we have upper and lower bounds $0 < r \leq |\zeta| \leq R$ on the magnitudes of the roots ζ of the $p_v(z)$, and Theorem 4.1, together with a corresponding result, with a similar proof, for upper bounds, implies that $r^2 \leq |\eta_j|^2 \leq R^2$. N_P is the size of the largest admissible configuration of occupied edges in G; let $M \subset E$ be an admissible configuration with $|M| = N_P$. Each edge of M is incident on a unique vertex of V_1, and every vertex of V_2 must be joined by an edge of E to one of these vertices, since if $v \in V_2$ were not so joined then two edges incident on v could be added to M. Thus $|V_2| \leq d_1 N_P$, and since $|E| \leq d_2|V_2|$, $N_P \geq |E|/d_1 d_2$. From (5.13) we thus have

$$\mathrm{Var}(X_P) \geq \frac{|E|}{d_1 d_2} \min \{r^2, R^{-2}\}. \tag{5.14}$$

Remark 5.4. Families of graphs described in Examples 5.3 and 5.6 may be used to model the absorption of dimers, trimers, or certain more complicated molecules on the two-dimensional square lattice (see, e.g., [27]) and thus obtain LCLTs for the associated graph counting polynomials. For example, let G_Λ be the graph whose vertices are the points of a rectangle $\Lambda \in \mathbb{Z}^2$, with edges connecting nearest-neighbor vertices; G_Λ is bipartite with partition determined by vertex parity. Subgraphs obtained from $C^{(1)} = \{0, 1\}$ and $C^{(2)} = \{0, 1, 2\}$ may be interpreted as configurations of absorbed dimers and trimers, with the trimers centered on vertices of V_2; the trimers, in contrast to those considered in [27], may be either straight or bent. Taking $C^{(2)} = \{0, 2\}$ as in Example 5.6 gives configurations involving trimers only. Other molecular shapes may be included by enlarging $C^{(2)}$.

6. A central limit theorem for graph-counting polynomials

To obtain the LCLTs proved in Section 5 we had to assume conditions guaranteeing that the zeros of a graph-counting polynomial P all lie in the open left half-plane. As an application of Theorem 2.1 we will here show that a CLT holds under a much less stringent condition, satisfied by a broad class of graph-counting polynomials P: that the zeros of P avoid a neighborhood of the point z_0 on the positive real line. To obtain a CLT from Theorem 2.1 we need also the condition that $\mathrm{Var}(X_P) \gg N_P^{2/3}$. We will show that this latter condition holds, with room to spare, when, as we assume throughout this section, $P(z)$ is the graph-counting polynomial for a graph G such that for each vertex v of G,

$$C_v = \{0, 1, \dots, c_v\} \tag{6.1}$$

for some $c_v \geq 1$.

Theorem 6.1. *Fix $z_0 > 0$ and suppose that for some δ with $0 < \delta < z_0$, $P(z) := \sum_{m=0}^{N_P} p_m z^m$ satisfies $P(z) \neq 0$ if $|z| < \delta$ or $|z - z_0| < \delta$. Then with $F_P(x)$, $G(x)$ as in (2.1), (2.2),*

$$\sup_{x\in\mathbb{R}} |F_P(x) - G(x)| \leq B N_P^{-1/6}, \tag{6.2}$$

where the constant B depends only on z_0, δ, and $d_{\max}(G)$.

Proof. From the given hypotheses and the fact that $p_0 = 1$ and $p_1 = |E(G)| \geq N_P$ we can apply Proposition 2.4 (with $c_1 = 1$) to conclude that $E[X] \geq B_1 N$, where B_1 depends on δ. Then we obtain (6.2) from Theorem 2.1 once we show that $\mathrm{Var}(X_P) \geq B_2 E[X_P]$, where B_2 may depend on $d_{\max}(G)$. For this we use

Lemma 6.2. *(See Ginibre [14].) Let X be a random variable taking nonnegative integer values and let $T_m := m!\,\Pr(X = m)$. If for some $A > -1$ and all m, $0 \leq m \leq N - 2$,*

$$\frac{T_{m+2}}{T_{m+1}} \geq \frac{T_{m+1}}{T_m} - A, \tag{6.3}$$

then

$$\mathrm{Var}(X) \geq \frac{E[X]}{1 + A}. \tag{6.4}$$

Proof. We give the proof for completeness. Observe first that

$$E\left[\frac{T_{X+1}}{T_X}\right] = \sum_{m\geq 0}(m+1)\Pr(X=m+1) = E[X]. \tag{6.5}$$

So

$$\begin{aligned}(1+A)^2E[X]^2 &= \left(E\left[\frac{T_{X+1}}{T_X}+XA\right]\right)^2 \leq E\left[\left(\frac{T_{X+1}}{T_X}+XA\right)^2\right]\\ &= E\left[\left(\frac{T_{X+1}}{T_X}\right)^2\right]+2A\,E\left[X\frac{T_{X+1}}{T_X}\right]+A^2E[X^2]\\ &=: R_1+R_2+R_3. \end{aligned}\tag{6.6}$$

Here, since $mT_{m+1}/T_m = (m+1)m\Pr(X=m+1)/\Pr(X_m)$,

$$R_2 = 2A\sum_{m\geq 0}(m+1)m\Pr(X=m+1) = 2A\,E\bigl[X(X-1)\bigr]. \tag{6.7}$$

Furthermore, using (6.3) and (6.5),

$$\begin{aligned}R_1 &\leq E\left[\frac{T_{X+1}}{T_X}\cdot\left(\frac{T_{X+2}}{T_{X+1}}+A\right)\right]\\ &= \sum_{m\geq 0}(m+2)(m+1)\Pr(X=m+2)+AE[X]\\ &= E\bigl[X(X-1)\bigr]+AE[X]. \end{aligned}\tag{6.8}$$

Combining (6.6), (6.7) and (6.8), we conclude that

$$(1+A)^2E[X]^2 \leq (1+A)^2\,E[X^2]-(1+A)E[X],$$

which is equivalent to (6.4). □

Naturally our next step is to prove that the distribution of X_P meets the condition of (6.3) of Lemma 6.2.

Proposition 6.3. *For all $z_0>0$ the quantities $T_m = m!p_m z_0^m/P(z_0)$ satisfy (6.3) with $A=(2\alpha+1)z_0$, where $\alpha := \max_{v\in V}[d_v-c_v]_+$.*

To prove Proposition 6.3 we first establish a lemma relating p_{m+1} and p_{m+2} to p_m. Let $\mathcal{M}_m$ be the set of admissible subgraphs with m edges, so that $p_m = |\mathcal{M}_m|$, and for each $M\in\mathcal{M}_m$ let $K_1(M)$ and $K_2(M)$ be the numbers of subgraphs in $\mathcal{M}_{m+1}$ and $\mathcal{M}_{m+2}$, respectively, which contain M; equivalently, we may introduce

$$E_1(M) = \{e \mid e \in E \setminus M, \{e\} \cup M \in \mathcal{M}_{m+1}\},$$
$$E_2(M) = \{\{e_1, e_2\} \mid e_1, e_2 \in E \setminus M, \{e_1, e_2\} \cup M \in \mathcal{M}_{m+2}\},$$

with $e_1 \neq e_2$ in the second line, and define $K_1(M) = |E_1(M)|$, $K_2(M) = |E_2(M)|$. We will regard K_1 and K_2 as random variables, furnishing $\mathcal{M}_m$ with the uniform probability measure $\mathrm{Prob}(M) = 1/p_m$. It turns out that the ratios p_{m+1}/p_m, p_{m+2}/p_m are proportional to the expectations $E[K_1]$ and $E[K_2]$ respectively.

Lemma 6.4.

$$p_{m+1} = \frac{1}{m+1} \sum_{M \subset \mathcal{M}_m} K_1(M) = \frac{E[K_1]}{m+1} p_m, \tag{6.9}$$

$$p_{m+2} = \frac{2}{(m+2)(m+1)} \sum_{M \subset \mathcal{M}_m} K_2(M) = \frac{2E[K_2]}{(m+2)(m+1)} p_m. \tag{6.10}$$

Proof. Let $S_1 = \{(M, e) \mid M \in \mathcal{M}_m,\ e \in E_1(M)\}$ and notice that $|S_1| = \sum_{M \in \mathcal{M}_m} K_1(M)$. S_1 may be put in bijective correspondence with $S_1' = \{(M', e) \mid M' \in \mathcal{M}_{m+1},\ e \in M'\}$, via the correspondence $(M, e) \leftrightarrow (M', e)$ with $M' = M \cup \{e\}$; here we use the fact that each $C(v)$ has the form (6.1), which implies that the subgraph obtained by deleting an edge from an admissible subgraph is admissible. Clearly $|S_1'| = (m+1)p_{m+1}$, and (6.9) follows from $|S_1| = |S_1'|$. Similarly, (6.10) is obtained from the correspondence of $S_2 = \{(M, \{e_1, e_2\}) \mid M \in \mathcal{M}_m,\ \{e_1, e_2\} \in E_2(M)\}$ with $S_2' = \{(M', \{e_1, e_2\}) \mid M' \in \mathcal{M}_{m+2},\ e_1, e_2 \in M',\ e_1 \neq e_2\}$. $\square$

Proof of Proposition 6.3. By Lemma 6.4 and the definition of T_m in Proposition 6.3,

$$\frac{T_{m+2}}{T_{m+1}} - \frac{T_{m+1}}{T_m} = z_0 \left(\frac{2E[K_2]}{E[K_1]} - E[K_1] \right).$$

Let us bound $E[K_2]$ from below. To this end notice that we may obtain $E_2(M)$ by choosing a pair $\{e_1, e_2\}$ of distinct edges from $E_1(M)$ and then rejecting this pair if $\{e_1, e_2\} \cup M$ is not admissible, which can happen only if e_1 and e_2 share a vertex v with $d_M(v) \geq c_v - 1$. Thus if we first choose e_1 with endvertices v, v' we will reject at most $d_v - c_v + d_{v'} - c_{v'}$ ordered edge pairs (e_1, e_2); this counts unordered edge pairs twice, and so we find that

$$K_2(M) \geq \binom{K_1(M)}{2} - \alpha K_1(M), \quad \alpha := \max_{v \in V}[d_v - c_v].$$

Consequently, as $E[K_1^2] \geq E[K_1]^2$,

$$2E[K_2] - E[K_1]^2 \geq E[(K_1)_2] - 2\alpha E[K_1] - E[K_1]^2 \geq -(2\alpha + 1)E[K_1],$$

and thus

$$\frac{T_{m+2}}{T_{m+1}} - \frac{T_{m+1}}{T_m} \geq -(2\alpha+1)z_0,$$

proving Proposition 6.3. □

By Ginibre's result, we then have

$$\mathrm{Var}(X_P) \geq \frac{E[X_P]}{1+(2\alpha+1)z_0}.$$

This completes the proof of Theorem 6.1. □

Corollary 6.5. *Suppose that $\mathcal{G}$ is a family of graphs such that for each vertex v of a graph $G \in \mathcal{G}$, $d_v \leq d_{\max}$ for some fixed $d_{\max}$ and C_v has the form (6.1) with $c_v \leq 4$. Then for $G \in \mathcal{G}$ and $P = P_G$,*

$$\sup_{x\in\mathbb{R}} |F_P(x) - G(x)| \leq B_0 N_P^{-1/6}, \tag{6.11}$$

where the constant B_0 depends only on z_0 and $d_{\max}$.

Proof. We must verify that the hypotheses of Theorem 6.1 are satisfied with some uniform choice of δ. First, as discussed in Example 5.3, it follows from $c_v \leq 4$ that there is then an angle $\phi_{\max}$ (which may depend on $d_{\max}$), with $0 \leq \phi_{\max} < \pi/2$, such that, for any v, each root ζ of $p_v(z)$ satisfies $|\arg(\zeta)| \in [\pi - \phi_{\max}, \pi]$. Thus taking $\phi = \phi_{\max}$ in Theorem 4.2(a) we see that the roots ζ_j of P satisfy $|\arg(\zeta_j)| \in [\pi - 2\phi_{\max}, \pi]$, and so for any $z_0 > 0$ there will be a neighborhood of z_0, which can be chosen uniformly in G, which is free from zeros of P. Moreover, the condition $d_v \leq d_{\max}$ implies that the roots of $p_v(z)$ are uniformly bounded away from zero, and then by Theorem 4.1 so are the roots of P. □

7. Applications to statistical mechanics

In this section we discuss briefly some applications of the results of Section 2 to the statistical mechanics of classical lattice systems; we refer the reader to [32] for the necessary background. For a system in a finite subset Λ of the lattice $\mathbb{Z}^d$, at inverse temperature β, the *partition function* $P(\beta, z; \Lambda)$, a polynomial in z of degree $|\Lambda|$, is a generating function which may, for example, count the number of particles present. One also is interested in the pressure

$$\Pi(\beta, z) = \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{\log P(\beta, z; \Lambda)}{|\Lambda|}; \tag{7.1}$$

the existence of the limit in (7.1) can be proved in many cases. In the limit the zeros of $P(\beta, z; \Lambda)$, called *Lee–Yang zeros*, can approach the positive z-axis and thus cause singularities in the pressure at these physically relevant values of z. However, if the positive fugacity z_0 is not an accumulation point of such zeros, or equivalently if $\Pi(\beta, z)$ is analytic at z_0, and we assume for the moment that

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} \mathrm{Var}(X_\Lambda)/|\Lambda|^{2/3} = \infty, \tag{7.2}$$

where X_Λ is the random variable obtained from $P(\beta, z; \Lambda)$ via (1.1) and (1.2), then Theorem 2.1 shows that the family $\{X_\Lambda\}$, as Λ increases, satisfies a CLT.

Remark 7.1. This approach to obtaining a CLT in statistical mechanics originated in [19], which considers only translation invariant systems with nearest-neighbor interactions. Theorem 2.1 strengthens and gives a complete proof of the result there. In contrast to other ways of proving such a CLT (see the discussion in Section 1), the method here applies even when the interactions are not translation invariant, although this was not noted in [19]. We also observe here that Dobrushin and Shlosman [8] proved a local "large and moderate deviation" result for X which implies a LCLT under a further *locality* condition, which rules out situations in which all the zeros are close to the imaginary axis.

Various cases are known in which there exist fugacities $z_0 > 0$ with a neighborhood free of Lee–Yang zeros; we briefly describe some of these.

- In a seminal paper [24], see also [38], Lee and Yang proved that, for Ising spin systems with ferromagnetic interactions, all the zeros of $P(z, \beta; \Lambda)$ lie on the unit circle, $|z| = 1$. Thus the family X_Λ, where in this case X_Λ is the number of up spins in Λ, satisfies a CLT for $z_0 \neq 1$. More recent references about Lee–Yang zeros can be found in [35,34].
- In general, one can show [32] that (i) $\Pi(\beta, z)$ is analytic on the positive real z-axis, if β is sufficiently small (no phase transitions at high temperature), and (ii) $P(\beta, z; \Lambda)$ is nonzero, and hence $\Pi(\beta, z; \Lambda)$ is analytic, in a disc $|z| \le R(\beta; \Lambda)$, with $R(\beta) := \inf_\Lambda R(\beta; \Lambda) > 0$, for all $\beta > 0$, so that $\Pi(\beta, z)$ is analytic for $|z| < R(\beta)$. Each of these results yields a CLT for the corresponding real fugacities z_0.
- The behavior of the zeros for other interactions has been investigated extensively, both analytically and numerically (see [22,23] and references therein). One can show [23], for certain classes of interactions $U(\underline{\sigma})$, that for some $\delta > 0$ each zero of $P(\beta, z; \Lambda)$ satisfies $\mathrm{Re}\, \zeta < -\delta$; for these systems, $X_{\beta,\Lambda}$ satisfies the conditions of Corollary 3.8 and thus an LCLT. In other cases one can prove [22,23] that for β large the zeros stay away from the positive z-axis and $X_{\beta,\Lambda}$ thus satisfies a CLT by Theorem 3.1. Such CLT have been obtained by other methods; see for example [9] and the discussion in [13].

In some cases in which the zeros do approach the real z-axis at some z_0 in the $\Lambda \nearrow \mathbb{Z}^d$ limit, it is known that the fluctuations in $X_{\beta,z_0;\Lambda}$ are in fact not Gaussian in the $\Lambda \nearrow \mathbb{Z}^d$ limit [25,1].

We finally want to indicate how the assumption (7.2) may be justified. From Proposition 2.4 we can conclude that $E[X] \geq M|\Lambda|$ for some $M > 0$, once we verify the hypotheses of that result. Condition (i), that $p_1 \geq c_1 p_0 |\Lambda|$, follows easily from the definition of $P(\beta, z; \Lambda)$ (see [32]). Condition (ii) follows from the fact, mentioned above, that no zeros of $P(\beta, z; \Lambda)$ lie in the disc $|z| < R(\beta)$. With this, Ginibre's result Theorem 6.2 gives $\mathrm{Var}(X_{\beta,\Lambda}) \geq M|\Lambda|/(1 + A)$. We need to know, of course, that (6.3) holds for the systems under consideration here. In fact this is true more generally, as we show in Appendix B (a weaker version of this result is quoted from a "private communication" mentioned in [14], but no proof is given).

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Appendix A. Grace's Theorem and Asano contractions

Theorem A.1 *(Grace's Theorem). Let $P(z)$ be a complex polynomial in one variable of degree at most n, and let $Q(z_1, \dots, z_n)$ be the unique multi-affine symmetric polynomial in n variables such that $Q(z, \dots, z) = P(z)$. If the n roots of P are contained in a closed circular region K and $z_1, \dots, z_n \notin K$, then $Q(z_1, \dots, z_n) \neq 0$.*

Here a *closed circular region* is a closed subset K of $\mathbb{C}$ bounded by a circle or a straight line. If P is in fact of degree k with $k < n$ then we say that $n - k$ roots of P lie at ∞ and take K noncompact. For a proof of the result see Polya and Szegö [30, V, Exercise 145]. (We remark that one should perhaps use the Riemann sphere here instead of the complex plane, but for notational simplicity it is convenient to work with $\mathbb{C}$. We leave to the reader the task of compactifying $\mathbb{C}$ by a point at infinity whenever useful.)

Lemma A.2 *(Asano–Ruelle Lemma). (See [2,31].) Let K_1, K_2 be closed subsets of $\mathbb{C}$, with $K_1, K_2 \not\ni 0$. If Φ is separately affine in z_1 and z_2, and if*

$$\Phi(z_1, z_2) \equiv A + Bz_1 + Cz_2 + Dz_1 z_2 \neq 0$$

whenever $z_1 \notin K_1$ *and* $z_2 \notin K_2$, *then*

$$\tilde{\Phi}(z) \equiv A + Dz \neq 0$$

whenever $z \notin -K_1 \cdot K_2$.

Here we have written $-K_1 \cdot K_2 = \{-uv \mid u \in K_1,\, v \in K_2\}$. The map $\Phi \mapsto \tilde{\Phi}$ is called *Asano contraction*; we denote it by $(z_1, z_2) \to z$.

Appendix B. Ginibre's theorem for particle systems

We consider a set Λ of N sites and populate these with a random configuration Y_m of distinguishable (but identical) particles, at most one particle per site, in such a way that the probability of having exactly m sites occupied is given as in (1.1) by $p_m z_0^m / P(z_0)$, where $P(z) = \sum_{m=0}^{N} p_m z^m$ and

$$p_m = \frac{1}{m!} \sum_{Y_m} e^{-U(Y_m)}. \tag{B.1}$$

In (B.1) the sum is over ordered m-tuples $Y_m = (y_1, \ldots, y_m) \in \Lambda^m$ with $y_i \neq y_j$ for $i \neq j$, and $U(Y_m) = U(y_1, \ldots, y_m)$ is the potential energy of the system when site y_i is occupied by particle i, $i = 1, \ldots, m$, and the remaining $N - m$ sites are empty. The energy U is invariant under permutation of its arguments. It will be convenient to allow sums such as that of (B.1) to run over all $Y_m \in \Lambda^m$, so we define $U(y_1, \ldots, y_m) = +\infty$ whenever $y_i = y_j$ for any i, j. Then the factor $m!$ in (6.3) accounts for the possible orderings, and

$$T_m = \frac{z_0^m}{P(z_0)} \sum_{Y_m \in \Lambda^m} e^{-U(Y_m)}. \tag{B.2}$$

Let us define functions $V(Y_m | x_{m+1})$ and $W(Y_m | x_{m+1}, x_{m+2})$ by the requirement that they be $+\infty$ when any two arguments, among x_{m+1}, x_{m+2}, and the y_j's, coincide, and otherwise satisfy

$$U(Y_{m+1}) = U(Y_m) + V(Y_m | y_{m+1}), \tag{B.3}$$

$$U(Y_{m+2}) = U(Y_m) + V(Y_m | y_{m+1}) + V(Y_m | y_{m+2}) + W(Y_m | y_{m+1}, y_{m+2}). \tag{B.4}$$

Note that

$$V(Y_{m+1} | y_{m+2}) = V(Y_m | y_{m+2}) + W(Y_m | y_{m+1}, y_{m+2}). \tag{B.5}$$

For any function F we define $F_+ = \max\{F, 0\}$ and $F_- = \min\{F, 0\}$. With this notation the two key hypotheses needed for the result are

$$D := \sup_{0\le m\le|\Lambda|-2}\ \sup_{Y_{m+1}\in\Lambda^{m+1}} \sum_{y_{m+2}\in\Lambda} \left(1 - e^{-\beta W_+(Y_m|y_{m+1},y_{m+2})}\right) dy < \infty, \tag{B.6}$$

and

$$-B := \inf_{0\le m\le|\Lambda|-1}\ \inf_{Y_{m+1}\in\Lambda^{m+1}} V(Y_m|y_{m+1}) > -\infty. \tag{B.7}$$

Note that it follows from (B.7) that for any m and $Y_{m+2}\in\Lambda^{m+2}$,

$$V(Y_m|y_{m+1}) + W_-(Y_m|y_{m+1}, y_{m+2}) \ge -B, \tag{B.8}$$

since if $W(Y_m|y_{m+1}, y_{m+2}) \ge 0$ then this comes directly from (B.7), while otherwise, with (B.5), it comes from (B.7) with m replaced by $m + 1$.

Remark B.1. These conditions look somewhat artificial for the general potentials we are considering here, but more natural in the case of pair interactions, when $U(Y_m) = \sum_{1\le i\ne j\le m}\phi(y_i, y_j)$. Then

$$D = \sup_{y\in\Lambda}\sum_{x\in\Lambda}\left(1 - e^{-\beta\phi(x,y)}\right) \quad\text{and}\quad -B = \inf_{x\in\Lambda}\ \inf_{\Lambda'\subset\Lambda} \sum_{y\in\Lambda',\, y\ne x}\phi(x, y). \tag{B.9}$$

The next result was stated in [14] but only for the pair potentials of Remark B.1; the proof was not given but was attributed to a private communication and a preprint.

Theorem B.2. *Suppose that (B.6) and (B.7) hold. Then for $m \le N - 2$,*

$$T_{m+1}^2 - T_m T_{m+2} \le z e^{\beta B} D\, T_m T_{m+1}. \tag{B.10}$$

Proof. We make a preliminary calculation:

$$\begin{aligned} e^{-\beta[V(Y_m|x)+W(Y_m|x,y)]} &= e^{-\beta V(Y_m|x)}\left[\left(e^{-\beta W(Y_m|x,y)} - 1\right) + 1\right] \\ &\ge e^{-\beta[V(Y_m|x)}\left[e^{-\beta W_-(Y_m|x,y)]}\left(e^{-\beta W_+(Y_m|x,y)} - 1\right) + 1\right] \\ &\ge e^{\beta B}\left(e^{-\beta W_+(Y_m|x,y)} - 1\right) + e^{-\beta V(Y_m|x)}, \end{aligned} \tag{B.11}$$

where we have used (B.8). Now with this,

$$\begin{aligned} T_{m+1}^2 - T_m T_{m+2} = \frac{z^{2m+2}}{P(z_0)^2} \sum_{X_m\subset\Lambda}\sum_{Y_m\subset\Lambda}\sum_{x,y\in\Lambda} e^{-\beta[U(X_m)+U(Y_m)+V(Y_m|y)]} \\ \times\left[e^{-\beta V(X_m|x)} - e^{-\beta[V(Y_m|x)+W(Y_m|x,y)]}\right] \end{aligned}$$

$$
\begin{aligned}
&\leq \frac{z^{2m+2}}{P(z_0)^2} \sum_{X_m \subset \Lambda} \sum_{Y_m \subset \Lambda} \sum_{x,y \in \Lambda} e^{-\beta[U(X_m)+U(Y_m)+V(Y_m|y)]} \\
&\qquad \times \left[\left(e^{-\beta V(X_m|x)} - e^{-\beta V(Y_m|x)}\right) - e^{\beta B}\left(e^{-\beta W_+(Y_m|x,y)} - 1\right)\right] \\
&:= R_1 + R_2, \qquad\qquad \text{(B.12)}
\end{aligned}
$$

where R_1 arises from the term $\left(e^{-\beta V(X_m|x)} - e^{-\beta V(Y_m|x)}\right)$ and R_2 from the term $-e^{\beta B}\left(e^{-\beta W_+(Y_m|x,y)} - 1\right)$. We may average the formula for R_1 given in (B.12) with the equivalent formula obtained by interchanging the X_m and Y_m summation variables to obtain

$$
\begin{aligned}
R_1 &= -\frac{z^{2m+2}}{2P(z_0)^2} \sum_{X_m \subset \Lambda} \sum_{Y_m \subset \Lambda} e^{-\beta[U(X_m)+U(Y_m)]} \\
&\qquad \times \left[\sum_{x \in \Lambda}\left(e^{-\beta V(X_m|x)} - e^{-\beta V(Y_m|x)}\right)\right]^2 \\
&\leq 0. \qquad\qquad \text{(B.13)}
\end{aligned}
$$

For R_2 we can use (B.6) to estimate the sum over x and thus obtain

$$
\begin{aligned}
R_2 &\leq e^{\beta B} D \frac{z^{2m+2}}{P(z_0)^2} \sum_{X_m \subset \Lambda} \sum_{Y_m \subset \Lambda} \sum_{y \in \Lambda} e^{-\beta[U(X_m)+U(Y_m)+V(Y_m|y)]} \\
&= z e^{\beta B} D T_m T_{m+1}. \qquad\qquad \text{(B.14)}
\end{aligned}
$$

Now (B.10) follows from (B.13) and (B.14). □

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