INTERACTING DIMERS ON A SIERPINSKI GASKET*

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Received 1 October 1985
Revised 20 February 1986

The different manners of embedding subgraphs of many disjoint edges in a parent graph arise in several different chemical and physical contexts. The problem of enumeration, or more generally of weighted summation, of such embeddings seems quite difficult to treat quantitatively, at least for general extended graphs. The special extended parent graph treated here with the inclusion of interaction between dimers is that of a Sierpinski gasket with a fractal dimension of \(\ln 3/\ln 2\). The manners of solution should extend to other fractal graphs with low 'ramification degree'.

1. Introduction

The combinatorial problem of enumerating ways of placing dimers on a surface to cover a certain fraction of the surface is of key importance for understanding physisorption, passivation and activation of surfaces, and catalysis. The associated counting polynomial (or generating function) not only is the statistical mechanical partition function for these surface science applications [14,2,24] but also is a molecular 'cluster function' for making correlations between chemical structure and molecular properties [11,8]. The special case of a complete covering not only corresponds to a molecular monolayer for the surface science applications, but also has special relevance in the theory of (electronic) resonance of conjugated hydrocarbons [8,25]. A colloquial example of such a combinatorial problem is the enumeration of the ways of placing a number of dominoes on a checkered board, each domino covering an adjacent pair of checker squares. In mathematics a given graph’s subgraphs comprised entirely of disjoint edges are termed matchings and clearly correspond to the dimer placements mentioned above. An issue of the Journal of Graph Theory has recently been devoted to the topic of matchings and factorizations.

Several special classes of such combinatorial dimer placement problems are exactly soluble. Evaluations [19,21] of the full matching polynomial have been carried out for a variety of finite graphs for the chemical-structure applications. Treatments

* Research supported by The Robert A. Welch Foundation of Houston, Texas.
of partial coverings for several one-dimensional graphs, with but a single direction of infinite (translationally symmetric) extent, have been made \([18, 10, 20, 3, 22, 12, 15, 1]\). For some such one-dimensional lattice strips a physically-relevant generalized problem of evaluating the generating (or partition) functions, with weights \(w^c\) for matchings with \(c\) nearest-neighbor contacts (or interactions) between dimers, has been solved \([26]\). Results of general matching problems for extended graphs of higher dimensions have been rather limited, though some qualitative aspects have been established \([9]\). The only 2-dimensional problems treated successfully seem to be for complete coverings \([15, 7, 13, 4, 16, 27]\) on a few regular lattices.

Here we illustrate a general solution for the dimer placement partition (or generating) function at variable dimer density and interaction weight on an extended graph with a fractal dimension of \(d = \ln 3/\ln 2 \approx 1.58496\). This extended graph is the so-called \([17]\) Sierpinski gasket, obtained as the \(n \to \infty\) limit of the construction of which the \(n = 0, 1,\) and 2 stages are depicted in Fig. 1. Since this structure has a dimension greater than 1, it might serve as a check on approximate methods applied to structures with dimensions in this range. Further, percolation clusters near threshold appear \([23]\) to have features in common with the Sierpinski gasket: fractal dimensions and low 'ramification' degrees, this last feature being that the removal of only a few vertices distant from each of any chosen pair of well-separated vertices is sufficient to disconnect these two chosen vertices. Thence aggregates that arise in nucleation and floculation might be represented \([5, 23]\) in terms of such clusters. But since such high-surface-area clusters occur often in catalytic processes, absorption thereon, say by dimers, becomes of crucial interest. The feature of low ramification degree also aids in establishing simple recurrence relations for successively higher stage \(n\) gaskets. Much the same approach should apply to many other dilation-symmetric fractal graphs of finite ramification degree.

### 2. Recurrence relations

Consider the various possible matchings on an \(n\)th stage Sierpinski gasket \(\Gamma_n\). Associate to each matching \(\gamma\) a weight \(u^{a(\gamma)}b^{b(\gamma)}w^{c(\gamma)}\) where \(a(\gamma)\) is the number of vertices of \(\Gamma_n\) not in \(\gamma\), \(b(\gamma)\) is the number of vertices in \(\gamma\), \(c(\gamma)\) is the number of edges of \(\Gamma_n\) which adjoin two different edges of \(\gamma\), and \(u, v, w\) are associated non-negative factors. In statistical mechanical applications these factors may be called *activities* and thought of as (local) Boltzmann factors \(e^{-e_u/kT}\), \(e^{-e_v/kT}\), \(e^{-e_w/kT}\). The
generating (or partition) function $Z_n$ is given in terms of a sum over all matchings

$$Z_n = \sum_{\gamma \in \Gamma_n} u^{a(\gamma)} v^{b(\gamma)} w^{c(\gamma)}.$$  \hfill (2.1)

The logarithm of this is proportional to a statistical mechanical free energy, and as such should scale with the size of the system, say as measured by the number $|\Gamma_n|$ of vertices in $\Gamma_n$,

$$|\Gamma_n| = 3(3^n + 1)/2.$$  \hfill (2.2)

The derivatives

$$Z_n^v = \frac{\partial Z_n}{\partial \ln v} = \sum_{\gamma \in \Gamma_n} b(\gamma) u^{a(\gamma)} v^{b(\gamma)} w^{c(\gamma)},$$

$$Z_n^w = \frac{\partial Z_n}{\partial \ln w} = \sum_{\gamma \in \Gamma_n} c(\gamma) u^{a(\gamma)} v^{b(\gamma)} w^{c(\gamma)}$$

are of interest because their ratios to $Z_n$ give the mean number of dimer sites occupied in $\Gamma_n$ and the mean dimer-interaction energy (at the given values of the activities $u, v, w$). Thus the quantities

$$p_n = Z_n^v/Z_n |\Gamma_n|, \quad \epsilon_n = Z_n^w/Z_n |\Gamma_n|$$

give the probability that a typical site of $\Gamma_n$ is occupied (by one end of a dimer) and the mean dimer-interaction energy per site of $\Gamma_n$.

Recurrence relations leading to the $Z_n$, $Z_n^v$, $Z_n^w$ are obtained in terms of several auxiliary generating functions. These recurrence relations involve a construction wherein three $n$th stage cells are ‘glued’ together as suggested in Fig.2 to form an $(n+1)$th stage cell. To carry out this ‘gluing’ in an acceptable fashion requires information concerning the occupancies of apex sites in the $n$th stage cells. Thus the relevant auxiliary functions are of the same form as the $Z_n$ of (2.1) but with a restriction on the sums to specify the manner of occupancy of the apex sites. The relevant local state for an apex site, say in the $n$th cell, is labelled by an index which takes one of three values: +1 if the apex is occupied by a dimer in the given cell; 0 if the apex is unoccupied and remains so when ‘glued’ to another cell; and −1 if the apex is unoccupied at the current stage but upon ‘gluing’ will become occupied by a dimer the other end of which occurs in the appended $n$th stage cell. The relevant $n$th stage auxiliary generating functions are denoted $G_n(q, \sigma, \tau)$ with $q, \sigma, \tau$ being
the local states for the three apex vertices. Many of these \( 3^3 \) \( n \)th stage \( G_n(\varnothing, \sigma, \tau) \) are equal since they are seen to be invariant under permutation of the \( \varnothing, \sigma, \tau \). The non-zero initial stage \((n = 0)\) functions are

\[
\begin{align*}
G_0(0, 0, 0) &= u^3, \\
G_0(0, 0, 1) &= G_0(0, 1, 0) = G_0(1, 0, 0) = u^3, \\
G_0(0, 1, 1) &= G_0(1, 0, 1) = G_0(1, 1, 0) = u^3 w, \\
G_0(1, 1, 1) &= u^3 w^3, \\
G_0(0, 1, 1) &= G_0(1, 0, 1) = G_0(1, 1, 0) = u^3 w^2
\end{align*}
\]

(2.5)

where the \( \bar{I} = -1 \) local states are temporarily associated with an activity \( u \), though nearest-neighbor contacts to these subsequently to-be-occupied sites are counted. The 'gluing' operation now entails adjoining apices with local states of opposite signs and is represented algebraically as

\[
G_{n+1}(\varnothing, \sigma, \tau) = \frac{1}{u^3} \sum_{\xi, \zeta, \eta} G_n(\varnothing, \xi, \eta) G_n(\xi, \sigma, \zeta) G_n(\eta, \zeta, \tau)
\]

(2.6)

where the \( 1/u^3 \) factor corrects for the weight of the three pairs of 'glued' sites that are condensed to just three single sites. Finally the desired partition function is obtained as

\[
Z_n = \sum_{\varnothing, \sigma, \tau} G_n(\varnothing, \sigma, \tau)
\]

(2.7)

where the sum is over non-negative local states.

Recurrence relations for the derivative quantities of (2.3) are also possible. One first introduces derivatives of the auxiliary functions

\[
G_n^s(\varnothing, \sigma, \tau) = \frac{\partial}{\partial \ln s} G_n(\varnothing, \sigma, \tau), \quad s = u, w
\]

(2.8)

and also

\[
A_n(\varnothing, \tau; \xi, \eta) = \frac{1}{u^3} \sum_{\zeta} G_n(\xi, \sigma, \zeta) G_n(\eta, \zeta, \tau).
\]

(2.9)

Then the desired recurrence relations result from taking derivatives of (2.6) to yield

\[
G_{n+1}^s(\varnothing, \sigma, \tau) = \sum_{\xi, \eta} A_n(\sigma, \tau; \xi, \eta) G_n^s(\varnothing, \xi, \eta) + \sum_{\zeta, \xi} A_n(\tau, \varnothing; \xi, \zeta) G_n^s(\varnothing, \eta, \zeta) + \sum_{\eta, \zeta} A_n(\varnothing, \sigma, \eta) G_n^s(\eta, \xi, \zeta)
\]

(2.10)

and the \( G_0^s(\varnothing, \sigma, \tau) \) are obtained upon differentiating (2.5). The quantities of (2.3) then are obtained by summing over \( G_n^s(\varnothing, \sigma, \tau) \) in parallel with (2.7).
3. Asymptotic behavior

The mathematical limit of large systems is of interest as a close approximation to macroscopically-sized physico-chemical samples. Because the logarithm of $Z_n$ is (proportional to) a free energy, the dominant $n$-dependence for $\ln Z_n$ should scale $\sim |F_n|$, with the proportionality constant being, say, $\ln \kappa$. Moreover, the ratio $Z_n/\kappa^{|F_n|}$ is expected to asymptotically approach a constant, since the number of (interacting) ‘surface’ sites scales as $\sim |F_n|^0$, i.e., as just the number 3 of apices. Thus we anticipate

$$Z_n \equiv C \kappa^{(3^n)}, \quad n \text{ large} \quad (3.1)$$

Similarly, arranging the stage-$n$ auxiliary generating functions as a vector $G$ with $(\sigma, \tau, \rho)$th element $G_{\sigma, \rho}^{(\tau, \eta)}$, we expect

$$G_n \equiv \kappa^{(3^n)} G, \quad n \text{ large} \quad (3.2)$$

this form being consistent with the recurrence relations of (2.6). The value of $\kappa$ depends, of course, on the activities $u, v, w$.

Given the anticipated asymptotic behavior of $G_n$ the behavior of the derivatives $G_n^\rho$ and $G_n^\sigma$ (with respect to $\ln \nu$ and $\ln \omega$) follows. To see this we start out by introducing square matrices $M_n$ with rows and columns labelled as for the vectors $G_n$,

$$M_n(\sigma, \tau; \rho, \chi, \zeta, \eta) = \kappa^{-2(3^n)} \{ A_n(\sigma, \tau; \rho, \chi, \zeta, \eta) \delta(\rho, \chi, \zeta, \eta) + A_n(\tau, \rho; \zeta, \eta, \chi, \sigma) \delta(\sigma, \eta) \\ + (A_n(\rho, \sigma; \eta, \chi, \zeta) \delta(\sigma, \chi, \zeta, \eta) \} \quad (3.3)$$

From (3.2) and (2.9) it follows that $M_n$ should approach a (nonzero) constant matrix $M$ as $n \to \infty$. Then since the derivative recurrence relations of (2.10) may be recast as

$$G_{n+1}^\rho = \kappa^{2(3^n)} M_n G_n^\rho$$

$$= \kappa^{2(3^n + 3^{n-1} + \cdots + 1)} M_n M_{n-1} \cdots M_0 G_0^\rho, \quad (3.4)$$

one finds

$$G_n^\rho \equiv \kappa^{(3^n)} \lambda^n G^\rho \quad (3.5)$$

where $\lambda$ is the maximum eigenvalue to the asymptotic matrix $M$ and $G^\rho$ is a multiple of the associated eigenvector. This eigenvalue may be determined if we first note that, from the definitions of $M_n$ and (2.9), the application of $M_n$ to $G_n$ essentially reproduces the original recurrence relations of (2.3),

$$\kappa^{2(3^n)} M_n G_n = 3 G_{n+1}$$

Hence $G$ is an eigenvector to the asymptotic matrix $M$, clearly also for the maximum eigenvalue (since all its components are non-negative and the Frobenius–Perron
theorem [6] applies to $\mathbb{M}$). Thus

$$G^s = C^s G, \quad \lambda = 3$$

(3.7)

with $C^s$ a constant, $s = v, w$.

Asymptotic expressions for quantities of direct physical relevance also follow. The probability that a typical site be occupied and the mean dimer interaction energy per site are

$$p_n = \frac{2C^v}{3}, \quad \varepsilon_n = \frac{2C^w}{3}, \quad n \text{ large.}$$

(3.8)

Also $-\ln \kappa$ is a free energy per site.

4. Numerical treatment

The recurrence relations (2.6) with the initial conditions of (2.5) allow the partition functions to be evaluated via (2.7), and recursion via (2.10) leads to $p_n$ and $\varepsilon_n$. An especially stable method of accurately estimating $\kappa$ of (3.1) may be implemented if first one notes that $Z_n$ is homogeneous of degree $|T_n|$ in the pair of activities $u$ and $v$. Thence, now explicitly including the $u, v, w$-dependence of $Z_n,

$$Z_n[u, v, w] = \kappa^{\frac{|T_n|}{n}} Z_n[u/\kappa, v/\kappa, w].$$

(4.1)

Thus $\kappa$ may be accurately estimated as that value such that $Z_n[u/\kappa, v/\kappa, w]$, and hence also the associated $G_n$, remain 'balanced' for as many iterations as possible, i.e., the contrasting behaviors of divergence or convergence to 0 are delayed to $n$-values as high as possible. An error of $\kappa \delta$ in $\kappa$ should lead to $Z_n$ varying at large $n$ as $(1 + \delta)^{3^{(3^n)}}$ which should become noticeable once $\delta \approx 3^{-n}$. Thence iteration up to $n \equiv p \ln 10/\ln 3 \approx 2p$ should lead to $\kappa$ accurate through $\sim p$ decimal places. Once $\kappa$ and the rescaled $u$ and $v$ are found, subsequent recurrence for the $G_n^s$ at these rescaled values of $u$ and $v$ next yields $Z_n[u/\kappa, v/\kappa, w]$, all of which can then be used directly in the simple formulas of (2.4) for $p_n$ and $\varepsilon_n$ to give their common values in both the rescaled and unrescaled cases. Since $\varepsilon_n$ and $p_n$ depend only upon the ratio $u: v$, we constrain

$$u + v = 1.$$  

(4.2)

The free-energy per site depends upon the sum $u + v$ only through an additional term $-\ln(u + v)$, since rescaling as in (4.1) holds for an arbitrary factor. Thence, the constraint of (4.2) affects the free-energy per site only in a trivial way.

Numerical results have been made for a range of activities for stages $n \leq 12$, whence the asymptotic larger $-n$ behavior is closely approached. The value of $\kappa$ was first determined through about 9 decimal places as explained above, then the $p_n$ and $\varepsilon_n$ calculated up through $n = 12$, whence they were found to be converged to $4$
or 5 decimal places. In fact, since the number of ‘surface’ sites (as noted in Section 3) is a fraction $-|r_n|^0/|r_n|$ of all the sites one might anticipate that corrections to the asymptotic values $\rho = \rho_\infty$ and $\epsilon = \epsilon_\infty$ should be roughly the size of this fraction. In Figs. 3 and 4 this expectation is seen to be bourne out, i.e., these plots of $p_n$ and $\epsilon_n$ versus $1/|r_n|$ approach linearity as $n$ becomes large. Finally Figs. 5, 6, and 7

Fig. 3. Manner of variation of the $p_n$, approaching the straight (solid) line as $n$ increases.

Fig. 4. Manner of variation of the $\epsilon_n$, close along a straight line, for larger $n$. 
show curves of $\kappa, p$, and $\varepsilon$ as a function of $v$, each curve at a different value of the dimer-interaction activity $w$. When $w$ is small ($w \ll 1$) there appears to be some 'singular' behavior as $v \to 1$: the curve of $p$ follows close to the $w = 0$ curve up till $v \approx 1 - w$, then $p$ jumps steeply up toward $p = 1$ at $v = 1$. Similar behavior may be seen for the $\varepsilon$ versus $v$ curve, again when $w$ is small.

In conclusion, it is seen that properties of interacting dimers on a Sierpinski gasket can be accurately computed (within a grand canonical ensemble formalism).

Fig. 5. Curves of $\kappa$ versus $v$ at three different values of $w$.

Fig. 6 Curves of $p$ versus $v$ at four different values of $w$. 
The construction of recurrence relations for other dilation-symmetric fractals of finite ramification degree should be a similar finite program, which however increases rapidly in complexity both with increases in the number of cells 'glued' together and with the number of 'gluing' points per cell. This approach yields solutions for the general problem of partial dimer coverings (with interaction too) for systems of higher dimension than previously accomplished. Solutions both to more random (e.g., more percolation-like) graphs and to regular lattices would be of much interest.

References