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ORIGINAL PAPER

Exact solutions of lattice polymer models

R. Brak · A. L. Owczarek · A. Rechnitzer

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Abstract We consider directed path models of a selection of polymer and vesicle problems. Each model is used to illustrate an important method of solving lattice path enumeration problems. In particular, the Temperley method is used for the polymer collapse problem. The ZL method is used to solve the semi-continuous vesicle model. The Constant Term method is used to solve a set of partial difference equations for the polymer adsorption problem. The Kernel method is used to solve the functional equation that arises in the polymer force problem. Finally, the Transfer Matrix method is used to solve a problem in colloid dispersions. All these methods are combinatorially similar as they all construct equations by considering the action of adding an additional column to the set of objects.

Keywords Interacting self-avoiding walks · Directed paths · Polymer adsorption · Polymer collapse · Vesicles · Exact solution · Combinatorics

1 Introduction

Over the years many models have been use to study polymer phase transitions, some more realistic than others. In this paper we consider the class of models which use

R. Brak · A. L. Owczarek
Department of Mathematics and Statistics, The University of Melbourne, Parkville, VIC 3052, Australia
e-mail: brak@ms.unimelb.edu.au

A. L. Owczarek
e-mail: aleks@ms.unimelb.edu.au

A. Rechnitzer (✉)
Department of Mathematics, University of British Columbia, Vancouver, BC, Canada V6T-1Z2
e-mail: andrewr@math.ubc.ca

directed lattice paths. Although these models are clearly not quantitative models of their respective systems they do capture the qualitative nature of the phase transitions. They also have the big advantage of frequently being exactly solvable. Thus we obtain the certainty provided by the mathematical solution that is lacking in approximate solutions. These models have also had an unexpected bonus: they have provided a large amount of new pure combinatorics. The method of (kernel) functional equations is a very good example [1–7] as is the connection between the Bethe Ansatz [8,9] and Gessel-Viennot involution [10,11]. All the methods discussed in this paper are combinatorially similar as they all construct equations by considering the action of adding an additional step (or steps) to the set of objects.

We consider two classes of path: discrete lattice paths and semi-continuous paths. A *discrete lattice path* of length n is a sequence of $n+1$ vertices $\pi = v_0 v_1 \dots v_n$ where $v_i \in \mathbb{Z}^2$ such that consecutive pairs of vertices, $s_i = v_i v_{i+1}$ satisfy the condition that $v_{i+1} - v_i \in \mathcal{S}$, where $\mathcal{S}$ is some set of allowed pairs $(a, b) \in \mathbb{Z}^2$, called the *step set*. Usually v_0 is set to the origin $(0, 0)$.

The paths may also be *weighted*. A real valued weight can be associated with pairs of vertices $w_{i,j} : v_i v_j \to \mathbb{R}$. The weight, $W(\pi)$, of a path π is the product of the weights,

$$W(\pi) = \prod_{0 \le i < j \le n} w_{i,j}. \tag{1}$$

This gives rise to a weight polynomial,

$$Z_n = \sum_{\pi \in \mathcal{P}_n} W(\pi), \tag{2}$$

where $\mathcal{P}_n$ is the set of all paths of length n taken from some class of paths. The weight polynomial turns out to be the partition function for several models. The length generating function for the weight polynomials is defined as

$$G(x) = \sum_{n \ge 0} Z_n \, x^n \tag{3}$$

The generating function has the advantage that it is frequently easier to compute than the weight polynomial. It also has the property that the thermodynamic limiting *free energy*,

$$F = -\lim_{n \to \infty} \frac{1}{n} \log Z_n \tag{4}$$

(we use units such that $k_B T = 1$) is related to the closest singularity of $G(x)$ on the positive real axis x_c, that is,

$$F = \log x_c. \tag{5}$$

2 Interacting partially directed paths by the Temperley method

We can model the polymer collapse transition with interacting partially directed paths. *Partially directed paths* are discrete lattice paths with step set $\mathcal{S}=\{(0,1),(0,-1),(1,0)\}$ with the constraint that the following two successive pairs of steps, $s_i = (0,1)$, $s_{i+1} = (0,-1)$ and $s_i = (0,-1)$, $s_{i+1} = (0,1)$, are forbidden (this ensures self-avoidance). The step $(0,1)$ is called a *north step*, $(0,-1)$ is a *south step* and $(1,0)$ is an *east step*. The *interaction* is modelled with a nearest-neighbour weight, $w_{i,j}$, given by

$$w_{i,j} = \begin{cases} \tau, & \text{if } v_j - v_i = (1,0) \text{ and } j \neq i+1 \\ 1. & \text{otherwise} \end{cases} \tag{6}$$

The pair of vertices having a nearest-neighbour weight τ is called a (nearest-neighbour) contact. An example of an interacting partially directed walk is illustrated in Fig. 1. If each contact corresponds to some force between the monomers of the polymer, then the weight τ becomes the Boltzmann factor associated with the contact and the weight polynomial,

$$Z_n = \sum_{\pi \in \mathcal{P}_n} W(\pi) \tag{7}$$

is the partition function for this model, where $\mathcal{P}_n$ is the set of length n partially directed paths.

We now have the problem of computing Z_n, or more easily, its generating function $G(x)$. This combinatorial problem was solved in [12] using the Temperley method [13].

The method begins with the generating function, g_r, for walks whose first step is an east step followed by exactly $r \geq 0$ steps in either the north or south direction,

$$g_r(x) = \sum_{n \geq 0} Z_n(r) x^n \tag{8}$$

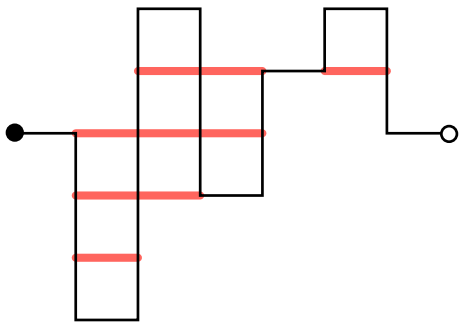

Fig. 1 An example of interacting partially directed walk with 24 steps and nine contacts

then

$$G(x) = \sum_{r \geq 0} g_r(x). \tag{9}$$

We can now write down recurrence relations for g_r as follows. Consider first paths whose last vertical step is length zero (i.e. those generated by g_0), these arise from either a single east step path, or, by appending an east step to g_0 paths, or to g_1 paths etc. Thus we get the equation,

$$g_0 = x + x(g_0 + g_1 + g_2 + \cdots) = x + xG(x). \tag{10}$$

Similarly, paths in the set generated by g_r, for $r > 0$, arise by appending an east step followed by either r north steps or r south steps on to paths in the sets g_k, for $k \geq 0$.

In order to account for the contacts we need to consider two cases. First, if the last sequence of vertical steps in g_k are in the opposite direction to those in g_r (in which case we get a weight $\tau^{\min\{k,r\}}$), or second, if they are in the same direction, in which case there is no contribution to the contact weight. Thus, for $r \geq 1$, we get the equations

$$g_r = x^{r+1}\left(2 + \sum_{k=0}^{r}(1+\tau^k)g_k + (1+\tau^r)\sum_{k>r} g_k\right). \tag{11}$$

By adding and subtracting appropriate multiples of g_{r-1} and g_{r+1} the following recurrence is obtained for $r \geq 1$,

$$g_{r+1} - x\left((1+\tau) - x(1-\tau)(\tau x)^r\right) g_r + \tau x^2 g_{r-1} = 0. \tag{12}$$

Because of the $(\tau x)^r$ term this is not a simple constant coefficient recurrence relation. To solve this equation let,

$$q = \tau x \tag{13}$$

and try the Ansatz,

$$g_r = \mu^r \sum_{m \geq 0} p_m(q)\, q^{mr}, \quad p_0(q) = 1. \tag{14}$$

Substituting leads to the characteristic equation

$$\mu^2 - (x+q)\mu + xq = 0 \tag{15}$$

and the first order recurrence relation

$$p_m(q) = \frac{\mu(-q)q^m}{(\mu q^m -)(\mu q^m - q)}\, p_{m-1}(q). \tag{16}$$

The general solution of (12) is the linear combination

$$g_r = A_1 g_r^{(1)} + A_2 g_r^{(2)}, \quad r \geq 1, \tag{17}$$

corresponding to the two solutions $\mu_1 = x$ and $\mu_2 = q$ of (15) and where

$$g_r^{(i)} = \mu_i^r + \mu_i^r \sum_{m\geq 1} \frac{\mu_i^m x^m (x-q)^m}{\prod_{k=1}^m (\mu_i q^k - x)(\mu_i q^k - q)} q^{m(m+1)/2+mr}. \tag{18}$$

The limiting behaviour of g_r as $r \to \infty$ requires $A_2 = 0$. To determine A_1, note $g_0 = A_1 g_0^{(1)}/2 = x + xG(x)$ and similarly $g_1 = A_1 g_1^{(1)} = p_1 + p_2 G(x)$ where

$$p_1 = 2 + x - q \tag{19}$$

$$p_2 = 1 + \tau + x - q \tag{20}$$

which gives a pair of equations for A_1. Solving then gives,

$$G(x) = -\frac{p_1 H(x) - 2}{p_2 H(x) - 2} \tag{21}$$

$$H(x) = x \frac{g_0^{(1)}}{g_1^{(1)}} \tag{22}$$

$$g_k^{(1)} = x^k + x^k J_k\left(\tau x^3 (1-\tau)\right) \tag{23}$$

where $J_r(t;q)$ is a q-Bessel function,

$$J_k(t;q) = \sum_{n\geq 0} \frac{t^n q^{n(n+3)/2}}{\prod_{k=1}^n (1-q^k)(1-xq^{k-1})} q^{kn}, \tag{24}$$

It is interesting to note that $H(x)$ can be represented as a continued fraction via

$$\tau \mathcal{H}(t) = 1 + \tau + \left(\frac{1}{\tau} - 1\right) q^2 t - \frac{1}{\mathcal{H}(qt)} \tag{25}$$

where $H(\tau, x) = \mathcal{H}(1)$.

3 Staircase vesicles by the ZL method

In this section we describe how to derive the exact solution [14] for the generating function of the semi-continuous analogue of staircase polygons (vesicles) using the method developed by Zwanzig and Lauritzen [15]. Its use was revived in [16] to consider the collapse phase transition of interacting partially directed walks. It is a continuous analogue of the Temperley method [17].

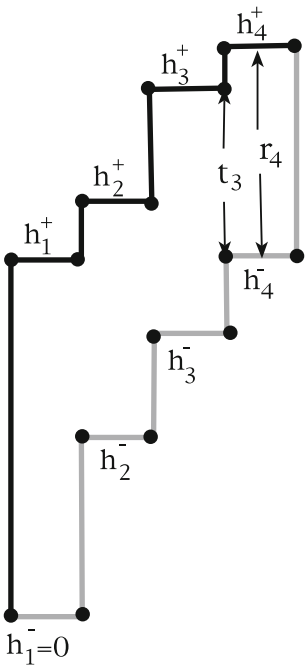

Fig. 2 A semi-continuous staircase polygon of $n = 4$ columns with upper horizontal steps at heights $h_1^+, h_2^+, h_3^+, h_4^+$ and lower horizontal steps at heights $0, h_2^-, h_3^-, h_4^-$. The overlap between columns 3 and 4 is shown as $t_3 = h_3^+ - h_4^-$ while the height of the right-most column is given as $r_4 = h_4^+ - h_4^-$. The upper path is shown in black while the lower path is shown in grey

The model can be defined as follows. Consider a plane, $\{(u, h) : (u, h) \in \mathbb{Z} \times \mathbb{R}\}$. Now consider a set of upper 'horizontal steps' at heights h_j^+, $j = 1, \ldots, n$, defined by the pairs of points $((j-1), h_j^+), (j, h_j^+)$, and a set of lower horizontal steps at heights h_j^-, $j = 1, \ldots, n$, defined by the pairs of points $((j-1), h_j^-), (j, h_j^-)$. We first impose the constraint $h_j^+ > h_j^-$ for $j = 1, \ldots, n$ and let $h_1^- = 0$ so that the first lower horizontal step is fixed. We also impose the *staircase constraints*, $h_j^- \geq h_{j-1}^-$ and $h_j^+ \geq h_{j-1}^+$ for $j = 2, \ldots, n$. An upper path defined by $(0, 0), (0, h_1^+), (1, h_1^+), (1, h_2^+), (2, h_2^+) \ldots (n-1, h_{n-1}^+), (n-1, h_n^+), (n, h_n^+)$ and a lower path defined by $(0, 0), (1, 0), (1, h_2^-), (2, h_2^-), \ldots, (n-1, h_n^-), (n, h_n^-), (n, h_n^+)$ begin and end at the same points, and so not otherwise intersect, thereby forming a polygon: a staircase polygon (Fig. 2).

We associate a length generating variable x with horizontal steps of the paths, a length generating variable $y = e^{-\tau}$ with the vertical steps of the two paths and an area generating variable $z = e^{-\varepsilon}$ with unit areas of the enclosed polygon (the area is also a continuous variable). Let

$$r_j = h_j^+ - h_j^- \tag{26}$$

be the height of each column of the polygon. Hence a polygon φ_n of n columns has weight

$$w(\varphi_n) = x^{2n}\, y^{\left[r_1 + \prod_{j=2}^{n} (h_j^+ - h_{j-1}^+) + (h_j^- - h_{j-1}^-) + r_n\right]}\, z^{\prod_{j=1}^{n} r_j}. \tag{27}$$

One further definition that will prove useful below is the overlap

$$t_j = h_j^+ - h_{(j+1)}^- \tag{28}$$

between successive columns j and $j+1$ with $j = 1, \ldots, (n-1)$.

The generating function of this polygon model of a vesicle is the integral over all configurations summed over all numbers of columns:

$$\mathcal{G}_T(x, \tau, \varepsilon) = \sum_{n=1}^{\infty} \int d\varphi_n \; w(\varphi_n), \tag{29}$$

where the single integral sign here represents multiple integrals over column heights for each polygon φ_n.

Consider polygons where the height of their right-most column is $r = h_n^+ - h_n^-$. The generating function can be written as a genuine single integral over all polygons that have the height of their right-most column as r:

$$\mathcal{G}_T(x, \tau, \varepsilon) = \int_0^{\infty} T(r) \, dr. \tag{30}$$

The major ingredient in the method of Zwanzig and Lauritzen is to find a integral equation for $T(r)$, which is the analogue of the recurrence relation of the Temperley method, by considering how configurations with their right-most column of height r can be constructed from configurations of one fewer columns and right-most column of height s. The method is then to solve this integral equation by turning it into a differential equation, and so solving for the generating function. Note that $T(r)$ depends on τ, ε and x. The resulting differential equation is one in the variable r rather than in one of the model parameters.

If a polygon is only a single column of height r then its total weight is

$$x^2 z^r y^{2r} \tag{31}$$

Now consider polygons of more than one column with right-most column of height r and how such a polygon can be constructed from polygons with one few columns and right-most column of height s. Clearly the contribution to the generating function can be written as

$$x^2 z^r \int_0^{\infty} ds \; T(s) f(r, s), \tag{32}$$

where $f(r, s)$ is the integral over the ways in which a column of height r can be added to a staircase polygon with right-most column of height s and obey the definition of a staircase polygon. Let t be the overlap of the two columns of height r and s (see Fig. 3). Now, the minimum value that the overlap can attain is 0 while its maximum

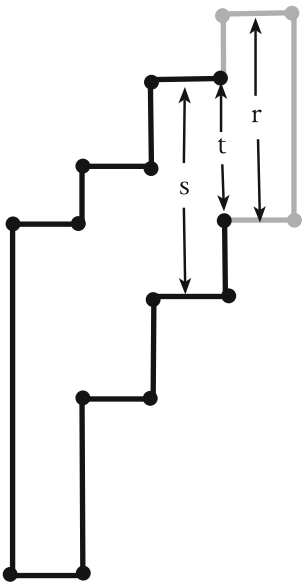

Fig. 3 A staircase polygon with a right-most column of height r, whose perimeter is shown in grey, and second-right-most column of height s. The perimeter of the rest of the polygon except the right-most column is shown in black. The weight of the configuration depends on the overlap t

value is $\min(r, s)$. Then the function $f(r, s)$ can be written as an integral over the values of the overlap t,

$$f(r, s) = \int_0^{\min(r,s)} dt\ y^{2(r-t)}, \tag{33}$$

since by adding a column of height r to one of height s one nominally gains vertical perimeter $2r$ but loses the overlap from both the new column and the one to which it attaches: that is, one loses vertical perimeter $2t$. By combining the above arguments and evaluating the integral for $f(r, s)$ we find the functional equation for the generating function $T(r)$ as

$$T(r) = x^2 z^r y^{2r} + x^2 z^r \int_0^{\infty} ds\ T(s) f(r, s), \tag{34}$$

where

$$f(r, s) = (2\tau)^{-1} \exp(-2\tau r) \left[\exp(\tau(r + s) - \tau|r - s|) - 1\right]. \tag{35}$$

To solve the integral equation it is more convenient to work with the function $g(r)$ defined as

$$g(r) = e^{\varepsilon r} e^{\tau r} T(r). \tag{36}$$

By differentiating the above integral equation we obtain the differential equation

$$\frac{d^2g}{dr^2} = (\tau^2 - x^2 e^{-\varepsilon r})g(r). \tag{37}$$

Making the substitutions $z = ae^{-\varepsilon r/2}$ and $h(z) = g(r)$ we obtain

$$z^2\frac{d^2h}{dz^2} + z\frac{dh}{dz} + \left(\frac{4x^2}{\varepsilon^2 a^2}z^2 - \frac{4\tau^2}{\varepsilon^2}\right)h(z) = 0. \tag{38}$$

This is Bessel's differential equation with

$$\nu = \frac{2\tau}{\varepsilon} \tag{39}$$

and

$$a = \frac{2x}{\varepsilon}. \tag{40}$$

The solution is given by

$$h(z) = C_1 J_\nu(z) + C_2 J_{-\nu}(z) \tag{41}$$

with C_j being constants that depend on the boundary conditions implicit in the integral equation. One can show (analogously to [18]) that $C_2 = 0$ and hence we can solve the boundary condition

$$g(0) = x^2 \tag{42}$$

to obtain

$$g(r) = x^2 \frac{J_{\frac{2\tau}{\varepsilon}}(\frac{2x}{\varepsilon}e^{-\varepsilon r/2})}{J_{\frac{2\tau}{\varepsilon}}(\frac{2x}{\varepsilon})}. \tag{43}$$

The boundary condition for $g'(r)$ can be written as

$$\mathcal{G}_T = x^{-2}g'(0) + \tau \tag{44}$$

and leads to

$$\mathcal{G}_T(x, \tau, \varepsilon) = \tau\left(1 - \sigma\frac{J'_\nu(\sigma\nu)}{J_\nu(\sigma\nu)}\right) \tag{45}$$

with

$$\sigma = \frac{x}{\tau} \quad \text{and} \quad \nu = \frac{2\tau}{\varepsilon}. \tag{46}$$

For the sake of completeness we give the solution with $z = 1$:

$$\mathcal{G}_T(x, \tau, 0) = \tau - (\tau^2 - x^2)^{1/2}. \tag{47}$$

The asymptotic behaviour of the model [14] can be derived from the generating function (45). Note that if the Temperley method is used to solve the discrete version [19], q-Bessel functions are obtained rather than Bessel functions.

So we have seen that a polygon model with continuous vertical lengths and with an area parameter can be solved by a method that is analogous to the Temperley method. Whereas we needed to solve a difference equation in the discrete case a integral/differential equation needs to be solved in the semi-continuous case. However, otherwise the method of solution follows the similar steps.

4 Adsorption of Dyck paths by partial difference equations

Polymer adsorption occurs when a polymer interacts with a surface. The system can undergo a phase transition from a phase where the polymer is desorbed from the surface to a phase where it is adsorbed. If the monomers have a attractive contact potential with the surface it will give rise to a Boltzmann factor, κ, associated with each monomer at the surface.

We can model this problem with weighted Dyck paths. However, to construct the partial difference equations we need ballot paths. *Ballot paths* of height $h \geq 0$ are discrete lattice paths $v_0 v_1 \dots v_n$, with $v_0 = (0, 0)$, $v_n = (n, h)$, step set $\mathcal{S} = \{(1, 1), (1, -1)\}$ and the constraint that the y coordinate of any vertex, $v = (x, y)$, must be non-negative. Thus the paths are always on or above the "surface" $y = 0$. *Dyck paths* are ballot paths of height zero. An example of each type of path is shown in Fig. 4.

To model adsorption we associate a weight κ with each step from $y = 1$ to $y = 0$. The weight polynomial, or partition function,

$$Z_n(h) = \sum_{\pi \in D_n} W(\pi) \tag{48}$$

is a sum over all Dyck paths of length n, D_n.

The method of solution we will consider for this model starts with the partial difference equations satisfied by the adsorption weight polynomial. The partial difference equations can then be solved by a constant term expression.

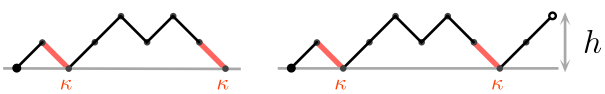

Fig. 4 An example of a Dyck path (*left*) with weight κ^2 and a ballot path (*right*) of height $h = 2$

The weight polynomial $Z_n(h)$ for ballot paths ending at height $h \geq 0$ satisfy the following system of partial difference equations

$$Z_n(h) = Z_{n-1}(h-1) + Z_{n-1}(h+1) \qquad h > 0 \qquad (49a)$$
$$Z_n(0) = \kappa\, Z_{n-1}(1) \qquad h = 0 \qquad (49b)$$
$$Z_0(h) = \delta_{0,h} \qquad h \geq 0 \qquad (49c)$$

These equations are obtained by consider how the weight polynomial changes when the length of the paths is increased by adding one additional step. Thus Z_n is expressed in terms of Z_{n-1}. Equation 49a is the "bulk" equation and is obtained by adding a down step to paths of height $h+1$ or by adding an up step to paths of height $h-1$. Equation 49b is the "boundary" equation obtained by adding a down step to paths of height one (and adding in the associated weight κ). Finally, Eq. 49c is the initial condition which ensures paths start at height zero.

We follow the method of solution given in [20]. A method using residues may be found in the earlier paper [21]. The bulk equation is satisfied by $Z_n{=}\lambda^n \rho^h$ so long as

$$\lambda = \rho + \frac{1}{\rho}. \qquad (50)$$

The boundary equation is satisfied by $Z_n(h) = \lambda^n \left(\rho^h - S(\rho)\rho^{-h}\right)$ where

$$S(\rho) = \frac{\lambda - \kappa\rho}{\lambda - \kappa/\rho}, \qquad (51)$$

which is found by taking the linear combination $A\rho^h + B\rho^{-h}$, substituting into the boundary equation, and then solving for the ratio B/A. Finally, the initial condition is satisfied if

$$Z_n(h) = \frac{1}{2}\mathrm{CT}_\rho \left[\lambda^n \left(1 - S(1/\rho)\right)\left(\rho^h - S(\rho)\rho^{-h}\right)\right]. \qquad (52)$$

Note, using induction the constant term expression is readily proved to satisfy all Eqs. 49a–49c. The constant term operator, CT_ρ acts on iterated Laurent power series in the field $\mathbb{Z}\langle\langle \rho, \kappa \rangle\rangle$ (see [22] for a more detailed explanation of iterated power series). Let $f(\rho, \kappa) \in \mathbb{Z}\langle\langle \rho, \kappa \rangle\rangle$ then $f(\rho, \kappa)$ is of the form

$$f(\rho, \kappa) = \sum_{n \geq n_0} a_n(\rho)\kappa^n, \quad n_0 \in \mathbb{Z}, \qquad (53)$$

with

$$a_n(\rho) = \sum_{m \geq m_0} a_{n,m}\rho^m, \quad m_0, a_{n,m} \in \mathbb{Z}. \qquad (54)$$

Then CT_ρ is defined as

$$\mathrm{CT}_\rho[f] = \sum_{n \geq n_0} a_{n,0}\, \kappa^n \tag{55}$$

Note, the rational function of ρ and κ in (52) must be expanded in κ first, then the coefficients of κ expanded in ρ. Expanding in the opposite order produces a constant term expression that does not satisfy the initial condition. In other words, the initial condition dictates the order of expansion and hence in which iterated field of Laurent power series the constant term is evaluated.

5 Adsorbing Dyck paths with a force by the kernel-functional method

The action of a vertical force pulling one end of a polymer adsorbing on to a surface can be modelled using ballot paths (see Sect. 4 for a definition). Of interest here is the effect the vertical force has on the adsorption phase diagram.

The interaction between the surface and the polymer is modelled in the same way as the adsorption problem discussed in Sect. 4, that is, associating a weight κ to a step returning to the surface. The vertical force is modelled by a Boltzmann factor s^h where h is the height of the end of the path. An example is shown in Fig. 5.

Thus we need to compute the generating function

$$f(s) = \sum_{n \geq 0} x^n \sum_{h \geq 0} Z_n(h) s^h \tag{56}$$

where $Z_n(h)$ is given by (48). The force exerted by a finite length polymer is

$$F_n(h) = -\log Z_n(h+1) + \log Z_n(h) = \log\left(\frac{Z_n(h)}{Z_n(h+1)}\right) \tag{57}$$

The thermodynamic behaviour is then obtained by taking the limit $\lim_{n\to\infty} F_n(h)/n$.

We shall construct a recursive functional equation for $f(s)$ by considering the process of adding a extra step to the end of the paths as illustrated in Fig. 6. The functional equation can then be solved by using the kernel method [23,24].

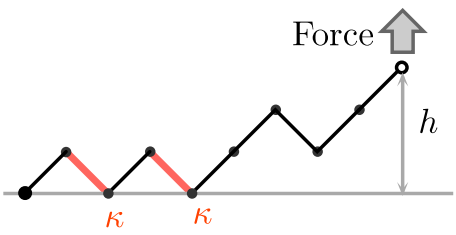

Fig. 5 An example of a ballot path with a surface interaction and a vertical force

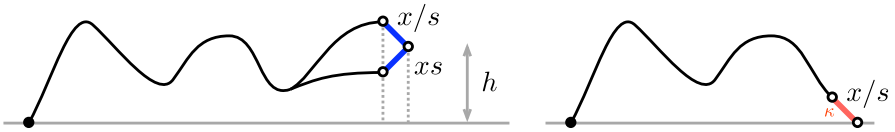

Fig. 6 The functional equation is constructed by considering the action of adding an extra step above the surface (left) and on the surface (right)

Consider paths ending at height h and partition the set of all weighted paths, $\mathcal{P}$ according to the height of the last step, thus $\mathcal{P} = \bigcup_{h\geq 0} \mathcal{P}_h$. Paths in $\mathcal{P}_h$ can be constructed from paths one step shorter in several ways.

Case $h = 0, n = 0$. This is the special case of a zero length path which cannot be constructed by adding a step to any other path.

Case $h = 0$. The set of paths length $n > 0$ ending at height $h = 0$, $\mathcal{P}_0$ can be constructed from the set of paths ending at height $h = 1$ by adding a down step which contributes a weight $\kappa x/s$.

Case $h > 0$. The set of all length $n > 0$ paths ending at some particular height $h > 0$, can be constructed from the set of all paths ending at height $h+1$, $\mathcal{P}_{h+1}$ by appending a down step and from the set of all paths ending at height $h-1$, $\mathcal{P}_{h-1}$ by appending an up step. The down step contributes a weight x/s and the up step xs.

Thus we have the weight preserving bijections.

$$\mathcal{P}_h \longleftrightarrow xs\,\mathcal{P}_{h-1} \cup \frac{x}{s}\,\mathcal{P}_{h+1}, \quad h > 0 \tag{58}$$

$$\mathcal{P}_0 \longleftrightarrow \{1\} \cup \kappa\frac{x}{s}\,\mathcal{P}_1, \quad h = 0 \tag{59}$$

and hence

$$\mathcal{P} = \{1\} \cup \kappa\frac{x}{s}\mathcal{P}_0 \cup \left(\bigcup_{h>0} xs\mathcal{P}_{h-1} \cup \frac{x}{s}\mathcal{P}_{h+1}\right) \tag{60}$$

$$= \{1\} \cup xs\mathcal{P}_0 \cup \left(\kappa\frac{x}{s} + xs\right)\mathcal{P}_1 \cup_{h\geq 2} \left(xs + \frac{x}{s}\right)\mathcal{P}_h. \tag{61}$$

Since $\{\mathcal{P}_h\}_{h\geq 0}$ is a partition, the generating function (56), which we shall write in the form,

$$f(s) = \sum_{h\geq 0} f_h s^h, \tag{62}$$

satisfies

$$f(s) = 1 + sxf_0 + x(\kappa/s + s)f_1 s + \sum_{h\geq 2} x(1/s + s)f_k s^k. \tag{63}$$

Since $f_0 = f(0)$ and also $f_0 = 1 + \kappa x f_1$, Eq. 63 can be written

$$f(s) = \frac{1}{\kappa} + \left(\frac{\kappa - 1}{\kappa} - \frac{x}{s}\right) f(0) + x\left(s + \frac{1}{s}\right) f(s) \tag{64}$$

To solve (64) for $f(s)$ we first need find $f(0)$. We can't multiply (64) by s and then put $s = 0$ as both sides of the equation vanish. We thus proceed as follows. Write (64) in the form

$$K(s) f(s) = \frac{1}{\kappa} + \left(\frac{\kappa - 1}{\kappa} - \frac{x}{s}\right) f(0), \quad K(s) = 1 - x\left(s + \frac{1}{s}\right), \tag{65}$$

where $K(s)$ is the kernel. The equation $K(s) = 0$ has two solutions,

$$s_\pm = \frac{1}{2x}\left(1 \pm \sqrt{1 - 4x^2}\right). \tag{66}$$

Note, $s_+ = \mathrm{O}(z^{-1})$ and $s_- = \mathrm{O}(z)$ as $z \to 0$. We now consider the limit $s \to s_\pm$ in Eq. 65. As we shall see, $f(s)$ is a quadratic algebraic function. The branch, $f_-(s)$ has a simple pole at s_- and hence diverges as $s \to s_-$ whilst the other branch, $f_+(s)$ has a pole at s_+. Thus, we assume

$$\lim_{s \to s_-} K(s) f_+(s) = 0 \quad \text{and} \quad \lim_{s \to s_+} K(s) f_-(s) = 0 \tag{67}$$

which gives two equations

$$0 = \frac{1}{\kappa} + \left(\frac{\kappa - 1}{\kappa} - \frac{x}{s_-}\right) f_+(0) \tag{68}$$

$$0 = \frac{1}{\kappa} + \left(\frac{\kappa - 1}{\kappa} - \frac{x}{s_+}\right) f_-(0) \tag{69}$$

and hence, substituting into (64) gives the two solutions

$$f_\pm(s) = \frac{s_\pm}{((\kappa - 1) - \kappa x s_\pm)} \frac{1}{(s - s_\pm)}. \tag{70}$$

Thus we see that $f_\pm(s)$ diverges as $s \to s_\pm$ which is consistent with (67).

The generating function $f(s)$ we require for the partition function (56), is a Taylor series in s and x and hence an element of the ring $\mathbb{Z}((\kappa, s, x))$. It is readily checked that of the two solutions $f_\pm(s)$, only the solution $f_+(s)$ is an element of $\mathbb{Z}((\kappa, s, x))$. The other solution, $f_-(s)$ is a Laurent series, that is, has negative powers of x and s and is an element of the ring $\mathbb{Z}[[\kappa, x, s]]$. Thus the partition function generating function (56) is given by

$$f(s) = \frac{s_+}{(\kappa - 1 - \kappa x s_+)(s - s_+)} = \frac{1}{(\kappa x - (\kappa - 1)s_-)(1 - s_- s)}, \tag{71}$$

From (71) we can readily extract the fixed height h length generating function,

$$G_n(x) = \sum_{n\geq 0} Z_n(\kappa)x^n = \frac{s_-^{h+1}}{\kappa x - (\kappa - 1)s_-} \tag{72}$$

where we used $s_+s_- = 1$.

6 Dyck paths in a strip by the Transfer Matrix method

The force induced between colloid particles by a dilute solution of polymers gives rise to the phenomena of steric stabilisation and sensitised flocculation of colloidal dispersions [25]. We can model the phase transitions associated with this problem by Dyck paths in a strip.

In Sect. 4 we defined Dyck paths. Dyck paths in a strip are Dyck paths which have the additional constraint that they cannot step above height $y = L$. We can use them to model polymers in a strip by adding an interaction energy for each step on to the lower surface ($y = 0$) and an interaction energy for each vertex on the upper surface $y = L$. This gives rise to two weights. A weight κ—the same as the adsorption problem—and a weight ω with steps from $v_i = (i, L-1)$ to $v_{i+1} = (i+1, L)$. An example is shown in Fig. 7. Note, although the physics naturally associates the Boltzmann factor with the vertex, it is mathematically more convenient to associate the weight with the *step* immediately preceding the vertex on the upper (or lower) surface.

We will solve this problem using the Transfer Matrix method. Let T be the transfer matrix. If the path has a weight or step from $y = i$ to $y = j$ then the matrix element $T_{i,j}$ is set to that weight (or one if it is an un-weighted step). The partition function for n step weighted Dyck paths in the strip can then be written in the form,

$$Z_n(\kappa, \omega) = \left(T^n\right)_{0,0}, \tag{73}$$

where the transfer matrix has elements

$$T_{i,j} = \begin{cases} \kappa & \text{if } i = 1,\ j = 0 \\ \omega & \text{if } i = L-1,\ j = L \\ 1 & \text{if } j = i+1,\ i \notin \{0, L-1\} \\ 0 & \text{otherwise.} \end{cases} \tag{74}$$

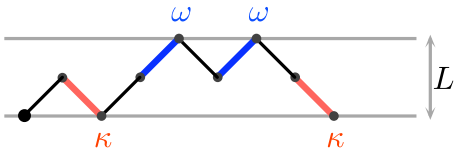

Fig. 7 A example of a Dyck path in a strip of width $L = 2$ showing the lower surface weights, κ, and the upper surface weights ω

This gives rise to a tri-diagonal or Jacobi matrix. As an example, the matrix for paths in a strip of width $L = 3$ is the 4×4 matrix,

$$T = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \kappa & 0 & 1 & 0 \\ 0 & 1 & 0 & \omega \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{75}$$

The mathematical problem now becomes that of finding the form of the matrix elements of the nth power of the transfer matrix. We do this by diagonalising the matrix and hence need the left and right eigenvectors, e_k^ℓ and e_k^r. The partition function can then be written,

$$Z_n(\kappa, \omega) = \sum_k e_k^r \, \lambda_k^n \, e_k^\ell, \tag{76}$$

where the sum is over all eigenvalues λ_k. The left eigenvectors satisfy the equations

$$\begin{aligned} \kappa e_1^\ell &= \lambda e_0^\ell \quad i = 0 \\ e_{i-1}^\ell + e_{i+1}^\ell &= \lambda e_i^\ell \quad 0 < i < L \\ \omega e_{L-1}^\ell &= \lambda e_L^\ell \quad i = L, \end{aligned} \tag{77a}$$

and for the right eigenvectors

$$\begin{aligned} e_1^r &= \lambda e_0^r \quad i = 0 \\ \kappa e_0^r + e_2^r &= \lambda e_1^r \quad i = 1 \\ e_{i-1}^r + e_{i+1}^r &= \lambda e_i^r \quad 0 < i < L \\ e_{L-2}^r + \omega e_L^r &= \lambda e_{L-1}^r \quad i = L - 1 \\ e_{L-1}^r &= \lambda e_L^r \quad i = L. \end{aligned} \tag{78a}$$

The left and right eigenvectors are closely related. In fact, Eqs. (77) are the same as (78) if we let

$$\kappa e_0^r = e_0^\ell \quad \text{and} \quad \omega e_L^r = e_L^\ell. \tag{79}$$

Thus we only need to solve the simpler set (77). Equations (77a) and (77a) are of the form

$$P_{-1} = 0 \tag{80a}$$

$$P_0 = 1 \tag{80b}$$

$$P_{k+1} = \lambda P_k - \mu_k P_{k-1}, \quad k \geq 0 \tag{80c}$$

$$P_{L+1} = 0, \tag{80d}$$

with $P_k := e_k^\ell$, $k > 0$ and

$$\mu_k = \begin{cases} 1, & \text{if } 0 \le k \le L-1 \\ \omega, & \text{if } k = L. \end{cases} \tag{81}$$

Thus we see that the components of the eigenvectors satisfy a three term recurrence and hence are orthogonal polynomials in λ. The first equation (77a) does not satisfy (80c) with the standard initial conditions (80a) and (80b) and thus must be solved separately.

Equations (80) are readily solved in a few simpler cases: $\kappa = \omega = 1$ and $\kappa\omega = \kappa + \omega$. The full (κ, ω) case is somewhat more difficult [20,26] and we shall only give the final result.

Case: $\kappa = \omega = 1$. This case is usually solved by the method of inclusion exclusion and not via eigenvectors. However, to solve the general (κ, ω) case it is still necessary to solve this simpler case. Thus, if $\kappa = \omega = 1$, then (77) are solved by Chebychev polynomials (of the second kind). In particular, $P_k = \rho^k - \rho^{-k}$ with $\lambda = \rho + 1/\rho$ and thus

$$e_k^\ell = e_k^r = \rho^k - \rho^{-k}, \quad \text{and} \quad \rho^{2L+2} = 1, \quad \kappa = \omega = 1. \tag{82}$$

The eigenvalues are given by the roots of unity, $\rho^{2L+2} = 1$.

Case: $\kappa\omega = \kappa + \omega$. For this more interesting case we can solve (77a) with $e_k^\ell = \rho^k - \rho^{-k}$ with $\lambda = \rho + 1/\rho$. To solve (78a) we try $e_k^\ell = A\rho^k + B\rho^{-k}$ and one finds that $B/A = -(\lambda - \kappa\rho)/(\lambda - \kappa/\rho)$. However, this form of the solution, whilst still satisfying (77a), only satisfies (77a) if $\kappa\omega = \kappa + \omega$. Thus we get

$$e_k^\ell = \rho^k - S(\rho)\rho^{-k}, \quad S(\rho) = \frac{\rho + 1/\rho - \kappa\rho}{\rho + 1/\rho - \kappa/\rho}, \quad \kappa\omega = \kappa + \omega. \tag{83}$$

The eigenvalues are now given by the roots of $e_{L+1}^\ell(\rho) = 0$.

Case: κ, ω **arbitrary.** We see from (80d) that the zeros of the $L+1$th polynomial are the eigenvalues and hence in order to evaluate the partition function in the form (76) we need to sum over the zeros of $P_{L+1}(\lambda_k) = 0$. Each term in the sum requires us to evaluate $P_m(\lambda_k)$ at that zero i.e. evaluate one orthogonal polynomial at a zero of another. Surprisingly for orthogonal polynomials this can be done. It turns out [20] that the sum (76) can be written as a constant term. One way of seeing this is to write the sum over zeros as a contour integral. The zeros translate into poles and the residue expansion is the partition function sum. The integral is then evaluated (after a suitable change of variable) in terms of the residue at infinity—it is this residue at infinity that can be written as a constant term.

Thus, to use get the constant term expression we must change variables to $\lambda = \rho + 1/\rho$. The sum can then be written as a constant term [26], in particular

$$Z_{2n}(\kappa, \omega) = \mathrm{CT}_\rho \left[\left(\rho + \frac{1}{\rho}\right)^{2n} \frac{1-\rho^2}{\rho^2 - \sum_{s=0}^{L} \beta_s \rho^{-2s}} \sum_{r=0}^{L} \alpha_r \rho^{-2r} \right] \tag{84}$$

where

$$\alpha_r = \begin{cases} 2-\omega & r \in \{1, \ldots, L-1\}, \\ 1 & r \in \{0, L\}, \end{cases} \tag{85}$$

$$\beta_s = \begin{cases} 2\kappa + 2\omega - \kappa\omega - 4 & s \in \{1, \ldots, L-2\}, \\ \kappa + \omega - 3 & s \in \{0, L-1\}\,, \\ -1 & s = L\,. \end{cases} \tag{86}$$

and hence

$$Z_{2n}(0,0) = \sum_{r=0}^{L} \sum_{s=0}^{n} {\sum_{s_0,\ldots,s_L}}' C_{2n,n^*} \binom{s}{s_0, \ldots, s_L} \alpha_r \prod_{m=0}^{L} \beta_m^{s_m} \tag{87}$$

where the multinomial sum has the constraint $s_0 + \cdots + s_L = s, s_i \in \{0, \ldots, s\}$, $C_{n,m}$ is the generalised Catalan number,

$$C_{n,m} = \binom{n}{m} - \binom{n}{m-1}.$$

7 Conclusion

We have considered several directed path models of some polymer and vesicle problems. Each model was used to illustrate an important method of solving lattice path enumeration problems. In particular, the Temperley method was used for the collapse problem in the discrete case and the ZL method for the semi-continuous vesicle model. The constant term method was used to solve a set of partial difference equations for the polymer adsorption problem. The Kernel method was used to solve the functional equation that arose in the polymer force problem. Finally, the Transfer Matrix method was used to solve the problem of colloid dispersions.

Each of these methods are in fact very similar in that they each rely on writing down equations for the partition function of various generating functions that occur when an extra step is added to the lattice path (or column in the case of the collapse and vesicle problems).

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