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Two-dimensional self-avoiding walks and polymer adsorption: critical fugacity estimates

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Abstract
Recently Beaton, de Gier and Guttmann proved a conjecture of Batchelor and Yung that the critical fugacity of self-avoiding walks (SAW) interacting with (alternate) sites on the surface of the honeycomb lattice is $1+\sqrt{2}$. A key identity used in that proof depends on the existence of a parafermionic observable for SAW interacting with a surface on the honeycomb lattice. Despite the absence of a corresponding observable for SAW on the square and triangular lattices, we show that in the limit of large lattices, some of the consequences observed for the honeycomb lattice persist irrespective of lattice. This permits the accurate estimation of the critical fugacity for the corresponding problem for the square and triangular lattices. We consider both edge and site weighting, and results of unprecedented precision are achieved. We also *prove* the corresponding result for the edge-weighted case for the honeycomb lattice.

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1. Introduction

Self-avoiding walks (SAWs) in a half-space, originating at a site on the surface, are well-known and useful models of polymer adsorption, see [11, 21] for reviews. It is known [20] that the connective constant for such walks is the same as for the bulk case. To model surface adsorption, one adds a fugacity $y = \mathrm{e}^{\alpha}$ to sites or edges on the surface. Let $c_n^+(m)$ be the number of half-space walks of n-steps, with m monomers on the surface, and define the partition function as

$$Z_n(\alpha) = \sum_{m=0}^{n} c_n^+(m)\mathrm{e}^{m\alpha},$$

with $\alpha = -\epsilon/k_BT$, where ϵ is the energy associated with a surface site (or edge), T is the absolute temperature and k_B is Boltzmann's constant. If ϵ is sufficiently large and negative, the

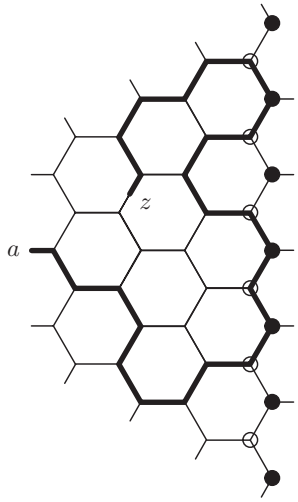

Figure 1. The two types of surface site on the honeycomb lattice as indicated by solid and empty circles. A SAW starting at a and finishing at z is also shown.

polymer adsorbs onto the surface, while if ϵ is positive, the walk is repelled by the surface. It has been shown by Hammersley, Torrie and Whittington [10] in the case of the d-dimensional hyper-cubic lattice that the limit

$$\lim_{n\to\infty} n^{-1} \log Z_n(\alpha) \equiv \kappa(\alpha)$$

exists, where $\kappa(\alpha)$ is the reduced, intensive, free-energy of the system. It is a convex, non-decreasing function of α, and therefore continuous and almost everywhere differentiable. Their discussion and proof apply *mutatis mutandis* to the honeycomb and triangular lattices.

In the case of the honeycomb lattice there are two types of surface sites, marked as solid and empty circles in figure 1. In most studies just one of the two types is weighted, namely those marked with solid circles in figure 1. In this study, we also allow for a surface weight on the second type of sites and we study the case where all surface sites carry the same weight.

For $\alpha < 0$, $\kappa(\alpha) = \log \mu$ [20], where μ is the connective constant for SAW on the given lattice. For $\alpha \geqslant 0$,

$$\kappa(\alpha) \geqslant \max[\log \mu, \alpha].$$

This behaviour implies the existence of a critical value α_c, such that for the hyper-cubic lattice, $0 \leqslant \alpha_c \leqslant \log \mu$. The situation as $\alpha \to \infty$ has only recently been rigorously established by Rychlewski and Whittington [19], who proved that $\kappa(\alpha)$ is asymptotic to α in this regime. As illustrated in figure 1, it is convenient to attach weights y to only half of the sites along the surface to allow for simplifications later on. In this case, the bounds on α_c become $0 \leqslant \alpha_c \leqslant 2 \log \mu$, or equivalently $1 \leqslant y_c = e^{\alpha_c} \leqslant \mu^2$.

Various other quantities exhibit singular behaviour at y_c. For example, the mean density of sites on the surface is given by

$$\rho_n(y) = \frac{1}{n} \frac{\sum_m m c_n^+(m) y^m}{\sum_m c_n^+(m) y^m} = \frac{1}{n} \frac{\partial \log Z_n(\alpha)}{\partial \alpha}.$$

In the limit of infinitely long walks one has

$$\rho(\alpha) = \frac{\partial \kappa(\alpha)}{\partial \alpha}.$$

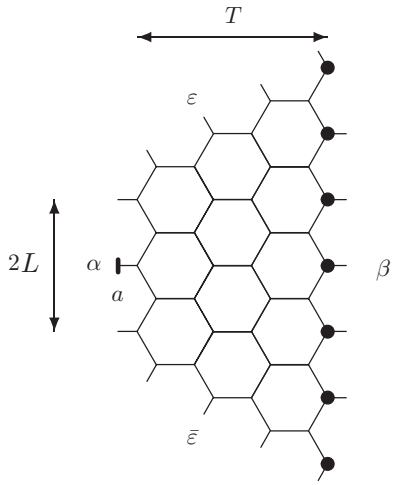

Figure 2. Finite patch $S_{3,1}$ of the honeycomb lattice with a boundary.

From the behaviour of κ given above, it can be seen that $\rho(\alpha) = 0$ for $y < y_c$ and $\rho(\alpha) > 0$ for $y > y_c$.

2. An identity for the honeycomb lattice with a boundary

In a recent paper, Beaton, de Gier and Guttmann [2] generalized a finite-lattice identity by Duminil-Copin and Smirnov [6] for the honeycomb lattice to the case where weights are introduced on alternating sites along a boundary as represented by the solid circles in figure 2. This resulted in a proof of a conjecture of Batchelor and Yung [1] that the critical surface fugacity of SAWs interacting with (alternate) sites on the surface of the honeycomb lattice is $1 + \sqrt{2}$. Here, we briefly outline the results.

Let H be the set of mid-edges on a half-plane of the honeycomb lattice. We define a *domain* $\Omega \subset H$ to be a simply connected collection of mid-edges. The set of sites adjacent to the mid-edges of Ω is denoted $V(\Omega)$. Those mid-edges of Ω which are adjacent to only one site in $V(\Omega)$ form $\partial\Omega$. Since surface interactions are the focus of this article, we will insist that at least one site of $V(\Omega)$ lies on the boundary of the half-plane.

Let γ be a SAW in a domain Ω. We denote by $\ell(\gamma)$ the number of sites occupied by γ and by $\nu(\gamma)$ the number of contacts with the boundary. Define the following observable, for $a \in \partial\Omega$, $z \in \Omega$, set

$$F(a, z; x, y, \sigma) := F(z) = \sum_{\gamma(a\to z)\subset\Omega} \mathrm{e}^{-\mathrm{i}\sigma W(\gamma(a\to z))} x^{\ell(\gamma)} y^{\nu(\gamma)},$$

where the sum is over all configurations $\gamma \subset \Omega$, for which the SAW goes from the mid-edge a to a mid-edge z. $W(\gamma(a \to z))$ is the winding angle of that SAW. See figure 1 for an example—the SAW shown there starts on the central mid-edge of the left boundary (shown as a) and ends at a mid-edge z. As the SAW runs from mid-edge to mid-edge, it acquires a weight x for each step and a weight y for each contact (shown as a solid circle) with the right-hand side boundary.

We define the following generating functions:

$$A_{T,L}(x,y) := \sum_{\substack{\gamma \subset S_{T,L} \\ a \to \alpha/\{a\}}} x^{\ell(\gamma)} y^{v(\gamma)},$$

$$B_{T,L}(x,y) := \sum_{\substack{\gamma \subset S_{T,L} \\ a \to \beta}} x^{\ell(\gamma)} y^{v(\gamma)},$$

$$E_{T,L}(x,y) := \sum_{\substack{\gamma \subset S_{T,L} \\ a \to \varepsilon \cup \bar{\varepsilon}}} x^{\ell(\gamma)} y^{v(\gamma)},$$

where the sums are over all configurations that have a contour from a to the α, β or $\varepsilon, \bar{\varepsilon}$ boundaries, respectively, for domains of height $2L$ and width T as shown in figure 2. For the SAW model in the dilute regime, the result proved in [2] for the n-vector model simplifies (in the case $n = 0$) to

$$1 = \cos\left(\frac{3\pi}{8}\right) A_{T,L}(x_c, y) + \cos\left(\frac{\pi}{4}\right) E_{T,L}(x_c, y) + \frac{y^* - y}{y(y^* - 1)} B_{T,L}(x_c, y), \tag{1}$$

where

$$y^* = \frac{1}{1 - 2x_c^2} = 1 + \frac{1}{\cos(\pi/4)}, \qquad y^* x_c^2 = (2)^{-1/2}.$$

A simple corollary of (1) is that at $y = y^*$ we have

Corollary 1.

$$1 = \cos\left(\frac{3\pi}{8}\right) A_{T,L}(x_c, y^*) + \cos\left(\frac{\pi}{4}\right) E_{T,L}(x_c, y^*). \tag{2}$$

The importance of this result is that the generating function $B_{T,L}$ for $y = y^*$ has disappeared from (2). In [2], we proved that the critical surface fugacity y_c is equal to y^*. Using this result and taking the limit $L \to \infty$, the geometry becomes a strip of width T, and the corollary then becomes

$$1 = \cos\left(\frac{3\pi}{8}\right) A_T(x_c, y_c) + \cos\left(\frac{\pi}{4}\right) E_T(x_c, y_c). \tag{3}$$

In [2], we also proved that $E_T(x_c, y) = 0$ for all $0 \leqslant y \leqslant y_c$. So (3) simplifies further to

$$1 = \cos\left(\frac{3\pi}{8}\right) A_T(x_c, y_c). \tag{4}$$

This is a remarkable equation in that it implies that y_c can be identified from the generating function $A_T(x_c, y)$ *for any width* T, simply by solving equation (4). To show the power of this observation, note that virtually by inspection one can write down the solution for strip width 0, which is

$$A_0(x,y) = \frac{2x^3 y}{1 - x^2}.$$

Solving $1/\cos\left(\frac{3\pi}{8}\right) = A_0(x_c, y)$, recalling $x_c = 1/\sqrt{2 + \sqrt{2}}$, gives $y = y_c = 1 + \sqrt{2}$, the exact value of the critical fugacity.

For other lattices, and even for the honeycomb lattice with interactions at every surface site, we do not have an equivalent identity, such as $1 = c_\alpha A_T(x_c, y_c)$. However, if one plots

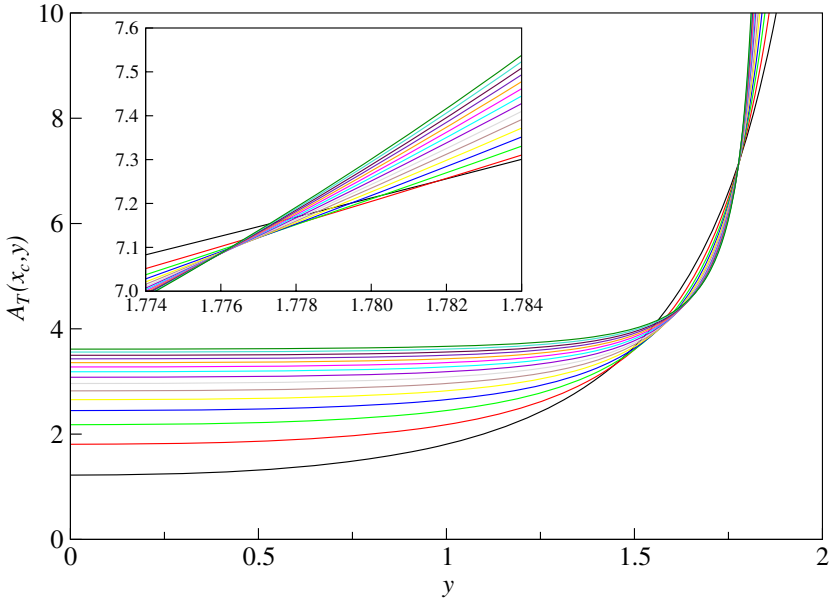

Figure 3. Square lattice with surface site interactions. $A_T(x_c, y)$ versus y for $T = 1, \ldots, 15$. Inset shows the intersection region on a finer scale.

$A_T(x_c, y)$ versus y in these cases, one might be forgiven for thinking that such an identity exists. In figure 3, we show a plot of $A_T(x_c, y)$ versus y, for a range of strip widths T. To graphical accuracy, it appears that there is a unique point of intersection for plots corresponding to higher values of T. Even finer resolution, see inset, suggests that this is the case. The actual small deviation can be seen from the data given in table 4.

We denote by $y_c(T)$ the point of intersection of $A_T(x_c, y)$ and $A_{T+1}(x_c, y)$. We observe that the sequence $\{y_c(T)\}$ is a monotone function of T. We argue, as in [3], that in the scaling limit all two-dimensional SAW models are given by the same conformal field theory. Since it is known for one of these models (i.e. honeycomb-lattice SAW with alternate site interactions) that the critical point can be found by requiring certain contour integrals to vanish, it follows that in the scaling limit the same should be true for all two-dimensional SAWs[1]. This is entirely consistent with our observations, and implies that $\lim_{T\to\infty} y_c(T) = y_c$.

This then suggests a potentially powerful new numerical approach to estimating y_c. One calculates the generating functions $A_T(x_c, y)$, for all strip widths $T = 0, 1, 2, \ldots T_{\max}$, uses these to calculate $y_c(T)$ for $T = 0, 1, 2, \ldots T_{\max-1}$ as defined above and then extrapolates this monotone sequence by a variety of standard sequence extrapolation methods. A similar idea was used to furnish estimates of x_c in [3].

In section 3, we describe the derivation of the generating functions $A_T(x_c, y)$ by the finite-lattice method for a range of strip widths T that are needed in this study. For the value of the critical step fugacity x_c, we use the exact result $x_c = 1/\sqrt{2+\sqrt{2}}$ for the honeycomb lattice, and the best available series estimates in the case of the square and triangular lattices. These are $x_c(\text{sq}) = 0.379\,052\,277\,76$ [13, 17], with uncertainty in the last digit, and $x_c(\text{tr}) = 0.240\,917\,5745$ [15], with similar uncertainty. We performed a sensitivity analysis of our critical surface fugacity estimates in order to determine how sensitive they are

[1] We thank John Cardy for this observation.

to uncertainties in our estimates of x_c. The estimates of x_c are sufficiently precise that a change in our estimate of x_c by a factor of 10 times the estimated uncertainty will not change our estimates of the surface fugacity y_c even in the least significant digit.

In section 4, we estimate the critical fugacity by extrapolating $y_c(T)$ using a range of standard extrapolation algorithms. These are Levin's u-transform, Brezinskii's θ algorithm, Neville tables, Wynn's ϵ algorithm and the Barber–Hamer algorithm. Descriptions of these algorithms, and codes for their implementation, can be found in [9]. However, we find that the most precise estimates are given by the Bulirsch–Stoer algorithm [4]. This algorithm requires a parameter w, which can be thought of as a correction-to-scaling exponent. For the purpose of the current exercise, we have set this parameter to 1, corresponding to an analytic correction, which is appropriate for the two-dimensional SAW problem [5]. Our implementation of the algorithm is precisely as described by Monroe [18], and we retained 50-digit precision throughout.

We used this method to estimate the critical fugacity for all cases of interest for two-dimensional SAWs. For the honeycomb lattice, discussed in subsection 4.1, we have already proved [2] that $y_c = 1 + \sqrt{2}$ for the alternate site interaction model, as conjectured by Batchelor and Yung [1]. It is a straightforward consequence of this result—the argument is given in subsection 4.1 below—that for the honeycomb lattice with surface edge interactions (rather than site interactions), the critical fugacity is $\sqrt{1+\sqrt{2}}$. For the honeycomb-lattice site interaction problem where every surface site interacts with the walk, we find the critical fugacity to be $y_c = 1.467\,67$, where the error in this estimate (and all such estimates given below) is expected to be confined to a few parts in the last quoted digit. We know of no other estimate of this quantity in the literature.

In subsection 4.2, we discuss the critical fugacity for site- and edge-weighted adsorption on the square lattice. The only previous estimates for the site-weighted case can be found in [12], where Monte Carlo methods were used to obtain the estimate $y_c = 1.76 \pm 0.02$. Our estimate, $y_c = 1.775\,64$ is three orders of magnitude more precise than this. For the edge-weighted case, a transfer matrix (TM) estimate is given in [8], and is $y_c = 2.041 \pm 0.002$. In [7], a Monte Carlo estimate of comparable precision is given, $y_c = 2.038 \pm 0.002$. Our estimate is $y_c = 2.040\,135$, again some three orders of magnitude more precise.

For the triangular lattice, discussed in subsection 4.3, we are unaware of any previous investigations of the critical fugacity. We find, in section 4.3, that $y_c(\text{site}) = 2.144\,181$ and $y_c(\text{edge}) = 2.950\,026$. We repeat that errors in our quoted estimates are expected to be confined to a few parts in the last quoted digit.

3. Enumeration of self-avoiding walks

The algorithms we use to enumerate SAW interacting with a surface on the honeycomb, square and triangular lattices are based on the algorithm outlined in our previous paper [3] and detailed descriptions can be found in these papers [14–16]. Suffice to say that the generating functions for a given strip were calculated using TM techniques. The most efficient implementation of the TM algorithm generally involves bisecting the finite lattice with a boundary (this is just a line in our case) and moving the boundary in such a way as to build up the lattice site by site. If we draw a SAW and then cut it by a line, we observe that the partial SAW to the left of this line consists of a number of loops connecting two edges in the intersection, and at most two unconnected or free edges. The other end of the free edge is an end point of the SAW; hence, there are at most two free ends.

Table 1. The estimated value of $y_c(9)$ from the crossing between $A_{10}(x_c, y)$ and $A_9(x_c, y)$ truncated at degree M and using strips of half-length from M up to $10M$.

M	$L = M$	$L = 2M$	$L = 5M$	$L = 10M$
100	1.832 547 814 756	1.778 376 701 255	1.778 024 722 094	1.778 024 722 094
250	1.776 250 937 231	1.775 990 603 337	1.775 990 594 686	1.775 990 594 686
500	1.775 990 340 341	1.775 990 291 271	1.775 990 291 271	
1000	1.775 990 291 271			

The sum over all contributing graphs is calculated as the boundary is moved through the lattice. For each configuration of occupied or empty edges along the intersection, we maintain a generating function G_S for partial walks with configuration S. In exact enumeration studies, G_S would be a truncated two-variable polynomial $G_S(x, y)$, where x is conjugate to the number of steps and y to the number of surface contacts (sites or edges). In a TM update, each source configuration S (before the boundary is moved) gives rise to a few new target configurations S' (after the move of the boundary line) and $n = 0$, 1 or 2 new edges and $m = 0$ or 1 new contacts are inserted leading to the update $G_{S'}(x, y) = G_{S'}(x, y) + x^n y^m G_S(x, y)$. Here, we are primarily interested in the case where $A(x, y)$ or $B(x, y)$ are evaluated at the critical point $x = x_c$. This actually makes life easier for us, since we can change to a single variable generating function $G_S(y)$ and update signatures as $G_{S'}(y) = G_{S'}(y) + x_c^n y^m G_S(y)$. Here, $G_S(y)$ is a polynomial in the contact fugacity y with real coefficients truncated at some maximal degree M. The calculations were carried out using quadruple (or 128 bit) floating-point precision (achieved in FORTRAN with the REAL(KIND=16)-type declaration).

In our calculations, we truncated $A(x_c, y)$ at degree $M = 1000$ and used strips of half-length $L = M$. In table 1, we have listed estimates for $y_c(9)$ obtained from strips of width 10 and 9 (the crossing between $A_{10}(x_c, y)$ and $A_9(x_c, y)$) for various values of M and L. Clearly, the choice $M = L = 1000$ suffices to estimate $y_c(9)$ to more than 10-digit accuracy.

The TM algorithm is eminently suited for parallel computations, and here we used the approach first described in [13] and refer the interested reader to this publication for further detail. The bulk of the calculations for this paper were performed on the cluster of the NCI National Facility, which provides a peak computing facility to researchers in Australia. The NCI peak facility is a Sun Constellation Cluster with 1492 nodes in Sun X6275 blades, each containing two quad-core 2.93 GHz Intel Nehalem CPUs with most nodes having 3 GB of memory per core (24 GB per node). It took a total of about 3300 CPU h to calculate $A_T(x_c, y)$ for T up to 15 on the square lattice. It is known [14] that the time and memory required to obtain the number of walks in a strip of width T grows exponentially as 3^T for the honeycomb and square lattices and as 4^T for the triangular lattice. So the bulk of the time was spent calculating A_{15} and B_{15}, which amounted to almost 2300 h in the square-lattice case. In this case, we used 48 processors and the split between actual calculations and communications was roughly 2 to 1 (with quite a bit a variation from processor to processor). Smaller widths can be generated more efficiently in that communication needs are lesser and hence not as much time is used for this task.

4. Data analysis

4.1. Honeycomb lattice

In [2], we proved that the critical fugacity for the case of interactions with alternate sites on the honeycomb lattice is $y_c = 1 + \sqrt{2}$. There are two other cases to consider. The first is the

Table 2. The value of $y_c(T)$ estimated from the crossing of $A_T(x_c, y)$ and $A_{T+1}(x_c, y)$ for the honeycomb-lattice surface site model.

T	$y_c(T)$	$A_T(x_c, y_c(T)) = A_{T+1}(x_c, y_c(T))$
1	1.474 342 684 974 343	2.758 023 465 753 132
2	1.471 231 066 324 457	2.699 581 979 117 133
3	1.469 859 145 369 675	2.671 309 655 463 187
4	1.469 144 651 946 551	2.655 387 366 045 945
5	1.468 728 339 703 417	2.645 467 247 042 683
6	1.468 465 540 675 101	2.638 829 094 236 329
7	1.468 289 428 840 316	2.634 145 423 791 235
8	1.468 122 140 755 486	2.629 489 693 948 282
9	1.468 008 309 717 543	2.626 054 066 036 805
10	1.467 956 382 495 343	2.624 432 487 387 554
11	1.467 915 603 443 970	2.623 117 304 368 586
12	1.467 883 002 922 926	2.622 033 892 173 660
13	1.467 856 536 243 392	2.621 129 346 334 020

case of interactions with every surface site, and the second is the case of interactions with every edge. We will deal with the second case first, as it is a straightforward consequence of the proof given in [2] that $y_c = \sqrt{1+\sqrt{2}}$ in the second case. The proof of this result, in outline, is the following. We denote the generating functions A and B, as defined in section 2, for the alternate site case considered in [2], by subscript a (for alternating). We denote the corresponding generating functions for the case with edge weighting with the subscript e. Then it is clear by inspection that $A_e(x_c, y) = A_a(x_c, y^2)$, as every time a walk contributing to the A generating function passes through n alternating surface sites, whether adjacent or not, it must pass through $2n$ surface edges.

By the same argument, every time a walk contributing to the B generating function passes through n alternating surface sites, whether adjacent or not, it must pass through $2n-1$ surface edges. This then gives rise to $B_e(x_c, y) = \frac{1}{y} B_a(x_c, y^2)$. From either of these two equations it follows that $y_c(\text{alternating}) = (y_c(\text{edge}))^2$; hence, $y_c(\text{edge}) = \sqrt{1+\sqrt{2}}$.

We now consider the first case, in which every surface site carries a fugacity y. We generated data for $A_T(x_c, y)$ for $T \leqslant 14$, as described in section 3, and found the intersection points where $A_T(x_c, y) = A_{T+1}(x_c, y)$, which defines $y_c(T)$. These data are tabulated in table 2. Extrapolating $y_c(T)$ as described above, we estimate

$$y_c = 1.467\,67.$$

We also find, by an identical method of extrapolation, that $A(x_c, y_c) = 2.613$, which is probably exactly $1/\cos(3\pi/8)$, as is the case when considering interactions with every alternate site, see (4).

4.2. Square lattice

We next consider data for the square lattice, with every surface site (vertex) carrying a fugacity y. We generated data for $A_T(x_c, y)$ for $T \leqslant 15$ as described in section 3, and found the intersection points where $A_T(x_c, y) = A_{T+1}(x_c, y)$, which defines $y_c(T)$. These data are tabulated in table 3. Extrapolating $y_c(T)$ as described above, we estimate

$$y_c = 1.775\,64.$$

We also find, by an identical method of extrapolation, that $A(x_c, y_c) = 2.678\,405$, which is $1.024\,981/\cos(3\pi/8)$. In [3] we found, for the non-interacting case (corresponding to $y = 1$),

Table 3. The value of $y_c(T)$ estimated from the crossing of $A_T(x_c, y)$ and $A_{T+1}(x_c, y)$ for the square-lattice surface site model.

T	$y_c(T)$	$A_T(x_c, y_c(T)) = A_{T+1}(x_c, y_c(T))$
1	1.781 782 909 906 119	2.748 677 355 944 862
2	1.778 386 591 113 354	2.715 115 253 913 871
3	1.777 378 005 442 640	2.704 018 907 440 273
4	1.776 850 407 093 364	2.697 681 121 136 133
5	1.776 527 700 942 633	2.693 512 738 663 579
6	1.776 316 359 764 735	2.690 608 915 840 792
7	1.776 170 974 231 462	2.688 500 944 397 294
8	1.776 066 934 443 028	2.686 918 847 615 982
9	1.775 990 033 953 699	2.685 698 355 993 929
10	1.775 931 645 420 429	2.684 735 010 917 280
11	1.775 886 299 456 907	2.683 959 815 456 866
12	1.775 850 398 954 429	2.683 325 675 630 414
13	1.775 821 502 307 431	2.682 799 521 958 416
14	1.775 797 906 369 155	2.682 357 553 489 197

Table 4. The value of $y_c(T)$ estimated from the crossing of $A_T(x_c, y)$ and $A_{T+1}(x_c, y)$ for the square-lattice surface edge model.

T	$y_c(T)$	$A_T(x_c, y_c(T)) = A_{T+1}(x_c, y_c(T))$
1	2.023 317 607 727 152	2.519 464 246 890 523
2	2.031 649 211 433 080	2.585 125 356 952 430
3	2.035 085 448 834 840	2.616 332 757 155 513
4	2.036 771 224 259 312	2.633 293 109 539 552
5	2.037 723 730 407 517	2.643 677 266 387 231
6	2.038 317 002 192 238	2.650 588 857 893 349
7	2.038 712 823 877 066	2.655 469 267 857 106
8	2.038 990 695 898 482	2.659 069 610 531 442
9	2.039 193 569 770 578	2.661 816 780 067 225
10	2.039 346 383 471 084	2.663 969 985 883 853
11	2.039 464 457 297 598	2.665 695 001 241 074
12	2.039 557 641 399 558	2.667 102 372 510 593
13	2.039 632 511 102 958	2.668 268 404 182 947
14	2.039 693 596 208 206	2.669 247 312 794 744

$A(x_c, 1) = 2.678\,365 = 1.024\,966/\cos(3\pi/8)$. Thus, there appears to be a very weak y dependence. (In the normalization of the generating function $A_T(x_c, y)$ used here, two extra half-steps are included, giving an extra factor of the step fugacity x_c, compared to the value that would be quoted if contributing walks started and ended *on* the surface. This explains the difference between the values quoted in table 3 and the ordinates in figure 3.)

Table 4 shows the corresponding data for the edge-weighted case. Extrapolating $y_c(T)$ as described above, we estimate

$$y_c = 2.040\,135.$$

We also find that $A(x_c, y_c) = 2.678\,405$, which is $1.024\,981/\cos(3\pi/8)$. In [3] we found, for the non-interacting case (corresponding to $y = 1$), $A(x_c, 1) = 2.6783 = 1.0249/\cos(3\pi/8)$. This is too imprecise to see any evidence of y dependence.

Table 5. The value of $y_c(T)$ estimated from the crossing of $A_T(x_c, y)$ and $A_{T+1}(x_c, y)$ for the triangular-lattice surface site model.

T	$y_c(T)$	$A_T(x_c, y_c(T)) = A_{T+1}(x_c, y_c(T))$
1	2.169 017 975 620 833	5.299 883 162 257 977
2	2.152 124 186 067 447	5.089 804 987 842 667
3	2.147 952 081 330 057	5.033 100 087 535 114
4	2.146 325 209 334 416	5.009 022 287 728 647
5	2.145 537 862 947 824	4.996 485 228 732 837
6	2.145 102 964 455 591	4.989 109 337 635 192
7	2.144 840 361 941 141	4.984 402 909 686 655
8	2.144 671 215 263 562	4.981 219 362 650 799
9	2.144 556 764 080 381	4.978 968 525 942 606
10	2.144 476 246 964 690	4.977 320 728 801 566

Table 6. The value of $y_c(T)$ estimated from the crossing of $A_T(x_c, y)$ and $A_{T+1}(x_c, y)$ for the triangular-lattice surface edge model.

T	$y_c(T)$	$A_T(x_c, y_c(T)) = A_{T+1}(x_c, y_c(T))$
1	2.933 665 548 671 216	4.793 416 679 321 919
2	2.939 352 607 034 002	4.841 229 819 027 843
3	2.942 788 011 875 285	4.873 934 294 210 283
4	2.944 814 166 604 381	4.895 179 517 868 169
5	2.946 090 146 548 846	4.909 648 090 189 844
6	2.946 944 189 466 541	4.919 989 731 979 732
7	2.947 544 335 340 955	4.927 679 988 442 194
8	2.947 982 663 246 637	4.933 582 932 189 477
9	2.948 312 910 101 248	4.938 231 892 866 670
10	2.948 568 146 735 367	4.941 971 526 310 544

Table 7. Estimated critical fugacity y_c for surface adsorption.

Lattice	Site weighting	Edge weighting
Honeycomb	1.467 67	$\sqrt{1+\sqrt{2}}$
Square	1.775 64	2.040 135
Triangular	2.144 181	2.950 026

4.3. Triangular lattice

We next consider data for the triangular lattice, with every surface site (vertex) carrying a fugacity y. We generated data for $A_T(x_c, y)$ for $T \leqslant 11$ as described in section 3, and found the intersection points where $A_T(x_c, y) = A_{T+1}(x_c, y)$, which defines $y_c(T)$. These data are tabulated in table 5. Extrapolating $y_c(T)$ as described above, we estimate

$$y_c = 2.144\,181.$$

We also find, by an identical method of extrapolation, that $A(x_c, y_c) = 4.970\,02$, which is $1.901\,944/\cos(3\pi/8)$. In [3] we found, for the non-interacting case (corresponding to $y = 1$), $A(x_c, 1) = 4.970\,111 = 1.901\,979/\cos(3\pi/8)$. Thus there again appears to be a very weak y dependence.

Table 6 shows the corresponding data for the edge-weighted case. Extrapolating $y_c(T)$ as described above, we estimate

$$y_c = 2.950\,026.$$

We also find that $A(x_c, y_c) = 4.9696$, which is $1.901\,78/\cos(3\pi/8)$. In [3] we found, for the non-interacting case (corresponding to $y = 1$), $A(x_c, 1) = 4.970\,111 = 1.901\,979/\cos(3\pi/8)$. Again, there is evidence of weak y dependence.

5. Conclusion

We have estimated the critical fugacity for surface adsorption for two-dimensional SAW on all regular lattices for both the case of site and edge interactions. Many of these estimates are new. Those that are not are several orders of magnitude more precise than pre-existing estimates. Uniquely for the case of the honeycomb lattice with edge interactions, we give the exact value of the critical fugacity, and also prove it. Our results are summarized in table 7.

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