# Crossover behavior for self-avoiding walks interacting with a surface

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Exact enumeration data have been analyzed by the partial-differential-approximation method for the adsorption (special) transition in self-avoiding walks attached to penetrable and impenetrable surfaces. Estimates of the crossover exponent  $\varphi$  are consistent with 0.28±0.05 (D=2) and 0.40±0.01 (D=3) for the penetrable surface, and 0.51±0.04 (D=2) and 0.54±0.07 (D=3) for the impenetrable surface.

### I. INTRODUCTION

The self-avoiding walk (SAW) on a D-dimensional lattice and interacting with a (D-1)-dimensional surface has been considered as a model for the study of polymer adsorption. The monomers of the SAW interact with the surface, which can be penetrable or impenetrable, with energy  $\omega$ . The impenetrable surface corresponds to the adsorption of polymers at a solid-liquid interface, while Hammersley et al.<sup>1</sup> suggest that the penetrable surface may correspond to the problem of polymer adsorption at a liquid-liquid interface. They have proved that the two models exhibit a phase transition at a (different) critical energy  $\omega_0$  with desorbed phase for  $\omega < \omega_0$  and adsorbed phase for  $\omega > \omega_0$ .<sup>1</sup> The crossover exponent  $\varphi$ , defined near the critical point in each model to describe the behavior of the phase transition,  $2^{-4}$  is believed to take different values for the two cases. (In the language of surface critical phenomena the singular behavior near  $\omega = \omega_0$ corresponds to the special transition.<sup>5</sup>) For impenetrable surfaces, series analysis,<sup>3</sup> the results of the transfermatrix approach<sup>6</sup> and conformal invariance theory<sup>7</sup> are consistent with a value for  $\varphi$  of 0.5 for D=2; for D=3, series analysis<sup>2</sup> and Monte Carlo estimates<sup>8</sup> give  $\varphi = 0.59$ . For penetrable surfaces, the scaling prediction  $\varphi = 1 - v$ gives  $\varphi = 0.25$  for D=2 and  $\varphi = 0.41$  for D=3. Nakanishi<sup>9</sup> obtains an estimate of 0.25 based on a small-cell renormalization-group calculation. The series analysis of Ishinabe<sup>4</sup> yields an estimate of  $\varphi = 0.5$  for D=2 and  $\varphi = 0.59$  for D = 3, inconsistent with the scaling prediction. His analysis seems to suggest that the two models have the same critical behavior for D=2 and D=3.

In this paper we analyze the available series for SAW's for the penetrable and impenetrable problems on a number of lattices in two and three dimensions for bond and site data. We analyze the two variable series using the method of partial-differential approximants (PDA) introduced by Fisher<sup>10</sup> in connection with spin systems. This method may be more appropriate for the analysis of multicritical behavior than a standard one-variable analysis. Our results indicate that the crossover exponent  $\varphi$  is different for the two models and consistent with the prediction of scaling. In Sec. II a scaling form for the twovariable generating function for the number of n step walks is given. Section III includes the result of the twovariable analysis based on the method of partialdifferential approximants (PDA) and a one-variable analysis to point out the possible source of the discrepancy in Ishinabe's analysis.<sup>4</sup>

# **II. THE SCALING FORM AT THE CRITICAL POINT**

Let  $a_{n,m}$  be the number of *n*-step SAW's in a *D*-dimensional lattice starting at the origin with *m* steps in the surface. We assign to each step of the walk a fugacity *x* in the bulk and a fugacity *y* in the (D-1)-dimensional surface. The generating function is

$$G(x,y) = \sum_{n} \sum_{m} a_{n,m} e^{m\omega}$$
(2.1)

or

$$G(x,y) = G(x,\omega) = \sum_{n} A_{n}(\omega) x^{n} , \qquad (2.2)$$

where  $e^{\omega} = y/x$  and

$$A_n(\omega) = \sum_m a_{n,m} e^{m\omega} .$$

The generating function is assumed to have singularities at  $x_c(\omega) = e^{-A(\omega)}$  of the form<sup>2-4,11</sup>

$$G(x,y) \sim [x_c(\omega) - x]^{\gamma(\omega)} .$$
(2.3)

 $A(\omega)$  is a convex nondecreasing function of  $\omega$  and nonanalytic at  $\omega_0$ , which is defined as the critical point.  $A(\omega)$  satisfies the inequalities

$$\max(\kappa, \kappa' + \omega) \le A(\omega) \le \max(\kappa, \kappa + \omega) , \qquad (2.4)$$

where  $\kappa$  and  $\kappa'$  are connective constants in *D*- and (D-1)-dimensional spaces, respectively. As  $\omega - \omega_0 \rightarrow 0^+$ ,  $A(\omega)$  behaves like

$$A(\omega) - A(\omega_0) \sim (\omega - \omega_0)^{1/\varphi} .$$
(2.5)

 $\varphi$  is the crossover exponent, which from the inequalities

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(2.4) is not greater than 1.

The trajectory of the singularities in the xy plane is then represented in terms of the parameter  $\omega$  by

$$x_c(\omega) = e^{-A(\omega)}, \quad y_c(\omega) = e^{\omega - A(\omega)}.$$
 (2.6)

From the property of  $A(\omega)$ , one can show the following.

(a) For  $\omega \le \omega_0$ , the trajectory is a vertical line corresponding to  $x_c(\omega) \equiv e^{-\kappa}$ . As  $\omega$  crosses  $\omega_0$ ,  $x_c(\omega)$  begins to decrease.  $\omega_0$  corresponds to the "special transition point"<sup>5</sup> defined by

$$x_c = x_c(\omega_0) = e^{-\kappa}, \quad y_c = y_c(\omega_0) = e^{\omega_0 - \kappa}.$$
 (2.7)

(b) Near the special point, we have as  $\omega - \omega_0 \rightarrow 0+$ ,

$$y - y_{c} = e^{\omega}x - e^{\omega_{0}}x_{c} = (e^{\omega} - e^{\omega_{0}})x + (x - x_{c})e^{\omega_{0}} \sim x_{c}e^{\omega_{0}}(\omega - \omega_{0}) + e^{\omega_{0}}(x - x_{c}) \\ \sim x_{c}e^{\omega_{0}}[A(\omega) - A(\omega_{0})]^{\varphi} + e^{\omega_{0}}(x - x_{c}) \sim x_{c}e^{\omega_{0}}(x_{c} - x)^{\varphi} + e^{\omega_{0}}(x - x_{c}) .$$
(2.8)

Since  $\varphi \leq 1$ , we may write

$$y - y_c = (x_c - x)^{\varphi} .$$
(2.9)  
(c) As  $\omega \to \infty$ ,  $x_c(\omega) = e^{-A(\omega)} \to 0$  and  
 $y_c(\omega) = e^{\omega - A(\omega)} \to \text{const} \le e^{-\kappa'} .$ 

Hence, (2.6) gives the phase boundary as has been previously described.<sup>12,13</sup>

In the limit  $N \rightarrow 0$ , it is well known that the problem of SAW's interacting with a surface is closely analogous to surface magnetism for either a semi-infinite N-component spin system or a system with a planar defect. The generating function G(x,y) for SAW's corresponds to the expansion of the high-temperature susceptibility  $\chi$ , while the fugacity x is the interaction parameter J/kT in the bulk and y is the coupling constant in the surface defined by y = Rx. Thus, R is related to  $\omega$  by identifying  $e^{\omega} = R$ .

From the assumption that G is a generalized homogeneous function near the special point, Binder<sup>5</sup> has given a scaling form of G in terms of R and  $t = (T - T_c)/T_c$ , that is,

$$G(R,t) \sim t^{-\gamma} Z((R-R_c)/t^{\varphi}) , \qquad (2.10)$$

and indicated that (2.5) and (2.10) define the same crossover exponent  $\varphi$ . From (2.8), the scaling form can be written, in terms of x and y, as

$$G(x,y) \sim (x_c - x)^{-\gamma} Z \left[ \frac{(y - y_c) + e^{\omega_0}(x_c - x)}{(x_c - x)^{\varphi}} \right]. \quad (2.11)$$

#### **III. ANALYSIS**

The two-variable series were analyzed using the method of partial-differential approximants. The method has been previously applied to spin systems.<sup>10</sup> However, this is (to the best of our knowledge) the first application to geometrical phase transitions, such as SAW's attached to an interacting surface. The series for the penetrable surface were also analyzed using a one-variable analysis.

## A. Partial-differential approximants

The method of partial-differential approximants is a generalization of d log Padé approximants for a function

f(x,y) of two variables with a truncated expansion around the origin. The assumed scaling form for the function near its multicritical point  $(x_c, y_c)$  is

$$f(x,y) \sim (\Delta \tilde{x})^{-\gamma} Z(\Delta \tilde{y} / (\Delta \tilde{x})^{\varphi}) , \qquad (3.1)$$

where  $\Delta \tilde{x} = \Delta x - (1/e_2)\Delta y$  and  $\Delta \tilde{y} = \Delta y - e_1\Delta x$ ;  $e_1$  and  $e_2$  are two scaling parameters to specify the derivative of x and y near the multicritical point and  $\varphi$  is the crossover exponent. Near the multicritical point, the scaling form satisfies

$$\left[ \left[ 1 - \frac{\varphi e_1}{e_2} \right] \Delta x - \frac{1 - \varphi}{e_2} \Delta y \right] \frac{\partial f}{\partial x} + \left[ e_1 (1 - \varphi) \Delta x - \left[ \frac{e_1}{e_2} - \varphi \right] \Delta y \right] \frac{\partial f}{\partial y} = \gamma \left[ 1 - \frac{e_1}{e_2} \right] f . \quad (3.2)$$

A partial-differential approximant  $F_{LMN}(x,y)$  to such a function f(x,y) is a solution of the linear partial-differential equation

$$Q_{M}(x,y)\frac{\partial F(x,y)}{\partial x} + R_{N}(x,y)\frac{\partial F(x,y)}{\partial y} = P_{L}(x,y)F(x,y) ,$$
(3.3)

where  $P_L(x,y)$ ,  $Q_M(x,y)$ , and  $R_N(x,y)$  are the defining polynomials with L, M, and N terms, respectively, and are chosen such that the series solutions of F(x,y) in powers of x and y agree with the known expansion of f(x,y) to some predetermined order.

The estimate for  $(x_c, y_c)$  is given by

$$Q_M(x_c, y_c) = 0$$
 and  $R_N(x_c, y_c) = 0$ ,

while the other parameters are determined by

$$e_{1}e_{2} = \frac{1}{2} \frac{R_{2} - Q_{1}}{Q_{2}} \pm \frac{1}{2} \left[ \left[ \frac{R_{2} - Q_{1}}{Q_{2}} \right]^{2} - 4 \frac{R_{1}}{Q_{2}} \right]^{1/2},$$
(3.4a)

$$\gamma = -P_c / (e_2 Q_2 - R_2)$$
, (3.4b)

$$\varphi = \gamma (Q_1 + R_2) / P_c - 1$$
, (3.4c)

 $\omega$ 

where

$$P_c = P_L(x_c, y_c) ,$$
  

$$Q_1 = -(\partial Q_M / \partial x)(x_c, y_c) ,$$
  

$$Q_2 = -(\partial Q_M / \partial y)(x_c, y_c) ,$$
  

$$R_1 = -(\partial R_N / \partial x)(x_c, y_c) ,$$

and

$$R_2 = -(\partial R_N / \partial y)(x_c, y_c)$$

(Refs. 10 and 14).

## **B.** Results

The analysis we report is for bond and site data for  $C_{n,m}$  on the square lattices and the simple cubic lattices and bond data on the triangular lattices. The source of our data includes Refs. 1–3 and previously unpublished data that we have generated (Tables III–VI). Generally, the results for site data on all lattices were worse for both the penetrable and impenetrable models. From (2.5), we have that

$$G(x,y) \sim (x_c - x)^{-\gamma} Z\left[\frac{(y - y_c) - e^{\omega_0}(x_c - x)}{(x_c - x)^{\varphi}}\right].$$
 (3.5)

Comparing with the generalized form (3.1), the two scaling axes for SAW's are

$$e_1 = e^{\omega_0}, \quad e_2 = \infty \quad . \tag{3.6}$$

A PDA depends on three labeling sets which define the polynomials P, Q, and R and a matching set which is a subset of the labeling set of F(x, y) specifying the powers of x and y of F(x,y) that are to be matched. We constructed the approximants in two ways: (1) We let the three labeling sets have full triangular forms with M = N = L. The matching set of F(x, y) is then selected to be as symmetrical as possible with the main diagonal of the labeling set of F(x, y). (2) We choose a full triangular subset as the matching set and if the number of entries is J, we let M = N and choose L such that M + N + L = J + 1. The entries for the polynomials were then chosen to be as close to the triangular form as possible. In all of our approximants,  $|e_2| \gg 1$ , while  $e_1$  varies in a rather large interval and depends on the estimate of  $(x_c, y_c).$ 

The estimates of  $y_c$ ,  $y_c/x_c$ ,  $\gamma$ , and  $\varphi$  are tabulated in Table I. Figures 1–3 are representative plots of  $y_c$  versus  $x_c$ ,  $\gamma$  versus  $\varphi$ , and  $\gamma$  versus  $y_c$  for a number of lattices for bond (or site) data as examples from which the estimates in Table I were obtained. The estimate for  $y_c$  as a function of  $x_c$  for all lattices lie on a curve resembling the critical phase diagram (Fig. 1). They do not converge to any particular value, as in a one-variable analysis. For values of y less than some critical  $y_c$ , the approximants concentrate around the bulk value for  $x_c$ . The point at which x begins to decrease is taken as the critical point  $(x_c, y_c)$ . The linear

TABLE I. The estimates of the critical parameters obtained using partial-differential approximants (PDA) for the square (SQ), triangular (T), and simple cubic (sc) lattices for (a) impenetrable and (b) penetrable surfaces.

Lattice	S	Q	Т	sc	
	Bond	Site	Bond	Bond	Site
Variable					
		(a) Impenetra	ble surface		
$x_c$	0.379 05ª	0.379 05ª	0.240 92 <sup>a</sup>	0.2135 <sup>a</sup>	
$y_c$	$0.780 {\pm} 0.050$	$0.690 \pm 0.010$	$0.688 {\pm} 0.015$	$0.314 {\pm} 0.040$	
$y_c/x_c$	$2.060 \pm 0.10$	$1.820 \pm 0.030$	$2.850 {\pm} 0.070$	$1.470 \pm 0.020$	
γ	$1.450 {\pm} 0.050$	$1.400 \pm 0.050$	$1.400 \pm 0.100$	$1.550 {\pm} 0.150$	
$\varphi(x_c)$	$0.500 {+0.050 \atop -0.030}$	0.520±0.020	$0.500 {+0.050 \atop -0.070}$		
$\varphi(y_c)$	$0.500 {+0.100 \atop -0.080}$		0.450±0.050		
$\varphi(\gamma)$	$0.500 {\pm} 0.090$	$0.520{\pm}0.030$	0.500±0.010	$0.540 {\pm} 0.070$	
		(b) Penetral	ole surface		
$\boldsymbol{x}_{c}$	0.379 05 <sup>a</sup>	0.379 05 <sup>a</sup>	0.240 92 <sup>a</sup>	0.2135 <sup>a</sup>	0.2135 <sup>a</sup>
y <sub>c</sub>	$0.380 {\pm} 0.010$	$0.400 {\pm} 0.020$	$0.250 \pm 0.010$	$0.200 {\pm} 0.020$	0.225±0.150
$y_c/x_c$	$1.000 \pm 0.020$	$1.050 {\pm} 0.050$	$1.030 {\pm} 0.050$	$0.940 {\pm} 0.080$	$1.050 {\pm} 0.050$
γ	$1.350 \substack{+0.050 \\ -0.100}$	$1.350^{+0.080}_{-0.100}$	1.340±0.040	$1.200 {+0.110 \atop -0.030}$	1.210±0.030
$\varphi(x_c)$	$0.260 {\pm} 0.060$		$0.400 \pm 0.200$	$0.400 {\pm} 0.010$	0.580±0.090
$\varphi(y_c)$	$0.250 {\pm} 0.030$	$0.260 {\pm} 0.060$		$0.420 {\pm} 0.020$	
$\underline{\varphi(\gamma)}$	0.270±0.040	0.350±0.100	0.350±0.150	0.450±0.090	0.045±0.100

<sup>a</sup>Reference 15.



FIG. 1. Plots of  $y_c$  against  $x_c$  for (a) square-lattice (site) impenetrable surface, (b) square-lattice (bond) penetrable surface, and (c) simple cubic lattice (bond) impenetrable surface.

FIG. 2. The exponent  $\gamma$  is plotted against the crossover exponent  $\varphi$  for (a) square-lattice (bond) impenetrable surface, (b) simple cubic (bond) penetrable surface, and (c) triangular lattice (bond) impenetrable surface.

correlation seen in the graphs of  $\varphi$  versus  $\gamma$  (Fig. 3) is that would be expected if G(x,y) is a general homogeneous function in the vicinity of  $(x_c, y_c)$  (Sec. II). The values of  $\varphi$ in Table I are read from a plot of the estimates of  $\varphi$  against the estimates of  $\gamma$  by assuming  $\gamma(D=2)=\frac{93}{64}$  (Ref. 6) and  $\gamma(D=3)=1.44$  (Ref. 8) for an impenetrable surface and  $\gamma(D=2)=\frac{43}{32}$  (Ref. 15) and  $\gamma(D=3)=1.162$  (Ref. 15) for a penetrable surface. Correlations of  $\varphi$  with  $x_c$  and  $y_c$  are consistent with these values.

For the impenetrable surface, our result of  $\varphi = 0.51 \pm 0.04$  in two dimensions is consistent with a value of  $\varphi = 0.5$ , obtained previously from transfer-matrix,<sup>6</sup> conformal invariance theory,<sup>7</sup> and one-variable exact enumeration work<sup>3</sup> on the square lattice. The value of  $\gamma$  (Fig. 2) is consistent with the result  $\frac{93}{64}$  given by Guim and Burkhardt.<sup>6</sup> The estimate of  $2.05\pm0.01$  for the ratio  $y_c/x_c$  agrees with Ishinabe's result for the square-lattice bond problem<sup>3</sup> and the estimate  $1.80\pm0.02$  agrees with



FIG. 3. The exponent  $\gamma$  is plotted as a function of  $y_c$  for (a) square-lattice (bond) impenetrable surface and (b) triangular lattice (bond) penetrable surface.

the estimate of Hammersley *et al.* for the site data.<sup>1</sup> In three dimensions,  $\varphi = 0.54 \pm 0.07$  for the simple cubic lattice is in accord with Monte Carlo results of  $\varphi = 0.59$  (Ref. 8) and our estimate of  $1.46 \pm 0.01$  for  $y_c/x_c$  agrees with 1.45 from Monte Carlo work (Ref. 11) and the estimate 1.50 by considering the zeros of the partition function.<sup>2</sup>

For the penetrable surface, our estimate of  $\varphi = 0.28 \pm 0.05$  in two dimensions is not consistent with Ishinabe's result ( $\varphi = 0.5$ ),<sup>4</sup> but is in accord with the scaling prediction ( $\varphi = 0.25$ ). Our value  $\varphi = 0.40 \pm 0.01$  for the simple cubic is consistent with the scaling prediction ( $\varphi = 0.41$ ), but does not agree with Ishinabe's result ( $\phi = 0.6$ ).<sup>4</sup>

For the simple cubic lattice, most of the approximants are either poorly conditioned or give good estimates for  $(x_c, y_c)$ ; however, because the argument under the square-root sign in (3.4) is negative, it is difficult to calculate all critical parameters.

Partial-differential approximants are useful in representing critical properties such as the critical line in a plane and the linear correlation of  $\gamma$  and  $\varphi$  near the special point. However, since an approximant depends on both the degree and form of the defining polynomials, convergence such as that obtained in a one-variable analysis is not easy to detect and accurate estimates are difficult.

#### C. One-variable analysis for penetrable surface

The problem of estimating  $\varphi$  may be reduced to a onevariable analysis if  $\gamma$  and the ratio  $y_c/x_c$  are known with sufficient accuracy, by differentiating the scaling function (3.1) with respect to y and setting the ratio y/x to its value at the critical point.<sup>16</sup> The resulting function has a power-law dependence on  $x_c - x$  which may be analyzed using standard one-variable analysis techniques:

$$\frac{\partial f(x,y)}{\partial y}\Big|_{y/x=y_c/x_c} \sim (x_c - x)^{-(\gamma + \varphi)} Z(0) .$$
 (3.7)

In the present case,  $y_c/x_c$  is belived to be 1 for the penetrable surface problem<sup>1</sup> and, consequently,  $\gamma$  has its bulk value, which is known to a high accuracy. We have applied a number of standard one-variable analysis techniques<sup>17</sup> to the resulting series to this case. The results are summarized in columns (a) to (d) of Table II. (We have included results for a number of lattices where the series are too short to allow a reasonable test of the PDA method or the PDA approximants are too scattered to give meaningful estimates. The data for these lattices are given in Ref. 4, Tables 7 and 8. In the case of the impenetrable surface, the ratio  $y_c/x_c$  is not known with sufficient accuracy to give us any confidence in this method.)

The results for  $\varphi$  in columns (a) to (d) of Table II show reasonable consistency amongst themselves for a given lattice dimensionality but are too high to be consistent with the predictions  $\varphi(D=2)=0.25$  and  $\varphi(D=3)$ 

TABLE II. The estimates of  $\varphi$  for the body-centered-cubic (bcc), face-centered-cubic (fcc), simple cubic (sc), diamond (Di), triangular (T), and square (SQ) lattices from the one-variable analysis of the series f'(x) described in Sec. III B by the method of (a) Neville tables, (b) d log Padé approximants, (c) biased d log Padé approximants, (d) Baker-Hunter confluent singularity analysis. Estimates of  $\varphi$ obtained by applying the Baker-Hunter method to the modified seires  $(x_c - x)^{\gamma} f'(x)$  are reported in column (e).

Method Lattice	а	b	С	d	е
		(a) Bor	nd		
bcc	$0.420 \pm 0.020$	0.450±0.01	$0.450 {+0.010 \atop -0.020}$	$0.480 {+0.030 \\-0.050}$	$0.380 {+0.030 \\ -0.040}$
fcc	$0.430 \pm 0.008$	0.463±0.005	0.450±0.020	0.480±0.060	$0.386 \substack{+0.002 \\ -0.014}$
sc	$0.413 \begin{array}{c} +0.030 \\ -0.015 \end{array}$	$0.444 {\pm} 0.003$	$0.440 {+0.020 \\ -0.030}$	$0.510 {+0.050 \atop -0.080}$	$0.350 \substack{+0.080 \\ -0.060}$
Т	0.3062±0.0035	0.3262±0.003	0.320 + 0.002 - 0.003	$0.323 {+0.002 \\ -0.003}$	$0.270 {+0.003 \\ -0.002}$
SQ	$0.307 \pm 0.004$	0.317±0.001	0.319±0.001	0.323 + 0.008 - 0.009	0.290±0.010
		(b)	Site		
Di	0.473 ±0.015	0.530±0.010	$0.500 {+0.030 \atop -0.010}$	0.510±0.060	$0.420 {+0.020 \\ -0.054}$
sc	$0.470 \pm 0.020$	$0.530 {\pm} 0.010$	$0.480{\pm}0.020$	$0.500 {\pm} 0.080$	$0.400 {\pm} 0.050$
SQ	0.356 ±0.005	0.370±0.010	0.375±0.010	0.263±0.013	0.270±0.040

=0.408±0.002, which result from the scaling relation  $\varphi = 1 - v$ .

The only exception to this is the analysis of the square-lattice site series by the Baker-Hunter method,<sup>18</sup> which is consistent with the predicted value of  $\varphi = 1 - v$ . Inspection of the approximants to the Baker-Hunter auxiliary function for the square-lattice site series showed that a second pole on the real positive axis was also resolved. This indicates that a confluent singularity is present and the position of this secondary pole provides an estimate of the exponent of this confluence.<sup>17,18</sup> By plotting the position of the secondary pole against the position of the primary pole for the approximants considered and using the expected value of the leading exponent  $\gamma + \varphi = \frac{51}{32}$ , we estimate that the confluence has an exponent approximately equal to  $\gamma$ . The existence of a confluence with exponent  $\gamma$  is not surprising and will, in fact, always occur if the crossover function  $Z(\Delta \tilde{\gamma}/(\Delta \tilde{x})^{\varphi})$  contains a multiplicative factor or additive term that is analytic in y.

To test the assumption that it is the influence of this confluence that results in the discrepancy with the expected value of  $\varphi$ , we have formed the series

$$f'(\mathbf{x}) = (\mathbf{x}_c - \mathbf{x})^{\gamma} \frac{\partial f(\mathbf{x}, \mathbf{y})}{\partial \mathbf{y}} \bigg|_{\mathbf{y}_c / \mathbf{x}_c = 1}, \qquad (3.8)$$

which is expected to have the form

$$f'(x) \sim (x_c - x)^{\varphi} + B(x)$$
, (3.9)

where B(x) is a (background) term which is not singular at  $x = x_c$ . Estimates of  $\varphi$  obtained by a Baker-Hunter analysis of this series are shown in column (e) of Table II. For both the two- and three-dimensional cases the results are in reasonably good agreement with the predicted value. That the central estimates in two dimensions are still a little high is perhaps not surprising since the singularity of the series analyzed in this case is somewhat weak. The weak nature of the singularity also leads to difficulty in analyzing the modified series by other methods. For example, if the Neville table method is used to analyze the square and simple cubic lattice series, the columns of the table do not converge (for the number of terms presently available). This may be attributed to a singularity at  $x = -x_c$  which, now, is stronger than the singularity at  $x = x_c$ . Applying a Euler transform, which moves the singularity on the negative axis to a position further from the origin, results in reasonably converged Neville tables with results consistent with those given in column (e) of Table II.

#### **IV. SUMMARY AND CONCLUSION**

In this paper our aim has been to analyze existing series<sup>1-3</sup> and new series (Tables III–VIII) to estimate the crossover exponent  $\varphi$  for a self-avoiding walk interacting with a penetrable and an impenetrable surface. We have used the method of partial-differential approximants to analyze the two-variable surface series. For the impenetrable problem, we estimate that  $\varphi=0.51\pm0.04$  (D=2) and  $\varphi=0.54\pm0.07$  (D=3), in agreement with other analyses. For the penetrable problem, unlike the analysis of Ishinabe,<sup>4</sup> our results [ $\varphi=0.28\pm0.05$  (D=2) and  $\varphi=0.40\pm0.01$ ] are consistent with the scaling prediction. For the penetrable surface in two dimensions, a one-

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TABLE III. Values of  $a_{n,m}$  (bond) on the square lattice for a penetrable surface.

m	0	1		2	3		4		5
<u>n</u>	2		,						
2	6	2	L	2					
3	18	12		4		2			
4	46	36	5	12		4	2		
5	122	104	ļ	40		12	4		2
6	330	272		116		44	12		4
7	882	768	3	328		128	48		12
8	2 342	2 068	3	932		364	140		52
9	6 2 4 6	5 656	Ĵ	2 648		1 088	404		152
10	16 602	15 168	\$	7 3 1 6		3 100	1 2 2 8		444
11	44 1 54	41 200	, )	20 336		8 880	3 596		1 384
12	117 154	110 304	ļ	55 824	2.	4 904	10 304		4 096
13	311 222	297 376	5	153 744	- 7	0.288	29 736		11 920
14	825.078	794 848	2 2	418 792	19	5072	84 368		34 636
15	2 189 434	2 134 516	ń	1 144 504	55	4076	239 372		100 160
16	5 800 702	5 695 960	ý	3 102 688	149	8712	671 140		285 636
17	15 380 494	15 252 188	2 2	8 432 552	4 14	4 040	1 885 316		814 488
18	40 728 794	40 648 592	, ,	22 773 776	11 34	8 3 2 0	5 241 608		2 299 768
10	107 924 642	108 614 813	,	61 637 628	31 17	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	14 600 576		6492 300
20	285 677 910	289 162 460	- 1	165 981 712	84.96	9 980	40 330 468		18 172 296
20	756 622 494	771 398 731	, ,	447 773 612	232.20	0.056	111 598 544		50 897 812
m	6	7		8	9	10	1	1	12
<i>n</i>									
6	2								
7	4	2		_					
8	12	4		2					
9	56	12		4	2	_			
10	164	60		12	4	2			
11	484	176		64	12	4		2	_
12	1 548	524		188	68	12		4	2
13	4 640	1 720		564	200	72		12	4
14	13 624	5216		1 900	604	212		76	12
15	40 192	15 464		5 824	2 088	644		224	80
16	117 092	46 208		17 424	6464	2 284		684	236
17	338 484	136 152		52 756	19 504	7 136	2	488	724
18	971 000	396 620		157 044	59 832	21 704	7	840	2 700
19	2 778 152	1 150 476		461 736	179 912	67 452	24	024	8 576
20	7 883 704	3 313 656	1	350 772	533 560	204 812	75	632	23 664
21	22 337 896	9 501 848	3	927 176	1 575 292	612 500	231	824	84 388
m n	13	14	15	16	17	18	19	20	21
13	2								
14	- 4	2							
15	12	- 4	2						
16	84	12	4	2					
17	248	88	12	- 4	2				
18	764	260	92	12	4	2			
19	2 920	804	272	96	12	4	2		
20	9 344	3 1 4 8	844	284	100	12	4	2	
21	29 024	10 144	3 384	884	296	104	12	4	2

(bond) on the simple cubic lattice for a penetrable surface.	

m	0	1	2	3	4			5	6
n	_	-	_	-				-	
1	2	4							
2	10	8	12						
3	50	40	24	36					
4	218	216	120	72		100			
5	962	1 008	720	360		200		284	
6	4 370	4 464	3 4 3 2	2 312		1 000		568	780
7	19 858	20736	15 776	11 408		7 040		2 840	1 560
8	90 968	95 288	74 424	53 032	3	5 1 7 6		21 288	7 800
9	414 394	441 888	351 088	257 584	16	7 272		108 672	63 168
10	1 900 130	2 034 848	1 647 016	1 233 832	82	7 208		520 168	325 000
11	8 716 706	9 430 480	7 719 520	5 904 128	406	5 336		2 636 048	1 578 216
12	40 085 154	43 542 544	36 113 618	27 976 960	19 69	6 800		3 146 528	8 127 992
13	184 421 418	201 863 216	168 975 024	132 908 352	95 06	9 344	6	4 839 408	41 409 568
14	849 948 160	933 698 304	789 458 080	627 622 944	456 50	2 592	31	6 327 064	206 471 376
m	7	8	9	10	11	12	13	14 15	16
7	2 172								
8	4 344	5 916							
9	21720	11 832	16268						
10	185 880	59 160	32 536	44 100					
11	971 248	541 296	162 680	88 200	120 292				
12	4 736 888	2 844 936	1 565 256	441 000	240 584	32	4932		
13	24 914 240	14 018 008	8 323 024	4 498 624	1 202 920	64	9 864	881 500	)
14	128 616 528	74 856 984	41 141 464	24 030 840	12 850 632	3 24	9 320	1 763 000	237 444

**TABLE V.** Values of  $a_{n,m}$  (bond) on the triangular lattice for penetrable surface.

m	0		1	2		3		4		5
n										
1	4		2							
2	20	)	8	2						
3	88	3	40	8		2				
4	376		188	44		8		2		
5	1616	5	840	216		48		8		2
6	6 896	5	3 724	1 0 2 0		244		52		8
7	29 264	ŀ	16356	4 7 3 6		1 188		272		56
8	123 884	ŀ	71 184	21 624		5 700		1 368		300
9	523 116	5	308 108	97 428		26 784		6 740		1 5 5 6
10	2 204 724	ŀ	1 327 200	434 816		123 964		32 408		7 868
11	9 278 108	3	5 694 880	1 925 424		567 128	1	53 232		36 668
12	38 995 816	5	24 358 312	8 471 768		2 568 944	7	15 296		186 484
13	163 726 848	3 1	03 909 128	37 075 332		11 543 752	33	01 632		886 276
14	686 803 808	3 4	42 262 148	161 518 020		51 521 408	150	99 600	4	159 572
15	2 878 788 104	18	78 736 624	700 915 740		228 612 464	68 5	16 376	19	322 788
m	6	7	8	9	10	11	12	13	14	15
n										
6	2									
7	8	2								
8	60	8	2							
9	328	64	8	2						
10	1 752	356	68	8	2					
11	9076	1 956	384	72	8	2				
12	45 556	10 364	2 168	412	76	8	2			
13	223 992	53 076	11732	2 388	440	80	8	2		
14	1 083 224	265 868	61 244	13 180	2616	468	84	8	2	
15	5 165 288	1 307 664	312 304	70 076	14 708	2 852	496	88	8	2

TABLE VI. Values of  $a_{n,m}$  (bond) on the triangular lattice for an impenetrable surface.

 m	0	1	·····	2	3	4		5		6
n	-	-		-	-			-		Ū
1	2	2	!							
2	10	4	Ļ	2						
3	40	20	)	4	2					
4	158	86	5	22	4		2			
5	642	350	)	96	24		4	2		
6	2 642	1 442	2	406	106		26	4		2
7	10 7 50	5 942	2	1 722	454		116	28		4
8	44 184	24 442	2	7 2 5 0	1 970		506	126		30
9	181 884	100 730	)	30 298	8 4 5 6		2 228	560		136
10	749 612	415 442	2	126 294	36 000		9 682	2 506		616
11	3 092 220	1 714 674	Ļ	525 436	152 516	4	1 732	11016		2 800
12	12 764 548	7 081 192	2	2 183 698	643 106	17	9 090	47 966		12 456
13	52 721 134	29 257 292	2	9 069 060	2 702 964	76	4 398	207 784		54 816
14	217 853 078	120 929 818	3	37 646 550	11 333 082	3 24	8 786	895 036		239 638
15	900 553 022	500 009 024	↓ 1	56 221 490	47 430 536	1375	8 970	3 838 360	1	040 542
16	3 723 882 338	2 067 981 806	6 6	48 115 682	198 220 204	58 10	2 162	16 396 674	4	495 834
m	7	8	9	10	11	12	13	14	15	16
n										
7	2									
8	4	2								
9	32	4	2							
10	146	34	4	2						
11	674	156	36	4	2					
12	3 1 1 0	734	166	38	4	2				
13	13 998	3 4 3 6	796	176	40	4	2			
14	62 268	15 644	3 778	860	186	42	4	2		
15	274 798	70 336	17 396	4 1 3 6	926	196	44	4	2	
16	1 203 070	313 338	79 042	19 256	4 5 1 0	994	206	46	4	2

TABLE VII. Values of  $a_{n,m}$  (bond) on the face-centered-cubic lattice for a penetrable surface.

m	0	1	2		3	4
n						
1	6	6				
2	66	36		30		
3	642	444		180	138	
4	6210	4 596		2 448	828	618
5	60 630	46 440	,	26 628	12 396	3 708
6	594 258	469 356	28	30 944	140 160	60 672
7	5 837 394	4 729 716	2 94	45 208	1 538 472	707 028
8	57 445 806	47 544 072	30 5	89 860	16 703 880	8 0 3 5 1 6 4
9	566 192 622	477 174 444	315 52	28 384	178 742 100	90 033 648
10	5 587 703 910	4 783 889 904	3 2 3 8 54	48 864	1 892 410 260	990 158 280
m	5	6	7	8	9	10
n						
5	273ª					
6	16 380	11 946				
7	290 772	71 676	51 882			
8	3 471 408	1 371 432	311 292	224 130		
9	40 701 408	16 704 696	6 387 708	1 344 780	964 134	
10	469 131 072	201 576 984	79 134 888	29 457 432	5 784 804	4 133 166

<sup>a</sup>Reference 18.

TABLE VIII. Values of a	(bond) on the bod	v-centered-cubic	lattice for a	penetrable surface.
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m	0	1	2	,	3	4
n						
1	4	4				
2	28	16		12		
3	180	128		48	36	
4	1 1 1 6	864		424	144	100
5	7 140	5 640		3 104	1 392	400
6	45 364	37 128		20 888	10 536	4 2 2 4
7	290 172	344 192	1	44 688	73 920	33 600
8	1 855 044	1 592 232	9	76 144	528 152	241 896
9	11 900 692	10 421 256	65	82 984	3 686 856	1 802 528
10	76 335 892	67 858 016	43 9	58 216	25 413 144	12 881 664
11	490 799 116	442 855 432	293 4	98 688	174 319 416	91 500 784
12	3 155 724 092	2 881 375 568	1 946 4	91 368	1 184 629 312	640 267 888
m	5	6	7	8	9	10
n						
5	284					
6	1 1 3 6	780				
7	12 960	3 1 2 0	2172			
8	105 344	38 304	8 688	5916		
9	782 584	321 928	113 920	23 664	16 268	
10	5 987 728	2 444 528	971 952	330 784	65 072	44 100
11	44 009 232	19 336 040	7 579 040	2 890 992	964 128	176 400
12	318 821 400	144 943 376	61 322 120	23 000 128	8 523 504	2 765 136
m	11	12				
n						
11	120 292					
12	481 168	324 932				

variable analysis that takes into account confluent terms also gives consistent results. The presence of these confluent terms may be the source of the discrepancy in the results of Ishinabe.<sup>4</sup>

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