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LETTER TO THE EDITOR

A six-vertex model as a diffusion problem: derivation of correlation functions

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Abstract. A cellular automaton which describes diffusion of particles with exclusion in one dimension is shown to be equivalent to a six-vertex model on a critical line. The arrow-arrow correlation function of the six-vertex model is calculated exactly on this line using a transfer matrix method.

A family of problems dealing with shrinking domains of Ising spins at T = 0 has been studied recently [1]. For a particularly simple geometry, that of a single corner of a domain of up spins in a sea of down, some interesting equivalences were established. Firstly this problem was shown to map onto that of many particles, with hard core repulsion, diffusing on a one-dimensional chain. This soluble problem [2] was then reformulated in a manner that utilises parallel dynamics, thereby turning it into a one-dimensional stochastic cellular automaton. Such an automaton, however, is equivalent to an equilibrium problem in d = 1 + 1 dimensions [3, 4]. It was shown that the resulting 2D equilibrium problem is that of the six-vertex model on one of its critical manifolds [5]. For completeness' sake we reproduce these mappings in full detail below, and then proceed to use them in order to calculate the arrow-arrow correlation function of this critical six-vertex model.

The symmetric six-vertex model may be considered the prototype of soluble vertex models. Many of the techniques for exact solutions have been developed or are demonstrated first on the six-vertex model [5-7]. Nevertheless, not very much is known exactly about its correlation functions, except in the free fermion limit [8]. Even when the eigenvectors and eigenvalues of the transfer matrix are known, the necessary analysis to extract even a two-point correlation function is a difficult task which has not been successfully completed. Of course in the regimes where the model is scale invariant, the large distance behaviour of the two-point functions is calculable with the aid of the renormalisation group, and of the more-point correlation functions with the use of conformal invariance. These results, however, do not contain information about the short distance behaviour, and are applicable only in the scaling regimes. In the present letter we show that the arrow-arrow correlation function can be calculated without difficulty in a subspace of the general symmetric six vertex model, in which the model is not conformally invariant. Note that some correlation functions were calculated previously on disorder subspaces for the two- and three-dimensional Ising models [3, 9].

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Consider a problem of many particles that execute random walks on a linear chain of N^{\max} sites. A hard-core interaction prevents occupation of any site r by more than one particle. The model we consider has parallel dynamics, with rules defined as follows. First, pair all neighbouring sites; this can be done in two ways, with either the odd or even indexed sites at the left side of every pair. These two ways of partitioning a linear chain are denoted, respectively, by A and B in figure 1(a), where presence of a particle is represented by a black dot, and empty sites are denoted by open circles. We choose pairing of type A at odd time steps (2t+1) and B at even ones (2t). The dynamic process allows, at every time step, motion of a particle within the pair to which it belongs at time t. If both sites of a pair are occupied, or both are empty, the state of the pair does not change. If one site is occupied and the other empty, the particle moves to the empty site with probability p, or stays where it was with probability 1-p. These (stochastic) rules are applied, in parallel, to all paired neighbouring sites.



Figure 1. (a) Two different partitions, A and B of a linear chain, occupied by particles (black sites) and holes (white sites), into paired neighbouring sites. (b) Representation of particles (holes) by up (down) pointing arrows. Every horizontal cut presents a snapshot of the particles at a given time step. The arrows are placed on line segments; segments associated with paired neighbouring sites meet at a vertex *above* the current time step. (c) At each vertex an exchange of particles and holes may take place, giving rise to a new configuration. The probabilities of all possible processes are identified as the standard weights of the corresponding six-vertex model.

The resulting probabilistic cellular automaton is equivalent to an equilibrium problem in d = 2 dimensions, which turns out to be a particular case of the six-vertex model. To show this, we *first* review the geometric aspects of this mapping. The coordinates (r, t) of site r at time t are placed at the centres of the edges of a square lattice, as indicated in figure 1(b). The r-axis is along one of the diagonals of this square lattice, and the t-axis (with time running upwards) along the other diagonal. The edges that go through two neighbouring points (r, t) and $(r \pm 1, t)$, meet above them if they belong to the same pair at time t. Hence at the vertices, where edges meet, exchange of a particle and a hole that belong to the same pair can take place. As we move up in time, the edge associated with a given site r will meet, alternatively, either the edge associated with site r-1 or r+1. This reflects the alternating pairing of site r at odd/even time steps.

Next, we demonstrate a mapping between particle and arrow configurations. To specify any spacetime history of the diffusing particles, an occupation number must be assigned to every point, n(r, t) = 1 (occupied) or n(r, t) = 0 (empty). There is a one-to-one correspondence between all possible n(r, t) assignments, consistent with our dynamic rule, and the arrow configurations of the six-vertex model. To realise this correspondence place on each site (r, t), with n(r, t) = 1, an arrow that points up (along its edge), and for n(r, t) = 0 an arrow that points down. Conservation of particles, built into our dynamic rule, translates to having an equal number of up arrows leaving a vertex from above as incident on it from below. This, however, ensures that only those arrow configurations that are allowed by the six-vertex model will occur.

The *final* step necessary to establish the mapping is to show that any spacetime history of particle configurations, i.e. occupation numbers n(r, t), will have the same statistical weight as that of the corresponding six-vertex model. It is easy to see that this is indeed the case if the following values are chosen for the (standard) vertex weights (see figure 1(c):

$$a=1 \qquad b=p \qquad c=1-p. \tag{1}$$

These weights correspond to a six-vertex model on one of its critical lines, a = b + c. This line is a limiting case (d = 0) of the disorder [4] variety a + d = b + c of the eight-vertex model [5].

The dynamic process described above is realised by a transition probability matrix (that plays the role of the transfer matrix, in a diagonal direction, for the six-vertex model). This matrix acts on occupation microstates denoted by $|A\rangle$. A basis of such states is formed by the direct products of single-site occupation states, characterised by occupation numbers $\{n_r^A\}$:

$$|A\rangle\rangle = \prod_{r} |n_{r}^{A}\rangle.$$
⁽²⁾

The transfer matrix can be written as

$$T = T^{\text{even}} T^{\text{odd}}.$$
(3)

The matrices operating at odd and even times are given by

$$T^{\text{odd}} = \prod_{j} \sum_{n',n} T(n'_{2j-1}, n'_{2j}; n_{2j-1}, n_{2j}) |n'_{2j-1}\rangle |n'_{2j}\rangle \langle n_{2j-1}|\langle n_{2j}|$$

$$T^{\text{even}} = \prod_{j} \sum_{n',n} T(n'_{2j}, n'_{2j+1}; n_{2j}, n_{2j+1}) |n'_{2j}\rangle |n'_{2j+1}\rangle \langle n_{2j}|\{n_{2j+1}|$$
(4a)

with

$$T(1, 1; 1, 1) = T(0, 0; 0, 0) = 1$$

$$T(1, 0; 0, 1) = T(0, 1; 1, 0) = p$$

$$T(1, 0; 1, 0) = T(0, 1; 0, 1) = 1 - p.$$
(4b)

It should be noted that whereas both T^{odd} and T^{even} are symmetric, T is not symmetric.

We now turn to calculate a spacetime correlation function for the diffusion model, which is trivially mapped into its six-vertex counterpart. We wish to calculate the quantity

$$G(r,t) = \langle n(r,t)n(0,0) \rangle.$$
(5)

For the six-vertex model the brackets mean average over an equilibrium ensemble. In the corresponding dynamic problem two averages are implied. First, average over realisations of all possible time developments, each with its proper statistical weight, starting from a given initial (t = 0) state. Second, average over an ensemble of initial states that is stationary with respect to the dynamic process. The equilibrium counterpart of this second averaging merits a brief explanation. In the equilibrium calculation one normally chooses in (5) two sites (0, 0) and (r, t) that are far from all boundaries. Hence a standard calculation of G(r, t) has the form

$$G(r, t) = \langle\!\langle 0 | \hat{O}(r, t) \hat{O}(0, 0) | 0 \rangle\!\rangle$$

where O is an operator, and $|0\rangle$ is that eigenvector of the transfer matrix which belongs to its largest eigenvalue. In the dynamic view of the problem, $|0\rangle$ represents the ensemble of initial states to be averaged over. Since the transfer matrix of the dynamic problem is one of transition probabilities its largest eigenvalue is 1, and therefore the ensemble represented by $|0\rangle$ is stationary, in that

$$T|0\rangle = |0\rangle. \tag{6}$$

The stationary state of a system of N particles is

$$|0\rangle = \frac{1}{\sqrt{N}} \sum_{\{n_r\}} \delta_{\Sigma n_r, N} \prod_r |n_r\rangle$$
(7)

where $\mathcal{N} = \binom{N_{N}^{\text{max}}}{N}$ is a normalisation constant. To see that (6) holds, operate on (7) with T^{odd} and next with T^{even} , as defined by (4). Note that since T does not change the total number of particles, it 'moves through' the δ -function in (7). In this way one can verify that $|0\rangle$ is also an eigenstate of each of the operators T^{odd} and T^{even} separately.

Similarly, it is easy to show that the corresponding left eigenvector of T, which has the largest eigenvalue is given by

$$\langle\!\langle 0| = \frac{1}{\sqrt{N}} \sum_{\{n_r\}} \delta_{\Sigma n_r, N} \prod_r \langle n_r|$$
(8)

with normalisation $\langle\!\langle 0|0\rangle\!\rangle = 1$. The correlation function we wish to calculate is given (after an even number of time steps t) by

$$G(r, t) = \langle\!\langle 0 | \hat{n}(r) T^{t/2} \hat{n}(0) | 0 \rangle\!\rangle.$$
(9)

Here $\hat{n}(r)$ is a number operator whose action on a microstate $|A\rangle$ is defined as

$$\hat{n}(r)|A\rangle = n^{A}(r)|A\rangle$$
(10)

i.e. it projects from any state the part in which site r is occupied. By definition of $|0\rangle$ and $\langle 0|$,

$$G(r,t) = \frac{1}{\mathcal{N}} \sum_{B,A} \left\langle \langle B | \hat{n}(r) T^{\prime/2} \hat{n}(0) | A \right\rangle$$
(11)

where the sum is over all microstates with N particles. This has the desired dynamic interpretation: from the stationary ensemble of initial states $\Sigma |A\rangle$ we project out those for which n(0) = 1, i.e. a particle is present at r = 0. These initial states are propagated an even number of t time steps, after which those microstates, which contain a particle at r, are projected out. This process is then summed over all possible final states $\langle B|$ of the system. To evaluate G(r, t), we introduce the following states:

$$|r\rangle = \hat{n}(r)|0\rangle = \frac{1}{\sqrt{N}} \sum_{\{n_r\}} \delta_{n_r,1} \delta_{\Sigma_{n_r},N} \prod_{r'} |n_{r'}\rangle$$
(12)

in terms of which (9) becomes

$$G(r, t) = \langle\!\langle 0 | \hat{n}(r) T^{t/2} | 0 \rangle\!\rangle.$$
(13)

Note that here $|0\rangle = |r = 0\rangle = \hat{n}(0)|0\rangle$.

We follow standard strategy, assuming that $|0\rangle$ can be expanded in the form

$$|0\rangle) = \sum_{\kappa} b_{0\kappa} |\kappa\rangle \tag{14}$$

where $|\kappa\rangle$ are (right) eigenfunctions of T, e.g.

$$T|\kappa) = \lambda(\kappa)|\kappa). \tag{15}$$

Then G(r, t) is given by

$$G(\mathbf{r},t) = \sum_{\kappa} C(\mathbf{r},\kappa) b_{0\kappa} [\lambda(\kappa)]^{1/2}$$
(16)

where $C(r, \kappa)$ is a matrix element,

$$C(\mathbf{r},\kappa) = \langle\!\langle 0|\hat{\mathbf{n}}(\mathbf{r})|\kappa\rangle. \tag{17}$$

We first calculate the eigenvalues $\lambda(\kappa)$ and the right eigenvectors $|\kappa\rangle$.

Acting with T, as defined by (3) and (4), on $|r\rangle$ given by (12), it is straightforward to get

$$T|r)) = (1-p)^{2}|r)) + p(1-p)[|r+1)) + |r-1)] + p^{2}|r-2(-1)^{\Delta(r)})$$
(18)

where we introduced a parity parameter

$$\Delta(r) = \begin{cases} 1 & \text{for } r \text{ odd} \\ 2 & \text{for } r \text{ even.} \end{cases}$$
(19)

The last term in (18) reflects the fact that due to our positioning of the chain, a particle on an odd site can move in two time steps two units to the right, but only one to the left. For an even site the situation is reversed. We can now combine states $|r\rangle$) to generate eigenstates of T, of the form[†]

$$|\kappa) = \sum_{r=1}^{N^{\max/2}} e^{i\kappa r} [u|2r-1) + v|2r)].$$
(20)

We find that (20) is indeed an eigenfunction (15) of T, provided u, v and λ satisfy the equation

$$\begin{bmatrix} (1-p)^2 + p^2 e^{-i\kappa}, & p(1-p)(1+e^{-i\kappa}) \\ p(1-p)(1+e^{i\kappa}), & (1-p)^2 + p^2 e^{i\kappa} \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \lambda \begin{bmatrix} u \\ v \end{bmatrix}.$$
 (21)

The eigenvalues $\lambda(\kappa)$ are given by the solutions of

$$\lambda^{2} - 2\lambda [(1-p)^{2} + p^{2} \cos \kappa] + (1-2p)^{2} = 0.$$
⁽²²⁾

As $\kappa \to 0$, for p < 1 the high branch can be written as

$$\lambda(\kappa) \simeq \exp\left[-\frac{p}{4(1-p)}\kappa^2\right] + O(\kappa^4).$$
(23)

This result already suffices to show that asymptotically $(t \gg 1)$ one has

$$G(0, t) \sim t^{-1/2} \tag{24}$$

a result that reflects the diffusive nature of the correlation function, and has the algebraic decay (albeit very anisotropic—see below) of a critical correlation function.

† With periodic boundary conditions $\kappa = 0, \pm l2\pi/N^{\max}, l \le N^{\max}/2$.

In what follows we concentrate on evaluating G(r, t) for the particular case $p = \frac{1}{2}$. For this value the algebra simplifies considerably, and we have reasons to believe that for $p \neq \frac{1}{2}$ qualitatively similar results are obtained (as long as special points such as p = 0, 1 are avoided).

For $p = \frac{1}{2}$ the two solutions of (22) are $\lambda(\kappa) = 0$ and

$$\lambda(\kappa) = \frac{1}{2}(1 + \cos \kappa). \tag{25}$$

The eigenstates corresponding to the $\lambda = 0$ solutions obviously (see (16)) do not contribute to G(r, t). The eigenvector that corresponds to (25) is

$$|\kappa) = \sum_{r}^{N^{\max/2}} e^{i\kappa r} [|2r-1\rangle] + e^{i\kappa} |2r\rangle].$$
(26)

To obtain G(r, t) by (16) we have to evaluate $b_{0\kappa}$, the coefficient of $|\kappa\rangle$ in the expansion of $|0\rangle$). In order to calculate this coefficient we need to construct states $(\kappa|$, such that

$$(\kappa'|\kappa) = \delta'(\kappa',\kappa) \tag{27}$$

since then we have

$$b_{0\kappa} = (\kappa|0)). \tag{28}$$

To do this, we first define states

$$((r) = \frac{1}{q\sqrt{N}} \sum_{\{n_r\}} \left[\delta_{n_{r,1}} - \delta_{n_{r,0}} \frac{q - (1/N^{\max})}{1 - q} \right] \delta_{\Sigma_{n_{r'}}, N} \prod_{r'} \langle n_{r'} |$$
(29)

where $q = N/N^{\text{max}}$. It is easy to see, using (12) and (29), that

$$((\mathbf{r}'|\mathbf{r})) = \delta(\mathbf{r}', \mathbf{r}). \tag{30}$$

The form (29) of the states ((r| is not going to any role in what follows. We are going to use the existence of such states and their property (30), but not their explicit form. The actual form of the states is given here only for the sake of completeness.

To obtain states with the property (27), we construct from ((r| left eigenstates of T, which have the form

$$(\kappa) = \sum_{r} e^{-i\kappa r} [\tilde{u}((2r-1) + \tilde{v}((2r))]$$
(31)

where (\tilde{u}, \tilde{v}) is the left eigenvector of the 2×2 matrix that appears in (21).

For $p = \frac{1}{2}$, the eigenvector that belongs to the non-vanishing eigenvalue (25), has $\tilde{u}(\kappa) = \tilde{v}(\kappa)$, and the normalisation factor $\tilde{u}(\kappa)$ is determined, using (26), (30) and (31), by

$$\delta(\kappa',\kappa) = (\kappa'|\kappa) = \tilde{u}(\kappa')(1+e^{i\kappa}) \sum_{r}^{N^{\max/2}} e^{i(\kappa'-\kappa)r}$$
(32)

so that

$$b_{0\kappa} = \tilde{u}(\kappa) = \left[\frac{1}{2}N^{\max}(1+e^{i\kappa})\right]^{-1} = \frac{1+e^{-i\kappa}}{2N^{\max}\lambda(\kappa)}.$$
(33)

Finally we have to calculate the matrix element $C(r, \kappa)$, given by (17). It has the form

$$C(r,\kappa) = \sum_{r'} e^{i\kappa r'} \langle\!\langle 0|\hat{n}(r)[u|2r'-1)\rangle + v|2r'\rangle \rangle]$$
(34)

which involves matrix elements that are easy to evaluate:

$$\langle\!\langle 0|\hat{n}(r)|r''\rangle = \langle\!\langle 0|\hat{n}(r)\hat{n}(r'')|0\rangle = q^2 + q(1-q)\delta(r,r'')$$
(35)

where we assumed the thermodynamic limit N, $N^{\max} \rightarrow \infty$ keeping $q = N/N^{\max}$ fixed. For $p = \frac{1}{2}$ we have u = 1, $v = e^{i\kappa}$, and find that

$$C(r,\kappa) = q^2 N^{\max} \delta(\kappa, 0) + q(1-q) e^{(1/2)i\kappa[r+\Delta(r)]}$$
(36)

where $\Delta(r) = 1$, 2 is the parity parameter (19). Finally substituting (25), (33) and (36) in (16) we get

$$G(r, t) = q^{2} + \sum_{\kappa \neq 0} \frac{q(1-q)}{2N^{\max}} (1 + e^{-i\kappa}) e^{(1/2)i\kappa[r+\Delta(r)]} \left(\frac{1+\cos\kappa}{2}\right)^{(1/2)t-1}$$

The first term is the squared average density of particles. The second term measures the correlation between an 'injected' particle, at r = t = 0, and presence of an extra particle at r, t. This 'net correlation function,' $G_c(r, t)$, is written, for the $N^{\max} \rightarrow \infty$ limit as an integral

$$G_{\rm c}(\mathbf{r},t) = \frac{q(1-q)}{8\pi} \int_{-\pi}^{\pi} \mathrm{d}\kappa (1+{\rm e}^{-{\rm i}\kappa}) \,{\rm e}^{(1/2){\rm i}\kappa(\mathbf{r}+\Delta)} \left(\frac{1+\cos\kappa}{2}\right)^{(t/2)-1}.$$
 (37)

Using trigonometric identities one can write the net correlation function in the form

$$G_{\rm c}(\mathbf{r},t) = \frac{q(1-q)}{2\pi} \frac{1}{2^t} \int_{-\pi}^{\pi} \mathrm{d}\kappa \; \mathrm{e}^{(1/2)\mathrm{i}\kappa(\mathbf{r}+\Delta-1)} (\mathrm{e}^{\mathrm{i}\kappa/2} + \mathrm{e}^{-\mathrm{i}\kappa/2})^{t-1}. \tag{38}$$

This integral can be solved after using the binomial expansion to simplify the integrand. The correlation function then takes the form:

$$G_{\rm c}(r,t) = \frac{q(1-q)}{2^t} \sum_{t=0}^{t-1} {t-1 \choose t} \delta_{2l,t-r-\Delta}.$$
(39)

As expected $G_c(r, t)$ vanishes outside the light cone defined by $t = r + \Delta$. Inside the light cone $(t \ge r + \Delta)$ we get a simple expression for the net correlation function:

$$G_{\rm c}(r,t) = \frac{q(1-q)}{2^t} \binom{t-1}{(t-r-\Delta)/2}.$$
(40)

To calculate the long time and large distance limit of $G_c(r, t)$ we use the Stirling formula to approximate factorials in expression (40). Assuming that the distance r is small compared with t we obtain the leading behaviour of the net correlation function:

$$G_{\rm c}(r,t) \sim q(1-q) \frac{{\rm e}^{-r^2/2t}}{\sqrt{2\pi t}}.$$
 (41)

To summarise, we calculated the arrow-arrow correlation function of a critical sixvertex model exactly. We showed that in the long time and large distance limit it behaves as a simple random walk, as one may expect from the solution of the equivalent dynamic model [1, 2] (diffusion of particles in one dimension with exclusion).

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