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LETTER TO THE EDITOR

Applications of Temperley–Lieb algebras to Lorentz lattice gases

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Abstract. Motivated by the study of motion in a random environment we introduce and investigate a variant of the Temperley–Lieb algebra. This algebra is very rich, providing us with three classes of solutions of the Yang–Baxter equation. This allows us to establish a theoretical framework to study the diffusive behaviour of a Lorentz lattice gas. Exact results for the geometrical scaling behaviour of closed paths are also presented.

The Temperley–Lieb (TL) algebra arose in the context of statistical mechanics and was used to map the q-state Potts model into the six-vertex model [1]. The relevance of this algebra to the theory of two-dimensional solvable models was further elaborated by Baxter [2] and the first detailed study of its mathematical structure was given by Jones [3]. In recent years, interest in TL algebras has been widespread in many branches of physics and mathematics, including quantum spin chains [4, 5], conformal field theory [6] and knot theory [7, 8] to name just a few.

In this letter, motivated by physical considerations, we introduce and investigate a variant of the TL algebra. Our physical motivation is to describe the diffusion behaviour of a Lorentz lattice gas, consisting of a dilute gas of particles moving in a random array of scatterers [9]. In the model we consider here, a particle moves along the bonds of the square lattice and its trajectory is changed when it hits scatterers which are either mirrors in different orientations or (right and left) rotators randomly placed at the sites of the lattice [9, 10]. These are perhaps the simplest nontrivial 'scattering rules' one can think of and they are illustrated in figure 1. To describe the statistical behaviour of these paths in a more general way, we assign a fugacity q to every closed trajectory. This then defines a loop model and its partition function is given by

$$Z = \sum_{\text{scatter configurations}} w_a^{n_a} w_b^{n_b} w_c^{n_c} w_d^{n_d} q^{\#\text{paths}} \tag{1}$$

where $w_a(w_c)$ and $w_b(w_d)$ are the Boltzmann weights probabilities of right and left mirrors (rotators) and $n_i(i = a, b, c, d)$ are the the number of weights in a given configuration. Setting $q = 1$ we recover the Lorentz gas model.

In the absence of rotators ($w_c = w_d = 0$), the partition function (1) can be interpreted as a graphical representation of the q^2-state Potts model, and therefore the algebraic structure

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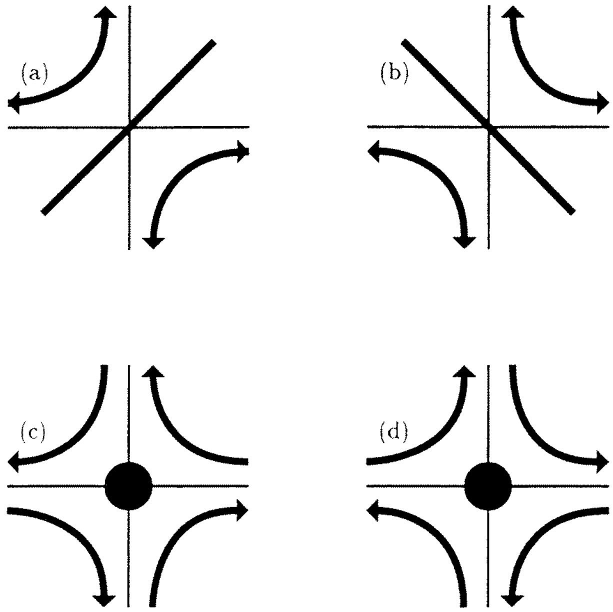

Figure 1. Scattering rules for (*a*) right mirrors; (*b*) left mirrors; (*c*) right rotators; (*d*) left totators on the square lattice.

underlying the mirror collision rules is the standard TL algebra. This is no longer valid if rotators are present, because a particle hitting a rotator does not behave exactly the same as when it hits a mirror. In fact, the algebra that mimics the behaviour of rotators is as follows. We associate to right and left rotators the elements R_i and L_i, acting on sites i and $i+1$ of a quantum spin chain of size L. We find that R_i and L_i are generators of the following associative algebra

$$R_i^2 = qR_i \qquad L_i^2 = qL_i \qquad [R_i, L_i] = 0 \tag{2}$$

$$L_i R_{i\pm1} L_i = L_i \qquad R_i L_{i\pm1} R_i = R_i \qquad [R_i, R_{i\pm1}] = [L_i, L_{i\pm1}] = 0 \tag{3}$$

$$[L_i, L_j] = [R_i, R_j] = [R_i, L_j] = 0 \qquad |i-j| \geqslant 2. \tag{4}$$

These relations can be seen as two commuting TL algebras whose generators alternate between R_i and L_i depending on the parity of the sites. This algebra has to be read in conjunction with the TL operator $E_i = R_i L_i$ and the identity I_i, which in the Lorentz gas corresponds to left and right mirrors, respectively. It is interesting to note that this algebra also allows us to define the braid operator $b_i = R_i + L_i - \mathrm{e}^{\theta} E_i - \mathrm{e}^{-\theta} I_i$ and its inverse $b_i^{-1} = R_i + L_i - \mathrm{e}^{-\theta} E_i - \mathrm{e}^{\theta} I_i$, where the parameter θ is related to the fugacity by $q = 2\cosh(\theta)$. The real surprise is the fact that the braid-monoid operators b_i, b_i^{-1} and E_i satisfy the Birman–Wenzel–Murakami (BWM) algebra [11]. More precisely, this connection occurs when the two independent parameters $\sqrt{Q}$ and c of the BWM algebra (we are using the notation of [8]) lie on the curve $\sqrt{Q} = 4\cosh^2(\theta)$ and $c = -\mathrm{e}^{3\theta}$. However, in the context of the Yang–Baxter equation, we find that the 'rotator' algebra (2)–(4) is richer than the BWM algebra (on the above curve), since the former gives us an extra integrable manifold.

To make further progress we look for possible integrable manifolds for the Boltzmann weights w_a, w_b, w_c and w_d. This not only allows us to establish a theoretical framework to study the Lorentz lattice gas but also prompts us to make exact predictions for its diffusive behaviour. The basic idea is to search for solutions of the Yang–Baxter equation by Baxterizing the ansatz $w_a I_i + w_b E_i + w_c R_i + w_d L_i$ with the help of the algebraic relations (2)–(4). Here we omit technical details, presenting only the final results. We find three different integrable manifolds given by

$$\text{(I)}\ w_a(\lambda) = \frac{\sinh(\theta-\lambda)}{\sinh(\lambda)} \qquad w_b(\lambda) = 1/w_a(\lambda) \qquad w_c(\lambda) = w_d(\lambda) = 1 \tag{5}$$

$$\text{(II)}\ w_a(\lambda) = \frac{\sinh(\theta-\lambda)}{\sinh(\lambda)} \qquad w_b(\lambda) = -\frac{\cosh(\theta-\lambda)}{\cosh(2\theta-\lambda)} \qquad w_c(\lambda) = w_d(\lambda) = 1 \tag{6}$$

$$\text{(III)}\ w_a(\lambda) = \frac{q}{e^{2\lambda}-1} \qquad w_b(\lambda) = \frac{q e^{2\lambda}}{q^2-1-e^{2\lambda}} \qquad w_c(\lambda) = 1 \qquad w_d(\lambda) = 0 \tag{7}$$

where λ is the spectral parameter of the Yang–Baxter equation. The third solution also admits $w_c(\lambda) = 0$ and $w_d(\lambda) = 1$, since the algebra (2)–(4) is invariant under the exchange of left and right rotators.

In order to interpret these solutions it is more appealing to work with a specific representation for the generators R_i and L_i. In the language of quantum spin chains, we find that these generators can be written as

$$R_i = \sigma_i^+ \tau_{i+1}^- + \sigma_i^- \tau_{i+1}^+ + \frac{\cosh(\theta)}{2}(1 - \sigma_i^z \tau_{i+1}^z) + \frac{\sinh(\theta)}{2}(\tau_{i+1}^z - \sigma_i^z) \tag{8}$$

$$L_i = \tau_i^+ \sigma_{i+1}^- + \tau_i^- \sigma_{i+1}^+ + \frac{\cosh(\theta)}{2}(1 - \tau_i^z \sigma_{i+1}^z) + \frac{\sinh(\theta)}{2}(\sigma_{i+1}^z - \tau_i^z) \tag{9}$$

where $\{\sigma_i^\pm, \sigma_i^z\}$ and $\{\tau_i^\pm, \tau_i^z\}$ are two commuting sets of Pauli matrices acting on the sites of a lattice of size L.

Considering this representation, it is not difficult to see that solution (I) behaves the same as two decoupled six-vertex models and therefore the underlying symmetry is based on the D_2 Lie algebra [12]. The second solution corresponds to a pair of six-vertex models coupled, in a finely tuned way, through their (total) energy–energy interaction. Its quantum group symmetry, after a canonical transformation, can be related to the twisted A_3^2 Lie algebra [12]. The third solution is clearly asymmetric in the spin variables and therefore cannot be interpreted in terms of the BWM algebra. This solution has also a number of unusual properties. For instance, the asymptotic braid limits $R(\pm\infty)$ are not invertible and for the special values $q = \pm 1$ we find a connection to a *singular* point ($t = 0$ in the notation of [11]) of the Hecke algebra. In the context of spin models, we have verified that the Boltzmann weights (7) can be related to an integrable non-self-dual manifold [13] of generalized Potts models introduced by Domany and Riedel [14] to model the adsorption of molecules on a crystal surface.

We now turn our attention to the Lorentz lattice gas. For $q = 1$ only the first two solutions turn out to be physically meaningful, since all the Boltzmann weights can be made positively definite. Thus, we shall concentrate our efforts on studying the critical behaviour of these two solutions with the expectation of making predictions for the geometrical scaling behaviour of closed particle paths in the Lorentz lattice gas. To this end, we study these models with generalized boundary conditions, in order to assure that closed loops on the cylinder pick up the correct Boltzmann weights. In general, these are twisted boundary conditions defined by

$$\sigma_{L+1}^\pm = e^{\pm i\psi_1}\sigma_1^\pm \qquad \tau_{L+1}^\pm = e^{\pm i\psi_2}\tau_1^\pm \qquad \sigma_{L+1}^z = \sigma_1^z \qquad \tau_{L+1}^z = \tau_1^z \tag{10}$$

where ψ_1 and ψ_2 are appropriate angles.

The critical behaviour of solution (I) is that of two decoupled XXZ spin chains and consequently the results for the central charge and anomalous dimensions can be read off directly from previous work in the literature [4]. This system is critical in the regime $q \in [2, -2]$ and it is more convenient to parametrize the fugacity by $q = 2\cos(\gamma)$. It turns out that the effective central charge behaviour is

$$c = 2 - \frac{3}{x_p(\gamma)} \sum_{i=1}^{2} [\psi_i/2\pi]^2 \tag{11}$$

while the conformal dimensions are given by

$$X^{m_1,m_2}_{n_1,n_2} = \sum_{i=1}^{2} \left[x_p(\gamma) n_i^2 + \frac{1}{4x_p(\gamma)} (m_i + \psi_i/2\pi)^2 \right] \tag{12}$$

where n_i and m_i are integers representing the spin-wave and the vortex excitations of two decoupled Coulomb gases—both having the same radius amplitude $x_p(\gamma) = \frac{\pi-\gamma}{2\pi}$. The finite-size corrections (11,12) are measured relative to the ground state of two *periodic* XXZ models [4].

The second solution corresponds to two nontrivially coupled XXZ models and it is possible to show that its Bethe ansatz solution is formally related to that of the A_3^2 vertex model [15]. The critical properties of the latter model has only been partially studied in the literature [16] and in a region that excludes the Lorentz lattice gas itself. We remark that here we have to perform the calculations in the presence of the seams ψ_1 and ψ_2, since they play a crucial role in the underlying critical behaviour. We find that the eigenvalues of the Hamiltonian associated to the second solution are given by

$$E_{II}(L) = \sum_{j=1}^{r_1} \frac{2\sin^2(\gamma)}{\cos(\gamma) - \cosh(\lambda_j^{(1)})} \tag{13}$$

and the corresponding Bethe ansatz equations are

$$\left[\frac{\sinh(\lambda_j^{(1)}/2 - \mathrm{i}\gamma/2)}{\sinh(\lambda_j^{(1)}/2 + \mathrm{i}\gamma/2)} \right]^L = -\mathrm{e}^{\mathrm{i}\psi_1} \prod_{k=1}^{r_1} \frac{\sinh(\lambda_j^{(1)}/2 - \lambda_k^{(1)}/2 - \mathrm{i}\gamma)}{\sinh(\lambda_j^{(1)}/2 - \lambda_k^{(1)}/2 + \mathrm{i}\gamma)}$$
$$\times \prod_{k=1}^{r_2} \frac{\sinh(\lambda_j^{(1)} - \lambda_k^{(2)} + \mathrm{i}\gamma)}{\sinh(\lambda_j^{(1)} - \lambda_k^{(2)} - \mathrm{i}\gamma)} \qquad j = 1, \ldots, r_1 \tag{14}$$

$$\mathrm{e}^{\mathrm{i}(\psi_1-\psi_2)} \prod_{k=1}^{r_1} \frac{\sinh(\lambda_j^{(2)} - \lambda_k^{(2)} + \mathrm{i}2\gamma)}{\sinh(\lambda_j^{(2)} - \lambda_k^{(2)} - \mathrm{i}2\gamma)} = -\prod_{k=1}^{r_2} \frac{\sinh(\lambda_j^{(2)} - \lambda_k^{(1)} + \mathrm{i}\gamma)}{\sinh(\lambda_j^{(2)} - \lambda_k^{(1)} - \mathrm{i}\gamma)} \qquad j = 1, \ldots, r_2. \tag{15}$$

The existence of the Bethe ansatz solution allows us to calculate, not only the thermodynamic limit, but also the dominant finite-size corrections for the eigenvalues of the Hamiltonian. For a conformally invariant system, these finite-size effects can be directly related to the central charge and scaling dimensions [17, 18], providing us with a way to study the universality class of solution (II). An essential step here is to determine the nature of the Bethe anstaz roots governing the ground state properties. In the regime that we are interested in, i.e. near $\gamma \sim \pi/3$, we find a mixture between one-string and two-string type of solutions. More precisely, the complex roots structure is given by

$$\lambda_j^{(1)} = \xi_j^{(1)} \pm \mathrm{i}(\pi/2 - \gamma) + \mathrm{O}(\mathrm{e}^{-L}) \qquad \lambda_j^{(2)} = \xi_j^{(2)} + \mathrm{i}\pi/2 \tag{16}$$

where $\xi_j^{(a)}$ are real numbers.

Table 1. Finite size sequences for the extrapolation of the effective central charge for $\gamma = \pi/3$.

L	$\psi_1 = \psi_2 = \pi/3$	$\psi_1 = \psi_2 = \pi/4$	$\psi_1 = \pi/3,\ \psi_2 = \pi/4$
8	1.556 67	1.788 90	1.672 53
16	1.518 57	1.630 17	1.630 17
24	1.510 21	1.731 59	1.620 83
32	1.506 83	1.727 37	1.617 05
40	1.505 06	1.725 16	1.615 07
Extrapolation	1.500 1(2)	1.718 6(2)	1.609 2(2)

Table 2. Finite size sequences for the extrapolation of the spin-wave anomalous dimensions $X_{1,0}^{0,0}$ and $X_{1,1}^{0,0}$ for periodic boundary conditions.

L	$X_{1,0}^{0,0}(\gamma = \pi/3)$	$X_{1,1}^{0,0}(\gamma = \pi/3)$	$X_{1,0}^{0,0}(\gamma = \pi/3.5)$	$X_{1,1}^{0,0}(\gamma = \pi/2.5)$
8	0.344 610	0.640 435	0.404 331	0.599 395
16	0.337 923	0.653 822	0.392 503	0.599 587
24	0.336 174	0.658 341	0.387 451	0.599 756
32	0.335 383	0.660 548	0.384 344	0.599 839
40	0.334 934	0.661 844	0.382 155	0.599 890
Extrapolation	0.333 30(2)	0.666 65(2)	0.357 5(3)	0.600 0(2)

In order to determine the finite-size corrections for the ground state, we have numerically solved the Bethe ansatz equations for several values of the lattice size up to $L \sim 40$. In table 1 we present our estimates for the effective central charge for general boundary conditions. Surprisingly, the behaviour is precisely the same of that given in formula (11) which suggests that the coupling between the two XXZ models becomes asymptotically irrelevant near $q = 1$. To give extra support to this scenario we have also investigated the low-lying spin-wave excitations. In table 2 we show some estimates for the exponents $X_{1,0}^{0,0}$ and $X_{1,1}^{0,0}$ and they are in accordance with the conformal dimensions (12). More generally, we verified that the critical behaviour for role region $q \in [0, \sqrt{2})$ is given in terms of two decoupled Coulomb gas models. However, in the regime $q \in [\sqrt{2}, 2]$ the coupling between the two XXZ models becomes relevant, and the criticality is governed by a $c = 3$ conformal field theory. We note that in the first branch all the Boltzmann weights probabilities can be positively defined while in the second one either w_b or w_a is necessarily negative. This is perhaps the physical reason behind these two different *antiferromagnetic* critical behaviour. Finally, we remark that our results complement and correct an early calculation in the literature [16].

We now have the basic ingredients to study the scaling properties of closed trajectories in the Lorentz lattice gas model. From our previous analysis we conclude that the critical behaviour, for both manifolds (I) and (II), is given in terms of two decoupled Coulomb gas in the presence of the background charges $\psi_1 = \psi_2 = 2\gamma = 2\pi/3$. Here we are interested in correlators that measure the probabilities that two points on the lattice separated by r belong to the same loop [19]. For large distances we expect the algebraic decay

$$\langle \Phi_l(r)\Phi_l(0)\rangle \sim r^{-2X_l} \tag{17}$$

where X_l is the scaling dimension of the conformal operator $\Phi_l(r)$ [20]. Equipped with equations (11) and (12) we can now calculate the dimensions X_l for the $q = 1$ model. The probability that $l = n_1 + n_2$ loop segments meet in the neighbourhood of two points in the lattice is associated to the conformal dimensions of the spin-wave excitations n_1 and n_2 with null vortex charges $m_1 = m_2 = 0$ [19, 20]. Due to the background charges, we also have to subtract the variation of the true ground state for the Lorentz lattice gas. We conclude that the value of these dimensions is

$$X_{n_1,n_2} = \sum_{i=1}^{2} \left[x_p(\pi/3) n_i^2 - \frac{(\frac{1}{3})^2}{4x_p(\pi/3)} (1 - \delta_{n_i,0}) \right] = \sum_{i=1}^{2} \left[\frac{n_i^2}{3} - \frac{(1 - \delta_{n_i,0})}{12} \right]. \tag{18}$$

The scaling behaviour of single paths is governed by the lowest conformal dimension $X_{1,0} = X_{0,1} = \frac{1}{4}$, predicting a fractal dimension [21] $d_f = 2 - \frac{1}{4} = \frac{7}{4}$. This is the same value found in numerical simulations of a fully occupied lattice of either mirrors or rotators [21, 22]. Therefore, our result brings an extra theoretical support to the fact that the scaling behaviour of single paths does not depend on whether the scatterers are mirrors or rotators. However, the situation changes drastically when we consider the probability for multi-loops, $l \geqslant 2$. In fact, in the case of a mixed rotator–mirror model the second lowest dimension occurs in the sector $n_1 = n_2 = 1$, and the corresponding fractal dimension is $d_f = 2 - \frac{1}{2} = \frac{3}{2}$. This value is double that expected ($d_f = 2 - \frac{5}{4} = \frac{3}{4}$) when we have only mirrors [20]. In general, formula (18) leads us to conclude that the multi-loops scaling behaviour is sensible to the details of the scattering mechanism. This can be understood when it is noted that a single particle scattered by a lattice full of rotators and mirrors can not distinguish the two types of scatterers. However, two particles in different orbits are capable of making the distinction. Finally, we remark that our findings are valid for rather distinct manifolds, suggesting that $w_c = w_d$ is indeed a critical surface in the Lorentz gas model.

In summary, we have introduced a variant of the TL algebra which generates three classes of solutions of the Yang–Baxter equation. We have applied the first two of them to study the diffusion behaviour of a Lorentz lattice gas whose scatterers are either mirrors or rotators. The third manifold seems to be relevant to the study of phase transition in adsorbed films [14], and we hope to investigate its critical properties in a future publication. Finally, we remark that after this paper had been written we noted the very recent work [23] in which the *third* manifold and its generalizations were obtained via Baxterization of Fuss–Catalan algebras.

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