Application of Operator Algebras to Stochastic Dynamics and the Heisenberg Chain

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Algebraic manipulations are used to reduce a new description of stochastic dynamics and quantum spin chains involving two nonlocal operators C, D. For the symmetric hopping of hard-core particles, and its associated Heisenberg chain, the operator algebra may be written in the reduced form $2\dot{D} = [[C, D], C^{-1}]$, $2D^2 = CDC^{-1}D + DC^{-1}DC$. These equations are shown to describe diffusive dynamics and phase change on interchange, respectively, and to lead to Bethe ansatz equations for the spectrum of the isotropic Heisenberg chain with symmetry-breaking boundary fields. This yields new exact results for the dynamics of boundary-driven systems.

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The representation of interacting stochastic particle dynamics by quantum spin systems has been providing valuable insights into nonequilibrium behavior and complex dynamics (see, e.g., [1–10], and references therein). In particular, it has given many new results by exploiting standard techniques for quantum spin models, such as Bethe ansatz and related approaches [1–5,11], spin wave theory [6,12], and global [7,8] and broken symmetry arguments [6]. Perhaps the simplest nontrivial example is the representation of symmetric diffusion of hard-core particles (known as the symmetric exclusion process [13,14]) by the Heisenberg model (see, e.g., [7] for a detailed discussion). Other stochastic processes whose representation by quantum spin systems has proved useful are asymmetric hopping [1–3,8] and related growth processes [15,16], multimer evaporation and deposition [6], and large classes of reaction-diffusion processes [3–5,9,10].

An elegant algebraic approach has recently been introduced for the treatment of ground states of quantum spin chains [17] and particularly for the steady states of one-dimensional stochastic exclusion processes [18,19]. These states correspond to the ground states of the related spin Hamiltonians, in the simplest case to the ferromagnetic Heisenberg Hamiltonian with suitably chosen boundary fields. In this algebraic approach particle and vacancy configurations are represented by strings of symbols, D or E. The steady state probability of such a configuration is given by a particular matrix element of the string, with the symbols now regarded as operators obeying a suitable associative algebra. The states involved in the selection of the matrix element(s) are determined by boundary conditions (e.g., particle injection), while the algebra of the operators is determined by the bulk dynamics (see below). It should be noted that in contrast to ordinary (equilibrium) statistical mechanics the boundary conditions are of major importance, since they may induce phase transitions [3,20] related to shock behavior [19,21]. This algebraic technique provides a very convenient and economic framework for the derivation of solvable recursion relations for the matrix elements of the operators and therefore for the calculation of steady state correlation functions. These recursions (and their solution) have been obtained directly from the master equation [22,23], but this approach is not readily generalizable to other models. Two conceptually most important questions raised by the algebraic treatment, however, remained open, namely, the conditions under which such a matrix ansatz is successful and how one can understand the algebra derived from the bulk dynamics of the process. Another question posed by this algebraic treatment is whether it can be generalized to describe time-dependent properties of the system.

Subsequently, a generalization of the technique to the full *dynamic* stochastic problem has been given [24]. This answers the third of the above-mentioned questions. As well as providing a new direct approach for the treatment of one-dimensional stochastic dynamics of interacting particle systems, it gives a new operator algebra description of the corresponding quantum spin model. The algebra has been briefly presented elsewhere, but without developing its consequences [24]. The purpose of this Letter is to exploit this algebra.

In particular it is used here to obtain by purely algebraic techniques new results for both stochastic and quantum spin systems, and to provide extremely efficient derivations of old ones, such as the Bethe ansatz. On the one hand, we derive explicitly the time evolution of the density profile in the symmetric exclusion process (hard-core hopping) driven by biased boundary injection and absorption, and starting from an arbitrary initial condition. We also discuss the time evolution of n-point density correlation functions on a cyclic chain with translationally invariant initial conditions. This second result is implicitly known from the Bethe ansatz, but the first result is new. On the other hand, our algebraic approach to the dynamic problem gives a partial understanding of the mathematical properties underlying the algebra in terms of results known from the quantum inverse scattering approach [25] and is a first step towards an understanding of the general applicability of the matrix method. Furthermore, it yields a physical understanding of the algebra as it is shown to

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describe free diffusive motion of the particles and phase change on interchange of two particles and the reduction of multiparticle interactions in terms of two-particle interactions. Contact is thus made with Yang-Baxter equations and with factorization properties of the scattering matrix.

The description employs three site-independent (nonlocal) operators C $(= D + E)$, D, and S, where D and S are time dependent. Probabilities (which in quantum language are wave functions) are given as in the stationary case by matrix elements of products of these operators. The algebra is determined so that the probability of finding any configuration satisfies the master equation (the Schrödinger equation in Euclidean time defined by the corresponding quantum Hamiltonian). This new approach has already been shown to give statements equivalent to the action of the spin-1/2 Heisenberg Hamiltonian on a complete basis of spin states [24]. An essentially different feature is the site independence of C, D, and S in contrast to the local description of the process in terms of site-dependent Pauli matrices in the Heisenberg chain. Whereas the Heisenberg problem turns out to be solvable by the Bethe ansatz, we derive the Bethe ansatz equations from the operator algebra. Moreover, we explicitly obtain the Bethe ansatz equations for the system with particle number breaking boundary conditions and use this to derive the time evolution of the density profile. These boundary conditions are known to retain the integrability of the system [26,27], but no concrete results have previously been derived.

The detailed description, which now follows, begins with asymmetric hard-core particle diffusion [14,18,22,23,28], with hopping rates p, q to the right and left, on a chain of L sites. We consider two types of boundary conditions: (a) open boundary conditions with particle injection and ejection (boundary driving) at the boundaries of a finite chain, and (b) periodic boundary conditions. In case (a) we allow for arbitrary initial conditions while in case (b) we restrict ourselves to translationally invariant initial conditions. We derive the time-dependent operator algebra, which illustrates the general strategy. The detailed results outlined above are then presented for the symmetric exclusion process $(p = q)$.

Following the discussion of the stationary problem [18], we represent an arbitrary state of the particle or spin system by a string of L operators, D or E, e.g., $EEDEDDD \ldots E$. Here D or E at the kth position in the string represent a particle or a vacancy (spin up or down) at site k. Using the master equation for the process, we have shown elsewhere [24] that the (unnormalized) time-dependent probability of the associated configuration can be expressed as a matrix element $\langle EEDEDDD \ldots E \rangle$ of the string. For this, $D \equiv D(t)$ and the time-independent operator $C = D + E$ have to be matrices satisfying the algebra

$$SC + \dot{D}C = \Lambda, \tag{1}$$

$$CS - C\dot{D} = \Lambda, \tag{2}$$

$$\dot{D}D + D\dot{D} = [D, S]. \tag{3}$$

Here the dot denotes the derivative with respect to time t, $\Lambda = qCD - pDC + (p - q)D^2$, and S is related to the current. The symbol $\langle \cdots \rangle$ denotes, in case (a), a matrix element between time-independent vectors $\langle W|$ and $|V\rangle$ determined by the boundary conditions, while in case (b) it denotes a trace. The conditions on $\langle W|$, $|V\rangle$ are

$$\langle W|\{(\alpha + \gamma)D - \alpha C - S + \dot{D}\} = 0, \tag{4}$$

$$\{(\beta + \delta)D - \delta C + S + \dot{D}\}|V\rangle = 0, \tag{5}$$

where α, γ are the rates for particle injection, ejection at the left hand boundary site 1, and δ, β are those for the right hand boundary site L, in case (a). To obtain normalized probabilities, the matrix element $\langle \cdots \rangle$ has to be divided by the factor $Z_L = \langle C^L \rangle$. The stationary problem corresponds to the special case $\dot{D} = 0$ with S an arbitrary c-number. Then (3)–(5) yield the algebra and conditions of Derrida *et al.* [18]. It is interesting to note that in this case the expectation values $\langle C^{n_1 - 1} \Lambda C^{n_2 - n_1 - 2} \Lambda \ldots \rangle$ are the current correlations between sites $n_1, n_2, \ldots$ on the chain. Equation (1) implies $\Lambda = SC$, which in turn implies that in this invariant matrix product measure k-point *current* correlators are space independent (for $|n_i - n_j| \geq 2$). In a usual c-number invariant product measure k-point *density* correlations are space independent (for $|n_i - n_j| \geq 1$).

In this Letter we consider the full dynamic problem. Introducing the inverse C^{-1} of C reduces (1)–(3) to

$$2\dot{D} = [\Lambda, C^{-1}] \overset{p=q=1}{\rightarrow} [[C, D], C^{-1}], \tag{6}$$

$$0 = \Lambda C^{-1} D - D C^{-1} \Lambda \overset{p=q=1}{\rightarrow} CDC^{-1}D + DC^{-1}DC - 2D^2, \tag{7}$$

$$2S = \Lambda C^{-1} + C^{-1}\Lambda \overset{p=q=1}{\rightarrow} CDC^{-1} - C^{-1}DC. \tag{8}$$

The arrows indicate the reduction, which occurs in the case of symmetric hopping. Relations (6) and (7) together with (4) and (5) in case (a) provide a complete description of the model in terms of just two nonlocal operators C and D together with the inverse C^{-1}.

From now on we discuss only the symmetric model $p = q = 1$. It turns out to be useful to construct operators $D_n = C^{n-1} D C^{-n}$ and their Fourier transforms $\mathcal{D}_q = \sum_n D_n \exp(iqn)$. The time dependence of $\mathcal{D}_q$ is now simply obtained from (6)

$$\mathcal{D}_q(t) = e^{-\epsilon_q t} \mathcal{D}_q(0), \tag{9}$$

$$\epsilon_q \equiv 1 - \cos q \tag{10}$$

in terms of the initial matrix $\mathcal{D}_q(0)$ and the "energy" ϵ_q. Moreover, (7) can be written as $0 = \int dq' \, \mathcal{D}_{q'} \mathcal{D}_{q-q'} (1 + e^{-iq} - 2e^{iq' - iq})$. Since this holds for all times (and all

q), it can be divided into separate time components, each of which must vanish. This leads to

$$\mathcal{D}_{q_1}\mathcal{D}_{q_2} = S(q_1, q_2)\mathcal{D}_{q_2}\mathcal{D}_{q_1}, \tag{11}$$

$$S(q_1, q_2) \equiv -\frac{1 + e^{iq_1+iq_2} - 2e^{iq_2}}{1 + e^{iq_1+iq_2} - 2e^{iq_1}}. \tag{12}$$

These results together with

$$C\mathcal{D}_q C^{-1} = e^{-iq}\mathcal{D}_q, \tag{13}$$

resulting from the definition of $\mathcal{D}_q$, have a direct and intuitive interpretation. C acts as a lattice translation operator. Equations (9) and (10) express the diffusive motion of the particles, and (11) and (12) express the phase change experienced on exchange of particles. In $S(q_1, q_2)$ one readily recognizes the two-particle scattering matrix element known from the Bethe ansatz and in the quantum inverse scattering method [25]. Indeed, (11) is just the algebra satisfied by the reflection matrices arising in the treatment of the nonlinear Schrödinger equation and the Heisenberg chain [25]. The associativity of the algebra (which guarantees that there are no separate equations for D^n, $n > 2$) is the analog of the factorization of the many-body S matrix into two-particle amplitudes. The new insight is that the whole system can be described in terms of just two (nonlocal) operators D, C and that this description does not depend on the system size.

As a specific application, consider the correlation function for m particles at positions $\{x_i\}$ at times $\{t_i\}$ for the symmetric exclusion process with periodic boundary conditions [case (b)]:

$$M_{\{x_i\}}(\{t_i\}) = Z_L^{-1}\mathrm{Tr}[D_{x_1}(t_1)\ldots D_{x_m}(t_m)C^L] \tag{14}$$

$$= \left(\prod_{i=1}^{m}\int \frac{dq_i}{2\pi}\, e^{-q_i x_i - \epsilon_{q_i} t_i}\right) T(\{q_i\}). \tag{15}$$

Here the normalization $Z_L = \mathrm{Tr}C^L$, and $T(\{q_i\}) = Z_L^{-1}\mathrm{Tr}\,[\mathcal{D}_{q_1}(0)\ldots\mathcal{D}_{q_m}(0)C^L]$. Using (11)–(13) and the invariance of the trace under cyclic permutation, one finds that $T(\{q_i\})$ vanishes unless $\sum_{i=1}^{m} q_i = 0$ and

$$e^{iq_i L} = \prod_{j=1}^{m}{}' S(q_j, q_i) \quad \forall\, i, \tag{16}$$

where the product excludes $j = i$. These are the well-known Bethe ansatz equations for total momentum zero [11], which arise directly and naturally from the operator algebra [particularly from (7) via (11)]. Matrix elements which are not determined by the operator algebra are given by the initial conditions by expressing $\mathcal{D}_q(0)$ in terms of $M_{\{x_i\}}(0)$. An explicit further calculation of the correlation function for general m is far from trivial, but the methods have been discussed elsewhere [29].

For a second application we turn to symmetric hard-core diffusion with injection and ejection at the boundaries [case (a)]. Here the relaxation will be towards a nontrivial nonequilibrium steady state. The m-point correlation function has the same form as in (15) but with $Z_L = \langle W|C^L|V\rangle$ and $T(\{q_i\}) = Z_L^{-1}\langle W|\mathcal{D}_{q_1}(0)\ldots\mathcal{D}_{q_m}(0)C^L|V\rangle$. To analyze this expression we extract from D_x the static parts [e.g., by using (9) and taking $q \to 0$]. These are $\mathcal{D}_0$ and I, where $I = \sum_n nC^{n-1}DC^{-n}$. As a result one may write

$$D_x = \mathcal{D}_0 + I - x\mathcal{D}_0 + \int' \frac{dq}{2\pi}\,\mathcal{D}_q e^{-iqx}, \tag{17}$$

where the integral now excludes $q = 0$. With $f_q(a, b) \equiv a + b - 1 + e^{iq}$ one obtains

$$0 = \langle W|C\{(\alpha + \gamma - 1)\mathcal{D}_0 + (\alpha + \gamma)I - \alpha\}, \tag{18}$$

$$0 = \langle W|C\{f_q(\alpha, \gamma)\mathcal{D}_q + f_{-q}(\alpha, \gamma)\mathcal{D}_{-q}\} \qquad (q \neq 0), \tag{19}$$

$$0 = \{(\beta + \delta - 1)\mathcal{D}_0 + (\beta + \delta)I - \delta\}|V\rangle, \tag{20}$$

$$0 = \{f_{-q}(\beta, \delta)\mathcal{D}_q + f_q(\beta, \delta)\mathcal{D}_{-q}\}|V\rangle \qquad (q \neq 0). \tag{21}$$

Using (13), (19), and (21), a cycling procedure readily gives $T(\{q_i\})$ vanishing unless

$$e^{2iq_i L} = B_{q_i}\prod_{j=1}^{m}{}' \frac{S(q_i, q_j)}{S(q_i, -q_j)} \quad \forall\, i, \tag{22}$$

$$B_q = f_{-q}(\alpha, \gamma)f_{-q}(\beta, \delta)/f_q(\alpha, \gamma)f_q(\beta, \delta). \tag{23}$$

These equations are the main result of this paper. They are the generalization of the known Bethe ansatz equations (16) for the Heisenberg chain with periodic boundary conditions to the system with open boundary conditions corresponding to generalized surface fields in spin language [24,26]. Via (10) they give the spectrum of the quantum Hamiltonian. Expressing $T(\{q_i\})$ in terms of the initial condition $M_{\{x_i\}}(0)$ and replacing the integral over q by a sum over the solutions of (22) gives then an explicit expression for the time evolution of the correlation function starting from an arbitrary initial state.

As an example, consider the density profile

$$M_x(t) = \rho_x + Z_L^{-1}\int' \frac{dq}{2\pi}\, e^{-iqx - \epsilon_q t}\langle W|\mathcal{D}_q C^L|V\rangle, \tag{24}$$

with $\rho_x \equiv M_x(\infty) = Z_L^{-1}\langle W|\{I - (x - 1)\mathcal{D}_0\}C^L|V\rangle$. This static part is clearly linear in the particle position x. With $[I, C] = C\mathcal{D}_0$ and (18) and (19) one obtains [24,30] ($L \to \infty$ at fixed x/L)

$$M_x(\infty) = \frac{\alpha}{\alpha + \gamma} - \frac{x}{L}\left(\frac{\alpha}{\alpha + \gamma} - \frac{\delta}{\beta + \delta}\right). \tag{25}$$

For the special case $\alpha + \gamma = \beta + \delta = 2$ the time-dependent profile turns out to have a simple expression in terms of modified Bessel functions:

$$M_x(t) = \rho_x - \sum_{y=1}^{L} a_y[C_{x-y}(t) - C_{x+y-1}(t)], \tag{26}$$

where $C_r(t) = \exp(-t)\sum_{m=-\infty}^{\infty} I_{r+2mL}(t)$ and the a_y are arbitrary constants defining the initial condition. In the generalization to m-point correlation functions, the static part $M_{\{x_i\}}(\infty)$ is easily seen to be a product of factors each linear in a given x_i [cf. (17)], and the effect of (11) in the cycling process also introduces the particle exchange phases into the time-dependent terms. This is a new result for the dynamics of the driven system.

The algebraic approach illustrated in the applications discussed above is only one method for exploiting the operator description provided by (1)–(3) [with (4) and (5) in the boundary driven case]. An obvious alternative is to find explicit matrix representations of the operators C, D, as has been done for the steady state problem [18]. A discussion has been given [24] of a matrix representation for the zero-current time evolution of the periodic system (b), and of the open system with injection rates chosen such that $\alpha\beta = \gamma\delta$. More general reaction-diffusion processes with $n > 2$ allowed states per site may be represented by an algebra of operators $A_1, \ldots, A_n$. A problem not yet fully understood is the relationship between such a generalized algebraic technique and the integrability of the system under consideration. The recovery of the algebra satisfied by the reflection matrices arising in the quantum inverse scattering method for the process studied here strongly suggests that an algebraic treatment of the kind proposed here for the dynamics or as discussed earlier for steady state properties of more general models is possible if, and only if, the system is integrable.

In conclusion, we have given a method for exploiting an operator algebra involving three nonlocal operators, which describes the full static and dynamic behavior of a stochastic interacting many-particle system and of its equivalent quantum spin model (the Heisenberg chain). Suitable operator manipulations clearly exhibit the physical characteristics of the system and provide an understanding of the relations satisfied by the operators. By such means correlation functions for periodic and open boundary-driven systems have been reduced, and the Bethe ansatz equations have been recovered (in the case of periodic boundary conditions) and generalized (to open boundary conditions with particle injection and ejection). This has led to a new result for the time-dependent density profile of the open stochastic system with arbitrary biased injection and absorption.

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