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Real-space renormalization for reaction–diffusion systems

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Abstract. The stationary state of stochastic processes such as reaction–diffusion systems can be related to the ground state of a suitably defined quantum Hamiltonian. Using this analogy, we investigate the applicability of a real-space renormalization group approach, originally developed for quantum spin systems, to interacting particle systems. We apply the technique to an exactly solvable reaction–diffusion system and to the contact process (both in $d = 1$). In the former case, several exact results are recovered. For the contact process, surprisingly good estimates of critical parameters are obtained from a small-cell renormalization.

1. Introduction

Reaction–diffusion systems and other interacting particle systems are relevant for the description of several phenomena in physics, chemistry and biology [1]. In the past, they have been mainly modelled by (nonlinear) partial differential equations [2], a description which implicitly contains a mean-field assumption. Such a description is, however, no longer appropriate in low dimensions where fluctuations are important. To take these into account one turns to a description of the reaction–diffusion system in terms of a stochastic process. This can, for example, be realized by adding a noise term to the partial differential equation. In recent years however, particular attention has been paid to models defined on a lattice. It has been found that these can be related to a number of interesting topics in modern statistical mechanics such as growing interfaces [3], phase transitions into an absorbing state [4], exactly solvable quantum spin chains [5], persistence exponents [6] and so on.

The systems which we will study here are defined on a lattice but evolve in continuous time. At each site of the lattice, one can have (hard core) 'particles' which can perform a random walk and/or can undergo one or several 'reactions'. In this paper we will limit ourselves to systems with one type of particle. Each lattice site can then be either empty ($\emptyset$) or be occupied by a particle (A). As an example, consider a system in which particles perform random walks and where two particles on neighbouring sites can 'annihilate' (i.e. undergo the reaction $A + A \to \emptyset + \emptyset$). In a simple mean field approach the density of particles $c(t)$ in this system decays asymptotically as $1/t$. It is common to introduce a critical exponent θ which describes the decay of the density ($c(t) \sim t^{-\theta}$) and which therefore in mean field theory equals 1. An exact solution of the diffusion–annihilation model in $d = 1$ (where it is equivalent to the $T = 0$ Glauber dynamics of an Ising model on the dual lattice) shows, however, that $\theta = \frac{1}{2}$ [7]. This latter value is also found experimentally in systems which are thought to be described by the diffusion–annihilation model. Moreover, θ shows a large universality across materials and initial conditions. The same value for θ is also found when the experimental situation is described more correctly by a diffusion–coagulation ($A + A \to \emptyset + A$, $A + A \to A + \emptyset$)

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model [8]. Hence, as in the theory of equilibrium critical phenomena one needs a scheme which at the same time explains the observed universality and gives precise values for critical exponents such as θ. One is therefore naturally led to a search for renormalization group (RG) approaches to stochastic systems.

Mathematically, the stochastic process is a continuous time Markov process. Using the formal equivalence between the master equation and the Schrödinger equation in imaginary time, one can set up a field theoretic formulation for stochastic systems which in turn can be used in the construction of a renormalization approach [9]. Critical exponents can then be calculated in an ϵ-expansion around the upper critical dimension, which in this case equals 2. This approach is by now well established and has been applied to many interesting systems. As an example, we mention the much studied branching and annihilating random walks (BARWs) [10], where besides diffusion and annihilation, particles can undergo branching processes ($A \rightarrow (m+1)A$). The competition between annihilation and branching leads to a non-equilibrium phase transition where the stationary state particle density $c_{\mathrm{st}}(\equiv \lim_{t\rightarrow\infty} c(t))$ goes to zero in a continuous way as a function of the rates of the different processes. Near this transition, several critical exponents (static and dynamic) can be introduced. It has been shown, both numerically and using the field theoretic RG, that the universality class of the transition for BARW is completely determined by the parity of m [11]. For m odd, the transition falls in the universality class of directed percolation (DP), whereas for m even a new universality class appears. On the basis of very precise simulations, Jensen [12] conjectured that $\theta = \frac{2}{7}$ and $\beta = \frac{13}{14}$ when m is even (β describes the way c_{st} goes to zero near the transition). So far, a precise analytical calculation of these exponents has, however, not been possible. Menyhárd and Ódor propose the value $\beta = 1$ on the basis of a perturbation around mean-field theory [13]. Using a loop expansion at fixed dimension, Cardy and Täuber find $\beta = \frac{4}{7}$ [11]. Given the existing uncertainty in exponent values, there is clearly room for the introduction of new, analytical approaches to the BARW and related models.

In this paper, we investigate the possibilities of a real-space RG approach to interacting particle systems. Our starting point is again the equivalence between a stochastic system and a quantum mechanical one. In the past, several real-space RG approaches to quantum lattice systems have been introduced. We must mention here as an example the *density matrix RG* (DMRG) which has been very successful [14]. Currently, several research teams in the world are investigating the applicability of the DMRG to stochastic systems [15–17]. Unfortunately, the name DMRG is a bit of a misnomer, since one rarely calculates RG flows in this approach and hence it is not easy to decide on questions of universality using this technique. Moreover, the approach is purely numerical. Instead in this paper, we will use the so-called standard (also called SLAC) approach [18]. We have applied this RG method to the study of the stationary state properties of some interacting particle systems. We found that the method works surprisingly well in several cases which we studied. These include a solvable reaction–diffusion model (with diffusion, coagulation and decoagulation) and the contact process, which has a transition which is also thought to be in the directed percolation universality class.

This paper is organized as follows. In section 2 we briefly introduce the description of stochastic processes in a quantum mechanical language. In section 3, we discuss the SLAC real-space approach to the ground state of quantum (spin or fermion) chains. We also discuss how critical exponents for stochastic systems can be obtained from such an approach. In section 4 we study properties of the stationary state of some solvable reaction–diffusion systems. In section 5, we give our results for the contact process. Finally, in section 6 we present some conclusions and an outlook on further applications of the real-space RG technique.

2. Quantum formalism of reaction–diffusion systems

In this section we discuss the relation between stochastic processes in continuous time on the one hand and quantum mechanics on the other hand [19,20]. This relation was (independently) discovered by several authors, and has been developed extensively in recent years (see, e.g., [21–24]). We only give a brief overview, with the aim of fixing our notation (which to a large extent is the one used in [5]).

Consider a one-dimensional lattice of L sites and let $\eta = \{\eta_1, \ldots, \eta_L\}$ ($\eta_i = 0(1)$ when no (a) particle is present at site i) be the microscopic configuration of the particle system. Furthermore, we denote by $P(\eta, t)$ the probability that the system is in configuration η at time t. The time evolution of $P(\eta, t)$ is determined by the transition rates $w_0, w_1, \ldots, w_s$ of the model. In general, one of these is used to fix the time scale (say $w_0 = 1$). We will collect the remaining rates in a vector $\vec{w} = (w_1, \ldots, w_s)$.

As a first step in turning the stochastic description into a quantum mechanical one, we associate with each state η a basisvector $|\eta\rangle$ of a 2^L-dimensional vector space. Next, we introduce a state vector $|P(t)\rangle$

$$|P(t)\rangle = \sum_{\eta} P(\eta, t)|\eta\rangle. \tag{1}$$

The time evolution of $|P(t)\rangle$ is described by the master equation

$$\frac{\mathrm{d}|P(t)\rangle}{\mathrm{d}t} = -H|P(t)\rangle \tag{2}$$

where H is a $(2^L \times 2^L)$ matrix which depends on all the transition rates of the system. In particular the matrix element $-H_{\zeta,\xi} \geqslant 0$ (for $\zeta \neq \xi$) equals the transition rate to go from configuration ξ to configuration ζ. Due to the conservation of probability the diagonal elements are given by

$$H_{\zeta,\zeta} = -\sum_{\xi \neq \zeta} H_{\xi,\zeta}. \tag{3}$$

This relation implies that the sum of the elements in a column of H equals zero, a condition which we will refer to as the *stochasticity condition*.

It is now common to consider (2) as a Schrödinger equation (in imaginary time) and call H the Hamiltonian. In contrast to the quantum mechanical situation H is not necessarily Hermitian. Hence, left and right eigenvectors are, in general, not related by simple transposition. In situations where there are only local interactions we can write H in terms of local operators. In the particular cases studied in this present paper, transitions involve at most two sites so that one can write

$$H = \sum_j 1_1 \otimes \cdots \otimes 1_{j-1} \otimes H_{j,j+1} \otimes 1_{j+2} \otimes \cdots \otimes 1_L$$

which is commonly abbreviated to $H = \sum_j H_{j,j+1}$.

For reaction–diffusion systems with one type of particle, it is common to interpret the model as a spin model (where a spin up (down) corresponds the absence (presence) of a particle) so that one writes H in terms of the four matrices

$$v = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad n = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \qquad s^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad s^- \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{4}$$

The stochasticity condition implies the existence of at least one eigenvalue which equals zero and an associated left eigenvector $\langle s|$ given by

$$\langle s| = \sum_{\eta} \langle \eta|. \tag{5}$$

Moreover, it can be shown that the real part of every eigenvalue is non-negative.

The formal solution of the master equation (2) is

$$|P(t)\rangle = \mathrm{e}^{-Ht}|P(0)\rangle. \tag{6}$$

With any physical quantity x (such as the density of particles) an operator (matrix) X can be associated in the following way. If $x(\eta)$ is the value of the physical quantity in the microstate η the matrix elements of X are defined as $\langle\eta|X|\eta'\rangle = \delta_{\eta,\eta'}x(\eta)$. As an example, the number of particles at site i is given by the operator

$$C_i = 1_1 \otimes \cdots \otimes 1_{i-1} \otimes n_i \otimes 1_{i+1} \otimes \cdots \otimes 1_L. \tag{7}$$

Hence we get

$$\begin{aligned}\langle X(t)\rangle &= \sum_\eta x(\eta)P(\eta,t) \\ &= \langle s|X|P(t)\rangle \\ &= \langle s|X\mathrm{e}^{-Ht}|P(0)\rangle.\end{aligned} \tag{8}$$

In this paper, we will be mainly interested in stationary state properties of the stochastic system. In that limit, (8) is determined by the ground state(s) $|0\rangle$ of H. In particular, (8) becomes

$$x_{\mathrm{st}} = \lim_{t\to\infty}\langle X(t)\rangle = \langle s|X|0\rangle \tag{9}$$

in the case of a non-degenerate ground state $|0\rangle$.

In summary, when we want to study properties in the stationary state of a stochastic system we are in need of a (real-space) RG which is suitable for the ground state of quantum spin systems. In the next section, such an approach will be presented.

3. Ground state renormalization for quantum spin systems

The real-space RG method which we will employ in this work is known as the standard or SLAC (after the Stanford Linear Accelerator, where the technique was introduced [18]) approach. It was used a lot in the early 1980s to study ground state properties of several quantum spin and fermion chains (for a review, see [29]). As usual in real-space RG methods, the lattice is divided into cells, each containing b sites. The Hamiltonian H is then divided into an intracell part H_0 and an intercell part V. If α labels the cells, one can in the particular case of one dimension write

$$H = \sum_\alpha (H_{0,\alpha} + V_{\alpha,\alpha+1}). \tag{10}$$

As a first step, the Hamiltonian within one cell $H_{0,\alpha}$ is diagonalized exactly. Let $H_{0,\alpha}$ have eigenvalues $E_{n,\alpha}$ with corresponding right (left) eigenvectors $|n\rangle_\alpha$ ($_\alpha\langle n|$). One then selects two low-lying eigenstates (for example, the ground state $|0\rangle_\alpha$ and the first excited state $|1\rangle_\alpha$) and considers them as effective spin states for the cell: $|+_\alpha\rangle' = |0\rangle_\alpha$ and $|-_\alpha\rangle' = |1\rangle_\alpha$. Renormalized lattice states $|\sigma\rangle'$ can then be constructed by making tensor products over all cells: $|\sigma\rangle' = \otimes_\alpha|\sigma_\alpha\rangle'$. These states span a $2^{L/b}$-dimensional vector space $\mathcal{W}$.

The renormalization transformation, which always involves an elimination of degrees of freedom, is now performed by projecting the original Hamiltonian onto $\mathcal{W}$. Mathematically this is achieved by introducing a $2^L \times 2^{L/b}$-matrix T_2 whose columns contain the vectors $|\sigma\rangle'$ together with a $2^{L/b} \times 2^L$-matrix T_1 whose rows contain the vectors $'\langle\sigma|$ (which are constructed

from the left eigenvectors of $H_{0,\alpha}$). In all the cases we have encountered it was possible† to normalize the left and right eigenvectors in such a way that

$$T_1 T_2 = 1 \tag{11}$$

where 1 is the identity operator on $\mathcal{W}$.

Then the renormalized Hamiltonian H' is defined as

$$H' = T_1 H T_2. \tag{12}$$

The transformation (12) will define a mapping in the parameter space $\vec{w}' = f(\vec{w})$, from which fixed points and critical exponents can be determined as we will explain further below.

The procedure which was defined above at first sight seems to be rather *ad hoc* and non-perturbative. Further insight into the method was obtained when its relation with more conventional real-space RG approaches was discovered [28]. These approaches [25, 26] work at finite temperature T and are a direct extension of the Niemeijer–Van Leeuwen [27] real-space approach to the case of quantum spin systems. As in the SLAC approach $H_{0,\alpha}$ is diagonalized exactly, while the intercell interaction is treated in a perturbative way, taking into account in an appropriate way the fact that H_0 and V generically do not commute. In [28] it was shown that if one starts from such a finite-temperature approach, makes an expansion *to first order* in V, and then takes the limit $T \to 0$, one recovers the SLAC approach. This relation is useful for several reasons. First and most importantly, it shows that the SLAC approach is perturbative and one obtains a procedure to calculate higher-order corrections. Secondly, since the finite-temperature RG is constructed to conserve the partition function, one is guaranteed that for $T \to 0$ the ground state energy is conserved. In practice however, any real calculation is limited to a finite order in V so that the ground state energy is only approximately conserved.

Going back to reaction–diffusion systems, which are non-equilibrium systems, we are thus guaranteed that our RG approach conserves the ground state energy. Using (9) this can be written as

$$\langle s|H|0\rangle = {}'\langle s|H'|0\rangle'. \tag{13}$$

In principle, we also have a recipe to calculate perturbative corrections to the SLAC approach. In this paper, we will limit ourselves to calculations in first order. Higher-order corrections usually lead to a proliferation of terms in the Hamiltonian. However, as we will discuss in our conclusions, the existence of these higher-order terms will be necessary for a proper study of the BARW with $m = 2$, or for any other model in which H contains terms involving three or more sites. Since our calculation only goes to first order, (13) only holds approximately.

We now turn to a discussion of how steady state properties can be determined from the RG mapping $\vec{w}' = f(\vec{w})$. To fix ideas, let us assume that this equation has a non-trivial fixed point at $\vec{w} = \vec{w}^\star$, with one relevant scaling field (which in linear approximation is proportional to $\Delta w_1 = w_1 - w_1^\star$) whose scaling dimension is y_{w_1}. From standard RG theory it then follows that, near criticality, the correlation length ξ will diverge as $\xi \sim |\Delta w_1|^{\nu_\perp}$ with $\nu_\perp = 1/y_{w_1}$.

In general, it will be so that after renormalization $w_0' \neq 1$. Hence time needs to be rescaled again, which is achieved by dividing H' by w_0'. The number $w_0'(\vec{w}^\star)$ therefore teaches us how time rescales under a rescaling of space. We can use this quantity to calculate the exponent z as

$$w_0'(\vec{w}^\star) = b^{-z}. \tag{14}$$

† In the case that the ground state of the cell Hamiltonian is degenerate this is trivial to do. Otherwise, it is necessary to work with a linear combination of the ground state and an excited state which amounts to performing a similarity transformation.

From $\nu_\perp$ and z, scaling [30] gives us the exponent $\nu_\parallel = \nu_\perp / z$ which determines the divergence of the relaxation time near the critical point.

Next, we turn to the calculation of the particle density $c_{\rm st}$. If we introduce a (non-stochastic) Hamiltonian $\tilde{H} = H + hC_i$ (i arbitrary) we can, for a *translationally invariant* system write

$$c_{\rm st} = \langle s|C_i|0\rangle = \frac{\partial \langle s|\tilde{H}|0\rangle}{\partial h}(h=0). \tag{15}$$

Next, we renormalize $\tilde{H}$, using (12). The simplest possible case is the one in which the renormalization of the operator C_i does not involve other operators so that $T_1 C_i T_2 = a(\vec{w})C_\alpha$. Thus $\tilde{H}' = H' + h'C_\alpha$ with $h' = a(\vec{w})h$. Inserting this result into (15), and using (13), we obtain (where we now explicitly denote the dependence of $c_{\rm st}$ on the transition rates)

$$\begin{aligned} c_{\rm st}(\vec{w}) &= \frac{\partial h'}{\partial h} \cdot \left[\frac{\partial' \langle s|\tilde{H}'|0\rangle'}{\partial h'}(h'=0) \right] \\ &= a(\vec{w}) c_{\rm st}(\vec{w}'). \end{aligned} \tag{16}$$

This relation can be iterated along the RG flow, and hence the density of particles can be obtained as an infinite product if one knows the density at the fixed point $\vec{w}_t^\star$ which attracts $\vec{w}$ (where the t reflects the fact that this attractive fixed point is trivial and not critical):

$$c_{\rm st}(\vec{w}) = \left[\prod_{i=0}^{\infty} a(\vec{w}^{(i)}) \right] c_{\rm st}(\vec{w}_t^\star). \tag{17}$$

In principle correlation functions can be calculated in a similar way.

Near the critical fixed point $\vec{w}^\star$ we get, from (16), for the singular part of $c_{\rm st}$ (to leading order in Δw_1)

$$c_{\rm st}(\Delta w_1) = a(\vec{w}^\star) c_{\rm st}(b^{y_{w_1}} \Delta w_1). \tag{18}$$

From this relation we see that $a(\vec{w}^\star)$ determines the rescaling of the particle density at criticality. We write $a(\vec{w}^\star) = b^{D-d}$ where D can then be interpreted as the fractal dimension of the sites that are occupied by particles at criticality. Finally, from (18) we get the behaviour of the particle density close to the critical point as

$$c_{\rm st}(\Delta w_1) \sim (\Delta w_1)^{(d-D)/y_{w_1}} \tag{19}$$

so that we obtain the scaling relation $\beta = (d - D)\nu_\perp$. Finally, θ can be obtained from the scaling relation $\theta = \beta/\nu_\parallel$ [30].

It is straightforward to extend these reasonings to the case where the transformation of C_i is more complicated.

We thus see that a complete characterization of the stationary state particle density and of all the critical properties of the system can be obtained from our RG approach. In the next two sections we test our method on simple stochastic systems. The first one is an exactly solvable reaction–diffusion system with a trivial transition. The second one is the well known contact process which has a non-trivial transition thought to be in the DP universality class.

4. Renormalization for a simple reaction–diffusion system

We consider a model with diffusion, decoagulation (which is the process $A + \emptyset \to A + A$, $\emptyset + A \to A + A$) and coagulation. We will use the diffusion rate to fix the time scale, so that our model has two independent rates which we will denote as w_1 (decoagulation) and w_2

(coagulation). The local Hamiltonian $H_{i,i+1}$ in this case can most conveniently be written as a 4×4-matrix:

$$H_{i,i+1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1+w_1 & -1 & -w_2 \\ 0 & -1 & 1+w_1 & -w_2 \\ 0 & -w_1 & -w_1 & 2w_2 \end{pmatrix} \tag{20}$$

or in terms of the matrices (4) as

$$\begin{aligned} H_{i,i+1} = {} & 2w_2(n_i n_{i+1}) + (1+w_1)(n_i v_{i+1} + v_i n_{i+1}) \\ & -s_i^+ s_{i+1}^- - s_i^- s_{i+1}^+ - w_2(s_i^+ n_{i+1} + n_i s_{i+1}^+) - w_1(n_i s_{i+1}^- + s_i^- n_{i+1}). \end{aligned} \tag{21}$$

With a similarity transformation this Hamiltonian can be mapped onto that of a free fermion system [31], from which many exact results can be obtained.

To renormalize this model, we take $b = 2$, so that $H_{0,\alpha}$ equals (21). The spectrum of $H_{i,i+1}$ can be calculated trivially. The ground state is doubly degenerate and we identify the corresponding eigenstates as effective spin states. In particular, we have (we use spin language where $|+\rangle$ ($|-\rangle$) denotes a vacancy (an A-particle))

$$\begin{aligned} |+\rangle' &= |++\rangle \\ {}'\langle +| &= \langle ++| \\ |-\rangle' &= \frac{1}{N}[|+-\rangle + |-+\rangle + r|--\rangle] \\ {}'\langle -| &= \langle +-| + \langle -+| + \langle --| \end{aligned} \tag{22}$$

where $r = w_1/w_2$ and $N = 2 + r$. Notice that we normalize the states as probability vectors (and not quantum mechanically).

Next, we calculate H' using (12). We find that the renormalized Hamiltonian contains the same terms as (21). Moreover, the transformation conserves the stochasticity condition. The renormalized diffusion rate is $1/N$. We divide the Hamiltonian by this factor (rescaling of time). Then H' has completely the same form as H but with renormalized values for w_1 and w_2. The RG equations for w_1 and w_2 are

$$w_1' = w_1 \frac{1 + w_1 + w_2}{w_2} \tag{23}$$

$$w_2' = w_2 \frac{1 + w_1 + w_2}{2w_2 + w_1}. \tag{24}$$

The flow generated by these equations is shown in figure 1. There is a fixed point at $w_2 = 1$, $w_1 = 0$ (pure coagulation fixed point). The line $w_2 = 1$ is an invariant line. The RG equations, linearized at the fixed point, have one relevant eigenvalue (which leads to $y_{w_1} = 1$), together with an irrelevant eigenvalue.

Next, we turn to a calculation of particle density in the stationary state using the scheme outlined in the previous section. Projecting C_i onto $\mathcal{W}$ we find the simple recursion

$$(C_i)' = \frac{1+r}{N} C_\alpha. \tag{25}$$

From this we have

$$a(w_1, w_2) = \frac{1 + w_1/w_2}{2 + w_1/w_2}.$$

Since also w_1'/w_2' depends only on the ratio w_1/w_2 we arrive at the conclusion that the particle density only depends on that ratio. Its precise value can then be calculated by making a product of $a(w_1, w_2)$ along the RG flow. From figure 1 we see that all points with $w_1 > 0$ flow to

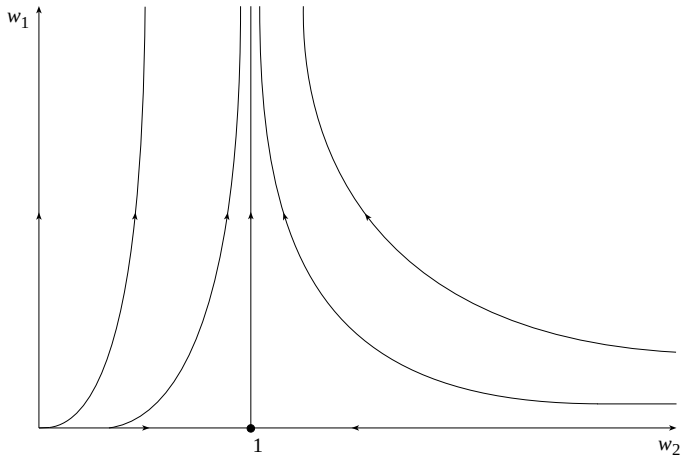

Figure 1. Schematic RG flow in the (w_1, w_2)-plane.

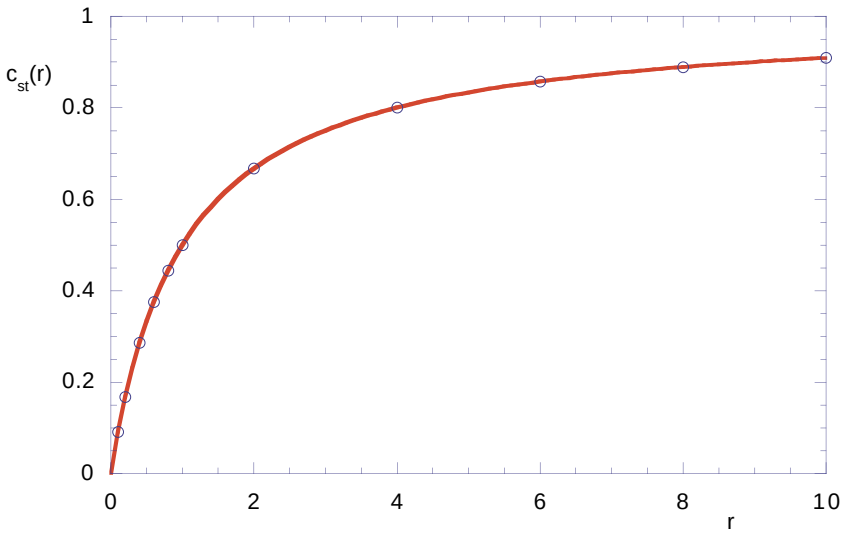

Figure 2. Particle density in the stationary state of the diffusion, coagulation, decoagulation model. The full curve represents the exact result, the circles are the RG results.

points where $w_1/w_2 \to \infty$. In that limit $c_{\rm st} = 1$. Then, using (17) we can obtain the particle density. In figure 2 we plot the result for $c_{\rm st}$ as a function of r together with the exact result [31]

$$c_{\rm st}(r) = \frac{r}{r+1}. \tag{26}$$

Within the numerical accuracy, both results coincide. Hence it seems that we recover the exact result! This might seem surprising since our calculation is only precise to first order in V. With hindsight the accuracy of our result can be understood by the fact that the ground state of the whole system is a product of one-particle states. Nevertheless, this calculation illustrates nicely the use of the method. Moreover, it gives an RG flow for the problem which cannot be obtained in any other way.

To conclude this section, we calculate the exponent β which determines the behaviour

of c_{st} near $r = 0$. From the exact result (26), one obviously has $\beta = 1$. On the other hand, from (25), we have $a(0, 1) = \frac{1}{2}$, hence $D = 0$ and using $y_{w_1} = 1$ we recover the exact result $\beta = 1$.

At this place it is appropriate to mention that for other simple reaction–diffusion systems we can also recover exactly known results. An example is a model with diffusion, decoagulation and death (which is the process $A + \emptyset \to \emptyset + \emptyset$, $\emptyset + A \to \emptyset + \emptyset$). This model undergoes a first-order transition [31]. When the decoagulation rate is greater then the death rate, $c_{st} = 1$, whereas when the opposite inequality holds, one has $c_{st} = 0$. The RG recovers this exact result. As usual, the first-order transition is controlled by a discontinuity fixed point.

We also recover an exact result for a model with diffusion, annihilation and pair creation $\emptyset + \emptyset \to A + A$. An exact solution, first obtained by Rácz [32], shows that c_{st} grows with the square root of the pair creation rate. The same power is found within our RG method.

5. The contact process

The contact process was originally introduced as a simple model for an epidemic [33]. In that interpretation a particle corresponds to a sick person, and a vacancy to a healthy individual. In the process particles can disappear ($A \to 0$) with a rate $w_0 = 1$. Empty sites can become occupied with a rate $\lambda z/2$, where z is the number of occupied neighbours of the empty site (this represents contamination in epidemic terms). This model cannot be solved exactly, but its critical exponents are known to high accuracy [4]. On the basis of numerical data, and from symmetry arguments, it is generally believed that the model is in the DP universality class [34, 35].

The Hamiltonian corresponding to this model contains one-site terms (for the process $A \to 0$) and two-site terms (for the contamination process). The local Hamiltonian for the model is

$$H_{i,i+1} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & \lambda/2 & 0 & -1 \\ 0 & 0 & 1+\lambda/2 & 0 \\ 0 & -\lambda/2 & -\lambda/2 & 1 \end{pmatrix}. \tag{27}$$

We will split the whole Hamiltonian in such a way that $H_{0,\alpha}$ contains the same number of two-site contribution as one-site terms. Then, the same holds for V. This guarantees, at least for the contact process, that the ground state of the intracell Hamiltonian is a doublet. These states are then the natural candidates to be used as effective cell spins.

We will perform a renormalization for this process using a cell with $b = 3$. The calculation is straightforward and can most effectively be done using Mathematica. It came as a surprise to us that also in this case, there is no proliferation of interactions in the renormalized Hamiltonian. The RG equation for λ is

$$\lambda' = \frac{\lambda^3(2+\lambda)(8+10\lambda+4\lambda^2+\lambda^3)}{4(16+40\lambda+37\lambda^2+18\lambda^3+4\lambda^4)}. \tag{28}$$

This equation has one non-trivial repulsive fixed point at $\lambda = \lambda^\star = 3.223\,19$. This value is surprisingly close to the best known numerical value for the contact process which is $\lambda_c = 3.2978$ (all numerical results are taken from [36]). From a linearization of the RG equation near the fixed point, we obtain $y_\lambda = 0.8886$, from which we obtain $\nu_\perp = 1.1253$, to be compared with the numerically determined value of 1.0972.

Finally, we need to determine D. As explained in section 3, one therefore has to renormalize the operator C_i. In a cell with $b \geqslant 3$ there is no translational invariance and hence the density of particles depends on the particular value of i that is chosen. This choice

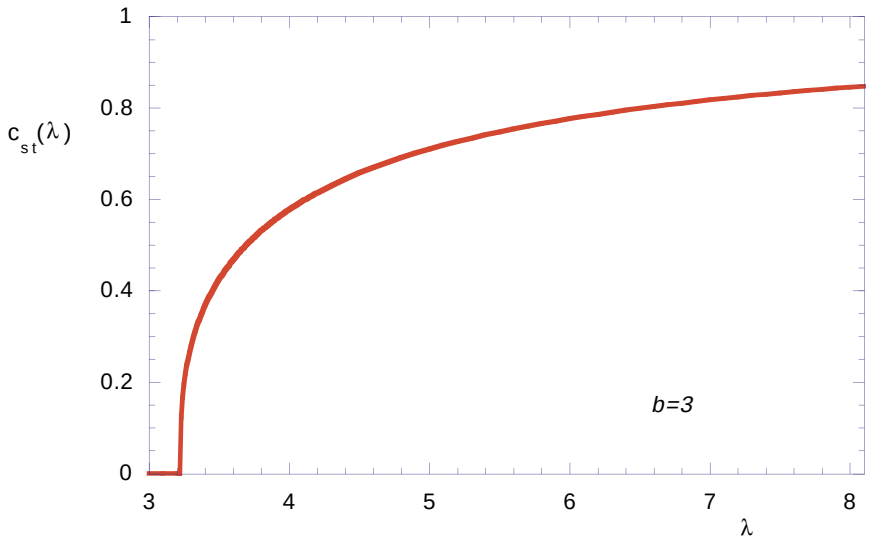

Figure 3. Particle density in the stationary state of the contact process as obtained from the RG approach.

can be made in several ways. Either one projects the operator C_m where m is a site at or near the middle of the cell. Alternatively we can take an 'average' operator C_a:

$$C_a = \frac{1}{b}\sum_{i=1}^{b} C_i.$$

We have performed both calculations. They give respectively $D = 0.6391$ and $D = 0.6940$, from which we obtain $\beta = 0.4061$, respectively $\beta = 0.3444$. These values should be compared with the precise numerical estimate $\beta = 0.2769$. Other exponents can be obtained using scaling relations. We get $\nu_\parallel = 1.6409, \theta = 0.2099$ whereas the best known values are $\nu_\parallel = 1.736, \theta = 0.1597$. We thus see that, taking into account the smallness of the cell considered, our estimates of λ_c and all critical exponents are close to the known values.

In figure 3 we finally plot $c_{\rm st}(\lambda)$ as obtained from our RG approach.

We are currently extending our calculations for the contact process to larger cell sizes. We hope that our approach, combined with suitable extrapolation techniques, is able to give very precise estimates of critical exponents.

6. Conclusions

In this paper we have investigated the applicability to reaction–diffusion processes of a quantum real-space RG method. We first studied simple processes for which exact information is available. In three cases, these exact results are reproduced in calculations done on very small cells.

For the contact process, which contains a non-trivial critical point, rather accurate estimates for the location of the critical point and for critical exponents are obtained from a calculation on a cell of three sites.

So far, we encountered one system in which the RG predicted wrong results. This is a model with diffusion, coagulation and birth ($\emptyset + \emptyset \to \emptyset + A$, $\emptyset + \emptyset \to A + \emptyset$). When

the diffusion rate equals the coagulation rate, this model belongs to a class which is, at least partially, integrable [37]. For small birth rates w_3, $c_{\rm st}$ is known to grow as $w_3^{1/3}$. The application of our technique to that model raised several difficulties. The ground state of $H_{0,\alpha}$ is a singlet, and for the first excited state there is a crossing of energy levels (in finite systems). Hence, there is no obvious choice for the effective cell states. For a specific choice we made, the renormalized Hamiltonian H' turns out to have a form different from the original Hamiltonian H, but there is a similarity mapping this H' onto H with renormalized couplings, and an extra decoagulation term. If we define the full RG as the projection (12), followed by the similarity we are able to obtain a flow in parameter space. Unfortunately, our results indicate that for cells with $b = 2$ and $b = 3$, $c_{\rm st}$ grows as $w_3^{1/2}$. We hope to clarify the RG for this model in the future.

Recently, several authors ([15–17]) applied the DMRG to non-equilibrium systems. The first two papers studied exclusion processes while in the third work two reaction–diffusion systems were studied. For the few cases studied so far, the DMRG is found to produce accurate results for correlation functions and critical exponents. In order to get results of the same accuracy using our real-space approach it is necessary to go to larger cell sizes. We are currently performing such a calculation for the contact process. It is our hope that in this way, and using good extrapolation techniques, it is possible to produce estimates for critical exponents of the same accuracy as that obtained from the DMRG. Moreover, our method allows the calculation of RG flows which are very helpful in deciding questions on universality, relations between different models and so on. To our knowledge such information cannot be obtained from the DMRG.

Another project we hope to carry through is a study of the BARW with $m = 2$. As stated in the introduction, there are few reliable analytical results on the critical properties of this system. A particularly nice model that is known to be in this universality class was introduced by Menyhárd. It is a non-equilibrium Ising model (NEKIM) with Glauber dynamics at zero temperature and Kawasaki dynamics at infinite temperature [38]. It was recently shown that this model is selfdual [39]. The ground state energy of the quantum Hamiltonian corresponding with this model is for all finite systems again doubly degenerated, so that effective cell states can be defined unambiguously. The quantum Hamiltonian for the NEKIM contains a three-site interaction term. Under the RG, performed to first order, such a term will be mapped onto a two-cell interaction term. However, by extending the SLAC-approach to second order in V, as discussed in section 3, one could generate a renormalized three-cell interaction. In fact, from a mathematical point of view, the Hamiltonian of the NEKIM is rather similar to that of a transverse Ising model with three spin interactions [40, 41]. That model also has a self-duality and was renormalized successfully by using our approach to second order [42]. An alternative model in the universality class of the even-m-BARW is a recently introduced variant of the contact process in which particles disappear and are contaminated in pairs [43]. Since this model does not involve any diffusion, it may be simpler to analyse.

While the technique presented here allows the calculation of some dynamic properties (such as the exponents z and θ) it is at present not at all clear whether it is possible to say anything about early time critical exponents. One must take into account that even for equilibrium critical phenomena no good real-space approach to dynamical aspects has been developed.

It has of course to be admitted that real-space RG methods in general involve some ill understood approximations. Furthermore, as the well known saying by K Wilson 'One cannot write a renormalization cookbook' indicates, it is not *a priori* possible to indicate for which systems an approach such as the one presented here can be succesful. For each model one has to investigate independently how to perform the RG, taking into account all known symmetries,

dualities and so on.

Nevertheless, it is our opinion that the results presented here give considerable hope that our RG can succesfully be used to further understand the critical behaviour of non-exactly-solved systems such as the BARW.

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Note added in proof. The steady state density c_{st} for the simple reaction–diffusion system considered in section 4 can be obtained exactly from the RG approach. The recursion relation for $r = w_1/w_2$ is $r^{(n+1)} = r^{(n)}(r^{(n)} + 2)$ (where $r^{(n)}$ is the nth iterate of r) while $a(r) = (1 + r)/(2 + r)$. Defining $G_n(r) = \prod_{i=0}^{n} a(r^{(i)})$ one can see that for $r > 0$

$$\frac{1+r}{r} G_n(r) = 1 + \frac{1}{r^{(n+1)}}.$$

Since $r^{(n)} \to \infty$ for $n \to \infty$, we recover the exact result (26) $c_{\mathrm{st}} = r/(r + 1)$. We thank an anonymous referee for pointing out this derivation.

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