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Abstract

We investigate the survival probability of immobile targets, which get annihilated by random walkers (RWs) at first encounter. We focus on scale-free networks (SFNs) and on small world networks (SWNs) as examples of irregular lattices. On SFNs we consider degree distributions (DDs) with long time tails. Interestingly, it turns out that the survival probability and the quality of its description through the average number of distinct sites visited, S_n, depend on the details of the DD: SFNs which are more ramified have survival probabilities which are more regular, whereas SFNs with long chain-like segments display decay laws similar to those of SWNs, where a description only in terms of S_n is rather poor.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Chemical reactions under diffusion-limited conditions have been extensively studied based on random walk models. Remarkably, such studies show spectacular deviations from the simple chemical decay laws, especially in low-dimensional spaces and on disordered lattices [1–8], as summarized in [9–13].

Of particular relevance in such studies is the $A + B \rightarrow B$ reaction, especially when one of the species is immobile. In the case that the As are immobile one has the target reaction [14] and in the case that the Bs are immobile the trapping reaction [4, 9, 10, 12, 15]. Mixed situations, in which both species move, have also been investigated [8–10]. The target problem can now be solved exactly on regular lattices of arbitrary dimensions [6, 14, 16, 17], and the solution can be extended to regular ultrametric spaces (UMSs) and to Cayley trees [10, 11, 18]. This situation contrasts strongly with the findings for the trapping problem where, apart from the one-dimensional case [9, 12], no exact solution in closed analytical form is known.

Recently, much interest arose in the study of complex graphs such as small world networks (SWNs) [19–29] and scale-free networks (SFNs) [15, 30–33], which are used to describe complex, disordered systems. SFNs are characterized by lacking a characteristic

node connectivity and by the presence of 'hubs', vertices with many bonds attached to them. Hence such hubs are connected to a large number of other vertices. In [34] we analysed the target problem on SWNs [19–29]. Interestingly, the target decay on SWNs turned out to be anomalous, in that at longer times the closed-form expressions valid for regular lattices do not hold anymore [34]. Even more interesting situations are found for target reactions on SFNs, as we proceed to show. In the following we determine numerically the target decay on SFNs and confront it to the results for other network types and for the trapping reaction [15].

2. Target problem

Let us recall the basic features of the target problem. As stated, it belongs to the $A + B \to B$ reactions, and in it the B molecules move independently of each other, while the A molecules are held fixed [14, 16–19, 35, 36]. Now, it turns out that for several regular lattice types the decay law Φ_n of the A targets as a function of the number n of steps can be determined analytically. Thus, if the Bs are initially randomly placed over the lattice, with average occupation q, their local spatial distribution is Poissonian, so that at each site the probability d_j of finding exactly j walkers is $d_j = q^j \exp(-q)/j!$. Then for translationally symmetric lattices the decay law of the targets is [6, 16]

$$\widetilde{\Phi}_n \equiv \exp[-q(S_n - 1)]. \tag{1}$$

In (1), S_n is the mean number of distinct sites visited by a walker in n steps. For regular lattices, in one dimension one has $S_n \sim \sqrt{n}$, and in dimensions higher than two, $S_n \sim n$. In the latter case S_n grows linearly with n, which implies that in the long run the probability for the random walker to visit a new site is constant and independent of n. As was shown in [19], a relation similar to (1) also holds approximately for target reactions on SWNs, for very small q and small to moderately large n. On the other hand, for larger values of q and longer times there are large discrepancies between the $\widetilde{\Phi}_n$ of (1) and the target decay Φ_n on SWNs [34].

The proof of the fact that (1) is exact on several types of regular lattice can be readily seen. Here we follow the approach given in [14, 16, 19, 34]. One starts from the probability that a particular immobile target (which is annihilated if any walker visits its site k) survives the first n time steps. Denoting by $H_{ki}(n)$ the probability that a walker which starts at i reaches the site k during the first n steps, the probability $\zeta_k(n)$ that the target at site k survives the first n time steps when initially there are j_i walkers at site i is [6, 16]

$$\zeta_k(n) = \prod_{i,i\neq k} [1 - H_{ki}(n)]^{j_i}. \tag{2}$$

Taking now that the j_i follow the distribution d_j leads for each term in the product of (2) to

$$\sum_{j=0}^{\infty} [1 - H_{ki}(n)]^j q^j \, \mathrm{e}^{-q}/j! = \mathrm{e}^{-1} \exp[q(1 - H_{ki}(n))] = \exp[-q H_{ki}(n)] \tag{3}$$

and $\zeta_k(n)$ averaged over all initial walker distributions reads

$$\phi_k(n) = \exp[-q\Theta_k(n)], \tag{4}$$

where the quantity

$$\Theta_k(n) \equiv \sum_{i,i\neq k} H_{ki}(n) \tag{5}$$

was introduced. In (4), as in [6, 16], the average over all initial walker distributions and their motion can be performed exactly. However, $\phi_k(n)$ depends on the particular lattice type and on the site k of the target. For a very regular network, on which both the site connectivities and

also the return probabilities to each site have site-independent values, the quantities $H_{ki}(n)$ are symmetric [14, 19], $H_{ki}(n) = H_{ik}(n)$. From this it follows that [14, 19]

$$\Theta_k(n) = \sum_{i,i\neq k} H_{ki}(n) = \sum_{i,i\neq k} H_{ik}(n) = S_n - 1, \tag{6}$$

where S_n, the mean number of distinct sites visited by a walker during the first n steps, is also independent of k. Inserting (6) into (4) (and noticing that all sites k are then equivalent) leads to (1), as claimed above. Now, on regular crystal lattices, on infinite Cayley trees, and also on regular ultrametric spaces, all sites are equivalent [16, 37–40]. Hence (1) holds for them exactly [6, 14, 16, 17]. On the other hand, the situation is different for SWNs and for SFNs.

3. Scale-free networks

Now, the degree k of a site is the number of bonds emanating from it (or, equivalently, the number of its nearest neighbours). For SFNs one usually assumes for the distribution of degrees (DD) a power-law:

$$\bar{p}_k \sim k^{-\gamma}, \tag{7}$$

where $\bar{p}_k$ is the probability that the degree is k and γ is a parameter that measures how densely connected the network is.

Now, there are many ways in which such a DD (which should obey (7) for large k) may be postulated. One may assume (7) to hold strictly for all $k = 1, 2, 3, \ldots$. Then

$$p_k = \frac{k^{-\gamma}}{\sum_{j=1}^{\infty} j^{-\gamma}}. \tag{8}$$

If on the other hand (7) holds starting from, say, only $k = 2$ (and also assuming, exemplarily, that $p_1 \equiv 0$) one obtains, instead of (8),

$$p_k = \frac{k^{-\gamma}}{\sum_{j=2}^{\infty} j^{-\gamma}}. \tag{9}$$

This DD also obeys (7). As we will see in the following, however, the properties of SFNs obtained from (8) and from (9) differ.

Let us now turn to the construction of a particular realization of an SFN. We start with vertex 1 and pick its degree randomly according to one of our specified DDs, say (8) or (9). Then we create new (open) vertices at the end of all the bonds. Picking one of such open vertices randomly, we continue the process until no new bonds can be added.

In figure 1 we display an SFN with $N = 36$ vertices obtained from (8). The numbering is according to the chronological order in which the vertices are created. We start from the position 1. From the DD given by (8) we pick the functionality of this vertex (which in figure 1 turns out to be one) randomly and we create one new open vertex, labelled 2. After this step we pick at random one of the open vertices present (now we have only one open vertex, namely vertex 2). Its functionality is then obtained from the distribution p_k, given by (8). If its functionality turns out to be one, then to this vertex no new vertex will be added and the vertex turns into a closed one. Otherwise, (as is the case here, since the functionality of vertex 2 is three) new open vertices are created. The process is iterated by picking another open vertex randomly.

In figure 2, for comparison, we display an SFN with $N = 35$ vertices, obtained from the DD (9). One can note that in figure 1 there are only two open vertices; on the other hand, by construction, in figure 2 all peripheral vertices are open. Also figure 1 is quite branched,

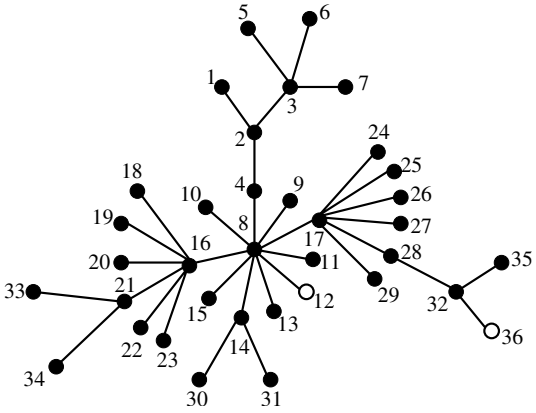

Figure 1. An example of a scale-free network with $N = 36$ and $\gamma = 2.5$. The construction follows the degree distribution (8); the white circles are the open vertices.

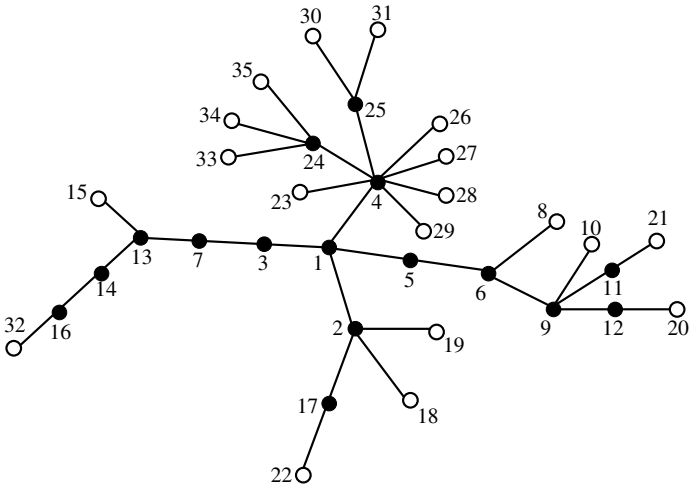

Figure 2. An example of a scale-free network with $N = 35$ and $\gamma = 2.5$. The construction follows the degree distribution (9); the white circles are the open vertices.

reminiscent of an irregular Cayley tree. Figure 2 has somewhat longer, chain-like segments between the branching points than figure 1.

Due to the limited time and memory resources available, we restrict the size of every SFN we use, i.e. the total number of its vertices, to a preset value $N_{\max}$. Now, under the DD (8) it often happens that the SFN construction stops at N vertices, with $N < N_{\max}$. This is due to the fact that with (8) many vertices have degree one. In such a case we discard the SFN with $N < N_{\max}$ and start the construction anew. On the other hand, under (9) every vertex has at least two neighbours, so that the construction never stops by itself. Then, when we reach $N_{\max}$ we stop the growth by assigning to all remaining open vertices the degree one. We remark that for $N_{\max}$ large the construction of SFNs using (8) is very time consuming, because many SFNs have to be discarded before we obtain a structure with $N = N_{\max}$.

In figure 3 we plot the degree distribution for 50 structures obtained from (8) and (9) for $\gamma = 2.5$ and $N = 100\,000$, leaving out for (9) the contribution of the peripheral beads of degree one. Figure 3 shows that the expected scaling (7) is well obeyed.

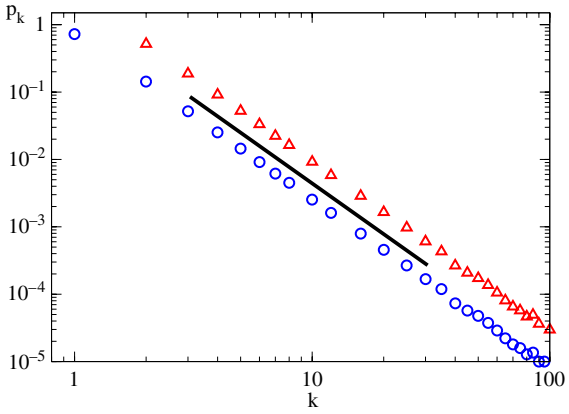

Figure 3. The degree distribution found by constructing 50 structures, containing each 100 000 vertices. The structures are obtained for $\gamma = 2.5$, using (8) (circles) or (9) (triangles). In the case (9) only the interior beads are accounted for; see the text for details. The slope 2.5 is indicated by a straight line.

4. Simulations and results

We evaluate the target decay Φ_n on SFNs through direct simulations, which we then compare to (1), calculated based on S_n. The simulations proceed in a direct way, by randomly placing walkers on the SFNs according to the parameter q. In the beginning all sites that are not occupied by walkers are taken to be targets. Each random walker moves at every time step from the site i which it occupies to one of its neighbouring sites j. We assume that all possibilities of leaving a given site are equally probable. A reaction act occurs at the first encounter of a target by any of the walkers. The survival probability Φ_n of the targets is given by simply counting the number of remaining targets after n steps. For the simulations we used the random number generator RANDOM_NUMBER, from FORTRAN. We took SFNs of size $N = 10^5$ and averaged over 50 different realizations of the process; for each realization, a new SFN was created, the walkers were randomly placed on it, unoccupied sites were assigned targets, and the walkers were then allowed to move. The decays obtained by this method are given in figure 4 for the DD (8) and in figure 5 for the DD (9). The results of the simulations are given by symbols, and we have indicated the standard deviations (vertical) obtained from the 50 realizations by error bars. In both figures γ is taken to be $\gamma = 2.5$, while for the average occupation we consider five cases, namely $q = 0.01$, $q = 0.02$, $q = 0.05$, $q = 0.1$ and $q = 0.2$.

For comparison we use $\widetilde{\Phi}_n$ given by (1). This expression, which for regular lattices is exact, will turn out to be only an approximation here. In the trapping process it is called the Rosenstock approximation [41, 42]. $\widetilde{\Phi}_n$ requires the knowledge of S_n, which we determine by averaging over 50 different realizations; over each of them 1000 different random walks are performed. Again we take the size of the SFNs to be $N = 10^5$ and randomly choose the starting position of the walker. In figure 4 the solid lines represent $\widetilde{\Phi}_n$. By comparing Φ_n to $\widetilde{\Phi}_n$ we can see that they agree rather well, especially for large values of q. This result is in good agreement with the study of the trapping problem over SFNs by Gallos [15], where it was shown that the Rosenstock approximation holds well. Gallos also used the DD (8) to create a set of vertices, which he then randomly combined into clusters, and chose as SFN the largest cluster from each realization [15]. It turns out that both for his construction and in our case here, with the DD (8), Φ_n provides a good description of the decay of the targets.

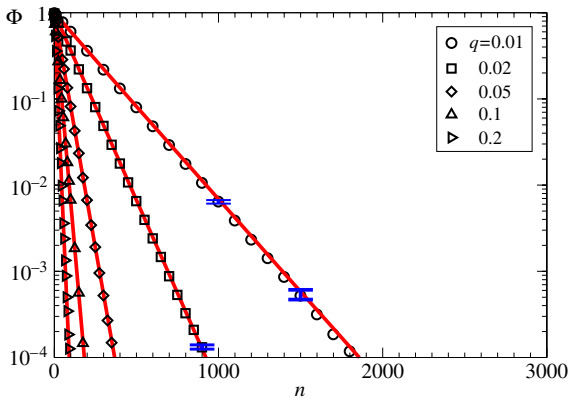

Figure 4. Target survival probabilities over SFNs (as a function of the number of steps n) determined by direct simulations (Φ_n, symbols) and by $\widetilde{\Phi}_n$, equation (1), solid lines. Here the degree distribution is given by (8) and the parameters are $N = 10^5$ and $\gamma = 2.5$. The average occupation is $q = 0.01, 0.02, 0.05, 0.1$ and 0.2 from above.

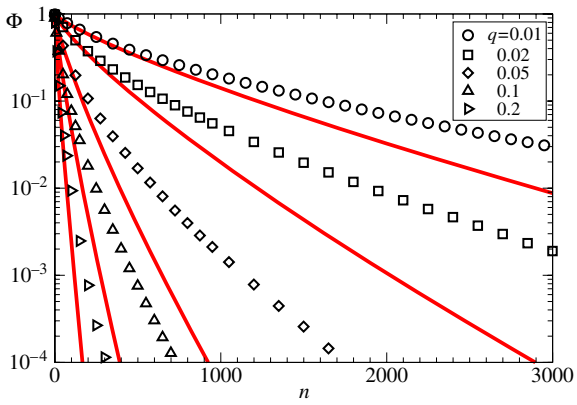

Figure 5. Same as in figure 4 for the degree distribution given by (9).

In figure 5, we plot the target decay Φ_n on SFNs using the DD (9). The procedure is similar to that leading to figure 4. To facilitate the comparison with the DD (8) we choose the same values for N, γ and q. In figure 5 the data for Φ_n are obtained from direct simulations for 50 different SFNs, while for the calculation of $\widetilde{\Phi}_n$ we took the same SFNs and performed 1000 random walks over each of them. We find that now the agreement between Φ_n and $\widetilde{\Phi}_n$ is considerably poorer. We attribute this fact mainly to the difference in the topologies obtained from the DD (8) and the DD (9). For example, under the DD (9) for internal vertices the degree two is dominant (see figure 3 and the sketch in figure 2), as is the case for a ring, which is the starting point of the SWNs to which we now turn.

For the target decay on SWNs we follow the steps of [19, 34, 43, 44]. The construction of the SWNs starts from a ring consisting of N vertices, where each vertex is connected to its two nearest neighbours and has thus degree two. Then to each vertex an additional link is added with probability p; this link ends with equal probability at any of the N sites of the ring (possibly the one it started from). Increasing p decreases the average (minimal) distance

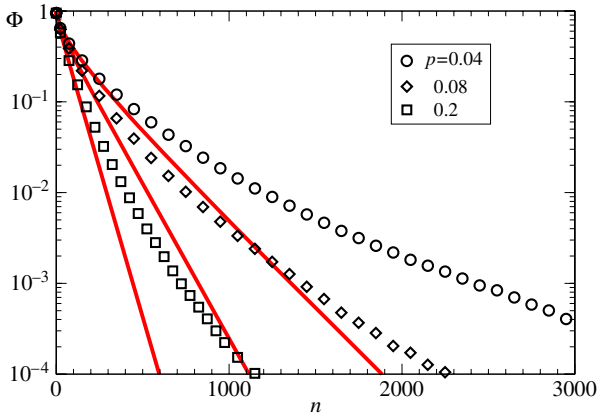

Figure 6. Target survival probabilities for SWNs (as a function of the number of steps n) determined by direct simulations (Φ_n, symbols) and by $\widetilde{\Phi}_n$, equation (1), solid lines. The parameters are $N = 10^5$, $p = 0.04, 0.08$ and 0.2 (from above) and the average occupation is $q = 0.05$.

between vertices on the ring. In figure 6 we plot the numerically determined Φ_n obtained from simulations over 50 SWNs of size $N = 10^5$, obtained by choosing $p = 0.04, 0.08$ and 0.2, while setting the average occupation equal to $q = 0.05$. We averaged over 50 different realizations of the target process, where for each realization a new SWN structure was created. The target decay obtained from simulations, Φ_n, is given by symbols, while we depict the decay of $\widetilde{\Phi}_n$ by solid lines. For $\widetilde{\Phi}_n$ we evaluated the corresponding S_n by taking the same SWNs and performing 1000 random walks over each structure. Our findings are in very good agreement with the previously published data (figure 1 of [34]), obtained using more extensive statistics. Noticeable is that under SWN conditions the departure of $\widetilde{\Phi}_n$ from Φ_n is considerable; this stresses the point that with increasing disorder one needs to go to higher cumulants of the decay distribution in order to represent Φ_n properly [34, 41].

5. Conclusions

In this work we focused on the target problem on scale-free networks (SFNs) and compared the obtained decay laws with the behaviour found for regular lattices and for SWNs. As in the case of SWNs and distinct from the situation for regular lattices, here we were not able to find the exact solution to the problem. The difficulty rests in the disorder inherent in the construction of SFNs, a situation akin to SWNs; such a disorder seems to preclude an exact solution along the lines of argument used for regular lattices. Distinct from the situation on SWNs, however, we sometimes find for SFNs decay forms which can be well understood in terms of S_n, the mean number of distinct sites visited by a random walk in n steps; this means that on particular SFNs the target problem is much closer to a mean-field behaviour than on SWNs. We hasten to note that a similar finding was reported in [15] with regards to the trapping problem. As is well known, the trapping problem is dominated at long times by rare events, which are notoriously difficult to handle. Here, for SFNs the target decay seems to follow the general pattern found for the decay due to trapping.

Evidently, the big problem is to determine (if possible, exact) solutions for chemical reaction schemes in the presence of disorder, as exemplified here by the underlying, irregular SWNs and SFNs.

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References

[1] Balagurov B Ya and Vaks V G 1973 *Zh. Eksp. Teor. Fiz.* **65** 1939
Balagurov B Ya and Vaks V G 1974 *Sov. Phys.—JETP* **38** 968 (Engl. Transl.)
[2] Donsker M D and Varadhan S R S 1975 *Pure Appl. Math.* **28** 525
Donsker M D and Varadhan S R S 1979 *Pure Appl. Math.* **32** 721
[3] Ovchinnikov A A and Zeldovich Ya B 1978 *Chem. Phys.* **28** 215
[4] Grassberger P and Procaccia I 1982 *J. Chem. Phys.* **77** 6281
[5] Toussaint D and Wilczek F 1983 *J. Chem. Phys.* **78** 2642
[6] Zumofen G, Blumen A and Klafter J 1985 *J. Chem. Phys.* **82** 3198
[7] Moreau M, Oshanin G, Bénichou O and Coppey M 2003 *Phys. Rev.* E **67** 045104
[8] Moreau M, Oshanin G, Bénichou O and Coppey M 2004 *Phys. Rev.* E **69** 046101
[9] Weiss G H and Rubin R J 1983 *Adv. Chem. Phys.* **52** 363
[10] Blumen A, Klafter J and Zumofen G 1986 *Optical Spectroscopy of Glasses* ed I Zschokke (Dordrecht: Reidel) p 199
[11] Blumen A and Köhler G H 1989 *Proc. R. Soc.* A **423** 189
[12] Weiss G H 1994 *Aspects and Applications of the Random Walks* (Amsterdam: North-Holland)
[13] ben-Avraham D and Havlin S 2000 *Diffusion and Reactions in Fractals and Disordered Systems* (Cambridge: Cambridge University Press)
[14] Blumen A, Zumofen G and Klafter J 1984 *Phys. Rev.* B **30** 5379
[15] Gallos L K 2004 *Phys. Rev.* E **70** 046116
[16] Zumofen G, Blumen A and Klafter J 1986 *J. Chem. Phys.* **84** 6679
[17] Szabo A, Zwanzig R and Agmon N 1988 *Phys. Rev. Lett.* **61** 2496
[18] Blumen A, Klafter J and Zumofen G 1986 *J. Phys. A: Math. Gen.* **19** L77
[19] Jasch F and Blumen A 2001 *Phys. Rev.* E **63** 041108
[20] Jasch F and Blumen A 2001 *Phys. Rev.* E **64** 066104
[21] Watts D J and Strogatz S H 1998 *Nature* **393** 440
[22] Newman M E J and Watts D J 1999 *Phys. Rev.* E **60** 7332
[23] Watts D J 1999 *Small Worlds: The Dynamics of Networks Between Order and Randomness* (Princeton, NJ: Princeton University Press)
[24] Moukarzel C F 1999 *Phys. Rev.* E **60** R6263
[25] de Menezes M A, Moukarzel C F and Penna T J P 2000 *Europhys. Lett.* **50** 574
[26] Barthélémy M and Amaral L A N 1999 *Phys. Rev. Lett.* **82** 3180
[27] Amaral L A N, Scala A, Barthélémy M and Stanley H E 2000 *Proc. Natl Acad. Sci. USA* **97** 11149
[28] Barrat A and Weigt M 2000 *Eur. Phys. J.* B **13** 547
[29] Monasson R 1999 *Eur. Phys. J.* B **12** 555
[30] Jasch F, von Ferber Ch and Blumen A 2004 *Phys. Rev.* E **70** 016112
[31] Newman M E J, Strogatz S H and Watts D J 2001 *Phys. Rev.* E **64** 026118
[32] Dorogovtsev S N, Mendes J F F and Samukhin A N 2001 *Phys. Rev.* E **63** 062101
[33] Albert R and Barabási A L 2002 *Rev. Mod. Phys.* **74** 47
[34] Jasch F and Blumen A 2002 *J. Chem. Phys.* **117** 2474
[35] Berezhkhovskii A M, Bicout D J and Weiss G H 1999 *J. Chem. Phys.* **110** 1112
[36] Argyrakis P and Kopelman R 2000 *Chem. Phys.* **261** 391
[37] Montroll E W and Weiss G H 1965 *J. Math. Phys.* **6** 167
[38] Köhler G H and Blumen A 1990 *J. Phys. A: Math. Gen.* **23** 5611
[39] Cassi D 1992 *Phys. Rev.* B **45** 454
[40] Cassi D 1989 *Europhys. Lett.* **9** 627
[41] Zumofen G and Blumen A 1982 *Chem. Phys. Lett.* **88** 63
[42] Rosenstock H B 1970 *J. Math. Phys.* **11** 487
[43] Blumen A and Jasch F 2002 *J. Phys. Chem.* A **106** 2313
[44] Jespersen S, Sokolov I M and Blumen A 2000 *J. Chem. Phys.* **113** 7652