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Survival Probability in One Dimension for the $A + B \rightarrow B$ Reaction with Hard-Core Repulsion

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We study the effect of hard-core repulsion (known as the bus effect) between B particles on the reaction-diffusion system $A + B \rightarrow B$ in the continuous-time random walk model in one dimension with the A particles stationary. We show rigorously that the survival probability of the A particles is asymptotically bounded as $C_1 \geqslant \lim_{t \rightarrow \infty}\{[-\log S(t)]/t^{0.5}\} \geqslant C_2$, where C_1 and C_2 are constants. We also do simulations to confirm our results.

KEY WORDS: Bus effect; random walk; survival probability; hard-core repulsion.

1. INTRODUCTION

The reaction $A + B \rightarrow B$ is one of the reaction-diffusion systems which has been extensively studied.[1-4] A point of interest in this system is the effect of the correlated motion of the particles on the survival probability of the A particles. An extreme case of this is the hard-sphere repulsion (also known as the bus effect) which prevents one particle from crossing over another.[5-7] Recently, Kuzokov and Kotomin[6] studied its effect in one dimension and came to the conclusion that the asymptotic survival probability gets appreciably altered from $\exp(-c\sqrt{t})$ without the bus effect to $1/t$ with the bus effect.

In this paper, we prove rigorously that the survival probability of A with the bus effect is less than or equal to that without the bus effect.

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Further, we obtain lower and upper bounds for the survival probability $S(t)$ of the A particles as

$$C_1 \geqslant \lim_{t \to \infty} \frac{-\log S(t)}{t^{0.5}} \geqslant C_2 \tag{1}$$

Here, C_1 and C_2 are constants depending on n_B, the concentration of B particles, but independent of time t. We also did simulations which confirm this result.

The system we consider is as follows. An A particle is kept stationary in a one-dimensional lattice. The B particles are initially randomly located at different lattice sites based on their concentration. They perform continuous-time random walks. These B particles make a transition to the lattice site at the right or left (with equal probability) with a transition rate of unity per unit time. Note that the results are valid for any transition rate D by using the dimensionless variable Dt. However, if the site to which the particle is to make a transition is already occupied by another B particle, the transition is forbidden and the former B particle remains wherever it was. Whenever an A and a B particle come onto the same lattice site, the A particle gets annihilated.

2. BOUNDS ON SURVIVAL PROBABILITY

Since it was not possible to obtain analytical results for the system mentioned above, we obtained bounds in terms of independent motion of the B particles. There are, therefore, two cases to be considered, first, the independent case where the B particles move independently, and second, the bus case where the B particles move with exclusion. In this section we prove that the probability of annihilation by time t using the bus effect is strictly greater than that without the bus effect. We also prove that this probability is smaller than that of independent particles using the rule that the jth particle (ordering the particles by their original placement from the origin) is annihilated when it reaches site $j-1$.

2.1. Upper Bound

We first prove that the survival probability of the A particle with the bus effect is in fact lower than that without it (that is, when the particles are executing independent motion). To prove this, let us take a stationary A particle at site 0 and two diffusing B particles B_1 and B_2 to its right. We define $\psi(t) = (\psi_1(t), \psi_2(t),..., \psi_i(t),...)^T$, where $i = (i_1, i_2)$ and $\psi_i(t)$ is the probability of finding B_1 at i_1 and B_2 at i_2 at time t. Then,

$$\frac{d\psi}{dt} = M'\psi \tag{2}$$

with $M' = M^T - I$. Here, M is the transition rate matrix for independent motion of the two B particles, I is the identity matrix, and M^T is the transpose of M. Here M is given by

$$M_{ij} = 0.5[\delta_{i_1, j_1}\delta_{i_2, j_2+1} + \delta_{i_1, j_1}\delta_{i_2, j_2-1} + \delta_{i_2, j_2}\delta_{i_1, j_1+1} + \delta_{i_2, j_2}\delta_{i_1, j_1-1}] \quad (3)$$

Equation (2) is to be solved with the boundary conditions $\psi_i(t) = 0$ for $i_1 = 0$ or $i_2 = 0$. For the case with the bus effect, let $\phi(t)$ and N' be the quantities corresponding to $\Psi(t)$ and M' above. Therefore,

$$\frac{d\phi}{dt} = N'\phi \quad (4)$$

with $N' = N^T - I$ and N is given by

$$N_{ij} \begin{cases} = M_{ij}, & i_2 \geqslant i_1 + 2 \\ = 0.5[\delta_{i_1, j_1}\delta_{i_2, j_2-1} + \delta_{i_2, j_2}\delta_{i_1, j_1+1} + 2\delta_{i_1, j_1}\delta_{i_2, j_2}], \\ \qquad i_2 = i_1 + 1 \\ = 0, & i_2 \leqslant i_1 + 1 \end{cases} \quad (5)$$

Defining $\Delta\psi = \psi - \phi$ and subtracting (4) from (2), we have

$$\begin{aligned} d\,\Delta\psi/dt &= M'\psi - N'\phi \\ &= M'\,\Delta\psi + (M' - N')\,\phi \\ &= M'\,\Delta\psi + (M^T - N^T)\,\phi \end{aligned} \quad (6)$$

This equation is similar to Eq. (2) except that it has a source term. Therefore, we have

$$\Delta\psi_i(t) = \sum_j \int G_{ij}(t, t')[(M^T - N^T)\,\phi(t')]_j\,dt' \quad (7)$$

Here, $G_{ij}(t)$ is the Green's function which satisfies the equation

$$dG_{ij}(t, t')/dt = \sum_k M'_{ik} G_{kj}(t, t') + \delta_{ij}\delta(t - t') \quad (8)$$

To verify that Eq. (7) is the solution of (6), we differentiate it with respect to t, to get

$$d\,\Delta\psi_i(t)/dt = \sum_j \int dG_{ij}(t, t')/dt\,[(M^T - N^T)\,\phi(t')]_j\,dt' \quad (9)$$

Substituting for $dG_{ij}(t, t')/dt$ from Eq. (8) and interchanging the summations in the first term, we get back Eq. (6) after some simplification.

$G_{ij}(t, t')$ is also the conditional probability of finding the B particles at i (that is, B_1 at i_1 and B_2 at i_2) at time t given that they were at j at time t'. Further, if we define the survival probability of the A particle at time t as $P_j(t, t')$, we have

$$P_j(t, t') = \sum_i G_{ij}(t, t') \tag{10}$$

Summing Eq. (7) over i, we get

$$\Delta\psi_0(t) = \sum_j \int P_j(t, t')[(M^T - N^T)\,\phi(t')]_j\,dt' \tag{11}$$

where $\Delta\psi_0(t) = \sum_i \Delta\psi_i(t)$ and is the excess survival probability without the bus effect over that with the bus effect. Now,

$$\begin{aligned}[(M^T - N^T)\,\phi(t')]_j &= \sum_k (M^T - N^T)_{jk}\,\phi_k(t') \\ &= \sum_k (M - N)_{kj}\,\phi_k(t') \end{aligned} \tag{12}$$

From Eqs. (3) and (5), we note that in Eq. (12) the matrices M and N differ from each other only for $k_2 \leqslant k_1 + 1$ $[k = (k_1, k_2)]$. Further, ϕ is the quantity corresponding to the bus effect and therefore is zero for values of $k_2 \leqslant k_1$. Therefore, the only contribution to the summation in Eq. (12) comes from $k_2 = k_1 + 1$. Using Eqs. (3) and (5) and the fact that ϕ_k is zero for $k_2 \leqslant k_1$, we have

$$\begin{aligned}\Delta\psi_0(t) &= 0.5 \sum_{k_1} \sum_{k_2} \int dt'\, P_{(j_1, j_2)}(t, t')\,\delta_{k_1, k_2 - 1}\,\phi_{(k_1, k_2)}(t') \\ &\quad \times [\delta_{k_1, j_1}\delta_{k_2, j_2 + 1} + \delta_{k_2, j_2}\delta_{k_1, j_1 - 1} - 2\delta_{k_1, j_1}\delta_{k_2, j_2}] \\ &= 0.5 \sum_{k_1} \int dt'\, \phi_{(k_1, k_1 + 1)}(t')[P_{(k_1, k_1)}(t, t') \\ &\quad \times P_{(k_1 + 1, k_1 + 1)}(t, t') - 2P_{(k_1, k_1 + 1)}(t, t')] \end{aligned} \tag{13}$$

Now, $P_{(k_1, k_2)}(t, t')$ is the survival probability at time t with independent motion of the two B particles given that the particles were at k_1 and k_2, respectively, at time t'. Equation (13) may be understood as follows. The difference between the case without the bus effect and that with it occur only when the two B particles are at the adjacent lattice sites (say k_1 and

k_1+1). At this stage, in the former case, transitions to k_1, k_1 as well as k_1+1, k_1+1 are allowed each with transition rate 1/2, while these are forbidden in the latter case. The difference between the two cases may therefore be thought of as a "difference source," one at k_1, k_1 plus one at k_1+1, k_1+1 minus twice the source at k_1, k_1+1. Since the particles are carrying out independent motion, the survival probability may be written as a product of the single-particle survival probabilities. Further, the transition rates are independent of time. Therefore, the survival probability depends only on the difference $t-t'$,

$$P_{(k_1,k_2)}(t, t') = p(k_1; t-t')\, p(k_2; t-t') \tag{14}$$

Here, $p(k_1; t)$ is the survival probability at time t given that there was a single B particle at k_1 at time $t=0$. Using Eq. (14) in Eq. (13), we get

$$\Delta\psi_0(t) = 0.5 \sum_{k_1} \int dt'\, \phi_{(k_1,k_1+1)}(t')[p^2(k_1; t, t') + p^2(k_1+1; t, t') - 2p(k_1; t, t')\, p(k_1+1; t, t')] \tag{15}$$

The quantity inside the square brackets is a perfect square and the ϕ's are all positive. Therefore $\Delta\psi_0$ is positive. Thus, we have proved that for a single A particle at 0 with two B particles at x and y, respectively, with $y>x>0$ the survival probability of the A particle with the bus effect is less than that without the bus effect. The extension of this result to an arbitrary number of B particles is straightforward. This further implies that the average survival probability $S(t)$ with the bus effect with a random initial distribution of B particles is less than the average survival probability $S_1(t)$ without the bus effect with the same initial distribution.[2]

$$S(t) \leqslant S_1(t) \tag{16}$$

2.2. Lower Bound

We follow a procedure very similar to the above for getting the lower bound. We again first consider the motion of two B particles to one side of a stationary A particle. The one-dimensional motion of the two B particles is equivalent to the two-dimensional motion of a single particle. The only difference is that in this case the absorbing boundaries are placed at $x=0$ and $y=1$. Note that the change in the boundary conditions does not in any way change the survival probability for the case with the bus effect,

[2] While we were revising our paper, we learnt that this result can be deduced from Lemma 4.12 of Chapter VIII of ref. 9. Also see ref. 10.

since particle B_2 cannot come to position 1 until particle B_1 has reached position 0. We can write equations similar to Eqs. (2) and (4) and again obtain an equation similar to Eq. (13):

$$\Delta\psi_0(t) = 0.5 \sum_{k_1} \int dt' \, \phi_{(k_1, k_1+1)}(t') [P'_{(k_1, k_1)}(t, t') + P'_{(k_1+1, k_1+1)}(t, t') - 2P'_{(k_1, k_1+1)}(t, t')] \tag{17}$$

The altered $P'_k(t, t')$ is given by

$$P'_{(k_1, k_2)}(t, t') = p(k_1, t-t') \, p(k_2 - 1, t-t') \tag{18}$$

The quantity in the square brackets of Eq. (17) therefore becomes

$$[P'_{k_1, k_1}(t, t') + P'_{k_1+1, k_1+1}(t, t') - 2P'_{k_1, k_1+1}(t, t')] = [p(k_1, \tau) \, p(k_1 - 1, \tau) + p(k_1 + 1, \tau) \, p^2(k_1, \tau)] \tag{19}$$

with $\tau = t - t'$. Now, using the method of images, it is easy to show that

$$p(j, \tau) = 2 \sum_{j'=0}^{j} q(j', \tau) - q(0, \tau) - q(j, \tau) \tag{20}$$

where $q(j', t)$ is the probability of finding a particle at j' at time t given that it started from $x = 0$ at time $t = 0$ and it was performing a continuous-time random walk on an infinite lattice with no absorbers. The term in the square brackets of Eq. (19) then reduces to $p(k_1, \tau)[q(k_1 + 1, \tau) - q(k_1 - 1, \tau)]$. Since q is a monotonically decreasing function of x, the total quantity is negative. Thus, we have proved that for a single A particle at 0 with two B particles respectively at x and y with $y > x > 0$, the survival probability with the bus effect is greater than that for the motion of a single particle executing a two-dimensional continuous-time random walk with absorbing boundaries at $x = 0$ and $y = 1$. The extension of this result to an arbitrary number of B particles yields

$$S(t) \geqslant S_2(t) \tag{21}$$

Here $S_2(t)$ is the survival probability of the A particle at time t for the independent case with the rule that the Jth B particle will annihilate the A particle if it reaches site $J - 1$. The ordering of the B particles is based on their initial positions. The initial conditions are the same as for the bus case, that is, any site is occupied with probability n_B and not occupied with probability $1 - n_B$ at $t = 0$.

3. ESTIMATES OF BOUNDS

In Section 2 we have shown that $S_1(t)$ and $S_2(t)$ are the upper and the lower bounds for the survival probability of an A particle with the bus effect for random initial distribution of B particles. In this section we estimate the values of these bounds.

3.1. Upper Bound

The $S_1(t)$ of Eq. (16) is the survival probability of the A particle with independent motion of the B particles put down without multiple occupancy. It is easier to estimate $\tilde{S}_1(t)$, which is the survival probability with multiple occupancy allowed. Let $\tilde{r}(j, t)$ be the probability that no B particle starting at j reaches 0 at time t. It is given by

$$\tilde{r}(j, t) = \sum_{k=0}^{\infty} \frac{n_B^k}{k!} e^{-n_B} p(j, t)^k = e^{-n_B(1-p(j,t))} \tag{22}$$

and hence

$$\tilde{S}_1(t) = \prod_{j=1}^{\infty} \tilde{r}(j, t) \tag{23}$$

Using the asymptotics for $p(j, t)$

$$\begin{aligned} \log \tilde{S}_1(t) &\sim \sum_{j=1}^{\infty} -n_B \left[1 - (2/\pi)^{1/2} \int_0^{j/\sqrt{t}} \exp(-x^2/2)\, dx \right] \\ &\sim -\sqrt{t}\, n_B \int_0^{\infty} \left[1 - (2/\pi)^{1/2} \int_0^{y} \exp(-x^2/2)\, dx \right] dy \\ &\sim -(2/\pi)^{1/2}\, n_B \sqrt{t} \end{aligned} \tag{24}$$

let $r(j, t)$ be the corresponding probability that no particle starting at j reaches 0 by time t for the case of no multiple occupancy (at $t=0$)

$$r(j, t) = (1 - n_B) + n_B\, p(j, t) \tag{25}$$

Hence

$$S_1(t) = \prod_{j=1}^{\infty} r(j, t) \tag{26}$$

The inequality $e^{-x} \geqslant 1-x$ immediately yields $\tilde{S}_1(t) \geqslant S_1(t)$. Using this along with Eqs. (16) and (23), we get

$$\lim_{t \to 0} \log S(t) \leqslant \log S_1(t) \leqslant \log \tilde{S}_1(t) \sim -\left(\frac{2}{\pi}\right)^{1/2} n_B \sqrt{t} \tag{27}$$

3.2. Lower Bound

Let $S_L(t)$ be the survival probability in the independent case for a finite lattice of size L with no multiple occupancy. Then

$$S_L(t) = \sum_{n=0}^{L} f_n Q(n, L, t) \tag{28}$$

where f_n is the probability of having exactly n particles in L sites

$$f_n = \frac{L!}{n!\,(L-n)!} (n_B)^n (1-n_B)^{L-n} \tag{29}$$

and

$$Q(n, L, t) = \frac{n!\,(L-n)!}{L!} \sum_{x_1=1}^{L_1} p(x_1, t) \sum_{x_2=Y_1}^{L_2} p(x_2-1, t) \times \cdots \sum_{x_n=Y_{n-1}}^{L_n} p(x_n-n+1, t) \tag{30}$$

Here $Y_i = x_i + 1$ and $L_i = L - n + i$. Note that

$$S_2(t) = \lim_{L \to \infty} S_L(t) \tag{31}$$

for any finite t. This is true even if we let $t \to \infty$, provided L is taken sufficiently large ($= \sqrt{t} \log t$, say). As shown in the Appendix

$$Q(n, L, t) \geqslant \langle p(l, t) \rangle^n \tag{32}$$

where $l = L - n + 1$ and

$$\langle p(l, t) \rangle = \frac{1}{l} \sum_{i=1}^{l} p(i, t) \tag{33}$$

We then let t and L both tend to infinity such that $L = \sqrt{t} \log t$. We now prove that for $l \to \infty$ and $t \to \infty$

$$\langle p(l, t) \rangle \sim 1 - (1/l)(2t/\pi)^{1/2} \tag{34}$$

Using the value of $p(j, t)$ from Eq. (20) in Eq. (33), we get

$$\langle p(l, t)\rangle = (1/l) \sum_{i=1}^{l} \left[2 \sum_{j=0}^{i} q(j, t) - q(0, t) - q(i, t) \right]$$
$$= (1/l)(2t/\pi)^{1/2} \int_0^{l/\sqrt{t}} dy \int_0^{y} dx \exp(-x^2/2) + E \tag{35}$$

E is the error term. It arises out of (a) use of the diffusion approximation for $q(j, t)$ and (b) the truncation error arising out of converting the double sum to a double integral. Both of them are $O(l/t^{3/2})$.

Integrating by parts, we have

$$\langle p(l, t)\rangle \sim (1/l)(2t/\pi)^{1/2} \left\{ \left[y \int_0^{y} dx \exp(-x^2/2) \right]_0^{l/\sqrt{t}} - \int_0^{l/\sqrt{t}} y \exp(-y^2/2)\, dy \right\} + E \tag{36}$$

If we take $l = \sqrt{t} \log(t)$, we can take the upper limit of each of the integrals to be infinity. We have

$$\langle p(l, t)\rangle \sim 1 - (1/l)(2t/\pi)^{1/2} + E$$

Defining

$$S'_L(t) = \sum_{n=1}^{L} \frac{L!}{n!\,(L-n)!} n_B^n (1-n_B)^{L-n} \langle p(l, t)\rangle^n \tag{37}$$

Taking $l_1 = Ln_B - kL^{0.5}$ and $l_2 = Ln_B + kL^{0.5}$, with k sufficiently large, we have

$$\log[S'_L(t)] \sim \log\left[\sum_{n=l_1}^{l_2} \frac{L!}{n!\,(L-n)!} n_B^n (1-n_B)^{L-n} \langle p(l, t)\rangle^n \right]$$
$$\sim \log\left\{ \sum_{n=l_1}^{l_2} \frac{L!}{n!\,(L-n)!} n_B^n (1-n_B)^{L-n} \times \left[1 - \frac{1}{L-n} \left(\frac{2t}{\pi}\right)^{1/2} + E \right]^n \right\} \tag{38}$$

Now,

$$\frac{1}{L-n} = \frac{1}{L(1-n_B) + Ln_B - n} \tag{39}$$

for $l_1 \leqslant n \leqslant l_2$ and $n_B \neq 1$,

$$\frac{1}{L-n} \sim \frac{1}{L(1-n_B)}\left(1-\frac{Ln_B-n}{L(1-n_B)}\right)$$
$$\sim \frac{1}{L(1-n_B)}\left[1-O\left(\frac{1}{\sqrt{L}}\right)\right] \tag{40}$$

Therefore,

$$\log[S'_L(t)] \sim \log\left\{\sum_{n=l_1}^{l_2} \frac{L!}{n!\,(L-n)!} n_B^n n_B^n (1-n_B)^{L-n} \times\left[1-\frac{1}{L(1-n_B)}\left(\frac{2t}{\pi}\right)^{1/2}\right]^n\right\}$$
$$\sim -\frac{n_B}{1-n_B}\left(\frac{2t}{\pi}\right)^{1/2} \tag{41}$$

Therefore, for t and L both tending to ∞ such that $L=\sqrt{t}\log t$ we get

$$\log S(t) \geqslant \log S_2(t) \sim \log S_L(t) \geqslant \log S'_L(t) \sim -\frac{n_B}{1-n_B}\left(\frac{2t}{\pi}\right)^{1/2} \tag{42}$$

This expression may be understood as follows. Our lower bound [obtained from Eq. (41)] is essentially a reduction of the average distance between successive B particles by unity. The average distance is nothing but $1/n_B$. Hence, the effective concentration becomes $1/(1/n_B-1)=n_B/(1-n_B)$.

The results of inequalities (27) and (42) are for the survival probability of the A particle with B particles on one side of it only. If there are B particles on both sides, the survival probability will be the square of the above quantity. Thus, we get

$$\lim_{t\to\infty} -2n_B(2t/\pi)^{0.5} \geqslant \log S(t) \geqslant \frac{-2n_B}{1-n_B}(2t/\pi)^{0.5} \tag{43}$$

4. RESULTS OF SIMULATIONS

We also did simulations to obtain the survival probability for $n_B<1$. The simulation procedure was as follows. A large lattice with a large number of sites in one dimension was randomly filled with A and B particles with concentrations n_A and n_B, respectively. The A particles were left stationary while the B particles were allowed to move to their nearest neighboring sites, provided these sites were not occupied by another B particle. The time at which the first B particle took a step was sampled from the distribution $\exp(-mt)$, where m is the total number of B particles in the lattice. Whether the step was to the right or to the left was then obtained by comparing a random number with 1/2. The particle was allowed to move if the particular step was permitted, that is, if the site was empty or occupied by an A particle. If it was occupied by an A particle, the A particle was annihilated. The random number generator used was a linear congruential generator used with the radiation transport code MCNP. It has a period of 2^{48}.

Figures 1 and 2 give the results of our simulations. In Fig. 1, the log of the survival probability (with the bus effect) is plotted against $\sqrt{t}$ for various concentrations of B. It is seen that the points fall quite well on a straight line. Figure 2 shows similar results for the survival probability without the bus effect for $n_B = 0.1$ and 0.5, respectively. Again, the survival probability shows a straight-line behavior and the slope correspond to $0.71 n_B$, which is very close to the expected behavior of $2(2/\pi)^{0.5} n_B D^{0.5}$ on theoretical grounds. The value of D used in the simulations was $D = 0.2$. A comparison of the two figures also shows that the survival probability without the bus effect is larger than that with the bus effect. The log of the survival probability goes as a function of n_B multiplied by $\sqrt{t}$. The statistical errors associated with the simulations were quite small except at very

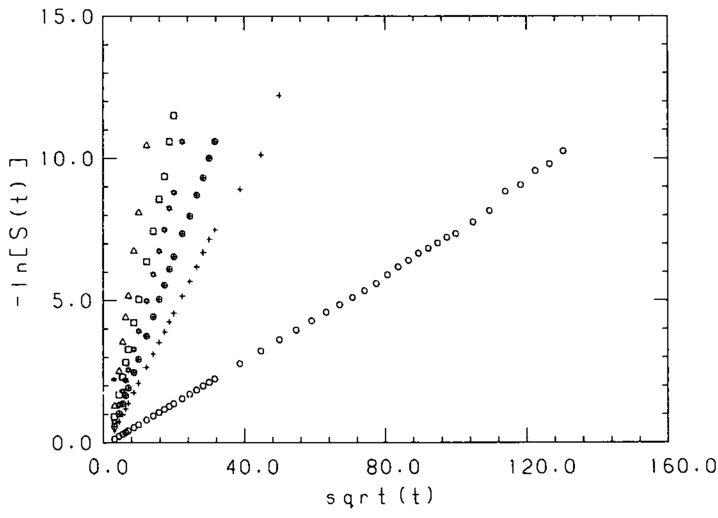

Fig. 1. Variation of the log of the survival probability with $t^{0.5}$, with the bus effect for concentration of the B particle $n_B = 0.8$ ($\triangle$), 0.6 ($\square$), 0.5 ($*$), 0.4 ($\oplus$), 0.3 ($+$), and 0.1 ($\bigcirc$).

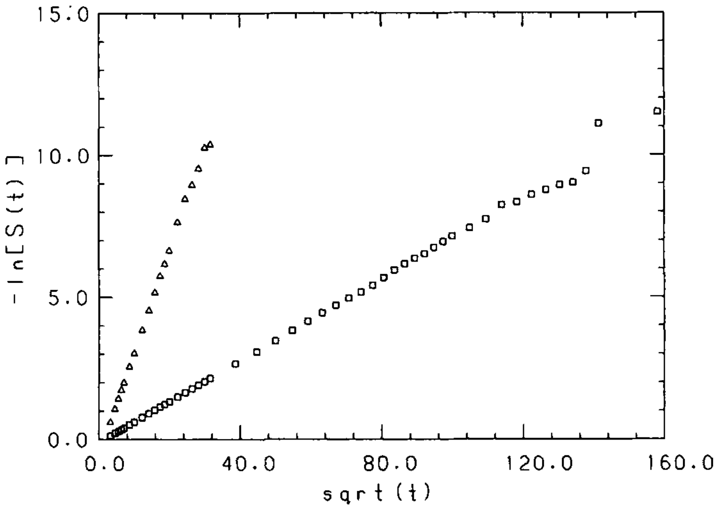

Fig. 2. Variation of the log of the survival probability with $t^{0.5}$, without the bus effect for concentration of the B particle $n_B = 0.5$ ($\triangle$) and 0.1 ($\bigcirc$).

low survival probabilities. To check finite-size effects, simulations were performed with three different sizes: 10^4, 10^5, and 10^6. The results indicate no finite-size effects for lattices of these sizes.

APPENDIX

To prove that $Q(n, L, t) \geqslant \langle p(l, t) \rangle^n$ we first prove the identity

$$n\tilde{q}(n, L, t) = \sum_{i=1}^{n} \sum_{x_1=1}^{L} p_1^i \tilde{q}(n-i, L, t) \tag{A1}$$

where

$$\tilde{q}(n, L, t) = \sum_{x_1=1}^{L} \sum_{x_2=x_1}^{L} \cdot \sum_{x_n=x_{n-1}}^{L} \prod_{k=1}^{n} p(x_k, t) \tag{A2}$$

and $p_j = p(x_j, t)$ and by definition $\tilde{q}(0, L, t) = 1$.

The proof is by induction on L and n.

The proposition is trivially true for $L=1$ for all n. Also, it can be easily verified to be true for $n=2$ for all L. We assume it to be true $\forall m\geqslant 1$ for $1\leqslant j\leqslant (n-1)$ and for $1\leqslant m\leqslant L$ for $j=n$ and then prove that

$$n\tilde{q}(n, L+1, t)=\sum_{i=1}^{n}\sum_{x_1=1}^{L} p_1^i\tilde{q}(n-i, L+1, t) \tag{A3}$$

Now,

$$\tilde{q}(n, L+1, t)=\sum_{x_1=1}^{L+1}\sum_{x_2=x_1}^{L+1}\cdots\sum_{x_n=x_{n-1}}^{L+1}\prod_{k=1}^{n} p_k \tag{A4}$$

We show that the coefficients of $(p_{L+1})^j$ are the same on both sides of Eq. (A3) for $1\leqslant j\leqslant n$. Let the coefficients on the lhs and the rhs be, respectively, C_j and D_j. Clearly

$$C_j=n\tilde{q}(n-j, L, t) \tag{A5}$$

since the only terms contributing to it are those with the first $(n-j)$ x's not equal to $L+1$ and the remaining equal to $L+1$.

The rhs of Eq. (A3) looks something like

$$\begin{aligned}&\sum_{x_1=1}^{L+1} p_1\sum_{x_2=1}^{L+1} p_2\sum_{x_3=x_2}^{L+1}\cdots\sum_{x_n=x_{n-1}}^{L+1} p_n\\ &\quad+\sum_{x_1=1}^{L+1} p_1^2\sum_{x_2=1}^{L+1} p_2\sum_{x_3=x_2}^{L+1}\cdots\sum_{x_{n-1}=x_{n-2}}^{L+1} p_{n-1}\\ &\quad+\cdots\sum_{1}^{L+1} p_1^i\sum_{1}^{L+1} p_2\sum_{x_{n-i+1}=x_{n-i}}^{L+1} p_{n-i+1}+\cdots\sum_{x_1=1}^{L+1} p_1^n\end{aligned}$$

The contribution to $(p_{L+1})^j$ comes from two kinds of terms.

(i) $x_1=L+1$; this will be for the first j terms only and each term contributes exactly $\tilde{q}(n-j, L, t)$.

(ii) $x_1\neq L+1$. Only the first $n-j$ terms contribute to this and the contribution of the ith term $(1\leqslant i\leqslant n-j)$ is $\sum_{x_1=1}^{L} p_1^i\tilde{q}(n-j-i, L, t)$.

We have

$$D_j=j\tilde{q}(n-j, L, t)+\sum_{i=1}^{n-j}\sum_{x_1=1}^{L} p_1^i\tilde{q}(n-j-i, L, t) \tag{A6}$$

But, by the induction hypothesis, the second term on the rhs is nothing but $(n-j)\,\tilde{q}(n-j, L, t)$, and

$$D_j = j\tilde{q}(n-j, L, t) + (n-j)\,\tilde{q}(n-j, L, t) \tag{A7}$$

Using Eqs. (A5) and (A7), we see that $C_j = D_j$. Thus Eq. (A1) is proved. We use this now to prove that

$$Q(n, L, t) \geqslant \langle p(l, t) \rangle^n \tag{A8}$$

From Eq. (30), we have that

$$\begin{aligned} Q(n, L, t) &= \frac{n!\,(L-n)!}{L!} \sum_{x_1=1}^{l} \sum_{x_2=x_1+1}^{l+1} \cdots \sum_{x_i=x_{i-1}+1}^{l+i-1} \cdots \sum_{x_n=x_{n-1}}^{l+n-1} \\ &\quad \times \prod_{k=1}^{n} p(x_k - k + 1, t) \\ &= \frac{n!\,(L-n)!}{L!} \sum_{1}^{l} \sum_{x_1}^{l} \cdots \sum_{x_{n-1}}^{l} \prod_{k=1}^{n} p(x_k, t) \end{aligned} \tag{A9}$$

We prove Eq. (A8) by induction on n. It can be easily seen to be true for $n=2$ for all $L \geqslant 2$. Using Eq. (A2) in Eq. (A9), we have

$$\begin{aligned} Q(n, L, t) &= \frac{n!\,(L-n)!}{L!}\,\tilde{q}(n, l, t) \\ &= \frac{(n-1)!\,(L-n)!}{L!} \sum_{i=1}^{n} \sum_{x_1=1}^{n} p_1^i \tilde{q}(n-i, l, t) \\ &= \frac{(n-1)!\,(L-n)!}{L!} \sum_{i=1}^{n} \sum_{x_1=1}^{n} p_1^i\, T(n-i, l) \\ &\quad \times Q(n-i, l_i, t) \end{aligned} \tag{A10}$$

where

$$T(i, l) = \frac{(l+i-1)!}{(l-1)!\,i!} \tag{A11}$$

and $li = l + n - i - 1$. Using the induction hypothesis, we have

$$Q(n, L, t) \geqslant \frac{(n-1)!\,(L-n)!}{L!} \sum_{i=1}^{n} \sum_{x_1=1}^{l} p_1^i \langle p(l, t) \rangle^{n-i}\, T(n-i, l) \tag{A12}$$

By the power mean inequality, we have

$$\sum_{x_1=1}^{l} p_1^i \geqslant l\langle p(l,t)\rangle^i \tag{A13}$$

Using Eq. (A13) in Eq. (A12) we have

$$Q(n,L,t) \geqslant \frac{(n-1)!\,(L-n)!}{L!}\, l\langle p(l,t)\rangle^n \sum_{i=1}^{n} T(n-i,l) \tag{A14}$$

It is easy to show that

$$l\sum_{i=1}^{n} T(n-i,l) = \frac{L!}{(n-1)!\,(L-n)!} \tag{A15}$$

Therefore,

$$Q(n,L,t) \geqslant \langle p(l,t)\rangle^n \tag{A16}$$

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