Comment on "Pair and Triple Correlations in the $A + B \rightarrow B$ Diffusion-Controlled Reaction"

In a recent Letter [1] Kuzovkov and Kotomin (KK) studied an important problem concerning the survival of an immobile target A in a 1D system with movable traps B. The new feature in Ref. [1], which makes it different from the earlier analysis [2–4], is that the traps' random walks (RW) follow hard-core exclusions (HCE): two B's cannot occupy simultaneously the same lattice site and cannot jump over each other [5]. In this situation A gets annihilated only through its nearest left (B_-) or right (B_+) trap. KK truncate the hierarchy of reaction-diffusion equations [6] on the level of three-particle correlations and solve the truncated equations numerically. Analyzing the numerical data, KK report the following result for the large-t behavior of the target's survival probability [1]:

$$P(t) \propto 1/t\,, \tag{1}$$

i.e., a result which is surprisingly different from that for the corresponding survival probability $P_0(t)$, in a 1D system without the HCE constraints [2–4],

$$P_0(t) \propto \exp(-n_B\alpha\sqrt{Dt}\,), \qquad t \gg t_D = 1/n_B^2 D\,, \tag{2}$$

where n_B is the mean concentration of B's, D is their diffusion coefficient, and α is a constant [2–4].

Here we argue that Eq. (1) appears due to only partial account of the HCE effects. Moreover, we claim that $P(t)$ in a 1D system with HCE is bounded at all times by

$$P(t) \leq P_0(t)\,. \tag{3}$$

The right hand side of Eq. (3) [Eq. (2)] decays quicker than Eq. (1), and thus contradicts it.

First we mention a possible explanation for Eq. (1). The truncation of correlations [1] takes into account that only the $B_\pm$ can annihilate the target, but disregards the influence of other B's on the motion of the $B_\pm$. This, in fact, reduces the original problem to a three-particle problem with the target and the pair $B_\pm$, whose RW's are unconstrained by other B's. Here $P(t)$ can be found analytically; letting $l_\pm$ be the initial separations between A and $B_\pm$, we have at sufficiently long times $P(t) \propto l_- l_+/Dt$. Averaging over $l_\pm$ yields $P(t) \propto 1/n_B^2 Dt$, $t \gg t_D$, i.e., Eq. (1).

However, in the original system with nonzero concentration of traps the motion of any B is *constrained* by its neighbors; thus the $B_\pm$ experience an effective pressure [7] from the rest of traps, which is directed towards A and leads to a quicker $P(t)$ decay. Below we prove this claim rigorously, by deriving the inequality in Eq. (3), which states that due to the HCE constraints the probability that traps, placed at $t = 0$ on the interval $]x_0, \infty[$ (or $]-\infty, x_0[$) remain within the same interval until time t, is less than or equal to that in the system without the HCE constraints. We focus on a 1D lattice with an immobile target placed at x_0 and the B's, whose dynamics obey the HCE (see Ref. [5], p. 361). The first step is to formulate the HCE in terms of a stirring system: For this an independent rate $\frac{1}{2}$ Poisson process is associated with each pair of neighboring sites $(x, x+1)$; at the event times of the stirring process the particles at x and $x+1$ are interchanged [5]. The stirring system is defined by ξ_t^x, which is the position at time t of the particle initially at x. For each x, ξ_t^x is an unconstrained RW on a 1D lattice. The motion of any B in the system with HCE, say, $B_\pm$, is related to the set of ξ_t^x by Lemma 4.10 of Ref. [5]. It follows then that for any realization of the initial B distribution, $P(t)$ is equal to the probability that neither of the RW's ξ_t^x visits x_0. Note that for $x \neq y$ the RW's ξ_t^x and ξ_t^y are not independent and have negative correlations [5], which reflect a mutual short range repulsion of the B's in the original system. Lemma 4.12 in Ref. [5] states that the probability for all RW's ξ_τ^x, whose initial positions x belong to a subset T of an interval X, to remain until time τ within X is smaller than or equal to the corresponding probability for the RW's without HCE constraints. We take the interval X to be the entire lattice with the exclusion of the site x_0 and T, the initial configuration, to be arbitrary. The averaging over all possible initial distributions does not change the inequality and leads to Eq. (3).

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