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Random Walks on Lattices. Influence of Competing Reaction Centers on Diffusion-Controlled Processes

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Abstract

We study diffusion-reaction processes on periodic simple cubic (sc) lattices and square planar lattices. We consider a single diffusing reactant undergoing an irreversible reaction upon first encounter with a static co-reactant placed at a given site ("one-walker problem"). We also allow for a competing reaction, namely, instantaneous trapping of the diffusing reactant at any other site (with probability s) before interacting with the static co-reactant. We use a generating function approach and Markov theory, as well as MC simulations, to determine the mean walklength $\langle n \rangle$ of the diffusing reactant before either of the two competing reactions takes place. To investigate the dependence of $\langle n \rangle$ on lattice size we compute the first, finite size corrections to the Green function of the sc lattice, correcting results reported in the literature. Using these results, space exploration properties and first-passage properties (e.g. walklength statistics, mean number of distinct sites visited, statistics of return to the origin, etc.) of both conventional (immortal) walks and mortal walks can be determined. In this context, we develop a novel approach based on a two-point Padé approximant for the Green function. Finally, we study by means of MC simulations the more complex case where both reactant and co-reactant undergo synchronous nearest-neighbor displacements ("two-walker problem"). Here, we assume that reactant and co-reactant can individually be trapped with probability s at any lattice site, or can undergo an irreversible reaction on first encounter at

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