Acta Physica Austriaca 53, 203–206 (1981)

Acta Physica Austriaca
EUROPHYSICS JOURNAL

On the Correlated Walks with Reflecting Walls*

By

Y. Okamura, M. Torres, E. Blaisten-Barojas, and S. Fujita*****
Instituto de Física, Universidad Nacional Autónoma de México, México

With 1 Figure

(*Received October 7, 1980*)

Summary

Exact expressions for the arrival probabilities with direction are obtained for correlated walks on an infinite line. The probability distribution exhibits a diffusive maximum, similar to that characteristic of random walks, *and* a runaway component which is associated with free passage (no scattering). The arrival probabilities for correlated walks on a finite line bounded by reflecting walls, are found to be expressed in terms of free-space probabilities.

In the usual random walks in one dimension [1], the walker is allowed to move right or left with step probabilities given at random. In 1951, Goldstein proposed and studied a correlated walk model in which the step probabilities depend on the direction of the preceding step [2]. Gillis and others obtained interesting results for the correlated walks in higher dimensions [3]. Manning applied the model for the study of atomic diffusion in crystals [4]. In our recent works, we reported the basic theory [5], and applications of correlated walks to various physical phenomena including the conformation of polymers [6], atomic diffusion in cubic crystals with impurities [7], the simulation of the dynamics of a Lorentz gas model [8].

In the present work we present exact expressions for the arrival probabilities with direction for the correlated walks on an infinite line *and* on a finite line bounded by reflecting walls.

* Work supported in part by the Programa Nacional de Ciencias Básicas (CONACYT, México) under project PNCB-0024.

** Present address: Department of Chemistry, McGill University, Montreal, PQ, Canada, H3A 2K6.

*** Permanent address: Department of Physics and Astronomy, SUNY Buffalo, Amherst, NY 14260, U.S.A.

0001 – 6713/81/0053/0203/$ 01.00

Let an object (walker) move in the same direction as that of the previous step with probability α and in the opposite direction with probability β. The step probabilities are normalized such that $\alpha + \beta = 1$. The probabilities of the walker arriving at the position m (integer) with the right (R) and left (L) step after N units of time will be denoted by $W_R(m, N)$ and $W_L(m, N)$, respectively. Consideration of two successive steps yields the following relations:

$$\begin{aligned} W_R(m, N) &= \alpha W_R(m-1, N-1) + \beta W_L(m-1, N-1), \\ W_L(m, N) &= \beta W_R(m+1, N-1) + \alpha W_L(m+1, N-1). \end{aligned} \tag{1}$$

We assume that the walker arrived at the position m_0 with the right step initially ($N = 0$). This condition can be represented by

$$W_R(m, 0) = \delta_{m,m_0}, \qquad W_L(m, 0) = 0. \tag{2}$$

The solutions of Eqs. (1) subject to (2) will be denoted by $W_j(m, N; m_0)$ with $j = R, L$. After lengthy calculations involving the generating function techniques [5], we obtain

$$\begin{aligned} &W_j(m, N; m_0) \\ &\equiv w_j(m - m_0, N) \\ &= \begin{cases} P_j[\frac{1}{2}(m - m_0 + N), N] & \text{if } m - m_0 + N \text{ is even and non-negative,} \\ 0 & \text{otherwise,} \end{cases} \end{aligned} \tag{3}$$

where

$$P_R(X, N) \equiv \begin{cases} \sum_{r=0}^{x} \binom{N-r-1}{X-1} \binom{X}{r} \alpha^N \left(\frac{\beta - \alpha}{\alpha^2}\right)^r, \\ \delta_{N,0}, \qquad 1 \leqslant X \leqslant N,\ X = 0, \end{cases}$$

$$P_L(X, N) \equiv \sum_{r=0}^{x} \binom{N-r-1}{X} \binom{X}{r} \beta \alpha^{N-1} \left(\frac{\beta - \alpha}{\alpha^2}\right)^r, \qquad 0 \leqslant X \leqslant N. \tag{4}$$

The probabilities of arrival from any direction, W, is the sum of $\{W_j\}$:

$$W(m, N; m_0) \equiv W_R(m, N; m_0) + W_L(m, N; m_0). \tag{5}$$

In Fig. 1 we show the probabilities $w(x, N)$, ($x = m - m_0$), for different values of the parameter α. The case of $\alpha = \beta = 0.5$ corresponds to that of random walks, where the distribution is symmetric about the starting point $m = m_0$. For the values of α close to unity there arises a diffusive maximum *and* a *runaway component* which is associated with free passage (no scattering). In between these two extremes, the diffusive maximum becomes flattened as α grows from one half to unity. The appearance of

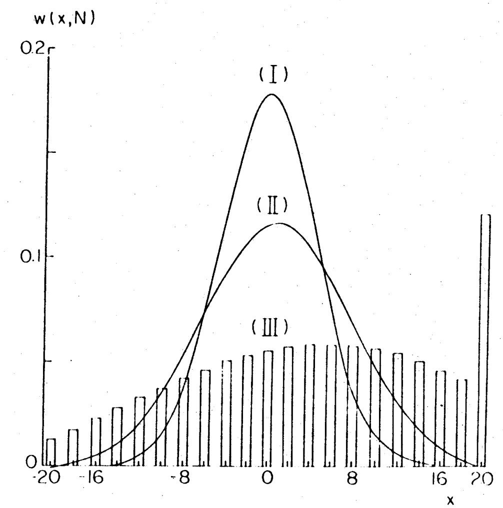

Fig. 1. The arrival probability distribution $w(x, N)$ for $x \equiv m - m_0$, $m_0 = 0$, $N = 20$, and different α-values: (I) $\alpha = 0.5$, (II) $\alpha = 0.7$ and (III) $\alpha = 0.9$. The case (III), represented by histograms, exhibits the runaway component at $x = 20$. Other cases are indicated by continuous curves rather than histograms

the runaway component is the most striking feature of correlated walks. The runaway component may even be greater than the diffusive maximum. In such a case, the average behavior cannot be described in terms of a few moments $\langle x \rangle$, $\langle x^2 \rangle, \ldots$, which are often used to characterize Gaussian-like distributions.

Let us now put two reflecting walls separated by a distance L and located half way between lattice points, say at $(\frac{1}{2}, L + \frac{1}{2})$. The motion of the walker is then restricted to the domain $(1, 2, \ldots, L)$. The condition of a reflecting wall dictates that every time the object arrives at the wall it will be rebounded to the previous position with the direction reversed. The exact solutions $W^{(\mathrm{ref})}$ for this case are obtained by the mirror methods [1], and are given by

$$W_j^{(\mathrm{ref})}(m, N; m_0)$$
$$= \sum_{k=-\infty}^{\infty} [W_j(2kL + m, N; m_0) + W_{j^*}(2kL - m, N; m_0)], \qquad (6)$$

where j^* denotes the conjugate of j, that is, $(1^*, 2^*) = (2, 1)$. If we take $L \to \infty$, we obtain the solution for a semi-infinite positive line, which is given by the single term with $k = 0$ on the right-hand side.

The correlated walks may be subjected to various types of boundary conditions. The periodic boundary, for instance, allows a simple solution:

$$W_j^{(\mathrm{per})}(m, N; m_0) = \sum_{k=-\infty}^{\infty} W_j(kL + m, N; m_0) \qquad (7)$$

where L is the period. The probabilities of eventual absorption at the absorbing walls, which limits the range of the correlated walks, were calculated earlier [9]. But other important properties of correlated walks with absorbing walls have not fully been explored. For example, the eventual absorption at the wall for semi-bounded Bernoulli walks critically depends on the value of the biased step probabilities. How this striking feature will change with introduction of the directional correlation is an important question.

As an application of the present work, we may discuss the evolution of the probabilities with direction, W_j, for a bounded space. The approach to the stationary state should depend on the step probabilities, the separation length between walls, and the boundary type.

The models treated here, if suitably extended for higher dimensions, will be useful for discussions of various phenomena including the sedimentation of particles in solution, atomic diffusion in crystals, and the diffusion of a Lorentz gas. Results of these and other studies however, will be reported in separate publications.

Acknowledgements

The authors wish to thank Professor P. A. Mello for fruitful discussions.

References

[1] Chandrasekhar, S.: Rev. Mod. Phys. **15**, 1 (1943); Wang, M. C., Uhlenbeck, G. E.: Rev. Mod. Phys. **17**, 90 (1945).
[2] Goldstein, S.: Quart. J. Mech. **4**, 129 (1951); Klein, G.: Proc. Roy. Soc. Edinb. **A63**, 268 (1952).
[3] Gillis, J.: Proc. Cambr. Philos. Soc. **51**, 639 (1955); Mohan, C.: Biometrica **42**, 486 (1955); Gupta, H. C.: Sankhya **20**, 295 (1958); Seth, A.: J. Roy. Stat. Soc. **B25**, 394 (1963); Jain, G. C.: Canad. Math. Bul. (3) **14**, 341 (1971), *ibid.* **16**, 389 (1973).
[4] Manning, J. M.: Diffusion Kinetics for Atoms in Crystals. New York: Van Nostrand. 1968.
[5] Fujita, S., Chen, J. T.: KINAM (Mexico) **1**, 177 (1979).
[6] Fujita, S., Chen, J. T., Okamura, Y.: J. Chem. Phys. **72**, 3993 (1980).
[7] Okamura, Y., Blaisten, E., Fujita, S., Godoy, S. V.: Phys. Rev. **B22**, 1638 (1980).
[8] Fujita, S., Okamura, Y., Blaisten, E., Godoy, S. V.: J. Chem. Phys. (accepted for publication).
[9] Simon, I., Fujita, S.: Acta Phys. Austr. **50**, 207 (1979).