Transport properties of a two-dimensional "chiral" persistent random walk

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The usual two-dimensional persistent random walk is generalized by introducing a clockwise (or counterclockwise) angular bias at each new step direction. This bias breaks the reflection symmetry of the problem, giving the walker a tendency to "loop," and gives rise to unusual transport properties. In particular, there is a resonantlike enhancement of the diffusion constant as the parameters of the system are changed. Also, in response to an external field, the looping tendency can resist or enhance the drift along the field and gives rise to a drift transverse to the field. These results are obtained analytically, and, for completeness, compared with Monte Carlo simulations of the walk. [S1063-651X(97)05310-5]

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INTRODUCTION

In this work I present a simple extension of the twodimensional (2D) persistent random walk [1] which gives rise to rather surprising transport properties. Among these is a resonantlike enhancement of the diffusion constant as the intrinsic parameters of the model are varied. The model under consideration consists essentially of a 2D persistent random walk with a clockwise (or counterclockwise) angular bias at each new step direction. This process can be thought of as the simplest description for the motion of a charged particle undergoing "soft" scattering by aligned magnetic domains. The angular bias only breaks the reflection symmetry of the problem, as the system continues to be homogeneous and isotropic, which motivates the name "chiral" persistent random walk. Thus, in this context, the chirality refers to the tendency of the random walk to "loop" in one or the other direction. This looping tendency gives rise to other phenomena in addition to the enhancement of the diffusion constant, for example, the presence of a field driving the particle induces also a drift in the transverse direction of the field, not unlike what happens in the Hall effect.

Some of the peculiar characteristics of the transport properties of this walk, in particular the enhancement of the diffusion constant, can be described in terms of the interplay between the two characteristic times present in the system, similar to what happens in resonant phenomena. These characteristic times are the correlation time associated with the persistence of the random walk, which roughly speaking is the time in which the random walk forgets its initial direction; and the looping time, i.e., the number of steps it would take a dispersionless random walk to close a loop. In short, the looping tendency of the walk makes the persistence length [2] a nonmonotonic function of the correlation time. Indeed the largest persistence length is that for which the correlation time is roughly half the looping time; as for longer correlation times, the looping tendency brings the walker back to its "starting" point.

In this paper I will focus on the simplest possible chiral persistent random walk, namely, the case in which the step lengths are all equal. The generalization to the case in which the step lengths are also a random variable is straightforward. In Sec. I the master equation for the problem without a driving field is posed, from which an analytic expression for the diffusion constant is obtained and discussed. Section II is devoted to the calculation of the linear response in the presence of an external field. Finally, Sec. III contains the concluding remarks and open questions of this problem.

I. DIFFUSION CONSTANT

The usual approach to describe persistence in random walks is via multistate random walks [1]; unfortunately in dimensions larger than 1, the general situation requires an infinite state random walk even for constant step lengths. In this vein I denote $P(x,y,n|\theta)dxdy$ the probability of arriving at a vicinity dxdy of position (x,y) after n+1 steps, the n step having been chosen in the direction θ (where θ denotes the angle of the step measured from the x axis). Thus θ works as the state label of the random walk. The probability of finding the random walk within dxdy of the point (x,y) after n steps is given by

$$P(x,y,n) = \int_{-\pi}^{\pi} P(x,y,n|\theta) d\theta.$$
(1)

The main ingredient in this problem will be $P(\Delta \theta)$, the distribution of changes of direction between steps, which in the approach taken in this work serves as the state transition distribution as well. It is clear that both the persistence and the chirality of the random walk are consequences of the shape of $P(\Delta \theta)$. If $P(\Delta \theta)$ is flat there is no correlation between successive step directions and we obtain what is known as a Pearson random walk [1]. On the other hand, if $P(\Delta \theta) = \delta(\Delta \theta)$, the random walker never changes direction and we obtain ballistic motion in the direction of the first step. If $P(\Delta \theta) = \delta(\Delta \theta - b)$ the walker will follow a polygonal trajectory. These polygons will eventually close or not, depending on whether *b* is a rational or irrational fraction of π . In any case they will certainly intersect themselves, and form a "loop," after $\approx 2 \pi/b$ steps.

The evolution of $P(x,y,n|\theta)$ in terms of $P(\Delta\theta)$ is given by

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$$P(x,y,n+1|\theta) = \int_{-\pi}^{\pi} P(x-L\cos\theta, y-L\sin\theta, n|\gamma)$$
$$\times P(\theta-\gamma)d\gamma, \qquad (2)$$

where *L* is the step size. The above equation merely expresses the fact that the probability of arriving within dxdy of (x,y) at step n+1, the *n* step having been chosen in the direction θ , is given by the probability of reaching the vicinity of $(x-L\cos\theta,y-L\sin\theta)$ in the intermediate "state" γ and changing to state θ , added over all possible intermediate states.

Fourier transforming Eq. (2) in space one obtains

$$P(w, \alpha, n+1 | \theta) = e^{iwL \cos(\theta - \alpha)} \\ \times \int_{-\pi}^{\pi} P(w, \alpha, n | \gamma) P(\theta - \gamma) d\gamma, \quad (3)$$

where w and α are the polar representation of the vector (w_x, w_y) of the transform variables associated with x and y, respectively. Finally, since the angular variables are cyclic, we can express $P(w, \alpha, n | \theta)$ and $P(\phi)$ as Fourier series of the form

$$P(w,\alpha,n|\theta) = \frac{1}{2\pi} \sum_{l=-\infty}^{\infty} P(w,\alpha,n|l) e^{-il\theta}.$$

The coefficients of the series then satisfy

$$P(w,\alpha,n+1|l) = \sum_{k=-\infty}^{\infty} (i)^{k} J_{k}(wL)$$
$$\times e^{-ik\alpha} P(w,\alpha,n|k+l) P(k+l), \quad (4)$$

where $P(w, \alpha, n|l)$ and P(l) are the amplitudes of the *l*th harmonic of $P(w, \alpha, n|\theta)$ and $P(\phi)$, respectively, and $J_k(wL)$ is the *k*th-order Bessel function. The wisdom of the above transformations might be doubtful, but they suffice for the purposes of this work.

While the exact solution of Eq. (4) appears to be very hard to obtain, it can be used to evaluate the moments of the displacement. To do this recall that the coefficients of the expansion in powers of w of the distribution $P(w, \alpha, n)$ [the Fourier transform of the distribution in Eq. (1)] are directly related to the moments of P(x, y, n). The w dependence on the right hand side of Eq. (4) is determined by the Bessel functions, thus, if one is interested in the second moment, one only needs to consider the terms k = -2, -1, 0, 1, 2 in the infinite sum.

Writing

$$P(w,\alpha,n|l) \approx q_0(\alpha,n|l) + iwLq_1(\alpha,n|l) - \frac{w^2L^2}{2}q_2(\alpha,n|l)...,$$
(5)

the second moment of the position of the walker can be expressed as

$$\langle r^2 \rangle_n = L^2[q_2(0,n|0) + q_2(\pi/2,n|0)] = \langle x^2 \rangle_n + \langle y^2 \rangle_n.$$

(6)

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Inserting Eq. (5) into Eq. (4), expanding the relevant Bessel functions [3], and collecting powers of w leads to the following recursion relations for the q_i 's:

$$q_0(\alpha, n+1|l) = P(l)q_0(\alpha, n|l),$$
 (7a)

$$q_{1}(\alpha, n+1|l) = P(l)q_{1}(\alpha, n|l) + \frac{1}{2}[e^{-i\alpha}P(l+1)q_{0}(\alpha, n|l+1) + e^{i\alpha}P(l-1)q_{0}(\alpha, n|l-1)], \quad (7b)$$

and

$$q_{2}(\alpha, n+1|l) = p(l)[q_{2}(\alpha, n|l) + \frac{1}{2}q_{0}(\alpha, n|l)] \\ + \frac{1}{2}[e^{-i\alpha}P(l+1)q_{1}(\alpha, n|l+1) \\ + e^{i\alpha}P(l-1)q_{1}(\alpha, n|l-1)] \\ + \frac{1}{4}[e^{-2i\alpha}P(l+2)q_{0}(\alpha, n|l+2) \\ + e^{2i\alpha}P(l-2)q_{0}(\alpha, n|l-2)].$$
(7c)

For simplicity, in what follows I will consider the distribution $P(\Delta \theta)$ to be symmetric around an angle *b*, thus $P(l) = e^{ilb}p(l)$ where p(l) = p(-l).

The solution of the above recursion relations is straightforward; it can be obtained using generating function techniques subject to any consistent initial condition (as the long time results will be independent of the initial condition). From the solution of Eqs. (7) and using Eq. (6), the diffusion constant turns out to be

$$D = \lim_{n \to \infty} \frac{\langle r^2 \rangle_n}{n} = L^2 \left(\frac{1 - p^2(1)}{1 - 2p(1)\cos b + p^2(1)} \right).$$
(8)

The extreme behaviors of this result are consistent with what one expects: if $P(\Delta \theta) = \delta(\Delta \theta - b)$, then p(1) = 1 and the walker moves along a polygon, which results in no diffusive transport (this is true as long as $b \neq 0$). On the other hand, if $P(\Delta \theta)$ becomes flat, i.e., $P(\Delta \theta) = 1/2\pi$, then p(1) vanishes and I obtain $D = L^2$, as expected for a Pearson random walk [1]. If b = 0, the usual diffusion constant for 2D persistent random walks is recovered [2,4–6].

This result for the diffusion constant has the feature of being a nonmonotonic function of p(1), having a maximum at $p_{\max}(1)=(1-\sin b)/\cos b$. The diffusion constant at its maximum value is $D_{\max}=1/\sin b$. This effect is illustrated in Fig. 1, where I show the diffusion constant obtained from Monte Carlo simulations of a random walker with $P(\Delta \theta)$ given by

$$P(\Delta \theta) = \begin{cases} \frac{1}{2a} & \text{if } b - a < \Delta \theta < b + a \\ 0 & \text{otherwise} \end{cases}$$
(9)

over the full range of a for various values of b, as well as the analytical prediction for each case.

The hesitation to call resonance the enhancement of the diffusion constant occurring in this system stems from the fact that there is no external signal to which the particle "hooks onto," as happens in most traditional stochastic resonance scenarios. Nevertheless, as mentioned above, the

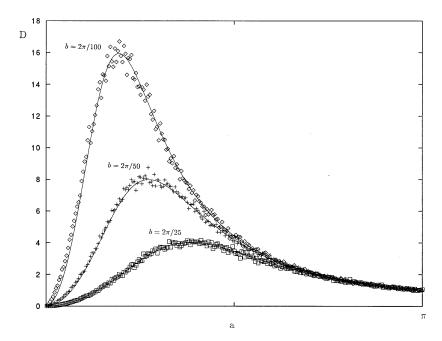


FIG. 1. Diffusion constant as a function of a, the width of the distribution of changes of direction [see Eq. (9)], for various values of the angular bias b. The large points correspond to the diffusion constant obtained from Monte Carlo simulations of the process, the lines to the result of the calculation.

enhancement does occur as a result of a particular relation between the two characteristic times present in the system. The qualitative explanation for this nonmonotonic behavior can be found by realizing that the step direction performs a random walk with constant drift b on the unit circle. The characteristic function [1] of this process is precisely $e^{ibl}p(l)$. Then the Fourier coefficients of the angular distribution function after n steps will be given by P(l,n) $=e^{inbl}p^{n}(l)$. Thus it is apparent that there are two main characteristic times: the "looping time" $\tau_{\rm loop} \sim 2 \pi/b$, and the correlation time $\tau_{\rm corr} \sim 1/\ln[1/|p(1)|]$. Now if the correlation time is large, $\tau_{corr} \ge \tau_{loop}$, the walker makes many loops before "forgetting" its initial direction. Since the net transport in each loop is small, the resulting process has a small diffusion coefficient. On the other hand, if $au_{
m corr} \!\!\ll\! au_{
m loop},$ then the steps are essentially uncorrelated, giving rise to a Pearson random walk. But if $\tau_{\rm corr} \sim \tau_{\rm loop}/2$ (as it turns out, for these definitions, the maximum diffusion constant is attained when $au_{
m corr} \approx au_{
m loop}/2\pi$ as $b \!
ightarrow \! 0$), then the walker makes "half" a loop before forgetting its initial direction. The resulting process can then be thought of as a random walker that gives uncorrelated "half loop'' steps. Since the loops can be quite large (for small *b*), this results in a large enhancement of the diffusion constant.

II. RESPONSE TO AN EXTERNAL FIELD

There appears to be no unique way to introduce the effect of an external field in this problem. For example, one way of introducing an external field would be to modify $P(\Delta \theta)$ so that steps with larger projections on the positive x axis are chosen with a higher probability. While this is a reasonable way of biasing the motion in the x direction, it complicates the formulation to no end. Instead, I have chosen a physically motivated approach which is simpler but perhaps slightly artificial. In what follows, the action of the field will be considered as a small deterministic addition to the x component of every step. The physical picture is that each change in direction is a scattering event, and that a weak external field acts on the particle between the scatterings. Thus the actual steps are calculated as the sum of the vector chosen at the outcome of the scattering event and a small constant vector in the x direction (see Fig. 2). The crucial aspect of the effect of the applied field is that not only the final position of each step is affected, but that the direction from which that position is reached must also be affected.

The master equation for the walk in the presence of this field becomes

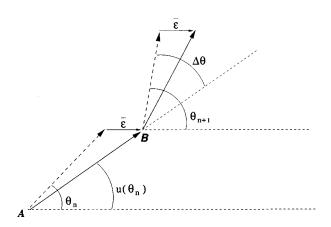


FIG. 2. The action of the external field on the random walk. At the "scattering point" A the direction θ_n is chosen. A small vector $\vec{\epsilon}$ in the x direction is then added to the step so the actual displacement is in the $u(\theta_n)$ direction. At the next step (from point B) the change of direction $\Delta \theta$ is taken with respect to the actual direction of arrival $u(\theta_n)$, and so on. In this way the field affects both the final position of the steps and the direction from which these positions are reached.

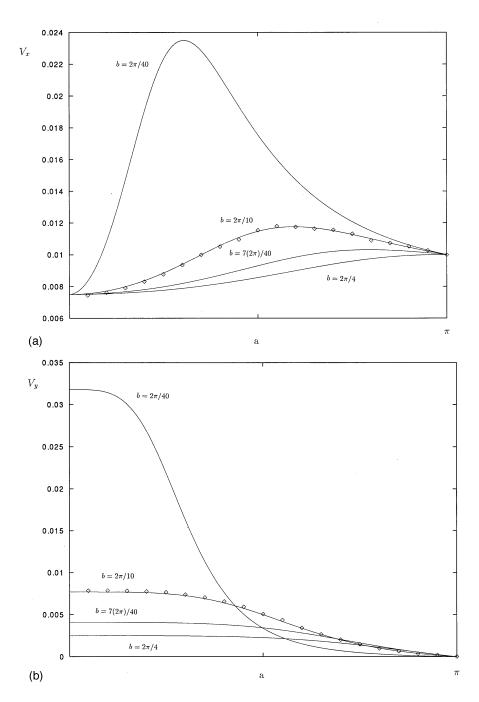


FIG. 3. Drift velocity parallel (a) and transverse (b) to the applied field as a function of the width of the distribution of changes of direction, for various values of the angular bias b. The large points correspond to the diffusion constant obtained from a Monte Carlo simulation of the process. The lines correspond to Eqs. (12a) and (12b), respectively.

$$P(x,y,n+1|\theta) = \int_{-\pi}^{\pi} P(x-L\cos\theta - \epsilon, y)$$
$$-L\sin\theta, n|\gamma(u))P(\theta-u) \frac{d\gamma}{du} du,$$
(10)

where $\epsilon \ll L$ is the size of the vector added in the *x* direction at each step. The interpretation of the quantities in Eq. (10) is a bit tricky: $P(x,y,n|\theta)$ is the probability of arriving in a vicinity dxdy of position (x,y), the last step having been *chosen* in the direction θ . This does not mean the the walker arrives at (x, y) from direction θ , but rather, that the direction chosen in the previous "scattering" was θ and the walker arrives at (x, y) from the direction resulting from the vector sum $(L \cos \theta, L \sin \theta) + (\epsilon, 0)$. In this context it proves convenient to return to the concept of state labels rather than angles; thus the right hand side of Eq. (10) denotes the summation over states γ which arrived at the position $(x - L \cos \theta - \epsilon, y - L \sin \theta)$ from the direction $u(\gamma)$ and scatter into the "state" θ . The factor $d\gamma/du$ is a Jacobian required for normalization.

Clearly there is little hope in carrying this calculation beyond linear order in ϵ . From symmetry considerations it is obvious that the diffusion constant will be unaffected to lin-

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ear order in ϵ , so only the response of the average position remains to be computed. Once again performing a Fourier transform in space and expanding in a Fourier series, one obtains from Eq. (10) the recurrence relations for the coefficients, correct to linear order in ϵ ,

$$P(w,\alpha,n+1|l) = \sum_{k=-\infty}^{\infty} (i)^{k} J_{k}(wL) e^{-ik\alpha} P(k+l)$$

$$\times \left(P(w,\alpha,n|k+l), -\frac{\epsilon}{2L} (k+l) \right)$$

$$\times [P(w,\alpha,n|k+l+1) - P(w,\alpha,n|k+l)]$$

$$(11)$$

In order to evaluate the average position of the random walk one needs the coefficient of the linear term in w in the expansion of $P(w, \alpha, n|0)$, so one needs to keep only the terms $k=0,\pm 1$ of the infinite sum. The procedure follows closely that for the determination of the diffusion constant. If one defines the field induced velocities v_x and v_y by

$$v_x \equiv \lim_{n \to \infty} \frac{\langle x \rangle_n}{n}, \quad v_y \equiv \lim_{n \to \infty} \frac{\langle y \rangle_n}{n},$$

one obtains that

$$v_{x} = \frac{\epsilon}{2} \left[\frac{2 - 3p(1)\cos b}{1 - 2p(1)\cos b + p^{2}(1)} \right]$$
(12a)

and

$$v_{y} = \frac{\epsilon}{2} \left[\frac{p(1) \sin b}{1 - 2p(1) \cos b + p^{2}(1)} \right],$$
 (12b)

where, for the sake of neatness, I have once again assumed that $P(\Delta \theta)$ is symmetrically centered about the angle *b*. These velocities are shown in Fig. 3 for the case in which $P(\Delta \theta)$ is given by Eq. (9) and $\epsilon = 0.01L$. Several features should be remarked. First of all, concerning the velocity parallel to the field (v_x) , one sees that for small distribution widths (in this case, small values of *a*), the looping tendency tends to "resist" transport. As the width increases this effect is reversed and the looping tendency enhances the transport in the direction of the field until a maximum is reached, beyond which the response falls to that of the Pearson random walk (namely, $v_x = \epsilon$). Transport transverse to the field (v_y) , as expected on geometrical grounds, has its maximum when the width is minimum, for at this point the looping tendency from which this component arises is maximum. As the width of $P(\Delta \theta)$ increases, the looping tendency gets "blurred" and transverse transport diminishes. It is worth noting that the curves cross as the width increases, implying that v_y is not a monotonous function of the bias angle.

III. CONCLUSIONS AND PERSPECTIVES

In this work I have shown that the transport properties of 2D persistent random walk are drastically altered by breaking the chiral symmetry of the system via the introduction of a tendency to "loop." This can give rise to a resonantlike behavior of the diffusion constant, as well as unexpected responses to an applied field. While these results suffice for the description of the process in the Gaussian approximation [1,5,6], the question of the actual distribution appears to be very hard to answer. Indeed, even in the continuous limit and in the absence of the angular bias, the Fokker-Planck equation [7] for this process is related to the Mathieu equation and appears to be intractable. Further, the equation for the marginal distribution of positions, independent of direction, cannot be obtained, for integration over the directions of the Fokker-Planck equation gives rise to an infinite hierarchy of equations involving the harmonics of the complete distribution (although it is a simple exercise to show that the first truncation of the hierarchy yields a two-dimensional telegrapher's equation). Nevertheless, interesting and important information should be analytically attainable, such as, for example, the correlations between direction and position.

Another interesting puzzle is the three-dimensional chiral random walk. This system differs from the present one in that it must be posed as a third-order Markov process; that is, the direction of each step depends on the directions of the *two* previous steps (and thus on the previous three positions). This makes dealing with the three-dimensional problem extremely hard. Clearly, enhancement of the diffusion constant as well as transverse transport are also expected in this case, and are worth pursuing, for it is in three dimensions where these models find most of their applications [1,2,5,6].

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- [1] G. H. Weiss, Aspects and Applications of the Random Walk (North-Holland, Amsterdam, 1994), and references therein.
- [2] P. J. Flory, Statistical Mechanics of Chain Molecules (Interscience, New York, 1969).
- [3] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972).
- [4] C. Tojo and P. Argyrakis, Phys. Rev. E 54, 58 (1996).
- [5] G. H. Weiss and R. J. Rubin, Adv. Chem. Phys. 52, 363 (1983).
- [6] A. H. Gamdjbakche and G. H. Weiss, Prog. Opt. XXIV, 333 (1995).
- [7] H. Risken, *The Fokker-Planck Equation* (Springer-Verlag, Berlin, 1989).