Phase transitions and superuniversality in the dynamics of a self-driven particle

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We study an active random walker model in which a particle's motion is determined by a self-generated field. The field encodes information about the particle's path history. This leads to either self-attractive or self-repelling behavior. For self-repelling behavior, we find a phase transition in the dynamics: when the coupling between the field and the walker exceeds a critical value, the particle's behavior changes from renormalized diffusion to one characterized by a diverging diffusion coefficient. The dynamical behavior for all cases is surprisingly independent of dimension and of the noise amplitude.

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Active walkers are random walkers whose motion is determined by a potential surface which is amenable to change by the walkers themselves [1]. They are one of several different classes of random walks in which walkers interact with their path history. The memory of these walkers leads to interesting properties, uncommon in pure random walks. Other common types of such self-interacting walks are the reinforced random walk [2,3] and the self-avoiding random walk [4,5].

Models based on active walkers have been used to study a number of phenomena, including ant foraging patterns [6], traffic [7], the formation of human and animal trail systems [8], animal mobility [9], chemotactic aggregation [10,11], and the self-assembly of networks [12]. The advantage of formulating problems in such a formalism is that it enables analytic study using methods from statistical physics and the general theory of stochastic processes. In this paper, we analyze in detail a fairly generic type of active walker model, in which a particle interacts with its path history by means of a self-generated field. This model is related to the self-driven many-particle system first introduced by Schweitzer and Schimansky-Geier [1], which studied it by means of a mean-field approximation applied on the stochastic model. Newman and Grima [11] analyzed the effect of fluctuations on the system's dynamics by means of a many-body theory approach. The spatiotemporal correlations make the problem difficult to understand, usually confining analysis to the case of weak coupling between particles and the generated field [11] or to the case of small noise [10]. Indeed even the case of a single self-driven particle is nontrivial (see, for example [5,10,13]) . We study a variant of the single self-driven particle model and develop a general theory to elucidate the particle's rich and complex dynamical behavior. This approach differs from the previous ones, in that it is valid for all coupling strengths and for both weak and strong noise. The model is potentially applicable to understanding a chemotactic biological system under certain conditions, a topic briefly discussed at the end of this paper.

Consider a random walker whose motion is described by the following coupled equations:

$$m\ddot{\mathbf{x}}_c(t) + \dot{\mathbf{x}}_c(t) = \xi(t) + \kappa\alpha \nabla \ln \phi(\mathbf{x}_c,t), \tag{1}$$

$$\partial_t \phi(\mathbf{x},t) = D_1 \nabla^2 \phi(\mathbf{x},t) - \lambda \phi(\mathbf{x},t) + \beta\delta(\mathbf{x} - \mathbf{x}_c(t)). \tag{2}$$

Equation (1) is a Langevin equation describing the motion of a walker with mass m. The stochastic variable ξ is white noise defined through the statistical averages $\langle \xi^i(t)\rangle = 0$ and $\langle \xi^i(t)\xi^j(t')\rangle = 2D_0\delta_{i,j}\delta(t-t')$, where i and j refer to the spatial components of the noise vectors. The mass is assumed to satisfy the condition $m \ll 1$, implying that in the absence of self-interaction the walker's dynamics are of the overdamped type. The walker's diffusion coefficient in this case is D_0. The self-generated field is denoted by ϕ; its temporal dynamics are determined by the reaction-diffusion equation (2). We shall refer to the field as a chemical field since this is most consistent with a physical interpretation of Eq. (2). Then the latter equation describes the continuous local release of chemical by the walker at a rate β, the diffusion of the chemical with diffusion coefficient D_1 and its decay at a constant rate λ.

The self-interaction comes from the second term on the right-hand side of Eq. (1). This term implies that the walker's motion is partly determined by the local gradient of the field. Note that the field encodes information about the walker's path history, meaning that the walker's motion at any given time is a complicated function of its previous whereabouts. The strength of the coupling between the field and the walker's motion is determined by α. The constant κ can take values 1 or −1: for $\kappa = 1$, the walker tends to explore regions already visited (a self-attracting walker) whereas for $\kappa = -1$ the opposite is true (a self-repelling walker). We assume that the initial chemical concentration is described by some function $\phi_0(\mathbf{x},t)$ which is greater than zero at all points in space.

The Langevin formulation is not usually considered the most convenient representation for the purposes of analytic calculations and so it is customary to derive a differential equation for the single-particle probability distribution (see Ref. [11], for example). For the problem at hand, this approach does not permit much analytic progress in understanding the walker's behavior. Applying a mean field approximation on the differential equation for the single-particle probability distribution one obtains a Fokker-Planck-type equation, which then permits a perturbative analysis in a coupling parameter. This approach ignores the important spatiotemporal correlations inherent in the problem and enables

one to understand the walker's behavior only when the coupling strength α is very small. The non-Markovian nature of the problem makes its solution a challenging task.

We here present a simple method to extract the asymptotic behavior of the active walker model. The results can also be reproduced by the method described in [10]. However, the method to be presented here is more transparent and gives a physically tractable picture of the complex underlying dynamics. Its main advantages are that spatiotemporal correlations are not ignored and that it enables an understanding of the motile behavior for all values of the coupling strength and of the other parameters. We start by switching to a description in discrete time $t=n\Delta t$ where $n \in \mathbb{N}$. Space is continuous. The walker's position at time $t+\Delta t$ is determined by the gradient of the logarithm of the chemical concentration it measures at time t. Since the walker secretes an amount of chemical $\beta\Delta t$ at every time step, then if the walker is at position $\mathbf{x}_c(t)$ at time t, the chemical field sensed by the walker at time t is given by

$$\phi = \sum_{n=1}^{t/\Delta t} \frac{\beta\Delta t}{(4\pi D_1 n\Delta t)^{d/2}} \times \exp\left[-\lambda n\Delta t - \frac{\sum_{i=1}^{d}[x_c^i(t)-x_c^i(t-n\Delta t)]^2}{4D_1 n\Delta t}\right] = \sum_{n=1}^{t/\Delta t}\phi_n, \tag{3}$$

and the gradient of the field is given by

$$\nabla\phi = -\sum_{n=1}^{t/\Delta t}\frac{[\mathbf{x}_c(t)-\mathbf{x}_c(t-n\Delta t)]}{2D_1 n\Delta t}\phi_n, \tag{4}$$

where $x_c^i(t)$ is the ith component of the particle position vector $\mathbf{x}_c(t)$ and d is the dimensionality of the space in which particle movement occurs. Since the chemical decays in a time of the order $1/\lambda$ then the concentration at time t will be approximately determined by the previous positions of the walker at times $t' > t-1/\lambda$. This implies that the sum in Eqs. (3) and (4) can be truncated at $n_{max}=1/\lambda\Delta t$. Now consider the term $x_c(t-n\Delta t)$. Since we are interested in the walker's behavior in the asymptotic limit $t \gg 1/\lambda$, then $n\Delta t \leqslant n_{max}\Delta t = 1/\lambda \ll t$. Thus it is possible to replace the term $x_c^i(t-n\Delta t)$ in the above two equations by its Taylor series expansion. Keeping terms only to first order in Δt we have

$$\nabla \ln \phi(\mathbf{x}_c,t) = \frac{\nabla\phi(\mathbf{x}_c,t)}{\phi(\mathbf{x}_c,t)} = -\frac{\dot{\mathbf{x}}_c(t)}{2D_1}. \tag{5}$$

Thus from Eq. (1) and the above equation, it follows that for long times the behavior of the walker is dominated by the effective Langevin equation

$$m\ddot{\mathbf{x}}_c(t) + \left(1+\frac{\kappa\alpha}{2D_1}\right)\dot{\mathbf{x}}_c(t) = \xi(t). \tag{6}$$

It is not possible to systematically calculate corrections to this equation by keeping more terms in the Taylor expansion of the position terms. It can however be shown that such corrections are negligible in high dimensions, $d \gg 2$. These issues are discussed more fully in the Appendix.

The modified Langevin equation (6) is clearly valid after some time t^* such that $t^* \gg 1/\lambda$. We define $\gamma=(1+\kappa\alpha/2D_1)/m$ and integrate Eq. (6) to get an equation for the time evolution of the ith component of the velocity vector:

$$\dot{x}_c^i(t) = \dot{x}_c^i(t^*)\exp[-\gamma(t-t^*)] + \frac{1}{m}\int_{t^*}^{t} dt' \exp[-\gamma(t-t')]\xi^i(t'). \tag{7}$$

Then it follows that the velocity autocorrelation function is given by

$$\langle \dot{x}_c^i(t)\dot{x}_c^i(s)\rangle = \dot{x}_c^i(t^*)^2 \exp[-\gamma(t+s-2t^*)] + \frac{D_0}{\gamma m^2}\{\exp(-\gamma|s-t|) - \exp[-\gamma(s+t-2t^*)]\}. \tag{8}$$

Using a Green-Kubo relation $D_R=\int_{t^*}^{t} dt' \langle \dot{x}_c^i(t)\dot{x}_c^i(t')\rangle$ it is possible to determine the effective (renormalized) particle diffusion coefficient D_R:

$$D_R = \frac{\dot{x}_c^i(t^*)^2}{\gamma}\exp[-\gamma(t-t^*)]\{1-\exp[-\gamma(t-t^*)]\} + \frac{D_0}{\gamma^2 m^2} \times \{1+\exp[-2\gamma(t-t^*)] - 2\exp[-\gamma(t-t^*)]\}, \tag{9}$$

which evaluated in the limit $t \to \infty$ leads us to the final set of results:

$$D_r = \begin{cases} D_0\left(1+\dfrac{\alpha}{2D_1}\right)^{-2}, & \kappa = 1, \quad \forall\,\alpha, \\ D_0\left(1-\dfrac{\alpha}{2D_1}\right)^{-2}, & \kappa = -1, \quad \alpha < 2D_1, \\ \infty, & \kappa = -1, \quad \alpha > 2D_1. \end{cases} \tag{10}$$

We defer a discussion of the physics behind these results for later. For the moment we focus on the numerical validation of the theory.

For the case of a self-attracting walker ($\kappa=1$) it is predicted that (i) the asymptotic behavior is diffusion with a renormalized diffusion coefficient whose magnitude decreases with increasing values of the coupling parameter α, and (ii) the behavior is independent of dimension (superuniversality in the velocity correlations). We test these predictions by numerically integrating the model equations (1) and (2) (see Fig. 1). The diffusion coefficient in all simulations is calculated from the slope of plots of the variance versus time for the time range $t \in (10, 1000)$. The initial chemical concentration is a Gaussian centered at the origin, though any nonzero function is suitable.

As expected, we find that the asymptotic behavior is diffusion characterized by renormalized diffusion coefficients which are relatively independent of the dimension (Fig. 1). However, there is some discrepancy between the theoretical values of D_R and the ones obtained from the numerics. Regression of the one-dimensional data in Fig. 1 shows that the numerical data is best fit by an equation of the form (see Fig. 2): $D_R=D_0(1+k\alpha/2D_1)^{-2}$ where $k=0.81\pm0.01$ (10^4 realizations). The difference between this value and the theoretical

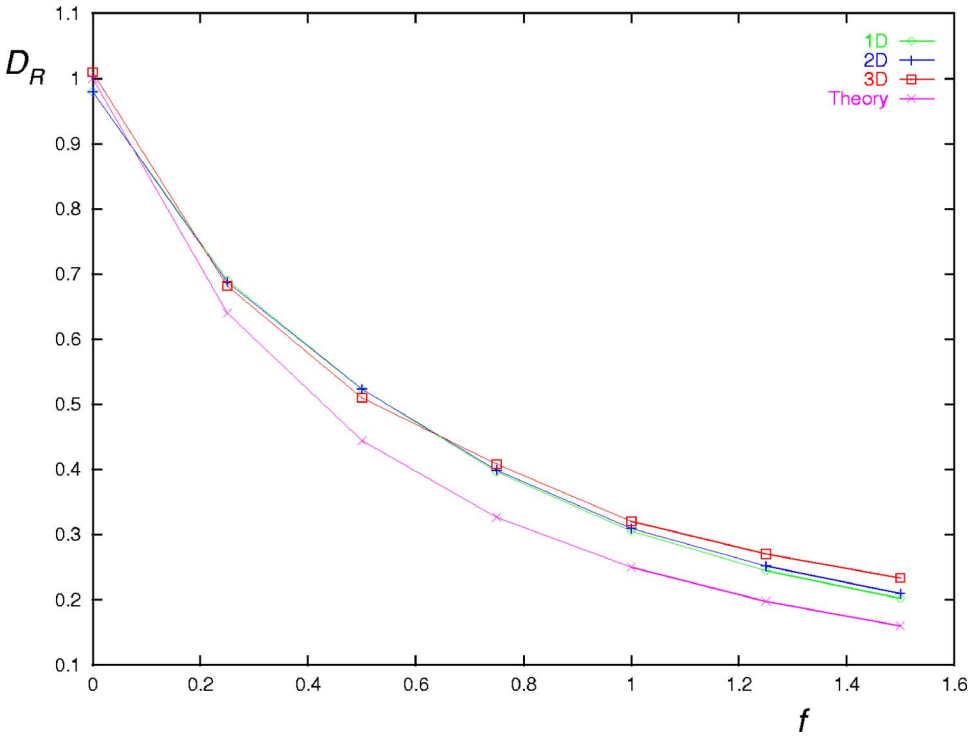

FIG. 1. (Color online) Plot of the renormalized diffusion coefficient D_R versus the nondimensional coupling parameter f, where $f=\alpha/2D_1$. The parameter κ equals 1, implying that the walker has a tendency to explore previously visited spatial regions. The other parameters are $m=10^{-6}$, $D_0=1$, $D_1=1$, $\lambda=1$, $\beta=1$, and $\delta t=0.1$ with 10^4 samples. As predicted, the renormalized diffusion coefficient is the same in one, two, and three dimensions.

value of unity, stems from a combination of the approximations used in deriving the effective Langevin equation (6) and numerical error due to a finite time step (note that the simulations are off-lattice and thus there is no numerical error due to a finite spatial step). As discussed in the Appendix, it is not possible to systematically calculate corrections to the effective Langevin equation. However, by repeating the simulations with a time step an order of magnitude smaller than those in Figs. 1 and 2, we find that the value of k increases to $k=0.87\pm0.02$ (2×10^3 realizations), which is closer to the theoretical value. Hence it is probable that the discrepancies between numerics and theory are in significant part due to numerical error rather than to the approximations implicit in deriving Eq. (6). This is plausible since the next-order correction to Eq. (6) is proportional to the walker's acceleration $\ddot{\mathbf{x}}_c(t)$ [see Eq. (A1) in the Appendix] which is negligible for a self-attracting walker since the dynamics are overdamped for small coupling ($m\ll1$) and become more

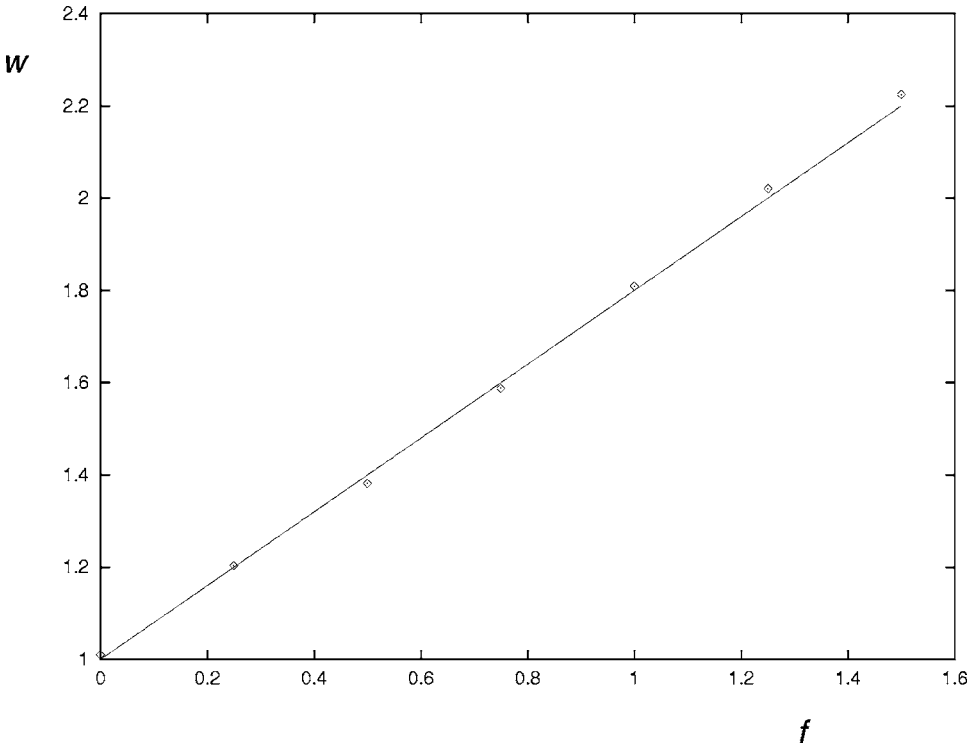

FIG. 2. Plot of $w=\sqrt{D_0/D_R}$ vs the nondimensional coupling parameter f, where $f=\alpha/2D_1$, for data obtained from one-dimensional simulations. Parameter values as in Fig. 1. This verifies the functional form predicted by theory. The solid line is the best fit through the data points. This line has a gradient of 0.81 and intercept of 0.99—theory predicts a gradient of 1.00 and an intercept of 1.00.

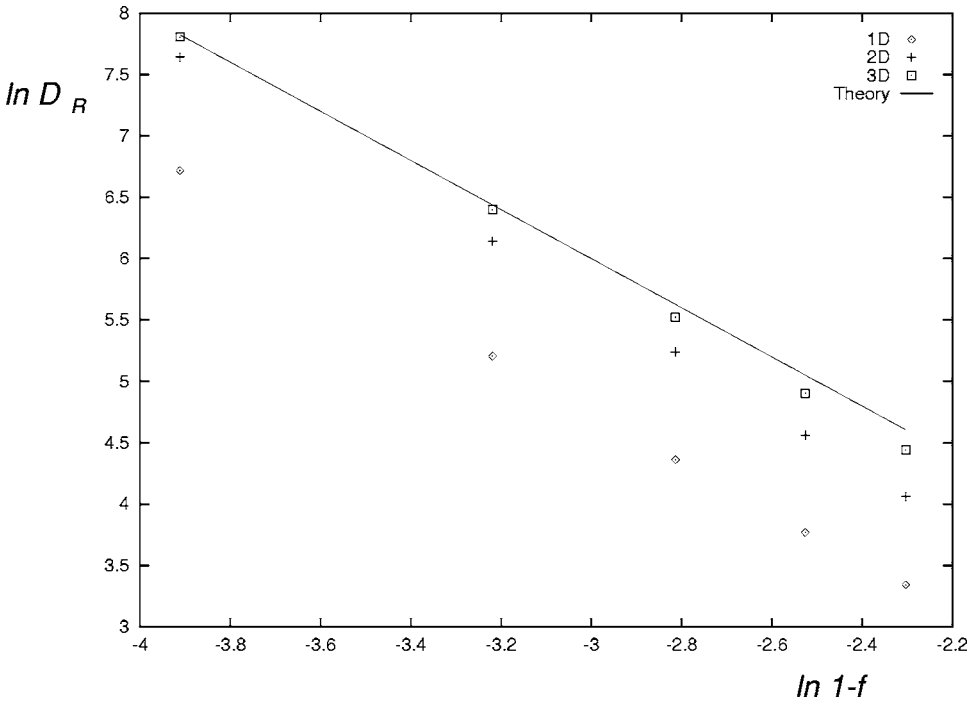

FIG. 3. Plot of the natural logarithm of the renormalized diffusion coefficient D_R versus the natural logarithm of the nondimensional parameter $1-f$, where $f=\alpha/2D_1$. Note that the f values in this plot vary between 0.9 and 0.98, meaning that we are exploring the walker's behavior near the theoretically predicted singularity at $f=1$. The parameter κ equals -1, implying that the walker has a tendency to explore previously unvisited spatial regions. The other parameter values are exactly as in Fig. 1. This graph confirms that $D_R \propto (1-f)^{-2}$, implying a singularity at $f=1$ in all dimensions.

strongly overdamped as the coupling increases [this is since the coefficient of the velocity term in Eq. (6) increases with the coupling].

For the case of a self-repelling walker ($\kappa=-1$) theory predicts that (i) if the coupling is less than a critical threshold, $\alpha<2D_1$, then the asymptotic behavior is diffusion with a renormalized diffusion coefficient, (ii) if the coupling is above this threshold, $\alpha>2D_1$, the particle diffusion coefficient diverges, and (iii) the behavior is independent of dimension. We tested these predictions by simulations. We find that near the predicted singularity, $0.9<\alpha/2D_1<1$, the variation of D_R with coupling is given by

$$D_R/D_0 \propto \left(1-\frac{\alpha}{2D_1}\right)^{-\zeta}, \tag{11}$$

where $\zeta=2.10\pm0.03$ in one dimension, 2.23 ± 0.02 in two dimensions, and 2.10 ± 0.02 in three dimensions (Fig. 3). These estimates agree well with the theoretical value of $\zeta=2$. The constant of proportionality in Eq. (11) is dependent on dimension, a feature not predicted by theory—interestingly, as shown in Fig. 3, the data in three dimensions is closest to the exact theoretical result. However, these features are not completely unexpected. This is since the coefficient of the velocity term in Eq. (6) decreases with increasing coupling, meaning that the acceleration of the walker becomes a determining factor as the critical coupling is approached. Thus the next-order correction to Eq. (6) [see Eq. (A1) in the Appendix] is probably not negligible (unlike in the case of a self-attracting walker). As discussed in the Appendix, these corrections are small in high dimensions and thus mostly significant in low dimensions. These theoretical arguments support the numerical data in Fig. 3.

Now we numerically explore the walker's asymptotic behavior for $\alpha/2D_1>1$. In this regime, the simulations break down after a few time steps. Using smaller values of the numerical time step does not help much and makes the numerical analysis computationally very expensive. This is overcome by simulating a model given by the equations

$$\dot{\mathbf{x}}_c(t) = \xi(t) - \alpha\frac{\nabla\phi(\mathbf{x}_c,t)}{\delta+\phi(\mathbf{x}_c,t)}, \tag{12}$$

$$\partial_t\phi(\mathbf{x},t) = D_1\nabla^2\phi(\mathbf{x},t) - \lambda\phi(\mathbf{x},t) + \beta\delta[\mathbf{x}-\mathbf{x}_c(t)]. \tag{13}$$

Since we are really interested in the case $\delta=0$, we obtained data for several small values of δ with the aim of extrapolating to the desired limit. As shown in Fig. 4, we find that for $\alpha/2D_1=3$ the renormalized diffusion coefficient clearly tends to infinity as $\delta\to0$. This is found to be generally true for $\alpha/2D_1>1$, meaning that the purported transition at $\alpha/2D_1=1$ is from finite D_R to $D_R=\infty$, in agreement with theory. Note that transitions in random walks with positive long correlations are known [14], though in this case the dynamical transition is from normal diffusion to superdiffusion in a one-dimensional space.

Now we discuss the theoretical results from a physical perspective. In the absence of self-interaction, the walker's motion is determined by the frictional force which is directly proportional to its velocity rather than by inertia (overdamped dynamics). For the case of a self-attracting walker ($\kappa=1$) it is expected that the walker spans space more slowly than for the case of no self-interaction: this typically means subdiffusive behavior or diffusive behavior with a renormalized diffusion coefficient smaller than D_0. We have shown that to a first approximation obtained by truncating the walker's memory to a time of the order $1/\lambda$, the self-interaction leads to a renormalization of the frictional force. This implies that the dynamics are always overdamped and that the

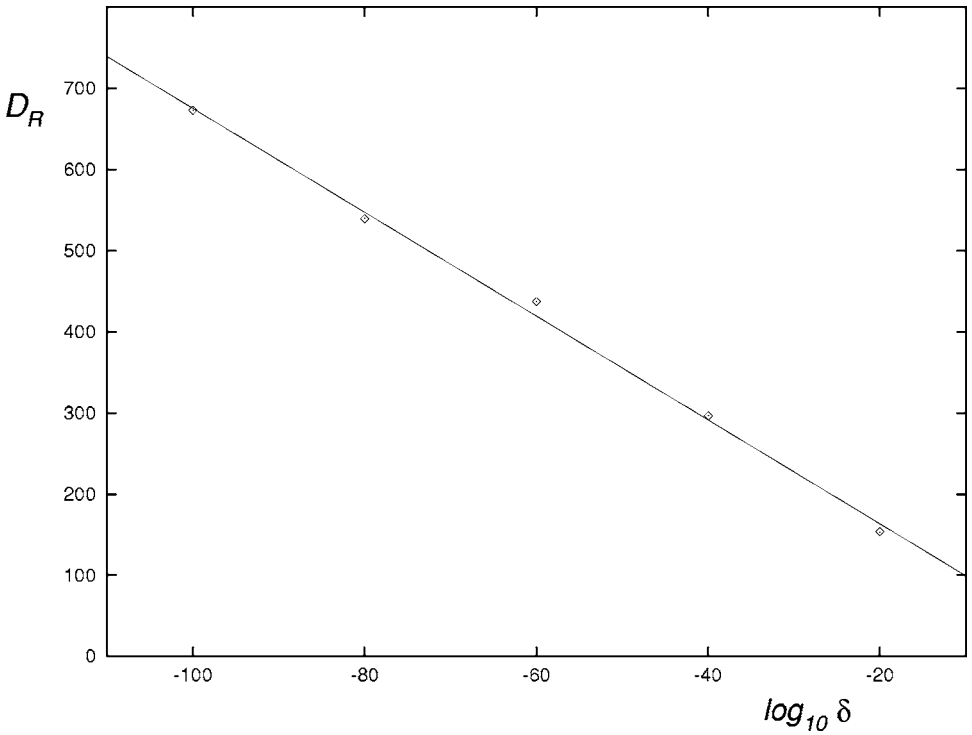

FIG. 4. Determination of the renormalized diffusion coefficient D_R for $f=3$ using the same parameters as in Fig. 3. The model simulated is that given by Eqs. (12) and (13). The solid line is the best fit through the data points, indicating that $D_R \propto \log_{10}(\delta^{-k})$ where k is some positive number. This suggests that in the limit $\delta \to 0$, $D_R \to \infty$ for $f>1$.

asymptotic behavior is that of renormalized diffusion, not subdiffusion.

For the case of a self-repelling walker ($\kappa=-1$) it is expected that the walker spans space faster than for the case of no self-interaction: this typically means superdiffusive behavior or diffusive behavior with a renormalized diffusion coefficient greater than D_0. We have shown that the self-interaction leads to a renormalization of the magnitude of the frictional force experienced by the walker. The frictional force decreases with increasing coupling α between the walker's motion and the chemical field until at a particular value of the coupling, $\alpha=2D_1$, the frictional force is exactly zero and the dynamics of the walker are purely determined by the inertial force. Thus the walker's behavior changes from one characterized by a low Reynolds number for weak self-interaction to behavior characterized by a high Reynolds number as one approaches the critical coupling. When the coupling exceeds the critical value, we find that the walker experiences a force that is proportional to the velocity but has the opposite effect of damping; the random fluctuations in the velocity due to the stochastic force are amplified rather than suppressed and thus the velocity of the walker increases uncontrollably with time, leading to an infinite velocity. This is the underlying reason for the divergence of the particle diffusion coefficient in this parameter regime.

It is worthwhile to compare the walker's behavior with logarithmic response to the behavior with linear response. The linear response model was studied by Grima [10], who found that if the particle diffusion coefficient (in the absence of self-interaction) is small then (i) for a self-attracting walker, the asymptotic behavior is that of renormalized diffusion, and (ii) for a self-repelling walker, the asymptotic behavior is renormalized diffusion below a critical threshold and ballistic diffusion above this threshold. The first difference to be emphasized between the two models with different responses is that for the logarithmic response the results are generally valid for any value of the particle diffusion coefficient and of the other parameters, whereas for the linear response model the results are restricted to small particle to chemical diffusion coefficients (small noise analysis). In other words the logarithmic response gives rise to behavior which is independent of the amplitude of the noise, an unusual property—for example, for intermediate to large noise, simulations indicate that the dynamics of a particle with linear response are not that of renormalized diffusion. It is also to be noted that the value of the critical coupling in the linear model is dimensionally dependent, unlike the superuniversal behavior in the present case. The logarithmic response $\nabla\phi/\phi$ is weaker than the linear response $\nabla\phi$ when $\phi>1$ and stronger otherwise. For the case of a self-attracting walker, the walker tends to stay in spatial regions that it has previously visited, meaning that the sampled chemical concentration ϕ at all times is significant and not small; thus in this case we expect the walker with linear response to exhibit a stronger or at least equally strong perturbation of its motion compared to that with logarithmic response. This reasoning agrees with our results. For the case of a self-repelling walker, the walker tends to avoid spatial regions that it has previously visited, meaning that the sampled chemical concentration tends to be very small; thus in this case we expect the walker with logarithmic response to exhibit a stronger or at least equally strong perturbation of its motion compared to that with linear response. This qualitatively explains the onset of the diverging diffusion regime for logarithmic response compared to the onset of ballistic diffusion for linear response.

As we mentioned in the Introduction, the model has potentially some applications in biology. The self-driven many-particle system is a model for chemotactic aggregation or

dispersion, behavior exhibited by a number of organisms, such as the slime mold [15]. The particles are then motile cells which secrete chemical and which simultaneously move up (or down) gradients of this chemical. The self-driven single particle can be thought of as a model for a chemotactic cell which is far away from the bulk of other cells; in that case the cell will predominantly sense its own chemical rather than that of other cells. In the linear response models studied by several authors, the cell's average velocity is assumed to be linearly proportional with the gradient of the local chemical field. In our model, the response is logarithmic which is known to be more realistic in some specific cases. This type of response is frequently referred to as the Weber-Fechner law and is thought to describe the sensory adaptation of a number of chemotactic cells to chemotactic signals, over certain concentration ranges [16–18]. With this proviso, our present model may perhaps be applicable to understanding some features of sensory adaptation at the micro-organism level.

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APPENDIX

It is in principle possible to calculate the next-order correction to Eq. (6) by retaining terms to second order in the Taylor series expansion of $x_c^i(t-n\Delta t)$ in Eqs. (3) and (4). Furthermore, since the exponent is slowly varying, the the sums over n can be approximated by integrals, leading to

$$\nabla \ln \phi(\mathbf{x}_c,t) = -\frac{\dot{\mathbf{x}}_c(t)}{2D_1} + \frac{\ddot{\mathbf{x}}_c(t)\Delta t}{4D_1} \times \left(\int_{n=1}^{n_{\max}} n^{1-d/2} f(n) \Big/ \int_{n=1}^{n_{\max}} n^{-d/2} f(n) \right), \tag{A1}$$

where

$$f(n) = \exp\left[-\Delta t \left(\lambda + \sum_{i=1}^{d} \frac{\dot{x}_c^i(t)^2}{4D_1} \right) n + \Delta t^2 \left(\sum_{i=1}^{d} \frac{\dot{x}_c^i(t)\ddot{x}_c^i(t)}{4D_1} \right) n^2 - \Delta t^3 \left(\sum_{i=1}^{d} \frac{\ddot{x}_c^i(t)^2}{16D_1} \right) n^3 \right]. \tag{A2}$$

The integrals in Eq. (A1) cannot be computed exactly and approximations are also hard to come by, since we do not *a priori* know the magnitude of the walker's velocity $\dot{\mathbf{x}}_c(t)$ and acceleration $\ddot{\mathbf{x}}_c(t)$, which appear in the argument of the exponent. The main problem here is that one has an implicit equation [given by Eq. (1) together with Eq. (A1)] in the walker's velocity. The only fact that can be safely deduced is that for $d \gg 2$, the two integrals are approximately equal; this implies that the second term in Eq. (A1) vanishes in the limit $\Delta t \to 0$ and that in high dimensions there are no further corrections to the modified Langevin equation (6). Clearly, in the formalism of the Langevin equation it is not easily possible to systematically calculate corrections to the modified Langevin equation (6). However, it is to be emphasized that the derivation of the latter equation (and the subsequent prediction of the phase transition) eludes a treatment based on the equation of motion of the walker's probability density function.

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