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A driven particle in a cloud of mobile impurities

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Abstract. The dynamics of a test particle interacting with diffusing impurities in one dimension is investigated analytically and numerically. In the absence of an applied external force, the dynamics of the particle can be characterized by a distribution of monotonic excursions Δx, which scales as a power law with an exponent $\tau_{\Delta x} = 4/3$. When the particle is driven at a slow constant velocity, there is again a power law distribution for the monotonic changes of the force ΔF, which is characterized by a similar exponent $\tau_{\Delta F} = 4/3$. These results can be understood from the theory of random walks.

Keywords: defects (theory), fluctuations (theory), stochastic processes (theory)

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Contents

1. Introduction

The interaction of driven particles, flexible lines and membranes etc. with disorder is an important topic in condensed matter physics [1]–[3]. Usually, this disorder is taken to be quenched, or frozen, such that its properties do not change within the relevant timescales. However, under certain conditions, this changes, as in the case of the diffusion of solute atoms in metallic alloys [4, 5] or oxygen vacancies in superconductors [6]. The mobile impurities play an important role in the dynamics of such systems, as evidenced for example by the Portevin–Le Chatelier (PLC) effect in solid solutions [7]. There, within a certain range of temperatures and applied strain rates, the dynamic interaction of lattice dislocations and diffusing solute atoms results in phenomena such as negative strain rate sensitivity of the flow stress, giving rise to macroscopic serrations in the stress–strain curve and strain localization in the form of bands of activity of various types [8]–[10].

Here, we consider the simple test problem of a single particle interacting with a cloud of diffusing impurities, with the dynamics constrained to one dimension (a line). We restrict ourselves to the region of the parameter space in which the impurities have a vanishingly small probability to escape from the vicinity of the particle within the timescale of the simulation. Thus, the particle is dragging an impurity cloud with a fixed number of impurity particles without escaping from it. Despite its apparent simplicity, such a system exhibits rich dynamics, but at the same time has features that make the problem analytically tractable. In the absence of external forces, we consider the statistics of monotonic excursions Δx of the particle, i.e. the distances the particle moves to a particular direction (here 'left' or 'right' along the one-dimensional line) without changing direction; see also figure 1. We find that these obey power law distributions $P(\Delta x) \sim (\Delta x)^{-\tau_{\Delta x}} f_c(\Delta x/\Delta x_0)$ with the exponent $\tau_{\Delta x} = 4/3$. The same is true for the monotonic changes of the external force ΔF when the particle is driven with a slow constant velocity. This paper is organized as follows. In the next section, we consider the interaction of a particle with a single mobile impurity, in the absence of external forces. Then we generalize this to the case with more impurity particles. In section 3, the effect of an external drive is studied. Finally, section 4 finishes the paper with conclusions.

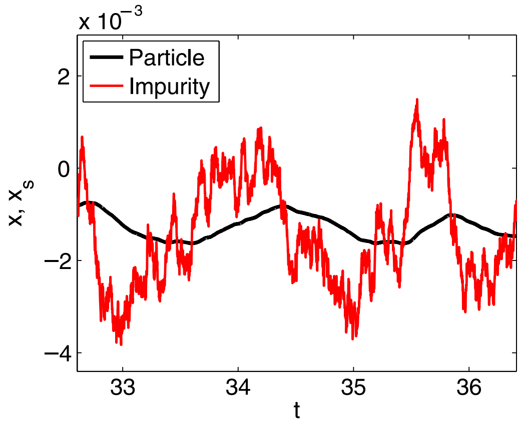

Figure 1. An example of the trajectories of the particle and a single impurity, in the absence of external forces. Notice that the monotonic excursions of the particle correspond to motion of the particle during time intervals that the impurity spends on a given side of the particle. Parameters of the simulation: $\mu = A = l = 1.0$, $\delta\eta = 0.1$.

2. A particle interacting with mobile impurities

2.1. Single impurity

As a starting point of our analysis, we consider for simplicity the dynamics of a single test particle interacting with one diffusing impurity particle. We take the test particle to be at zero temperature, as our main motivation for the present work is to study a simplified model of a dislocation interacting with diffusing solute atoms. As thermal fluctuations acting on the segments of the dislocation line tend to average out on the scale of the whole dislocation line, the test particle which can be thought of as a projection of the dislocation line to a single point can be regarded as noise free. Moreover, even in the case of a truly two-dimensional crystal with a large number of diffusing solutes, the magnitude of the total interaction force due to all the solute atoms acting on the point-like dislocation would dominate the noise term, whereas for solute atoms interacting only with the dislocation (they are assumed to be pure misfit solutes) the same is not true.

Consequently, we take the equations of motion for the system with a single impurity particle to be of the form

$$\mu\partial_t x = f(x - x_\mathrm{s}) \qquad \partial_t x_\mathrm{s} = -f(x - x_\mathrm{s}) + \eta, \tag{1}$$

where x and x_s are the positions of the particle and the impurity particle, respectively. $f(z)$ is the interaction force between the particle and the impurity particle, μ defines the relative mobilities of the impurity and the particle and η is Gaussian white noise with standard deviation $\delta\eta$.

The dynamics of the particle can be analyzed by considering the stochastic process for the velocity $\partial_t x$. By differentiating the equation of motion of the particle with respect to time and using the equation of motion for x_s, one obtains

$$\mu\partial_t^2 x = \partial_z f(z)\left[(1+\mu)\partial_t x - \eta\right]. \tag{2}$$

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Close to $z = x - x_s = 0$, the force $f(z)$ can be taken to be linear in z and thus the derivative of the force can be approximated by a constant, $\partial_z f(z) \approx -C$, with $C > 0$. With $\lambda = C(1+\mu)/\mu$ and $\xi = -(C/\mu)\eta$, equation (2) can then be rewritten in the form of an Ornstein–Uhlenbeck process for $\partial_t x$,

$$\partial_t^2 x = -\lambda \partial_t x + \xi. \tag{3}$$

For the process $\partial_t x$, equation (3) describes Brownian motion pushed toward the origin by a linear damping term. This problem has been considered e.g. in [11], and the scaling exponents are known. In particular, the first return times T, to the origin of $\partial_t x$, have a probability distribution scaling as

$$P(T) \sim T^{-\tau_T} f_c\left(\frac{T}{T_0}\right), \tag{4}$$

with $\tau_T = 3/2$ and the cut-off scale $T_0 \sim 1/\lambda$. Similarly, the average shape of an excursion, $\langle \partial_t x(t)\rangle_T$, scales for $t, T - t \ll 1/\lambda$ as $\langle \partial_t x(t)\rangle_T = T^{\gamma-1} f_{\mathrm{shape}}(t/T)$, with $\gamma = 3/2$. Then, by using the scaling relation $\gamma = (\tau_T - 1)/(\tau_{\Delta x} - 1)$ [12], one obtains the distribution of the lengths $\Delta x = \int_0^T \partial_t x \,\mathrm{d}t$ of monotonic excursions of the particle,

$$P(\Delta x) \sim (\Delta x)^{-\tau_{\Delta x}} f_c\left(\frac{\Delta x}{\Delta x_0}\right), \tag{5}$$

with $\tau_{\Delta x} = 4/3$. The cut-off scaling can be found as follows. The cut-off of the first return time distribution of equation (3) is given by $T_0 \sim 1/\lambda$ [11]. Here, both λ and ξ in equation (3) depend on C and μ. Due to the relation $\Delta x_0 \sim T_0^\gamma$ with $\gamma = 3/2$, Δx_0 is expected to scale like

$$\Delta x_0 = \left(\frac{1}{\lambda}\right)^{3/2} \delta\xi = \sqrt{\frac{\mu}{C}} \frac{\delta\eta}{(1+\mu)^{3/2}}. \tag{6}$$

We check this result in numerical simulations, where we take for simplicity $f(z)$ to be of the form $f(z) = -Az\exp\left(-(1/2)(z/l)^2\right)$, corresponding to $\partial_z f(z)|_{z=0} = -A$, i.e. $C = A$. We integrate the equations of motion (1) with the Euler algorithm. The strength of the thermal noise was chosen to be sufficiently weak compared to the strength of the particle–impurity interaction such that the impurity will not escape from the neighborhood of the particle within the timescales of the simulation. Figure 1 shows an example of the trajectories of the particle and the impurity. Figure 2 displays the distribution of Δx for various values of A. For a weak enough interaction strength A, the distributions exhibit the expected scaling with $\tau_{\Delta x} = 4/3$. The cut-off is found to scale as $\Delta x_0 \sim A^{-1/2}$, in agreement with our results above.

This implies that the motion of the particle is reminiscent of truncated Levy flights, with a step length distribution given by equation (5). However, the steps are not instantaneous—their durations T exhibit power law scaling as well; equation (4). If one were to interpret these step durations as waiting times between instantaneous steps, independent from the step lengths, one would obtain for early times the scaling $\langle x^2\rangle(t) \sim t^{2(\tau_T-1)/(\tau_{\Delta x}-1)} = t^{2\gamma} \sim t^3$ [13]. However, here Δx and T are not independent

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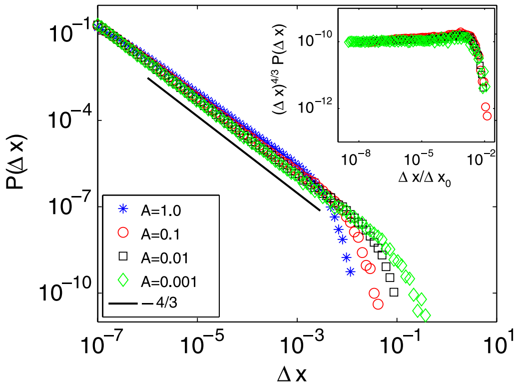

Figure 2. Main figure: the probability distributions of monotonic excursions of the particle interacting with a single impurity, for various strengths A of the interaction force. For sufficiently low A values, the distribution scales with the exponent $\tau_{\Delta x} = 4/3$, indicated by the solid line. Inset: a scaling plot of the distributions. The cut-off is observed to scale as $\Delta x_0 \sim \sqrt{1/A}$, in agreement with equation (6). Other parameters: $l = 1$, $\mu = 1$ and $\delta\eta = 0.1$.

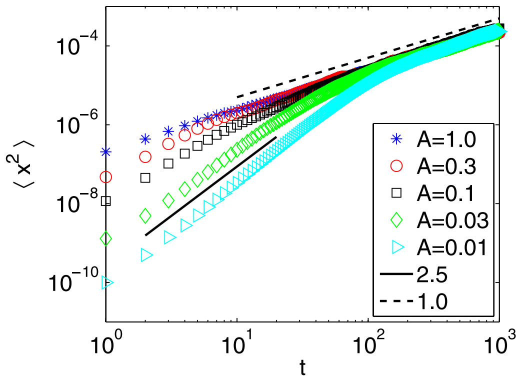

Figure 3. The mean square displacement of the particle interacting with a single impurity in the absence of external forces, for different strengths A of the particle–impurity interaction. The early times are characterized by superballistic motion with $\langle x^2\rangle(t) \sim t^{5/2}$ (solid line), while for longer times a crossover to diffusive dynamics is observed (dashed line). Parameters of the simulation: $\mu = l = 1.0$, $\delta\eta = 0.1$.

(they are coupled through the relation $\langle\Delta x\rangle \sim T^{\gamma}$). As the early time behavior is dominated by a single large step, one must consider instead the effect of a single step given its duration, yielding

$$\langle x^2\rangle(t) \sim \int_0^t [\Delta x(T)]^2 P(T)\,\mathrm{d}T = \int_0^t T^{2\gamma-\tau_T}\,\mathrm{d}T \sim t^{2\gamma-\tau_T+1}, \tag{7}$$

corresponding to $\langle x^2\rangle(t) \sim t^{5/2}$ for the exponent values at hand. Due to the cut-offs in the distributions of T and Δx, one expects a crossover to diffusive behavior with $\langle x^2\rangle(t) \sim t$ for long times. This is verified in figure 3.

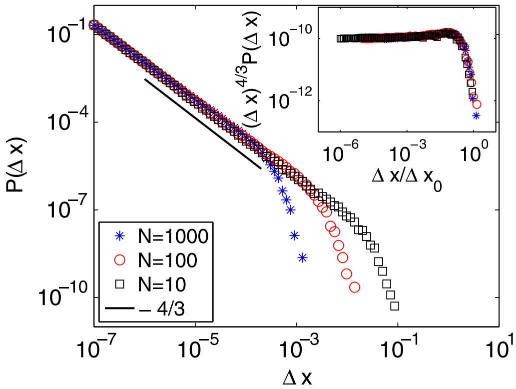

Figure 4. Main figure: the probability distributions of monotonic excursions of the particle interacting with N impurities. The distribution scales with the exponent $\tau_{\Delta x} = 4/3$, indicated by the solid line. Inset: a scaling plot of the distributions. The cut-off is observed to scale as $\Delta x_0 \sim 1/N$, in agreement with equation (9). Parameters of the simulation were $A = 0.01, l = 1$, $\mu = 1$ and $\delta\eta = 0.1$.

2.2. Several impurities

The case of a fixed number $N > 1$ of impurity particles is a straightforward generalization of that presented in the previous subsection. The equations of motion become

$$\mu \partial_t x = \sum_i f(x - x_{s,i}) \qquad \partial_t x_{s,i} = -f(x - x_{s,i}) + \eta_i. \tag{8}$$

From these, with the same procedure as above, one obtains an equation of the form of equation (3) by setting $\lambda = C(N + \mu)/\mu$ and $\xi = (C/\mu)\sum_i \eta_i$. Thus, the same scaling, i.e. $P(\Delta x) \sim (\Delta x)^{-4/3}$, is expected. One should notice, however, that the cut-off scale Δx_0 is getting smaller with increasing N. With arguments similar to the above, one finds that

$$\Delta x_0 = \left(\frac{1}{\lambda}\right)^{3/2} \delta\xi = \sqrt{\frac{\mu N}{C}} \frac{\delta\eta}{(N + \mu)^{3/2}}. \tag{9}$$

This is verified by the numerical results presented in figure 4.

3. Constant velocity drive

Next we proceed to study the effect of a weak external force F on the dynamics of the particle. In this context a constant velocity drive is perhaps the more interesting form of driving as a small constant force with $\partial_t F = 0$ does not change the dynamics from the non-driven case: equation (2) remains the same even if a constant force term is introduced in equation (1). In particular, we consider a particle driven by a force given by $F = K(Vt - x)$, where V is the driving velocity and K is a spring constant characterizing the response of the driving mechanism. The equations of motion read

$$\mu \partial_t x = \sum_i f(x - x_{s,i}) + F \qquad \partial_t x_{s,i} = -f(x - x_{s,i}) + \eta_i. \tag{10}$$

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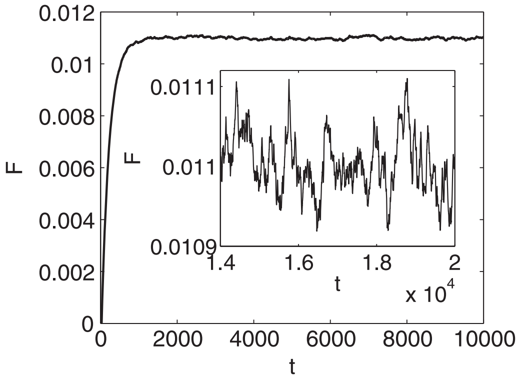

Figure 5. An example of the behavior of the force as a function of time. The inset shows a magnification of a part of the signal in the steady state. Parameters of the simulation: $\mu = l = 1.0$, $A = 0.01$, $N = 10$, $K = 0.1$, $\delta\eta = 0.1$ and $V = 0.001$.

In systems like this driven with a constant velocity, the interesting quantity is the statistics of the external force fluctuations. To this end, we consider the stochastic process $\partial_t F$. With an approach similar to the above, one can write

$$\partial_t^2 F = -K\partial_t^2 x = -\left[\frac{K}{\mu} + \frac{C}{\mu}(N+\mu)\right]\partial_t F + \frac{KC}{\mu}\sum_i \eta_i + \frac{KC}{\mu}\left[V(N+\mu) - F\right], \qquad (11)$$

where the relation $\partial_t x = V - \partial_t F/K$ has been used. In the steady state, the last term in equation (11) has a zero mean, as one can write for the average steady state force $F_\mathrm{s} = \langle \mu\partial_t x - \sum_i f(x - x_{\mathrm{s},i})\rangle = \mu V + N f_\mathrm{s}$, where f_s is the magnitude of the average retarding force acting on the particle due to a single impurity. In the steady state the condition $\langle \partial_t x_{\mathrm{s},i}\rangle = f_\mathrm{s} = V$ holds, and thus $\langle V(N+\mu) - F\rangle = 0$. Assuming that the fluctuations $\delta[V(N+\mu) - F] = \delta F$ are small compared to those of the white noise term in equation (11), i.e. $\delta F \ll \sqrt{N}\delta\eta$, equation (11) can be approximately written as

$$\partial_t^2 F = -\left[\frac{K}{\mu} + \frac{C}{\mu}(N+\mu)\right]\partial_t F + \frac{KC}{\mu}\sum_i \eta_i, \qquad (12)$$

which is again of the same form as equation (3). Thus, the monotonic changes of the external force $\Delta F = \int_0^T \partial_t F\,\mathrm{d}t$ are expected to be distributed according to a power law $P(\Delta F) = (\Delta F)^{-\tau_{\Delta F}} f_c(\Delta F/\Delta F_0)$, with the exponent $\tau_{\Delta F} = 4/3$ and the cut-off scale ΔF_0 scaling as

$$\Delta F_0 = \frac{KC\sqrt{\mu N}\delta\eta}{[K + C(N+\mu)]^{3/2}}. \qquad (13)$$

Notice that the condition $\delta F \ll \sqrt{N}\delta\eta$ implies that

$$\frac{KC\sqrt{\mu}}{[K + C(N+\mu)]^{3/2}} \ll 1. \qquad (14)$$

For most of the relevant parameter values condition (14) is fulfilled; only for $KC \gg 1$ is this not the case.

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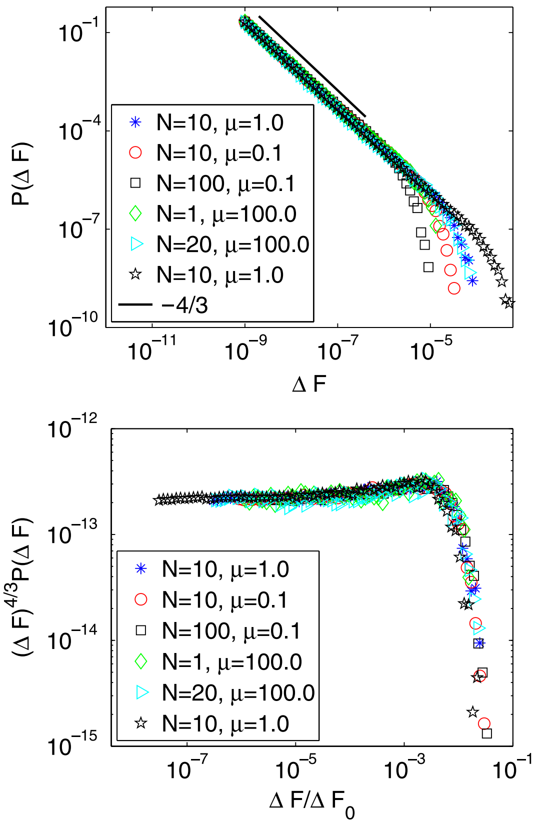

Figure 6. Distributions of the monotonic changes of the external force ΔF (upper panel) for various values of the parameters. The lower panel shows a data collapse of the distributions, with ΔF_0 computed from equation (13). All other cases have $\delta\eta = 0.1$, while the data shown with black stars have $\delta\eta = 1.0$. Other parameters of the simulations: $K = 0.1$, $A = 0.01$ and $V = 0.001$.

Next we check these predictions numerically for different values of the parameters satisfying the condition (14). Figure 5 shows an example of the behavior of the force as a function of time. After an initial transient, the system reaches a steady state in which the force fluctuates around a constant average value. In figure 6, we show the distributions of the monotonic changes of the external force ΔF in the steady state, for different values of the various parameters. Power law scaling of the distributions consistent with the exponent value $\tau_{\Delta F} = 4/3$ is observed, with a cut-off of the distributions in agreement with equation (13). The different ΔF values appear to be uncorrelated in time.

4. Conclusions

In this paper we have studied the dynamics of a single particle interacting with a cloud of diffusing impurities. In the absence of external forces, the problem can be mapped to Brownian motion in a potential within the harmonic approximation of the attractive particle–impurity interaction. Thus, the monotonic excursions of the particle are distributed as a power law, $P(\Delta x) \sim (\Delta x)^{-\tau_{\Delta x}}$, with $\tau_{\Delta x} = 4/3$. For a particle driven with a small constant velocity (such that the particle is dragging the impurity cloud without escaping from it), the external force fluctuations follow the same dynamics, which makes it possible to derive the probability distribution for the monotonic changes of the external force scaling as $P(\Delta F) \sim (\Delta F)^{-\tau_{\Delta F}}$, again with $\tau_{\Delta F} = 4/3$.

While a typical experimentally relevant scenario would correspond to either a higher dimensional object such as a flexible line or a large number of interacting particles interacting with mobile impurities, the simple setup of the present study serves as a convenient starting point for such considerations illustrating the relevant phenomena in a transparent manner. One interesting observation is that already at the level of a single particle interacting with one or more mobile impurities the dynamics has scale free features, arising from the properties of simple random walks. Physical situations in which such considerations could be relevant include dislocations interacting with solute atoms, a subject that has recently attracted considerable attention [14]–[16]. In many of these studies, more realistic interaction forces between dislocations and solute atoms have been used, but instead of the fluctuations studied here, the focus has been on different quantities such as the average velocity of the dislocation. Also, in classical studies on moving dislocations dragging a solute cloud, such fluctuations have been ignored [17].

The most intriguing phenomena associated with the presence of diffusing impurities are the collective effects arising from the simultaneous interaction of large number of entities with each other and with mobile impurities. An example of such a system is provided by interacting dislocation ensembles interacting with diffusing solute atoms in solid solutions, giving rise to phenomena such as the Portevin–Le Chatelier effect. In the PLC effect, large numbers of dislocations synchronize their motion to form macroscopic deformation bands of various kinds. As this is widely believed to be due to the dynamic interaction of the dislocations with the diffusing solute atoms, a natural future line of research would be to study such effects by considering numerically the dynamics of a large number of interacting dislocations interacting with diffusing impurities. One further motivation for such studies could be the recent observation that purely stochastic effects can induce switching between collective motion states [18].

Acknowledgments

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