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LETTER TO THE EDITOR

Long-time asymptotics of diffusion in random media and related problems

Hajo Leschke and Siegfried Wonneberger

Institut für Theoretische Physik, Universität Erlangen-Nürnberg, D-8520 Erlangen, Federal Republic of Germany

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Abstract. For n-dimensional diffusion in Gaussian random fields, with continuous and singular covariances, the leading long-time behaviour of the averaged population is derived by estimating Brownian motion expectations. It is shown how these results are related to the leading low-energy behaviour of the density of states for a particle in a corresponding random potential and to the strong-coupling limit of the free energy of the Pekar–Frölich polaron.

Diffusion in random media [1–3] is relevant in various fields of physics and also in chemistry and biology. While recently a first attempt has been made to derive intermediate-time aspects of the averaged population [4], the more accessible long-time asymptotics is still actively debated [5–8]. Our goal in the present letter is to contribute to the latter issue by solving a generalisation of a problem considered in [6, 8] and to eastablish its relation to important problems of condensed matter physics. Basically, our method of solution consists in constructing appropriate bounds for the averaged population. Some of the non-asymptotic bounds have an independent significance because they provide an elucidating control already for finite times.

Now we are going to state our main assertions. For the fundamental solution $P(t, x)$ of the linear reaction-diffusion equation in n-dimensional Euclidean space

$$\left(\frac{\partial}{\partial t} - D\nabla^2 + V(x)\right)P(t, x) = 0 \qquad P(0, x) = \delta(x) \qquad x \in \mathbb{R}^n \tag{1}$$

with diffusion constant $D > 0$ and the homogeneous Gaussian random field V characterised by the moments

$$\overline{V(x)} = 0 \qquad \overline{V(x)V(x')} \equiv C(x - x') \tag{2}$$

we present the leading long-time behaviour of its average for two different types of covariances C.

For *continuous* covariances the behaviour is

$$\lim_{t\to\infty} t^{-2} \ln \overline{P(t, x)} = C(0)/2. \tag{3}$$

For the *singular* covariance

$$C(x) = \nu^2 \begin{cases} \delta(x) & \text{for } n = 1 \\ |x|^{-1} & \text{for } n \geq 2 \end{cases} \tag{4}$$

the behaviour is

$$\lim_{t\to\infty} t^{-3} \ln \overline{P(t,x)} = \frac{\nu^4}{4D} \gamma_n \tag{5}$$

with the numerical constant

$$\gamma_n := \sup_f \left\{ \int_{\mathbf{R}^n} \mathrm{d}x \int_{\mathbf{R}^n} \mathrm{d}x' \frac{C(x-x')}{\nu^2} f^2(x) f^2(x') - \int_{\mathbf{R}^n} \mathrm{d}x (\nabla f)^2(x) \right\}. \tag{6}$$

The supremum has to be taken over real-valued functions f satisfying the normalisation

$$\int_{\mathbf{R}^n} \mathrm{d}x f^2(x) = 1.$$

Before giving the proofs, we offer several remarks in order to make contact to earlier results in the literature and to show interesting implications for two problems of condensed matter physics. Moreover, we will give information on the numerical value of the constant γ_n.

Remark 1. Equation (3) confirms a result in [2] obtained there by a discrete-space approach. We note that C does not need to be smooth. An example is $C(x) = \exp(-a|x|^{1/2})$ ($n=1, a>0$), which indeed has a non-negative Fourier transform by Pólya's condition [9]. We stress that the super-exponential asymptotic growth $\bar{P} \sim \exp(t^2)$ is independent of the diffusion constant and the dimension.

Remark 2. Of course, if $C(0)$ is infinite, the asymptotic growth must be even stronger. An example of considerable physical relevance (see also remarks 5 and 6 below) is given by (4). Here the scaling relation

$$C(\lambda x) = C(x)/\lambda \qquad \lambda > 0 \tag{7}$$

leads to the asymptotic growth $\bar{P} \sim \exp(t^3)$. It is interesting to note that in higher dimensions a long-range-correlated random field causes the same long-time behaviour as the short-range-correlated white noise in one dimension. We also note that the inequality

$$\overline{P(t,0)} \geqslant (4\pi D t)^{-n/2} \exp\left(\frac{t^3 \nu^4}{4D} \gamma_n\right) \tag{8}$$

according to [10, 11] already reflects the right asymptotic behaviour.

Remark 3. Specialising (5) or (8) to $n=1$ shows that the assertion of [6] is wrong. The inaccuracy of that assertion has also been observed in [8]. There, an asymptotic result essentially equivalent to

$$\lim_{t\to\infty} t^{-3} \ln \int_{\mathbf{R}} \mathrm{d}x \overline{P(t,x)} = \frac{\nu^4}{4D} \gamma_1 \tag{9}$$

was found by using plausible arguments. This result is sufficient to disprove [6], as can be seen by integrating the inequality

$$\overline{P(t,x)} \leqslant \overline{P(t,0)} \exp(-x^2/4Dt) \tag{10}$$

over x.

A derivation of (10) for general covariances and dimensions is given below. We will also show that the local result (5) is equivalent to the global result (9) (generalised to $n \geqslant 1$) which, in its turn, we show to be a consequence of the Donsker–Varadhan large-deviation theory.

Remark 4. The paper by Tao *et al* [7], dealing with delta-function covariances in dimensions $n \geqslant 2$, is wrong too, because in these cases it is known [12] that $\overline{P(t,0)}$ is infinite for any t.

Remark 5. By a saddle point argument, the results (3) and (5) for $x=0$ are equivalent to the leading low-energy behaviours

$$\lim_{E\to-\infty} |E|^{-2} \ln \rho(E) = -\frac{1}{2C(0)} \tag{11}$$

$$\lim_{E\to-\infty} |E|^{-3/2} \ln \rho(E) = -\left(\frac{16D}{27\nu^4\gamma_n}\right)^{1/2} \tag{12}$$

of the density of states (inverse Laplace transform of $\overline{P(t,0)}$)

$$\rho(E) = \frac{1}{2\pi i}\int_{\beta-i\infty}^{\beta+i\infty} dt\, e^{tE}\overline{P(t,0)} \qquad \beta>0 \tag{13}$$

of a particle (with mass $1/2D$, Planck's constant $\hbar \equiv 1$) in a Gaussian random potential V with the respective covariances. Equation (11) is well established in the literature [13]. For the white-noise potential in one dimension the density of states is known explicitly for all energies [14]. As it must do, its asymptotic evaluation agrees with (12) for $n=1$.

Remark 6. Result (5) for $x=0$ implies the strong-coupling limit

$$\lim_{\alpha\to\infty} \alpha^{-2} F(\alpha, t) = -\gamma_n \tag{14}$$

of the free energy $F(\alpha, t)$ of the Pekar–Frölich model for the large polaron [15–17] generalised to n dimensions [18, 19] (electron–phonon coupling constant α, temperature $1/k_B t$, Boltzmann's constant k_B, phonon energy $\hbar\omega \equiv 1$). In order to show this we start from the inequalities

$$-t^{-1}\ln Z\left(\frac{t}{2}\coth\frac{t}{2}, (\alpha^2 t)^{1/3}\right) \leqslant F(\alpha, t) \leqslant -t^{-1}\ln Z(1, (\alpha^2 t)^{1/3}). \tag{15}$$

Here we have used a scaling argument and the notation

$$Z(\alpha, t) := \overline{P(t,0)} \qquad \text{for} \qquad \nu^2 = \alpha(4D)^{1/2} \tag{16}$$

and identified the bare electron mass with $1/2D$. Then (14) follows from (5) and the fact that $F(\alpha, t)$ is increasing in t (cf [16]).

Remark 7. From the topics in remarks 5 and 6, we collect the known information about the value of the numerical constant (6) occurring in (5):

$$\gamma_1 = \tfrac{1}{2} \qquad \gamma_2 \approx 0.4047 \qquad \gamma_3 \approx 0.108\,513 \tag{17}$$

to be found in [11, 18, 15] respectively. In addition, the following inequalities:

$$\frac{1}{4n}\left(\frac{\Gamma((n-1)/2)}{\Gamma(n/2)}\right)^2 \leqslant \gamma_n \leqslant \frac{1}{(n-1)^2} \tag{18}$$

hold for $n \geqslant 2$, with Γ denoting Euler's gamma function. The lower bound has been obtained by varying over Gaussian functions f only. The upper bound is the negative ground-state energy of a particle (with mass $\hbar^2/2$) in the $-|x|^{-1}$ potential in $n \geqslant 2$ dimensions.

For the proofs we set out from the Feynman-Kac formula [20]

$$P(t, x)=\left\langle\delta(b(t)-x)\exp\left(-\int_0^t \mathrm{d}s\, V(b(s))\right)\right\rangle. \tag{19}$$

Here the angular brackets denote the average over n-dimensional Brownian motion $b(t)$ $(t \geq 0)$ starting at the origin, which is the continuous random process in $\mathbb{R}^n$ with $b(0)=0$ and independent increments $b(t+\tau)-b(t)$ $(\tau>0)$ having the stationary probability density

$$\langle\delta(b(t+\tau)-b(t)-x)\rangle=(4\pi D\tau)^{-n/2}\exp(-x^2/4D\tau). \tag{20}$$

In other words, the angular brackets serve as a streamlined notation for Wiener-type path integration. Averaging (19) over the random field yields

$$\overline{P(t, x)}=\langle\delta(b(t)-x)\mathrm{e}^{\Phi_t}\rangle \tag{21}$$

with the non-negative path functional

$$\Phi_t := \frac{1}{2}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s' C(b(s)-b(s')). \tag{22}$$

Our proofs of the inequality (10) and the assertions (3) and (5) are all based on formula (21).

We first turn to the proof of (10). In view of (20) it is sufficient to show that

$$\frac{\langle(\delta(b(t)-x)\Phi_t^m\rangle}{\langle\delta(b(t)-x)\rangle} \leq \frac{\langle\delta(b(t))\Phi_t^m\rangle}{\langle\delta(b(t))\rangle} \qquad m \in \mathbb{N} \tag{23}$$

for each power Φ_t^m in the Taylor expansion of $\exp(\Phi_t)$. But this follows from two facts. First, as a covariance C has a non-negative Fourier transform. Second, the explicit expression (e.g. [21]) for the characteristic functional

$$G(t, x, \eta) := \frac{\langle\delta(b(t)-x)\exp[\mathrm{i}\int_0^t \mathrm{d}s\, \eta(s) b(s)\rangle}{\langle\delta(b(t)-x)\rangle} \tag{24}$$

of pinned Brownian motion implies

$$|G(t, x, \eta)| \leq G(t, 0, \eta) \tag{25}$$

for each function $\eta:[0, t] \rightarrow \mathbb{R}^n$.

We now turn to the proof of (3). Since $|C(x)| \leq C(0)$ and C is continuous, for every $\varepsilon>0$ there is $\kappa>0$ such that

$$C(0)(1-\varepsilon-\kappa x^2) \leq C(x) \leq C(0) \tag{26}$$

holds for all $x \in \mathbb{R}^n$. We note that if C is twice continuously differentiable, κ can be chosen as $-(\nabla^2 C)(0)/2C(0)$ independent of ε. Inserting (26) into (22) and (21) yields the estimates

$$\exp\left(\frac{t^2 C(0)}{2}(1-\varepsilon)\right)\left\langle\delta(b(t)-x)\exp\left(-\frac{C(0)\kappa}{2}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s'(b(s)-b(s'))^2\right)\right\rangle$$
$$\leq \overline{P(t, x)} \leq \exp(t^2 C(0)/2)\langle\delta(b(t)-x)\rangle. \tag{27}$$

The average on the left-hand side can be performed explicitly to give [21, 22]

$$(4\pi Dt)^{-n/2}\left(\frac{\sigma}{\sinh\sigma}\right)^n \exp\left(-\frac{x^2}{4Dt}\sigma\coth\sigma\right) \qquad \text{where } \sigma := (DC(0)\kappa t^3)^{1/2}. \tag{28}$$

Asymptotically the logarithm of expression (28) is of the order $O(t^{3/2})$ as $t\to\infty$. Hence (27) together with (20) implies

$$\frac{C(0)}{2}(1-\varepsilon) \leqslant \lim_{t\to\infty} t^{-2}\ln\overline{P(t,x)} \leqslant \frac{C(0)}{2}. \tag{29}$$

Finally, performing the limit $\varepsilon\downarrow 0$ completes the proof of (3).

Clearly, the proof (5) requires a different method because $C(0)$ for C of (4) is not defined. It will be carried out in two steps. First we show the equality

$$\lim_{t\to\infty} t^{-3}\ln\overline{P(t,x)} = \lim_{t\to\infty} t^{-3}\ln\langle e^{\Phi_t}\rangle \tag{30}$$

and then calculate the limit

$$\lim_{t\to\infty} t^{-3}\ln\langle e^{\Phi_t}\rangle = \frac{\nu^4}{4D}\gamma_n. \tag{31}$$

Since C of (4) is non-negative, $\Phi_{t+4} \geqslant \Phi_t$ for $\tau > 0$, and therefore according to (21)

$$\begin{aligned}\overline{P(t+\tau,x)} &\geqslant \langle\delta(b(t+\tau)-x)\, e^{\Phi_t}\rangle \\ &= \int_{\mathbb{R}^n} dy \langle\delta(b(t+\tau)-b(t)-x+y)\rangle\langle\delta(b(t)-y)e^{\Phi_t}\rangle\end{aligned}$$

where we have used the fact that Brownian motion has independent increments. We restrict the y-integration to the ball $B(x,r) := \{y\in\mathbb{R}^n : |y-x|\langle r, r\rangle 0\}$ and use (20) to further estimate the right-hand side of (32). The resulting inequality

$$\overline{P(t+\tau,x)} \geqslant (4\pi D\tau)^{-n/2}\exp(-r^2/4D\tau)\int_{B(x,r)} dy\langle\delta(b(t)-y)e^{\Phi_t}\rangle \tag{33}$$

leads to

$$\lim_{t\to\infty} t^{-3}\ln\overline{P(t,x)} \geqslant \lim_{t\to\infty} t^{-3}\ln\int_{B(x,r)} dy\,\langle\delta(b(t)-y)\, e^{\Phi_t}\rangle. \tag{34}$$

For $r\to\infty$ we achieve

$$\lim_{t\to\infty} t^{-3}\ln\overline{P(t,x)} \geqslant \lim_{t\to\infty} t^{-3}\ln\langle e^{\Phi_t}\rangle. \tag{35}$$

To get the reverse inequality, we make use of the fact that for $t>0$ one can find a point $\xi\in B(x,r)$ such that

$$\overline{P(t,\xi)}\int_{B(x,r)} dy \leqslant \int_{B(x,r)} dy\,\overline{p(t,y)} \leqslant \int_{\mathbb{R}^n} dy\,\overline{p(t,y)} = \langle e^{\Phi_t}\rangle. \tag{36}$$

This implies

$$\lim_{t\to\infty} t^{-3}\ln\overline{P(t,\xi)} \leqslant \lim_{t\to\infty} t^{-3}\ln\langle e^{\Phi_t}\rangle. \tag{37}$$

The limit $r\downarrow 0$ together with (35) proves (30).

Due to the stochastic scaling relation $b(\lambda t) = b(t)\sqrt{\lambda}$ of Brownian motion [20] and the scaling relation (7) of the covariance (4), the identity

$$\langle \exp(\Phi_t) \rangle = \langle \exp(\lambda^{-3/2} \Phi_{\lambda t}) \rangle \tag{38}$$

holds for all $\lambda > 0$. Choosing $\lambda = t^2$ in (38) allows for the application [16] of a theorem of Donsker and Varadhan [17, 23]

$$\lim_{T \to \infty} T^{-1} \ln \langle \exp(T^{-1} \Phi_T) \rangle = \frac{\nu^4}{4D} \gamma_n \tag{39}$$

to prove (31), which together with (30) proves (5).

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