

Correlation Effects in the Trapping Problem: General Approach and Rigorous Results

L. V. Bogachev, S. A. Molchanov, Yu. A. Makhnovskii,
and A. M. Berezhkovskii

Dedicated to Professor Sergio Albeverio on occasion of his sixtieth birthday.

ABSTRACT. The problem of Brownian survival among randomly located traps is considered with emphasis on the role of trap correlations. We proceed from the general representation of the survival probability as the expected value of the emptiness probability function applied to the Wiener sausage. Using the definition of (pure) trap attraction vs. repulsion in terms of the emptiness probability function, we prove the physical conjecture about the trapping slowdown or acceleration, according to the “sign” of correlations. Two specific models are studied along this line, in which the emptiness probability can be found explicitly; in particular, the long-time survival asymptotics is derived. A remarkable correlation effect of the survival probability dependence on the trap size in one dimension is also discussed.

1. Introduction

The problem of Brownian particle’s survival among randomly located killing traps, usually referred to as the *trapping problem*, is well known in the general theory of transport processes in disordered media (see, e.g., [16] and the bibliography therein). Of primary interest is the time dependence of the survival probability $P(t)$. The case of *noncorrelated* trapping medium, where the traps are distributed in space according to a Poisson law, has been studied rather extensively (see [17] for a survey of analytic, approximation and simulation methods and results, and a recent monograph [27] for a rigorous mathematical treatment). Although the exact solution is available only in one dimension [2], two important general features of the trapping kinetics have been revealed in the noncorrelated situation:

1. At small and intermediate times, the decay of the particle species basically follows the conventional theory dated back to Smoluchowski [25]. In particular, an exponential decrease of the survival probability $P_{\text{nc}}(t)$ is predicted in dimensions $d \geq 3$. (Here and below, the subscript “nc” refers to the case of noncorrelated

1991 *Mathematics Subject Classification*. 60J70, 60J65, 60G55.

This work was supported in part by DFG Grant # 436 RUS 113/534, RFBR Grant # 99-01-00298, and NSF Grant # DMS-9971592.

traps.) The conventional approach is based on the mean-field approximation by neglecting the many-body effects due to “competition” between the traps (for an up-to-date account of this theory, see [4], [20]).

2. At long times ($t \rightarrow \infty$) the mean-field approach breaks down, since the behavior of the $P_{\text{nc}}(t)$ is governed by the particle’s untypical survival in untypically big “holes” in the Poisson cloud. This leads to a fractional-exponent form of the survival tail [2], [22]. More precisely, Donsker and Varadhan [12] proved that

$$(1.1) \quad \lim_{t \rightarrow \infty} t^{-d/(d+2)} \log P_{\text{nc}}(t) = -\gamma_d c^{2/(d+2)},$$

where c is the intensity of the Poisson law (i.e., the trap concentration) and $\gamma_d > 0$ is an explicit dimension-dependent constant (see also [27, § 4.5B]).

The problem of allowing for *trap correlations* has attracted considerable interest in the last 15 years (see [3], [6]–[9], [19], [23], [28], [29] and further references therein). In particular, it was argued, mainly on physical grounds, that trap *attraction* (*repulsion*) induces the *slowdown* (respectively, *acceleration*) of the trapping as compared to the case of noncorrelated traps¹ [6]–[8], [23], [28]. This conjecture was also supported by the calculation of the long-time survival tail in some models [1], [9], [19], [26], [29], which is of mathematical interest in its own right. We would like to point out a result proved by Sznitman [26] (see also an earlier paper by Kayser and Hubbard [19]) stating that for Gibbsian trap distribution (with finite-range interaction potential Φ), the asymptotical behavior of the survival probability $P(t)$ follows the law (1.1), but with concentration c replaced by the quantity βp , where β is the inverse temperature and p is the pressure [24, § 3.4].²

In the present contribution, we pursue a systematic approach to this problem. Analysis of the qualitative influence of correlations is of our main concern, complemented whenever possible by the calculation of the survival asymptotics. We proceed from the general representation of the survival probability as the expectation of a certain Brownian functional, in which the trapping medium enters through the *emptiness probability function* applied to the corresponding Wiener sausage (Sect. 2). On the other hand, a “phenomenological” definition of pure attraction vs. repulsion of traps can also be given in terms of the emptiness probabilities (Sect. 3), which essentially amounts to distinguishing between positive vs. negative correlations in the distribution of the trap point process.³ Using this link, we are able to prove the aforementioned general conjecture about the qualitative role of trap correlations.

We consider along this line two concrete models where the distribution of traps is determined by a Poisson cluster point process (Sect. 4) or by a one-dimensional renewal process (Sects. 5, 6). These models are exactly solvable in that the emptiness probability function can be found in a closed form, which paves the way for studying the survival probability in some detail. It is worth pointing out that in the Poisson cluster model, correlations prove to be of attractive type, regardless of the intra-cluster interaction. The renewal model, specified by the choice of the gamma distribution for distances between the adjacent traps, exhibits both types

¹In such a comparison, it is implied that the trap concentration c is fixed.

²In the Gibbsian framework, the noncorrelated case corresponds to the ideal gas with null interaction, $\Phi \equiv 0$. The pressure p_{nc} is easily identified as c/β .

³Of course, in general the qualitative character of the trap “interaction” may not be universal, that is, *purely* attractive or repulsive.

of correlations, depending on the distribution parameter. The long-time survival asymptotics is derived for these models as well. We also discuss some novel correlation effects arising in one dimension, in particular a remarkable dependence of the trapping rate upon the trap size (Sect. 6).

2. Survival probability

Let us briefly recall the setting of the trapping problem (see [1] for more details). Consider a standard Brownian motion $(B_t, t \geq 0)$ on \mathbf{R}^d ($d \geq 1$) starting from the origin, and let P_0 and E_0 stand for the corresponding Wiener measure and expectation, respectively. The trapping medium is constituted by random configuration of spherical traps of radius b centered at the points of a background random point process $Z = \{Z_i\}$. In other words, the trapping set is of the form $\cup_i \{Z_i + V_b\}$, where V_b is the closed ball of radius b centered at the origin (note that, generally speaking, the traps may overlap). The traps are supposed to be perfectly absorbing, which means that the particle is terminated at the first contact with a trap.

The law of the process Z denoted by \mathbb{P} is assumed to be independent of B_t , and therefore the trapping process is governed by the product probability measure $\mathbb{P} \otimes P_0$. We also suppose that Z is *simple* (i.e., without multiple points) and *stationary* (i.e., \mathbb{P} is invariant under space shifts). For a Borel subset $S \in \mathcal{B}(\mathbf{R}^d)$, let N_S stand for the number of points $Z_i \in S$. We assume that the expectation $\mathbb{E}[N_S]$ is finite for all bounded $S \in \mathcal{B}(\mathbf{R}^d)$. Thanks to stationarity, $\mathbb{E}[N_S]$ is proportional to the Lebesgue volume of S ,

$$\mathbb{E}[N_S] = c|S|,$$

where the constant c is called the *trap concentration*.

In this work, we are concerned with the *survival probability* $P(t)$ defined as

$$(2.1) \quad P(t) := \mathbb{P} \otimes P_0\{T > t\} = \mathbb{E}[P_0\{T > t|Z\}],$$

where $T := \min \{t \geq 0 : B_t \in \cup_i (Z_i + V_b)\}$ is the particle's lifetime. Note that generally $P(0) \leq 1$, since the origin where the particle is born may be covered by a trap. Hence, somewhat more natural is the *normalized survival probability*

$$\tilde{P}(t) := \mathbb{P} \otimes P_0\{T > t | T > 0\} = \frac{P(t)}{P(0)}.$$

The following basic representation of the function $P(t)$ is obtained from its definition (2.1) via interchanging the order of averages (see [1], [8], [9]):

$$(2.2) \quad P(t) = E_0[g(S_b(t))].$$

Here $S_b(t) := \cup_{0 \leq s \leq t} \{B_s + V_b\}$ is the b -tubular neighborhood of a Brownian path on time interval $[0, t]$ (referred to as the *Wiener sausage*, due to M. Kac [18]), and $g(\cdot)$ called the *emptiness probability function*⁴ is a set function defined as

$$(2.3) \quad g(S) := \mathbb{P}\{N_S = 0\}, \quad S \in \mathcal{B}(\mathbf{R}^d).$$

In particular, $P(0) = E_0[g(S_b(0))] = g(V_b)$, and therefore

$$(2.4) \quad \tilde{P}(t) = \frac{E_0[g(S_b(t))]}{g(V_b)}.$$

⁴In the general theory of point processes, where $g(\cdot)$ is also called the *avoidance function*, it is proved that this function completely characterizes the process distribution (see [11, § 7.3]).

In the case of noncorrelated traps where $Z = \{Z_i\}$ is a Poisson point process (with intensity c), the emptiness probability is explicitly given by

$$(2.5) \quad g_{\text{nc}}(S) = e^{-c|S|}, \quad S \in \mathcal{B}(\mathbf{R}^d).$$

As a result, equation (2.2) takes the form

$$(2.6) \quad P_{\text{nc}}(t) = E_0[\exp(-c|S_b(t)|)].$$

We would like to remark here that the Smoluchowski approximation amounts to carrying the expectation sign in (2.6) through the exponent:

$$(2.7) \quad P_{\text{nc}}(t) \approx \exp(-cE_0|S_b(t)|),$$

which in fact yields a lower bound for $P_{\text{nc}}(t)$ [4]. Evaluation of the expected volume of the Wiener sausage and related topics have been addressed in many papers (see, e.g., [5]). The corresponding expression is of particularly simple form for $d = 1$ and $d = 3$:

$$(2.8) \quad E_0|S_b(t)| = \begin{cases} \frac{4}{\sqrt{2\pi}} t^{1/2} + 2b, & d = 1, \\ 2\pi b t + 4\sqrt{2\pi} b^2 t^{1/2} + \frac{4\pi b^3}{3}, & d = 3. \end{cases}$$

In one dimension, the general formula (2.2) for the survival probability $P(t)$ reads as follows:

$$(2.9) \quad P(t) = \int_0^\infty g(\ell + 2b) f(\ell; t) d\ell,$$

where $g(\ell)$ is the probability that an interval of length ℓ is free from points $\{Z_i\}$,⁵ and $f(\ell; t)$ is the probability density of the range of a Brownian motion on $[0, t]$:

$$(2.10) \quad R(t) := \max_{0 \leq s \leq t} B_s - \min_{0 \leq s \leq t} B_s,$$

that is the ‘‘volume’’ of the one-dimensional Wiener sausage (with $b = 0$). It is well known [5], [13] that the function $f(\ell; t)$ can be expressed in either of the two forms:

$$(2.11) \quad f(\ell; t) = \frac{8}{\sqrt{2\pi t}} \sum_{k=1}^{\infty} (-1)^{k-1} k^2 \exp\left(-\frac{k^2 \ell^2}{2t}\right)$$

$$(2.12) \quad = \frac{8t}{\ell^3} \sum_{k=1}^{\infty} \left[\frac{(2k-1)^2 \pi^2 t}{\ell^2} - 1 \right] \exp\left(-\frac{(2k-1)^2 \pi^2 t}{2\ell^2}\right).$$

Accordingly, the normalized survival probability $\tilde{P}(t)$ is represented as

$$(2.13) \quad \tilde{P}(t) = \int_0^\infty \tilde{g}(\ell) f(\ell; t) d\ell,$$

where the function

$$(2.14) \quad \tilde{g}(\ell) := \frac{g(\ell + 2b)}{g(2b)}$$

can be viewed as an effective emptiness probability (a detailed discussion of formulas (2.13), (2.14) is deferred to Sect. 6).

⁵Thanks to stationarity of the point process Z , this probability does not depend on the position of the interval.

For noncorrelated traps, one has $\tilde{g}_{\text{nc}}(\ell) = g_{\text{nc}}(\ell) = e^{-c\ell}$ (see equations (2.5), (2.14)). Using representation (2.11), from (2.13) one then arrives, after some transformations, to the known Balagurov–Vaks expression [2]

$$(2.15) \quad \tilde{P}_{\text{nc}}(t) = \frac{4}{\pi^2} \int_0^\infty \exp\left(-\frac{\pi^2 c^2 t}{2x^2}\right) \frac{x}{\sinh x} dx.$$

As would be expected, at short times ($t \rightarrow 0$) the survival probability (2.15) is reduced to the Smoluchowski-type form (cf. (2.7), (2.8))

$$(2.16) \quad \tilde{P}_{\text{nc}}(t) = 1 - \frac{4c}{\sqrt{2\pi}} t^{1/2} + O(t).$$

It should be noted that this result is not restricted by the explicit formula (2.15) and can be derived directly from the basic equation (2.13). Indeed, substituting $\tilde{g}_{\text{nc}}(\ell) = 1 - c\ell + O(\ell^2)$ into (2.13) and using expression (2.12) for the probability density $f(\ell; t)$ of the Brownian range $R(t)$ (see (2.10)), we obtain

$$\begin{aligned} \tilde{P}_{\text{nc}}(t) &= \int_0^\infty f(\ell; t) d\ell - c \int_0^\infty \ell f(\ell; t) d\ell + O(1) \int_0^\infty \ell^2 f(\ell; t) d\ell \\ &= 1 - c\mathbb{E}[R(t)] + O(t). \end{aligned}$$

In view of (2.8) (with $d = 1$ and $b = 0$), this yields (2.16).

The long term asymptotics of $\tilde{P}_{\text{nc}}(t)$ (as $t \rightarrow \infty$) can be derived via the Laplace method from (2.15) or, alternatively, directly from (2.9) using (2.12) [2]:

$$(2.17) \quad \tilde{P}_{\text{nc}}(t) \sim 8 \left(\frac{2c^2 t}{3\pi}\right)^{1/2} \exp\left(-\frac{3}{2}(\pi^2 c^2 t)^{1/3}\right).$$

As compared to the general Donsker–Varadhan result (1.1) (for $d = 1$), this is a more precise formula since it identifies the pre-exponential factor.

3. Taking account of trap correlations

Representations (2.2) and (2.4) show that the emptiness probability function $g(\cdot)$ is the sole characteristic of the trap distribution that enters the survival probability. In particular, the influence of trap correlations on the particle's survival is determined by the difference between the corresponding emptiness probability functions, $g(\cdot)$ and $g_{\text{nc}}(\cdot)$.

On the other hand, the emptiness probabilities furnish a convenient tool to characterize the trap interaction (at least on a qualitative level). We give the following basic definition (cf. [1]):

DEFINITION 3.1. A random point process $\{Z_i\}$ is called (*purely*) *attractive* or *repulsive* if for any disjoint (bounded) Borel sets $S_1, S_2 \in \mathcal{B}(\mathbf{R}^d)$, the emptiness probability function $g(\cdot)$ defined in (2.3) satisfies respectively

$$(3.1) \quad g(S_1 \cup S_2) \geq g(S_1) \cdot g(S_2) \quad (\text{attraction})$$

$$(3.2) \quad g(S_1 \cup S_2) \leq g(S_1) \cdot g(S_2) \quad (\text{repulsion})$$

and, moreover, these inequalities do not degenerate to identity. Furthermore, we say that attraction or repulsion is *strict* if the equality sign in (3.1), (3.2) is only possible with $|S_i| = 0$, $i = 1, 2$, so that both sides amount to 1.

REMARK. The requirement for S_1, S_2 to be disjoint can be relaxed to the condition that $|S_1 \cap S_2| = 0$.

In fact, the above definition is just a suitable reformulation of the property for a random point process to have positive or negative correlations. Indeed, introducing the indicator random variables $\delta_S := I\{N_S \geq 1\}$, so that $\mathbb{E}[\delta_S] = 1 - g(S)$, it is straightforward to check that the condition $\text{Cov}(\delta_{S_1}, \delta_{S_2}) \geq 0$ (or ≤ 0) amounts to inequality (3.1) (or (3.2), respectively).

Note that in the noncorrelated case, due to (2.5) we have identically

$$g_{\text{nc}}(S_1 \cup S_2) \equiv g_{\text{nc}}(S_1) \cdot g_{\text{nc}}(S_2), \quad S_1 \cap S_2 = \emptyset,$$

and therefore the deviation from the equality is an evidence of some dependence. To get more insight why the specific inequality sign in (3.1) and (3.2) is relevant to a common notion of “attraction” and “repulsion”, let us introduce the *conditional emptiness probability* $g(S|x_0)$, conditioned on the presence of a “probe” trap center at point $x_0 \in S$:

$$g(S|x_0) := \mathbb{P}\{\delta_{S \setminus \{x_0\}} = 0 | \delta_{\{x_0\}} = 1\}.$$

Obviously, in the Poisson case the two emptiness probabilities coincide, $g_{\text{nc}}(S|x_0) \equiv g_{\text{nc}}(S)$. Moreover, it is easy to check that each of the hypotheses (3.1), (3.2) implies for all S and $x_0 \in S$ respectively

$$(3.3) \quad g(S|x_0) \leq g(S) \text{ (attraction) or } g(S|x_0) \geq g(S) \text{ (repulsion),}$$

which is in agreement with an intuitive understanding of the qualitative types of “interaction” [1], [9].

The following theorem provides a rigorous basis for the physical conjecture mentioned in Sect. 1.

THEOREM 3.1. *Suppose that the random point process $\{Z_i\}$ is purely attractive or repulsive, in the sense of Definition 3.1, and let c be its concentration. Then the emptiness probability $g(S)$ for all (bounded) Borel sets S satisfies respectively*

$$(3.4) \quad g(S) \geq g_{\text{nc}}(S) \text{ (attraction) or } g(S) \leq g_{\text{nc}}(S) \text{ (repulsion),}$$

where $g_{\text{nc}}(S) = \exp(-c|S|)$ is the emptiness probability of the Poisson point process with intensity c . In the case of strict attraction and repulsion, the inequalities (3.4) are strict provided $|S| > 0$.

PROOF. We give an outline of the proof. By induction, inequalities (3.1), (3.2) are readily extended to finite unions of disjoint sets. Therefore, via an appropriate approximation of S we obtain accordingly $g(S) \geq \prod_i g(\Delta S_i)$. It remains to make use of Korolyuk’s theorem (see [11, § 7.2]), which implies that for a “small” set ΔS one can write $g(\Delta S) = 1 - c|\Delta S| + o(|\Delta S|)$. \square

Applying Theorem 3.1 to (2.2), we arrive at our main claim in this section.

THEOREM 3.2 (Correlation Conjecture). *Suppose that the trap ensemble $\{Z_i\}$ is purely attractive or repulsive, according to Definition 3.1, and let c denote its concentration. Then the survival probability $P(t)$ for each $t \geq 0$ satisfies*

$$P(t) \geq P_{\text{nc}}(t) \text{ (attraction) or } P(t) \leq P_{\text{nc}}(t) \text{ (repulsion),}$$

where $P_{\text{nc}}(t)$ corresponds to the Poisson trap ensemble with intensity c . The same is valid for the normalized survival probabilities, that is, for all $t \geq 0$

$$\tilde{P}(t) \geq \tilde{P}_{\text{nc}}(t) \text{ (attraction) or } \tilde{P}(t) \leq \tilde{P}_{\text{nc}}(t) \text{ (repulsion).}$$

In case attraction or repulsion be strict, so are the above inequalities for all $t > 0$.

PROOF. To prove the statement for the normalized probabilities, being less evident, we use Definition 3.1 and Theorem 3.1 to write

$$\frac{g(S_b(t))}{g(V_b)} \geq g(S_b(t) \setminus V_b) \geq \exp(-c|S_b(t) \setminus V_b|) = \frac{\exp(-c|S_b(t)|)}{\exp(-c|V_b|)} = \frac{g_{\text{nc}}(S_b(t))}{g_{\text{nc}}(V_b)},$$

whence in view of (2.4) the result follows. \square

REMARK. Theorems 3.1, 3.2 can be extended to the nonstationary case where the expected number of points is determined by a certain (non-constant) concentration function $c(x)$ via the formula $\mathbb{E}[N_S] = \int_S c(x) dx$.

4. Poisson cluster model

We now proceed to studying a few specific models. In this section, we analyze the trapping problem in a locally inhomogeneous trapping environment, in which correlations are displayed in the presence of *trap clusters* [1], [3], [9], [21]. More precisely, suppose that each trap is attached to a certain group (cluster), to the effect that the process $\{Z_i\}$ can be represented in the form $\{X_i + Y_j^{(i)}, j = 1, \dots, \nu_i\}$, where X_i denotes the cluster “center” and a random aggregate of random vectors $\mathbf{Y}^{(i)} := \{Y_1^{(i)}, \dots, Y_{\nu_i}^{(i)}\}$ determines the positions of ν_i traps belonging to the cluster, relative to its center.

Let us consider the simplest model of such kind, the *Poisson cluster point process* [11, § 8.3], in which $\{X_i\}$ is a Poisson point process (with intensity c_0) and the aggregates $\{\mathbf{Y}^{(i)}\}$ are assumed to be independent both of each other and of $\{X_i\}$, and identically distributed. The total trap concentration for such an ensemble is $c = c_0 \bar{\nu}$, where $\bar{\nu} := \mathbb{E}[\nu]$ is the expected number of traps in a cluster. For $\nu \equiv 1$, our model obviously reduces to the noncorrelated one, since the Poisson process is invariant under independent identically distributed random shifts of its points (see [11, § 8.2]).

THEOREM 4.1 ([1, Proposition 3.10]; cf. [11, § 8.3]). *For the Poisson cluster process, the emptiness probability $g(S)$ has the form*

$$(4.1) \quad g(S) = \exp \left(-c_0 \int_{\mathbf{R}^d} \mathbb{P} \left(\bigcup_{j=1}^{\nu} \{x + Y_j \in S\} \right) dx \right),$$

where $\{Y_1, \dots, Y_{\nu}\} =: \mathbf{Y}$ represents the random structure of a generic cluster.

The survival probability $P(t)$ can now be obtained by substituting expression (4.1) into the general formula (2.2). However, via interchanging the order of the integration and expectation in the exponent, one can rewrite the equation for $P(t)$ in a more suggestive way (cf. (2.6)).

THEOREM 4.2 ([1, p. 173], [9]). *The survival probability $P(t)$ for the Poisson cluster trapping model can be represented as*

$$(4.2) \quad P(t) = E_0[\exp(-c_0 \mathbb{E}|S_b^*(\mathbf{Y}; t)|)],$$

where $S_b^*(\mathbf{Y}; t) := \cup_{j=1}^{\nu} (S_b(t) - Y_j)$, $S_b(t)$ being the Wiener sausage.

That is to say, $S_b^*(\mathbf{Y}; t)$ is a random region in \mathbf{R}^d defined as the union of ν identical copies of the Wiener sausage $S_b(t)$ shifted at $-Y_1, \dots, -Y_{\nu}$. We call such an object the *bunch of Wiener sausages*, or simply the *Wiener bunch*. This concept is useful in the trapping context [3], [21] and is of mathematical interest in itself.

Let us now cite some known general results for the Poisson cluster model. We assume henceforth that the cluster point process under consideration is proper, that is, $1 < \bar{\nu} < \infty$.

THEOREM 4.3 ([1, Proposition 4.1]). *The Poisson cluster process is purely attractive, regardless of the inner structure of the clusters.*

In accordance with Theorem 3.2, this leads to the trapping slowdown.

THEOREM 4.4 ([1, Propositions 5.2, 5.2']). *The survival probability (4.2) for all $t > 0$ satisfies the inequality $P(t) > P_{\text{nc}}(t)$. Moreover, the same inequality holds for the normalized survival probabilities: $\tilde{P}(t) > \tilde{P}_{\text{nc}}(t)$.*

Note that the inequalities in this theorem are strict, although attraction itself may not be strict (cf. Theorem 4.3) and therefore the last statement of Theorem 3.2 cannot be directly applied.

Physical discussion of the trapping slowdown predicted by Theorem 4.4 can be found in [3], [21], where the “transparency” of individual clusters is shown to be an important characteristic responsible for the manifestation of the effect at short and intermediate times.

The behavior of the survival probability $P(t)$ as $t \rightarrow \infty$ is described by the following theorem ([1, Proposition 5.3]; see also [3], [9]).

THEOREM 4.5. *The long-time asymptotics of the survival probability $P(t)$ in the Poisson cluster model is of the form*

$$(4.3) \quad \lim_{t \rightarrow \infty} t^{-d/(d+2)} \log P(t) = -\gamma_d c_0^{2/(d+2)},$$

where γ_d is the same constant as in (1.1).

Thus, the form of the long-time survival tail in the Poisson cluster model reproduces that in the noncorrelated case, but with parameter c replaced by c_0 . Expressing this in a picturesque way: at long times the Brownian particle “feels” the concentration of clusters, c_0 , rather than the total trap concentration, c . Note also that the limit (4.3) does not depend on the inner structure of clusters.

The remainder of this section is devoted to a particular one-dimensional version of the Poisson cluster model which illuminates the role of the clusters’ overlapping. Assume that each cluster is a segment of length L containing $n \geq 2$ pointwise traps ($b = 0$). More specifically, let two traps be attached to the segment ends and the remaining $n - 2$ traps be distributed over the segment completely at random, that is, uniformly and independently of each other.

Adapting the general formula (4.1) to this particular case, we obtain

THEOREM 4.6. *The emptiness probability function in this model is of the form*

$$g(\ell) = \exp \left\{ -\rho \left[1 + \frac{\ell}{L} - \left(1 - \frac{\ell}{L} \right)_+^{n-1} \right] \right\},$$

where $u_+ := \max(u, 0)$ and $\rho := c_0 L$.

Let Λ_k be the random subset of the line \mathbf{R} consisting of the points “covered” by exactly k clusters ($k = 0, 1, \dots$). Obviously, once the Brownian particle has been born in the Λ_k , it will henceforth stay there until being trapped. Let us point out that via cutting out those intervals on \mathbf{R} which are not in Λ_k and gluing together

the remaining segments, one can realize Λ_k as an *effective k -layer trapping medium* in which the distribution of the new traps is induced by the cutting procedure (cf. [10]). In the next theorem, we find the basic characteristics of Λ_k .

THEOREM 4.7. *The probability π_k for a given point to occur in the k -layer medium Λ_k follows the Poisson distribution with parameter $\rho = c_0 L$:*

$$(4.4) \quad \pi_k = \frac{\rho^k}{k!} e^{-\rho}, \quad k = 0, 1, 2, \dots$$

The conditional emptiness probability $g_k(\ell)$, conditioned on Λ_k , equals

$$(4.5) \quad g_k(\ell) = \left(1 - \frac{\ell}{L}\right)_+^{k(n-1)} e^{-\rho\ell/L}, \quad k = 0, 1, 2, \dots,$$

where expression u_+^0 is understood to be equal to 1. Finally, the inner concentration of traps in Λ_k is given by

$$(4.6) \quad c_k = c_0 \left(1 + \frac{k(n-1)}{\rho}\right), \quad k = 0, 1, 2, \dots$$

PROOF. In order for a given point to occur in Λ_k , its two-sided $(L/2)$ -vicinity must contain exactly k cluster centers, which has the probability (4.4).

Furthermore, it is easy to verify that the probability for an interval I of length ℓ to lie in Λ_k is given by the expression

$$e^{-2c_0\ell} \cdot \frac{c_0^k (L-\ell)_+^k}{k!} e^{-c_0(L-\ell)}.$$

To ensure the emptiness of I , this has to be multiplied by $(1 - \ell/L)_+^{k(n-2)}$, that is the probability that none of the $k(n-2)$ inner traps belonging to the k covering clusters (“layers”) occurs in I . Conditioning on Λ_k , which amounts to dividing by π_k , then yields (4.5).

Equation (4.6) follows from the observation that due to each of the k layers, the “ground” concentration c_0 is increased by $(n-1)/L = c_0(n-1)/\rho$ traps per unit length. To check (4.6) more formally, we find the probability distribution function of a random spacing $\Delta \subset \Lambda_k$ between two adjacent traps, which can be done similarly to the above calculation, and then compute the concentration c_k as the reciprocal of the conditional expectation $\mathbb{E}[\Delta | \Delta \subset \Lambda_k]$. We omit the details. \square

Note that for $k = 0$, one has $g_0(\ell) \equiv e^{-c_0\ell}$, which is actually due to the fact that the 0-layer medium Λ_0 is noncorrelated (cf. Sect. 2 and also Sect. 6 below). Using (4.5) and (4.6), one can also verify that for each $k \geq 1$ and all $\ell > 0$

$$g_k(\ell) < e^{-c_k\ell}.$$

That is to say, the emptiness probability inside Λ_k appears to be smaller than that in a Poisson medium with the same concentration c_k . In view of Theorem 3.1, this is an evidence of the inner trap *repulsion* in each Λ_k , $k \geq 1$. On the other hand, the clusterized medium on the whole exhibits trap *attraction* (cf. Theorem 4.3).

5. One-dimensional renewal model

In the remaining two sections we assume that $Z = \{Z_i\}$ is a stationary *renewal process* on the line⁶ \mathbf{R} , so that random spacings $\{\Delta_i\}$ between adjacent points are independent and identically distributed. In this section we consider the case of pointwise traps ($b = 0$). Let $\varphi(x)$, $x > 0$, be a common probability density of Δ_i 's. Due to the classical renewal theorem (see, e.g., [14, § XI.1]), the concentration c is equal to the reciprocal mean spacing, $1/\mathbb{E}[\Delta]$:

$$(5.1) \quad c = \left(\int_0^\infty x \varphi(x) dx \right)^{-1}.$$

Furthermore, the emptiness probability function $g(\ell)$ is explicitly given by the expression (see [14, § XI.4])

$$(5.2) \quad g(\ell) = c \int_0^\infty x \varphi(x + \ell) dx.$$

Let us now take $\varphi(x)$ in the form of the gamma density, first proposed in the trapping context in [6]:

$$(5.3) \quad \varphi_\alpha(x) = \frac{\alpha c}{\Gamma(\alpha)} (\alpha c x)^{\alpha-1} e^{-\alpha c x}, \quad x > 0,$$

where $\alpha > 0$ and $\Gamma(\alpha) = \int_0^\infty x^{\alpha-1} e^{-x} dx$ is the gamma function. (The parameter c here plays the role of the concentration, since $\varphi_\alpha(x)$ satisfies the relation (5.1).) Equation (5.2) then takes the form

$$(5.4) \quad g_\alpha(\ell) = \frac{e^{-\alpha c \ell}}{\Gamma(\alpha + 1)} \int_0^\infty x (x + \alpha c \ell)^{\alpha-1} e^{-x} dx.$$

Note that for $\alpha = 1$ the process Z reduces to a Poisson one. For $\alpha \neq 1$, the behavior of the density $\varphi_\alpha(x)$ at zero suggests that $\alpha < 1$ and $\alpha > 1$ correspond to trap attraction and repulsion, respectively. This is made precise by the following theorem which can be proved by a direct analysis of equation (5.4).

THEOREM 5.1. *The gamma ensemble governed by the density (5.3) is strictly attractive or repulsive, in the sense of Definition 3.1, according as $\alpha < 1$ or $\alpha > 1$. Therefore, by Theorem 3.1 one has $g_\alpha(\ell) \geq g_1(\ell) \equiv g_{\text{nc}}(\ell)$ whenever $\alpha \leq 1$. Moreover, $g_\alpha(\ell)$ is strictly decreasing as a function of α .*

This amounts to saying that the deviation of the emptiness probability $g_\alpha(\ell)$ from its noncorrelated counterpart $g_1(\ell) \equiv g_{\text{nc}}(\ell)$ becomes bigger as $|1 - \alpha|$ grows, while the sign of $1 - \alpha$ determines the “direction” of correlations. Note that in the limit $\alpha \uparrow \infty$, corresponding to the infinitely strong repulsion, from (5.3) we have $\varphi_\alpha(\cdot) \rightarrow \delta_{1/c}(\cdot)$, which means the formation of a regular lattice of traps on the line \mathbf{R} with period c^{-1} . Hence, the limiting emptiness probability $g_\infty(\ell) = (1 - c\ell) \mathbf{1}_{\{c\ell \leq 1\}}$ provides the minimal possible value of $g_\alpha(\ell)$, and thus the lattice appears to be the most unfriendly environment for the surviving particle.

The next result following from Theorem 5.1 specifies the general Theorem 3.2.

⁶Such a process can be directly constructed on the whole line \mathbf{R} (see [11, § 12.3]), without referring to the limit regime arising for the renewal process on a half-line as the starting point is moved to $-\infty$.

THEOREM 5.2. *For each $t > 0$ the survival probability $P_\alpha(t)$ is a strictly decreasing function of α . In particular, for all $t > 0$ one has $P_\alpha(t) \geq P_{\text{nc}}(t)$ whenever $\alpha \leq 1$. Moreover, the same is valid for the normalized survival probability $\tilde{P}_\alpha(t)$.*

The long-time survival asymptotics can be found from equations (2.13), (5.4) using representation (2.12) (cf. (2.17)):

THEOREM 5.3. *As $t \rightarrow \infty$,*

$$(5.5) \quad \tilde{P}_\alpha(t) \sim 8\sqrt{\frac{2}{3}} \frac{\pi^{-3/2}}{\Gamma(\alpha+1)} (\pi^2 \alpha^2 c^2 t)^{(2\alpha+1)/6} \exp\left(-\frac{3}{2} (\pi^2 \alpha^2 c^2 t)^{1/3}\right).$$

REMARK. Comparing (5.5) with the result for Gibbsian traps mentioned in Sect. 1 suggests that the quantity αc here is related to the ‘‘pressure’’ as $\alpha c = \beta p$, which can be viewed as the equation of state. In fact, the gamma ensemble can be embedded into a Gibbsian framework by picking the nearest-neighbor interaction potential $\Phi(x) = (1 - \alpha) \log(cx)$ (see [15]). Note that for $\alpha < 1$ (attractive case) this potential appears to be non-stable in the sense of Ruelle [24, § 3.2]. However, the ‘nearest-neighbor’ constraint prevents the system from the collapse.

6. Role of the trap size in one dimension

In this section, we analyze the dependence of the trapping rate upon the trap size b in one dimension. Contrary to the common opinion that the (normalized) survival probability is independent of b , we show that such a dependence does arise provided the traps are correlated (for the physical discussion, see [10]).

Recalling (2.13), we have⁷

$$(6.1) \quad \tilde{P}(t; b) = \int_0^\infty \tilde{g}(\ell; b) f(\ell; t) d\ell,$$

where $f(\ell; t)$ is specified in (2.11)–(2.12) and (cf. (5.2))

$$(6.2) \quad \tilde{g}(\ell; b) = \frac{g(\ell + 2b)}{g(2b)}$$

is a new emptiness probability function determined according to (5.2) by the conditional probability density

$$(6.3) \quad \tilde{\varphi}(\ell; b) = \frac{\varphi(\ell + 2b)}{\int_0^\infty \varphi(x + 2b) dx}.$$

Such a conditioning can also be realized as passing from the original ensemble of spacings $\{\Delta_i\}$ between the adjacent trap centers $\{Z_i\}$ to an effective ensemble of *void* intervals $\{\tilde{\Delta}_i\}$ which do not intersect with any trap $[Z_i - b, Z_i + b]$.⁸ It is not difficult to check that the random variables $\{\tilde{\Delta}_i\}$ are again independent and identically distributed, so that the ensemble $\{\tilde{Z}_i\}$ of effective pointwise traps generated by $\{\tilde{\Delta}_i\}$ is a renewal process as well.

As mentioned in Sect. 2, in the noncorrelated case one has $\tilde{g}_{\text{nc}}(\ell; b) \equiv \tilde{g}_{\text{nc}}(\ell; 0)$ ($= e^{-c\ell}$), so that actually the survival probability does not depend on b :

$$\tilde{P}_{\text{nc}}(t; b) \equiv \tilde{P}_{\text{nc}}(t; 0).$$

⁷We introduce b in the notation in order to emphasize the presence of this parameter.

⁸In terminology of Sect. 4, the void intervals $\{\tilde{\Delta}_i\}$ constitute the 0-layer medium Λ_0 .

Formulas (6.1) and (6.2) indicate that in general such a dependence does take place. Moreover, physical arguments suggest [10] that the effective trap concentration

$$(6.4) \quad \tilde{c}(b) = \left(\int_0^\infty x \tilde{\varphi}(x; b) dx \right)^{-1}$$

is likely to be smaller (attraction) or greater (repulsion) than the original concentration $c \equiv \tilde{c}(0)$. Accordingly, one can expect that nonzero trap radius b either promotes or inhibits the Brownian survival, depending on the qualitative type of trap interaction. For short times, $t \rightarrow 0$, this is justified by the Smoluchowski-type formula

$$\tilde{P}(t; b) = 1 - \frac{4\tilde{c}(b)}{\sqrt{2\pi}} t^{1/2} + o(t^{1/2}),$$

which can be derived from (6.1) in much the same way as (2.16); in so doing, one only needs to apply Korolyuk's theorem (mentioned in the proof of Theorem 3.1) to write $\tilde{g}(\ell; b) = 1 - \tilde{c}(b)\ell + o(\ell)$ for $\ell \rightarrow 0$.

The following general theorem makes these considerations precise.

THEOREM 6.1. *Suppose that the renewal (one-dimensional) point process $\{Z_i\}$ is purely attractive or repulsive, according to Definition 3.1. Then for all $t \geq 0$*

$$\tilde{P}(t; b) \geq \tilde{P}(t; 0) \quad (\text{attraction}) \quad \text{or} \quad \tilde{P}(t; b) \leq \tilde{P}(t; 0) \quad (\text{repulsion}).$$

Moreover, the deviation of the effective concentration is as predicted:

$$\tilde{c}(b) \leq c \quad (\text{attraction}) \quad \text{or} \quad \tilde{c}(b) \geq c \quad (\text{repulsion}).$$

PROOF. To be definite, consider the case of attraction. Using (6.2) and applying condition (3.1) of Definition 3.1, we can write

$$\tilde{g}(\ell; b) = \frac{g(\ell + 2b)}{g(2b)} \geq g(\ell) = \tilde{g}(\ell; 0),$$

whence the first assertion of the theorem immediately follows due to (6.1). In view of (6.4) and (6.3), in order to prove the second assertion we have to check that

$$(6.5) \quad \int_0^\infty \varphi(x + 2b) dx \leq c \int_0^\infty x \varphi(x + 2b) dx.$$

According to (5.2), the right-hand side of (6.5) coincides with $g(2b)$, whereas the left-hand side is equal to

$$\mathbb{P}\{\Delta > 2b\} = \mathbb{P}\{N_{(0, 2b]} = 0 \mid \delta_{\{0\}} = 1\} = g(2b|0).$$

Thus, inequality (6.5) amounts to $g(2b|0) \leq g(2b)$. But from (3.3) it follows that the last inequality is true, and we are done. \square

For the gamma model introduced above, the b -dependence can be studied in more detail. Substituting (5.4) into (6.2), we find the emptiness probability

$$(6.6) \quad \tilde{g}_\alpha(\ell; b) = \frac{\int_0^\infty x(x + \alpha\ell + 2\alpha cb)^{\alpha-1} e^{-x} dx}{\int_0^\infty x(x + 2\alpha cb)^{\alpha-1} e^{-x} dx} e^{-\alpha\ell},$$

whereas the trap concentration is given by (see (6.4), (6.3))

$$(6.7) \quad \tilde{c}_\alpha(b) = c \left(1 - 2bc \left[1 - (2\alpha bc)^{\alpha-1} \frac{e^{-2\alpha bc}}{\Gamma(\alpha, 2\alpha bc)} \right] \right)^{-1},$$

where $\Gamma(\alpha, z) = \int_z^\infty x^{\alpha-1} e^{-x} dx$ is the incomplete gamma function.

The following two results are proved similarly to Theorems 5.1, 5.2 using the explicit expressions (6.6), (6.7).

THEOREM 6.2 (cf. Theorem 5.1). *The emptiness probability $g_\alpha(\ell; b)$ is strictly decreasing in α . For a fixed $\alpha \neq 1$, both $\tilde{g}_\alpha(\ell; b)$ and $1/\tilde{c}_\alpha(b)$ monotonically increase or decrease as functions of b , depending on whether $\alpha < 1$ or $\alpha > 1$, respectively.*

THEOREM 6.3 (cf. Theorem 5.2). *For a fixed $\alpha \neq 1$, the probability $\tilde{P}_\alpha(t; b)$ is a strictly increasing or decreasing function of b , whenever $\alpha < 1$ or $\alpha > 1$, respectively.*

Combined with Theorem 5.2, this means that the effect of the trapping slowdown ($\alpha < 1$) or acceleration ($\alpha > 1$) is enhanced as the trap size b grows. This result may prove useful in experimental detecting of trap correlations in real one-dimensional systems.

References

- [1] S. Albeverio and L. V. Bogachev, *Brownian survival in a clusterized trapping medium*, Rev. Math. Phys. **10** (1998), 147–189.
- [2] B. Ya. Balagurov and V. G. Vaks, *Random walks of a particle on lattices with traps*, Zh. Eksp. Teoret. Fiz. **65** (1973), 1939–1945 (Russian). English translation: Soviet Phys. JETP **38** (1974), 968–970.
- [3] A. M. Berezhkovskii, Yu. A. Makhnovskii, L. V. Bogachev, and S. A. Molchanov, *Brownian-particle trapping by clusters of traps*, Phys. Rev. E **47** (1993), 4564–4567.
- [4] A. M. Berezhkovskii, Yu. A. Makhnovskii, and R. A. Suris, *Kinetics of diffusion-controlled reactions*, Chem. Phys. **137** (1989), 41–49.
- [5] ———, *Wiener sausage volume moments*, J. Statist. Phys. **57** (1989), 333–346.
- [6] A. M. Berezhkovskii, Yu. A. Makhnovskii, R. A. Suris, L. V. Bogachev, and S. A. Molchanov, *Trap correlation influence on Brownian particle death. One-dimensional case*, Phys. Lett. A **161** (1991), 114–117.
- [7] ———, *Diffusion-limited reactions with correlated traps*, Chem. Phys. Lett. **193** (1992), 211–214.
- [8] ———, *Trap correlation influence on diffusion-limited process rate*, Phys. Rev. A **45** (1992), 6119–6122.
- [9] L. V. Bogachev and Yu. A. Makhnovskii, *Brownian motion with absorption in a clusterized random medium*, Dokl. Akad. Nauk **340** (1995), 300–302 (Russian). English translation: Russian Acad. Sci. Dokl. Math. **51** (1995), 51–53.
- [10] L. V. Bogachev, Yu. A. Makhnovskii, and A. M. Berezhkovskii, *Trapping rate dependence on the trap size in one dimension*, Phys. Rev. E **52** (1995), 6900–6903.
- [11] D. J. Daley and D. Vere-Jones, *An introduction to the theory of point processes*, Springer, New York, 1988.
- [12] M. D. Donsker and S. R. S. Varadhan, *Asymptotics for the Wiener sausage*, Comm. Pure Appl. Math. **28** (1975), 525–565.
- [13] W. Feller, *The asymptotic distribution of the range of sums of independent random variables*, Ann. Math. Statist. **22** (1951), 427–432.
- [14] ———, *An introduction to probability theory and its applications*, Vol. 2, 2nd ed., Wiley, New York, 1971.
- [15] F. Gürsey, *Classical statistical mechanics of a rectilinear assembly*, Proc. Cambridge Philos. Soc. **46** (1950), 182–194.
- [16] S. Havlin and D. Ben-Avraham, *Diffusion in disordered media*, Adv. in Phys. **36** (1987), 695–798.
- [17] F. den Hollander and G. H. Weiss, *Aspects of trapping in transport processes*, Contemporary Problems in Statistical Physics, G. H. Weiss, ed., SIAM, Philadelphia, PA, 1994, pp. 147–203.
- [18] M. Kac, *Probabilistic methods in some problems of scattering theory*, Rocky Mountain J. Math. **4** (1974), 511–537.
- [19] R. F. Kayser and J. B. Hubbard, *Reaction diffusion in a medium containing a random distribution of nonoverlapping traps*, J. Chem. Phys. **80** (1984), 1127–1130.

- [20] E. Kotomin and V. Kuzovkov, *Modern aspects of diffusion-controlled reactions*, Elsevier, Amsterdam, 1996.
- [21] Yu. A. Makhnovskii, L. V. Bogachev, and A. M. Berezhkovskii, *The effect of trap grouping on the decay kinetics of Brownian particles*, Chem. Phys. Rep. **14** (1995), 710–728.
- [22] A. A. Ovchinnikov and Ya. B. Zeldovich, *Role of density fluctuations in bimolecular reaction kinetics*, Chem. Phys. **28** (1978), 215–218.
- [23] P. M. Richards, *Diffusion to nonoverlapping or spatially correlated traps*, Phys. Rev. B **35** (1987), 248–256.
- [24] D. Ruelle, *Statistical mechanics: Rigorous results*, Benjamin, Reading, Mass., 1969.
- [25] M. von Smoluchowski, *Versuch einer mathematischen Theorie der Koagulationskinetik kolloider Lösungen*, Z. Phys. Chem. **29** (1917), 129–168.
- [26] A. S. Sznitman, *Brownian survival among Gibbsian traps*, Ann. Probab. **21** (1993), 490–508.
- [27] ———, *Brownian motion, obstacles and random media*, Springer, Berlin, 1998.
- [28] S. Torquato, *Concentration dependence of diffusion-controlled reactions among static reactive sinks*, J. Chem. Phys. **85** (1986), 7178–7179.
- [29] G. H. Weiss and S. Havlin, *Trapping of random walks on the line*, J. Statist. Phys. **37** (1984), 17–25.

FACULTY OF MECHANICS AND MATHEMATICS, MOSCOW STATE UNIVERSITY, MOSCOW 119899, RUSSIA

E-mail address: `lvb@mech.math.msu.su`

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF NORTH CAROLINA AT CHARLOTTE, CHARLOTTE, NC 28223, USA

E-mail address: `smolchan@uncc.edu`

TOPCHIEV INSTITUTE OF PETROCHEMICAL SYNTHESIS, RUSSIAN ACADEMY OF SCIENCES, MOSCOW 117912, RUSSIA

E-mail address: `yuam@tips-gw.ips.ac.ru`

KARPOV INSTITUTE OF PHYSICAL CHEMISTRY, MOSCOW 103064, RUSSIA

E-mail address: `berezh@cc.nifhi.ac.ru`