Target searches of interacting Brownian particles in dilute systems

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We study the target searches of interacting Brownian particles in a finite domain, focusing on the effect of interparticle interactions on the search time. We derive the integral equation for the mean first-passage time and acquire its solution as a series expansion in the orders of the Mayer function. We analytically obtain the leading order correction to the search time for dilute systems, which are most relevant to target search problems and prove a universal relation given by the particle density and the second virial coefficient. Finally, we validate our theoretical prediction by Langevin dynamics simulations for the various types of the interaction potential.

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I. INTRODUCTION

Target search by random walkers is a fundamental process in a host of phenomena such as diffusion-controlled reactions [1–10], binding of DNA transcription factors [11–14], animal foraging [15], the spread of infectious diseases, and fluctuations of stock prices [16]. A central quantity characterizing the process is the first-passage time, namely, the time taken for a random walker or a diffusing particle to encounter a target for the first time. Over the past decades, the random-search problem has received considerable attention [17–22], in particular, in the context of optimal search strategies [23–28] and universal properties in scale-invariant processes [19]; see, e.g., recent reviews [29,30] and references therein.

While most studies rely on a single-particle picture, often a group of particles simultaneously search for a common target. In this case, the search time manifests the many-body properties even when searchers are noninteracting: The order statistic of the first-passage times recorded by individual searchers determines the search time and leads to the characteristic dependence on the number of searchers [22,23,30–38]. Moreover, searchers often interact with each other. One example is Mongolian gazelles utilizing acoustic communication to explore better habitat areas [39]. For such interacting searchers, one of the fundamental questions is how intersearcher interaction affects the first-passage time. There have been several theoretical efforts, mainly in the context of diffusion-limited reactions, to understand this interaction effect [40–46]. Most of them are effective coarse-grained theories, employing several assumptions at hydrodynamic regimes [40–44], and thus are limited in applicability (which will be detailed below).

To address the search problem in interacting systems, we consider the dynamics of N Brownian particles:

$$\dot{\mathbf{r}}_j = -\mu \nabla_{\mathbf{r}_j} U + \sqrt{2D}\,\boldsymbol{\xi}_j(t), \tag{1}$$

where $\mathbf{r}_j$ is the position of the jth particle, μ is its mobility, $D = \mu k_B T$, and $\boldsymbol{\xi}_j(t)$ denotes the Gaussian white noise. The particles interact with each other via pairwise interaction $v(\mathbf{r})$, and the total interaction energy reads as $U(\mathcal{R}) = \sum_{i<j}^{N} v(\mathbf{r}_i - \mathbf{r}_j)$ with $\mathcal{R} = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$. We regard the target as being found when one of the searchers reaches the target. Direct simulations of Eq. (1) for particles, with uniform initial distribution, interacting via exponential potential show that the relative change of averaged search time depends on whether the interaction is attractive or repulsive (see Fig. 1). However, this observation is a case-specific numerical result and gives little insight into other situations, for example, where particle interaction has both attractive and repulsive parts, as observed in colloidal particles, or where searcher distribution is nonuniform.

In what follows, we present a solution to the target search problem of interacting particles in dilute regimes. To this end, we obtain the integral equation for the mean first-passage time (MFPT), which explicitly includes the interaction potentials. The potential is introduced in the form of the Mayer function, which allows us to treat the potentials even if they diverge due to hardcore repulsions at short distances. Then, by solving the equation iteratively, we find that in the dilute limit the leading order correction to the MFPT of systems of arbitrary initial distributions due to interactions is given in the form of virial expansion, and is independent of the other details of potentials and search domain shapes.

This paper is organized as follows. In Sec. II, we define the problem and introduce key quantities. In Sec. III, we introduce the expansion of the MFPT in terms of the interaction strength, the validity of which is limited to weakly interacting

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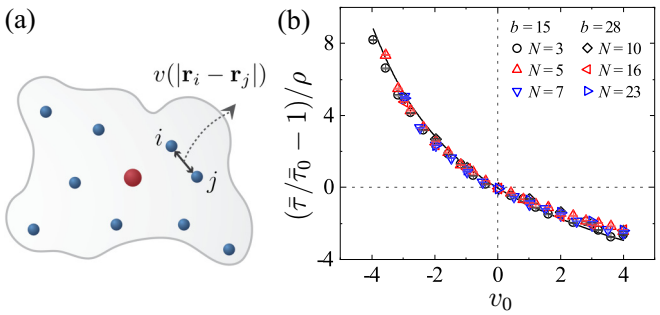

FIG. 1. (a) Schematic illustration of Brownian particles (blue circles) in search of a target (red circle), where the particles interact with each other via a pairwise interaction $v(r)$. (b) The normalized relative change in the global mean first-passage time, $(\bar{\tau}/\bar{\tau}_0 - 1)/\rho$, vs the interaction strength v_0 when $v(r) = k_B T v_0 e^{-r/\sigma}$ with $\sigma = 0.5a$. $\bar{\tau}(\bar{\tau}_0)$ is the search time averaged over a uniform initial searcher distribution in the presence (absence) of interactions, and $\rho \equiv (N-1)/V$. The solid line represents the theoretical prediction given by Eq. (23) (see the main text), and symbols are the search times obtained from Langevin dynamics simulations with N searchers in a two-dimensional circular domain of radius b, with a target of unit radius a located at the domain center. Error bars indicate the scale of statistical error.

systems. To consider arbitrary interaction potentials including hardcore repulsions, the low-density expansion of the MFPT is presented in Sec. IV. Assuming short-ranged potential, the leading-order correction to the MFPT for interacting particles is explicitly given in Sec. V. Comparison to simulation and discussion are given in Sec. VI, followed by conclusions in Sec. VII.

II. SETUP

We consider N Brownian particles searching for a small-size target $\mathcal{T}$ in a d-dimensional finite domain $\mathcal{D}$ of volume V. A schematic presentation of the system is given in Fig. 1(a), where the Brownian particles and the target are drawn with blue and red circles, respectively. The stochastic trajectories of the Brownian particles that start from the initial positions $\mathcal{R}_0 = (\mathbf{r}_{0;1}, \mathbf{r}_{0;2}, \ldots, \mathbf{r}_{0;N})$ are characterized by the N-particle probability density function (PDF) $P_N(\mathcal{R}, t|\mathcal{R}_0)$ of the particle positions $\mathcal{R}$ at time t. The PDF obeys the Fokker-Planck equation [47–49]:

$$\partial_t P_N(\mathcal{R}, t|\mathcal{R}_0) = \mathcal{L}_{\rm FP}(\mathcal{R}) P_N(\mathcal{R}, t|\mathcal{R}_0) \tag{2}$$

with the time derivative $\partial_t = \partial/\partial t$ and the forward Fokker-Planck operator

$$\mathcal{L}_{\rm FP}(\mathcal{R}) = \beta D \nabla \cdot [\nabla U(\mathcal{R})] + D\nabla^2, \tag{3}$$

where $\beta = 1/k_B T$ and $\nabla = \sum_{i=1}^{N} \nabla_{\mathbf{r}_i}$.

The search process terminates when any of the searchers reach the target boundary, and the particles are restricted from crossing the domain boundary throughout the process. To implement these conditions, an absorbing boundary condition is applied at the target boundary $\partial\mathcal{T}$ specified as $P_N(\mathcal{R}, t|\mathcal{R}_0) = 0$ when $\mathbf{r}_i \in \partial\mathcal{T}$ for any i. Additionally, a reflecting boundary condition is imposed on the domain boundary $\partial\mathcal{D}$ as $\hat{\mathbf{n}} \cdot \mathbf{j}(\mathcal{R}, t|\mathcal{R}_0) = 0$ when $\mathbf{r}_i \in \partial\mathcal{D}$ for any i. Here, $\hat{\mathbf{n}}$ represents a unit vector normal to the domain boundary, and $\mathbf{j}(\mathcal{R}, t|\mathcal{R}_0) = -D(\beta\nabla U(\mathcal{R}) + \nabla) P_N(\mathcal{R}, t|\mathcal{R}_0)$ denotes the probability current.

As mentioned in the introduction, we define the search time as the MFPT $\tau(\mathcal{R}_0)$, which is a function of the initial searcher position according to the setup provided above. It is well known that $\tau(\mathcal{R}_0)$ can be obtained by integrating the PDF over $\mathcal{R}$ and t as

$$\tau(\mathcal{R}_0) = \int_0^\infty dt \int d\mathcal{R}\, P_N(\mathcal{R}, t|\mathcal{R}_0). \tag{4}$$

To analyze $\tau(\mathcal{R}_0)$, it is convenient to use the backward Fokker-Planck equation:

$$\partial_t P_N(\mathcal{R}, t|\mathcal{R}_0) = \mathcal{L}^\dagger_{\rm FP}(\mathcal{R}_0) P_N(\mathcal{R}, t|\mathcal{R}_0) \tag{5}$$

with the adjoint Fokker-Planck operator

$$\mathcal{L}^\dagger_{\rm FP}(\mathcal{R}_0) = -\beta D \nabla_0 U(\mathcal{R}_0) \cdot \nabla_0 + D\nabla_0^2, \tag{6}$$

where ∇_0 is the del operator applied on $\mathcal{R}_0$. Integrating Eq. (5) over $\mathcal{R}$ and t, we obtain an adjoint equation for $\tau(\mathcal{R}_0)$ [47–49]:

$$\mathcal{L}^\dagger_{\rm FP}(\mathcal{R}_0)\tau(\mathcal{R}_0) = -1, \tag{7}$$

In deriving Eq. (7), we have used the fact that the target is eventually found in a finite domain, i.e., $\lim_{t\to\infty} \int d\mathcal{R}\, P_N(\mathcal{R}, t|\mathcal{R}_0) = 0$. Then the MFPT can be calculated by solving Eq. (7) with the boundary conditions given as $\tau(\mathcal{R}_0) = 0$ if $\mathbf{r}_{0,i} \in \partial\mathcal{T}$ and $\hat{\mathbf{n}} \cdot \nabla_0 \tau(\mathcal{R}_0) = 0$ if $\mathbf{r}_{0,i} \in \partial\mathcal{D}$, which can be derived from the boundary conditions imposed on the PDF [47].

Solving Eq. (7) directly is challenging due to the interaction potential in the adjoint Fokker-Planck operator Eq. (6). We aim to make progress in this direction. Before proceeding, we note that for noninteracting particles, the equation simplifies to $D\nabla_0^2 \tau(\mathcal{R}_0) = -1$, and its solution can be written as [18]

$$\tau_0(\mathcal{R}_0) = -\frac{1}{D} \int d\mathcal{R}\, G(\mathcal{R}|\mathcal{R}_0), \tag{8}$$

where $G(\mathcal{R}|\mathcal{R}_0)$ is a dN-dimensional Green function of the Laplace operator satisfying $\nabla^2 G(\mathcal{R}|\mathcal{R}_0) = \delta(\mathcal{R} - \mathcal{R}_0)$ and the boundary conditions $G(\mathcal{R}|\mathcal{R}_0) = 0$ if $\mathbf{r}_{0;i} \in \partial\mathcal{T}$ and $\hat{\mathbf{n}} \cdot \nabla_0 G(\mathcal{R}|\mathcal{R}_0) = 0$ if $\mathbf{r}_{0;i} \in \partial\mathcal{D}$ [50].

III. INTERACTION STRENGTH EXPANSION

In order to address the interacting searcher problem, we first introduce a formal expansion of the MFPT in terms of the interaction strength as follows:

$$\tau(\mathcal{R}_0) = \sum_{n=0}^{\infty} \tau_n(\mathcal{R}_0), \tag{9}$$

where $\tau_n = O(\tilde{U}^n)$ with $\tilde{U} = \beta U$ and thus the subindex specifies the order of expansion. By plugging this into Eq. (7) and collecting the terms according to the order of $\tilde{U}$, we obtain

$$\nabla_0^2 \tau_n(\mathcal{R}_0) = \begin{cases} -D^{-1} & \text{if } n = 0, \\ \nabla_0 \tilde{U}(\mathcal{R}_0) \cdot \nabla_0 \tau_{n-1}(\mathcal{R}_0) & \text{if } n \geqslant 1. \end{cases} \tag{10}$$

This relationship allows us to establish a mapping between the search time of interacting searchers to the electrostatic

problem. As is well known, the search time of noninteracting searchers corresponds to the electrostatic potential arising from a uniformly distributed charge density, which is captured by Eq. (10) with $n = 0$. Moreover, the solution to the order n equation can also be regarded as the electrostatic potential generated by the charge distribution prescribed by the interaction potential $\tilde{U}(\mathcal{R}_0)$ and the solution $\tau_{n-1}(\mathcal{R}_0)$ of the order $n-1$ equation, given as

$$\tau_n(\mathcal{R}_0) = \int d\mathcal{R}\, G(\mathcal{R}|\mathcal{R}_0)[\nabla\tilde{U}(\mathcal{R})\cdot\nabla\tau_{n-1}(\mathcal{R})]. \tag{11}$$

By recursively applying Eq. (11) starting from $n = 1$, the solution for τ_n with an arbitrary n can be found [51].

If the interaction strength is weak, the impact of interaction on the MFPT can be systematically evaluated by calculating τ_n order by order. However, particles in most realistic setups exert excluded volume interactions at close distances, which are described by diverging potentials. With such potentials, the integral in Eq. (11) also diverges, and evaluating the MFPT using a truncated sum of the series Eq. (9) can no longer be justified. In the following section, we suggest an alternative approach to resolve this issue.

IV. DENSITY EXPANSION

To evaluate the MFPT of particles interacting with hard-core potentials, we perform resummation of Eq. (9) in order to convert it into a perturbative expansion with respect to density, instead of interaction strength. We accomplish this goal through two independent approaches. First, we perform recursive integration by parts on Eq. (11) and isolate the leading-order term in the dilute density limit. By summing the terms collected over all orders of n, to our surprise, we arrive at an expression including the Mayer function of the interaction potential. This can be achieved via a straightforward but lengthy algebra, which we detail in Appendix A.

Here we instead present a more concise and elegant way to perform the low-density expansion. To do so, we use the following identity for the MFPT:

$$\tau(\mathcal{R}_0) = \tau_0(\mathcal{R}_0) + \beta\int d\mathcal{R}\, G(\mathcal{R}|\mathcal{R}_0)\nabla U(\mathcal{R})\cdot\nabla\tau(\mathcal{R}), \tag{12}$$

which is obtained by rearranging Eq. (7) as $\nabla_0^2\tau(\mathcal{R}_0) = -D^{-1} + \beta\nabla_0 U(\mathcal{R}_0)\cdot\nabla_0\tau(\mathcal{R}_0)$ then by solving it using the Green function. Defining $\tau(\mathcal{R}_0) - \tau_0(\mathcal{R}_0) \equiv \tau_U(\mathcal{R}_0)$, we rewrite τ_U in a manner akin to the virial expansion using $M(\mathcal{R}) \equiv e^{-\beta U(\mathcal{R})} - 1 = \prod_{i<j}(1+f_{ij}) - 1$ with the Mayer function $f_{ij} = e^{-\beta v(\mathbf{r}_i-\mathbf{r}_j)} - 1$:

$$\begin{aligned}\tau_U(\mathcal{R}_0) = &-\beta\int d\mathcal{R}\, G(\mathcal{R}|\mathcal{R}_0)M(\mathcal{R})\nabla U(\mathcal{R})\cdot\nabla\tau(\mathcal{R})\\ &-\int d\mathcal{R}\, G(\mathcal{R}|\mathcal{R}_0)\nabla M(\mathcal{R})\cdot\nabla\tau(\mathcal{R}).\end{aligned} \tag{13}$$

Exploiting the relation $-\beta\nabla U(\mathcal{R})\cdot\nabla\tau(\mathcal{R}) = -\nabla^2\tau(\mathcal{R}) - 1/D$ and integrating by parts, we get

$$\begin{aligned}\tau_U(\mathcal{R}_0) = &-\frac{1}{D}\int d\mathcal{R}\, G(\mathcal{R}|\mathcal{R}_0)M(\mathcal{R})\\ &+\int d\mathcal{R}\, M(\mathcal{R})\nabla G(\mathcal{R}|\mathcal{R}_0)\cdot\nabla\tau(\mathcal{R})\end{aligned} \tag{14}$$

and obtain the integral equation for MFPT as

$$\tau(\mathcal{R}_0) = \tau_0(\mathcal{R}_0) + \int d\mathcal{R}\, M(\mathcal{R})\mathcal{G}(\mathcal{R}|\mathcal{R}_0), \tag{15}$$

where $\mathcal{G}(\mathcal{R}|\mathcal{R}_0) = -G(\mathcal{R}|\mathcal{R}_0)/D + \nabla G(\mathcal{R}|\mathcal{R}_0)\cdot\nabla\tau(\mathcal{R})$.

Our basic strategy for solving the integral equation (15) is to expand the search time in the powers of M, whereby we let $\tau(\mathcal{R}_0) = \sum_{n=0}\tau^{(n)}(\mathcal{R}_0)$ with $\tau^{(n)}$ containing the nth power of M. First, neglecting the inter-particle interactions, the zeroth-order approximation for the MFPT is $\tau^{(0)}(\mathcal{R}_0) = \tau_0(\mathcal{R}_0)$. Replacing τ on the right-hand side of Eq. (15) with $\tau^{(0)}$, we obtain

$$\tau^{(1)}(\mathcal{R}_0) = \int d\mathcal{R}\, M(\mathcal{R})\nabla\cdot(G(\mathcal{R}|\mathcal{R}_0)\nabla\tau_0(\mathcal{R})). \tag{16}$$

This agrees with the result of direct resummation presented in Appendix A [see the derivation of Eq. (A24)]. Continuing iteration as such, we find $\tau^{(n\geqslant 2)}$ as

$$\tau^{(n\geqslant 2)}(\mathcal{R}_0) = \int d\mathcal{R}_1\,\mathcal{O}_1\cdots\int d\mathcal{R}_n\,\mathcal{O}_n\tau_0(\mathcal{R}_n), \tag{17}$$

where $\mathcal{O}_i = M(\mathcal{R}_i)\nabla_i G(\mathcal{R}_i|\mathcal{R}_{i-1})\cdot\nabla_i$. Summing up, the modifications of the search time caused by intersearcher interactions rest on Eqs. (16) and (17), and one can truncate the series upon the degree of pursued accuracy.

In the following sections, we explicitly evaluate the leading order correction, Eq. (16), and compare it to the results of the Langevin dynamics simulation.

V. THE LEADING-ORDER CORRECTION TO MEAN FIRST-PASSAGE TIMES

The Mayer function $f(\mathbf{r})$ becomes negligible at distances greater than the interaction range σ. Consequently, for dilute systems (or, equivalently, short-range interactions) where $n\sigma^d \ll 1$ with density n, the expansion using the Mayer function f_{ij} is quickly convergent [52]. Collecting terms linear in f, which only appear in $\tau^{(1)}(\mathcal{R})$, we obtain

$$\tau(\mathcal{R}_0) \simeq \tau_0(\mathcal{R}_0) + \int d\mathcal{R}\sum_{i<j} f_{ij}\nabla\cdot[G(\mathcal{R}_0|\mathcal{R})\nabla\tau_0(\mathcal{R})]. \tag{18}$$

This equation is one of the main results of our study, which directly accounts for the impact of interaction on the MFPT in terms of the Green function, the MFPT of noninteracting searchers, and the interaction potential. The interaction potential is introduced in the form of the Mayer function, the validity of which is not restricted to weakly interacting systems.

To tackle the analytic evaluation of Eq. (18), an instrumental element is $\tau_0(\mathcal{R})$ determined by the Green function $G(\mathcal{R}'|\mathcal{R})$ through the relation (8). The exact expression of $G(\mathcal{R}'|\mathcal{R})$ reads as

$$G(\mathcal{R}'|\mathcal{R}) = \sum_{n_1,\ldots,n_N=1}^{\infty}\left(\frac{-1}{\sum_{i=1}^N\lambda_{n_i}}\right)\prod_{i=1}^N(\psi_{n_i}(\mathbf{r}_i')\psi_{n_i}(\mathbf{r}_i)),$$

where $\psi_k(\mathbf{r})$ and λ_k are kth eigenfunction and eigenvalue of the Laplace operator, respectively [53]. The eigenvalues are organized in ascending order of magnitude. Noting that

in the limit of $V \to \infty$, the eigenvalue λ_1 with the smallest magnitude approaches zero, while other eigenvalues remain finite [54]. Consequently, we can simplify the above expression considerably if the search domain is much larger than the target size as

$$G(\mathcal{R}'|\mathcal{R}) \simeq -\frac{1}{N\lambda_1}\prod_i \psi_1(\mathbf{r}_i')\psi_1(\mathbf{r}_i). \tag{19}$$

This asymptotic expression of the Green function leads to the search time of non-interacting searchers as

$$\tau_0(\mathcal{R}) \simeq \frac{V^{N/2}}{ND\lambda_1}\prod_i^N \psi_1(\mathbf{r}_i), \tag{20}$$

where we let $\int d\mathbf{r}\,\psi_1(\mathbf{r}) \simeq V^{1/2}$, using the fact that the normalized eigenfunction ψ_1 is nearly constant, except in the region close to the target. Integrating $\tau_0(\mathcal{R})$ over a uniform initial distribution, one obtains the well-known expression of the first-passage time of noninteracting searchers given as $1/(N\lambda_1 D)$ [22].

By substituting Eq. (19) into Eq. (18) and performing the integrations, the interaction effects can be estimated. For interactions with a range shorter than the system size, $\sigma \ll L \sim V^{1/d}$, by following the steps detailed in Appendix B, we obtain the second main result, an expression of the MFPT for searchers with a given $\mathcal{R}_0$:

$$\tau(\mathcal{R}_0) \simeq \tau_0(\mathcal{R}_0)\left[1 - \frac{4}{3}\frac{N-1}{V}B_2\right], \tag{21}$$

where B_2 is the second virial coefficient defined as

$$B_2 \equiv -\frac{1}{2}\int d^d\mathbf{r}\,[e^{-\beta v(|\mathbf{r}|)} - 1]. \tag{22}$$

As a corollary, the same relation holds for the global mean first-passage time (GMFPT), i.e., MFPT averaged over arbitrary initial distributions of searchers: $\bar{\tau} \equiv \int d\mathcal{R}_0\,\tau(\mathcal{R}_0)\mathcal{P}_0(\mathcal{R}_0)$ with an initial distribution $\mathcal{P}_0(\mathcal{R}_0)$:

$$\bar{\tau} \simeq \bar{\tau}_0\left[1 - \frac{4}{3}\frac{N-1}{V}B_2\right]. \tag{23}$$

It is important to note that our formulation considers *arbitrary* initial distributions of interacting searchers, and we find that the correction due to interactions is given in a *universal* way: Remarkably, the initial position dependence and the interaction effect are decoupled and appear in the factorized form in determining MFPT. Moreover, the correction arising from interaction is in the form of a virial expansion, proportional to the particle density and the second virial coefficient of the interaction potential, whereby other details, such as domain shapes, play no role.

The relation (21) predicts how the sign of interaction affects the search time. For repulsive interactions, the second virial coefficient is positive, and the search time is shorter than the noninteracting, ideal case and further decreases with increasing interaction strength. Attractive interactions act oppositely and slow down the search process. This is consistent with our numerical results presented in Fig. 1(b) and can be intuitively understood by considering how the particle distribution close to the target boundary changes as the interaction turns on. The target area is a cavity devoid of particles, causing an imbalance in force distributions. Therefore, particles repelling one another are pushed toward the target, shortening MFPT, whereas attracting particles get shoved away from the target and take longer MFPT.

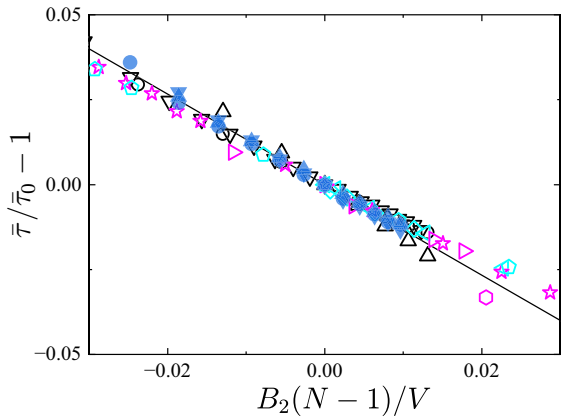

FIG. 2. GMFPT vs the second virial coefficient B_2 times the searcher density. Open symbols represent simulation results of GMFPT for systems with a uniform searcher distribution for three different types of interactions: exponential (black), hardcore (cyan), and Sutherland (magenta). In comparison, inhomogeneous searcher distributions are considered as Gaussian with the width of $16a$ and varying center positions (0, $9a$, and $18a$ from the domain center). The solid line represents our theoretical prediction, Eq. (23). Simulations were performed over a broad range of parameters, including $N =$ 3–23 and various interaction values of v_0 and σ, in a two-dimensional circular domain of radius $b = 15a$–$35a$ with a target of radius a (unit length). For each point, the statistical average is taken over more than 10^7 ensembles, giving error bars typically smaller than symbol sizes.

VI. SIMULATIONS AND DISCUSSIONS

To verify our prediction quantitatively, we perform the overdamped Langevin dynamics simulations, considering N particles with different initial distributions in a domain with a small target at the center. In simulations, we consider three different potentials: (i) exponential, $v(\mathbf{r}) = v_0 k_B T \exp(-|\mathbf{r}|/\sigma)$ with an interaction strength v_0 and a decay length σ; (ii) hardcore potential of radius σ, $v(\mathbf{r}) = \infty$ for $|\mathbf{r}| < \sigma$ and 0 otherwise; and (iii) Sutherland potential, $v(\mathbf{r}) = \infty$ for $|\mathbf{r}| < \sigma$ and $-v_0 k_B T(\sigma/r)^6$ otherwise. In simulating hardcore interactions, we let the particles repel along the line connecting their centers until there is no overlap between them. To investigate the dependence on initial searcher distributions, we consider not only a homogeneous uniform distribution (open symbols) but also an inhomogeneous Gaussian distribution (filled symbols) with its center lying at different radial distances. While GMFPTs change significantly depending on the initial distribution [55], the relationship between the search time of interacting particles and noninteracting particles still holds. In simulations, we consider the effective volume fraction $\phi = n\sigma^d$ up to the order of 10^{-1}, which covers the most relevant range in target search problems. To demonstrate the universal feature, we plot the relative changes in GMFPTs together in Fig. 2 for all

different distributions and potentials. For various values of the searcher number N, the domain size b, the interaction range σ, and the interaction strength v_0 considered here, all data points show a good agreement with the theoretical prediction, Eq. (23), represented as a straight line, clearly demonstrating the validity of our theory. Formulated in terms of the Mayer function, our theory applies to potentials diverging at short distances, such as the hardcore potential. Intermolecular potentials usually consist of a short-range hardcore repulsion and a smooth, relatively long-range attraction, as in Derjaguin-Landau-Verwey-Overbeek (DLVO) theory. For the potential of such type combining repulsive and attractive interactions, it is not obvious, even at a qualitative level, to predict the effect of interactions on the search time. Our result of Eq. (23), however, provides an explicit answer: the second virial coefficient determines the search time.

There exists an approach similar to ours called the generalized Smoluchowski theory [40–43]. This approach introduces the collective diffusion coefficient to account for interactions and relates it to the osmotic pressure derived for equilibrium [56]: $D(\rho) = M(\rho)\, d\Pi(\rho)/d\rho$ with a density-dependent mobility $M(\rho)$ and the equilibrium osmotic pressure $\Pi(\rho)$ [40–43]. Then, assuming a steady state, $\partial_t \rho = 0 = -\nabla \cdot \mathbf{J}$ with hydrodynamic flux $\mathbf{J} = -D(\rho)\nabla_{\mathbf{r}}\rho(\mathbf{r}, t)$, one defines the stationary reaction rate $\kappa = c_d(r)J(r)$ with $c_d = 2\pi r$ for two dimensions (2D) and $c_d = 4\pi r^2$ for 3D. Integration of this equation leads to $2\pi D\beta\Pi(\rho_\infty)/\ln(b/a)$ for 2D and $\kappa = 4\pi Da\beta\Pi(\rho_\infty)$ for 3D with a bulk density ρ_∞ [41–43], which gives the inverse of the mean first-passage time.

The approach described above cannot seize the initial configuration $\mathcal{R}_0$ dependence such as Eq. (21) obtained in our theory, and consequently fails to provide a correct understanding of the simulation results. The reason is apparent. As formulated using the homogeneous steady-state solution, this approach cannot incorporate (i) nonstationary distributions and (ii) the contribution of the transient state. In this aspect, we note that the main result, Eq. (21), provides an essential picture of the first-passage time of interacting searchers beyond the diffusion-limited reaction theory.

Our main result considers the search time in the large volume limit, or equivalently, the dilute density regime, which is most relevant in the context of the target search. If the particle density or the Mayer function is large (e.g., due to strong attractive interaction), our results are no longer valid, and alternative approaches are necessary. In semidilute regimes, the GMFPT deviates from the linear, leading order behavior, and the higher-order terms neglected in Eq. (18) would contribute. For the case of strongly attracting particles, the aggregation occurs as particle density increases, and the searching dynamics may show abrupt changes as a result of the clustering of the particles, as reported in Ref. [46]. In deriving Eq. (21), we also assumed the short-ranged interaction decaying faster than r^{-d}. Otherwise, the integral in evaluating B_2 is dominated by large distances and may diverge [52]. Therefore, in the case of long-range interactions such as Coulomb potential, the search time cannot be expressed in the form of a virial series.

VII. CONCLUSION

We have studied random target searches by interacting Brownian particles with arbitrary initial distributions in a confined space. Target searches become important when the searcher density is low; therefore, we have considered expansion using the Mayer function and derived the leading order correction to MFPT in the dilute searcher density limit. The universal features of the MFPT acquired from such consideration are as follows: The second virial coefficient determines the correction due to intersearcher interaction, and the effect of initial searcher distribution appears in the factorized form. We have verified our theory by comparing the theoretical expectations with the Langevin dynamics simulations for various forms of interactions and different initial distributions. In future studies, it would be interesting to extend the formalism presented in the current work to consider the random target searching by polymers and Kramers barrier crossing problem for interacting particles.

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APPENDIX A: RESUMMATION OF INTERACTION STRENGTH EXPANSION

In this section, through algebraic manipulations and volume-order counting, we show that the leading-order term of the Mayer function expansion, Eq. (16), can be reproduced by resuming the terms obtained from the interaction strength expansion, Eq. (11). We start by performing integration by parts on Eq. (11) and obtain

$$\tau_n(\mathcal{R}_0) = I_1 + I_2 \tag{A1}$$

with

$$I_1 = -\int d\mathcal{R}\, \tilde{U}(\mathcal{R})\nabla G(\mathcal{R}|\mathcal{R}_0) \cdot \nabla\tau_{n-1}(\mathcal{R}), \tag{A2}$$

$$I_2 = -\int d\mathcal{R}\, \tilde{U}(\mathcal{R})G(\mathcal{R}|\mathcal{R}_0)\nabla^2\tau_{n-1}(\mathcal{R}). \tag{A3}$$

For terms of order $n \geqslant 2$, we plug Eq. (11) for τ_{n-1} into I_1 and I_2, which gives

$$I_1 = -\int d\mathcal{R} \int d\mathcal{R}'\, \tilde{U}(\mathcal{R})[\nabla G(\mathcal{R}|\mathcal{R}_0) \cdot \nabla G(\mathcal{R}'|\mathcal{R})][\nabla'\tilde{U}(\mathcal{R}') \cdot \nabla'\tau_{n-2}(\mathcal{R}')],$$

$$I_2 = -\int d\mathcal{R}'\, \tilde{U}(\mathcal{R}')G(\mathcal{R}'|\mathcal{R}_0)\nabla'\tilde{U}(\mathcal{R}') \cdot \nabla'\tau_{n-2}(\mathcal{R}').$$

Here, $\mathcal{R}' = (\mathbf{r}'_1, \mathbf{r}'_2, \cdots, \mathbf{r}'_N)$ and $\nabla' = \sum_{i=1}^{N} \nabla_{\mathbf{r}'_i}$.

In the following, we show that I_1 can be neglected in comparison to I_2 in the large domain volume V limit. To achieve this, we track how I_1 and I_2 scale with V by employing the large volume asymptotic expression of the Green function, Eq. (19) of the main text. This leads to

$$I_1 \simeq -\frac{1}{N^2\lambda_1^2}\Psi_1(\mathcal{R}_0)\left[\int d\mathcal{R}\,\tilde{U}(\mathcal{R})\nabla\Psi_1(\mathcal{R})\cdot\nabla\Psi_1(\mathcal{R})\right]\left[\int d\mathcal{R}'\,\Psi_1(\mathcal{R}')\nabla'\tilde{U}(\mathcal{R}')\cdot\nabla'\tau_{n-2}(\mathcal{R}')\right],$$
$$I_2 \simeq \frac{1}{N\lambda_1}\Psi_1(\mathcal{R}_0)\left[\int d\mathcal{R}'\,\Psi_1(\mathcal{R}')\nabla'\left(\frac{1}{2}U^2(\mathcal{R}')\right)\cdot\nabla'\tau_{n-2}(\mathcal{R}')\right], \tag{A4}$$

where $\Psi_1(\mathcal{R}) = \prod_{i=1}^N \psi_1(\mathbf{r}_i)$. Here, $\lambda_1 = \mathcal{O}(V^{-1})$ and $\Psi(\mathcal{R}_0) = \mathcal{O}(V^{-N/2})$ according to the scaling properties of the principal eigenvalue and eigenfunction (with an additional logarithmic factor in two dimensions). For both I_1 and I_2, the integrands for $d\mathcal{R}'$ have an identical structure of

$$\Psi_1(\mathcal{R}')\nabla F(U)\cdot\nabla'\tau_{n-2}(\mathcal{R}'),$$

where $F(U)$ is a function of U. Since we consider short-ranged interactions, $F(U)$ does not contribute to the scaling with the volume, and the volume scaling exponents of the integrals of $\mathcal{R}'$ are the same.

In the meantime, I_1 has an additional factor that includes integration over $d\mathcal{R}$ as shown in Eq. (A4). The integrand of this part can be written as

$$\begin{aligned}&\int d\mathcal{R}\,U(\mathcal{R})\nabla\Psi_1(\mathcal{R})\cdot\nabla\Psi_1(\mathcal{R})\\ &= \int d\mathcal{R}\sum_{i<j}\tilde{v}_{ij}[\nabla\Psi_1(\mathcal{R})\cdot\nabla\Psi_1(\mathcal{R})],\\ &= \phi^{(1)}+\phi^{(2)},\end{aligned}$$

with

$$\phi^{(1)} = N(N-1)\int d\mathcal{R}\,\tilde{v}_{12}\nabla_{\mathbf{r}_1}\Psi_1(\mathcal{R})\cdot\nabla_{\mathbf{r}_1}\Psi_1(\mathcal{R}), \tag{A5}$$
$$\phi^{(2)} = \frac{N(N-1)(N-2)}{2}\int d\mathcal{R}\,\tilde{v}_{12}\nabla_{\mathbf{r}_3}\Psi(\mathcal{R})\cdot\nabla_{\mathbf{r}_3}\Psi(\mathcal{R}). \tag{A6}$$

Here $\tilde{v}_{ij} \equiv \beta v(\mathbf{r}_i - \mathbf{r}_j)$. In the following, we evaluate how these factors scale with the volume by going through detailed calculations.

1. $\phi^{(1)}$

We perform the integration of Eq. (A5) and obtain

$$\begin{aligned}\phi^{(1)} &= N(N-1)\left[\int d\mathbf{r}\,\psi_1^2(\mathbf{r})\right]^{N-2}\\ &\quad\times\int d\mathbf{r}_1 d\mathbf{r}_2\,\tilde{v}_{12}|\nabla_{\mathbf{r}_1}\psi_1(\mathbf{r}_1)|^2\psi_1^2(\mathbf{r}_2), &\text{(A7)}\\ &= N(N-1)\int d\mathbf{r}_1 d\mathbf{r}_2\,\tilde{v}_{12}|\nabla_{\mathbf{r}_1}\psi_1(\mathbf{r}_1)|^2\psi_1^2(\mathbf{r}_2). &\text{(A8)}\end{aligned}$$

Next, we approximate the short-ranged interaction as $\tilde{v}(|\mathbf{r}|) = \tilde{v}_0\delta(|\mathbf{r}|)$ in the large volume limit with

$$\tilde{v}_0 \equiv \int d\mathbf{r}\,\tilde{v}(|\mathbf{r}|). \tag{A9}$$

Lastly, we use the following asymptotic relations for the principle eigenfunction in the large volume limit:

$$\int d\mathbf{r}\,|\nabla\psi_1(\mathbf{r})|^2\psi_1^2(\mathbf{r}) = -\frac{\lambda_1}{3}\int d\mathbf{r}\,\psi_1^4(\mathbf{r}), \tag{A10}$$
$$\int d\mathbf{r}\,\psi_1^4(\mathbf{r}) \simeq \frac{1}{V}, \tag{A11}$$

To obtain Eq. (A10), we have performed integration by parts and have used the eigenvalue equation $\nabla^2\psi_1(\mathbf{r}) = -\lambda\psi_1(\mathbf{r})$. For Eq. (A11) we have used the relation $\psi_1(\mathbf{r}) \simeq 1/\sqrt{V}$ in the large V limit. Using Eqs. (A11) and (A10), we obtain

$$\phi^{(1)} \simeq -\frac{\lambda_1\tilde{v}_0 N(N-1)}{3V}. \tag{A12}$$

2. $\phi^{(2)}$

Next, we perform integration of Eq. (A6), which leads to

$$\begin{aligned}\phi^{(2)} &= \frac{N(N-1)(N-2)}{2}\left[\int d\mathbf{r}\,\psi_1^2(\mathbf{r})\right]^{N-3}\\ &\quad\times\left[\int d\mathbf{r}_1 d\mathbf{r}_2\,\tilde{v}_{12}\psi_1(\mathbf{r}_1)\psi_1(\mathbf{r}_2)\right]\int d\mathbf{r}_3\,|\nabla_{\mathbf{r}_3}\psi_1(\mathbf{r}_3)|^2, &\text{(A13)}\\ &= \lambda_1\frac{N(N-1)(N-2)}{2}\int d\mathbf{r}_1 d\mathbf{r}_2\,\tilde{v}_{12}\psi_1(\mathbf{r}_1)\psi_1(\mathbf{r}_2), &\text{(A14)}\\ &\simeq \frac{\lambda_1\tilde{v}_0 N(N-1)(N-2)}{2V}. &\text{(A15)}\end{aligned}$$

Note that both $\phi^{(1)}$ and $\phi^{(2)}$ are $O(V^{-2})$.

Gathering all the factors in I_1 and I_2, we conclude that

$$\frac{I_1}{I_2} = \mathcal{O}(V^{-1}), \tag{A16}$$

and thus I_1 can be neglected in the large volume limit: In sum, it is sufficient to keep I_2 in $\tau_n(\mathcal{R}_0)$. Next, we rewrite I_2 as

$$I_2 = \int d\mathcal{R}\,G(\mathcal{R}|\mathcal{R}_0)\nabla\left[-\frac{1}{2}\tilde{U}^2(\mathcal{R})\right]\cdot\nabla\tau_{n-2}(\mathcal{R}). \tag{A17}$$

By comparing Eq. (11) and (A17), we conjecture that the dominant part of $\tau_n(\mathcal{R}_0)$ can be written as

$$\tau_n(\mathcal{R}_0) \simeq -\int d\mathcal{R}\,G(\mathcal{R}|\mathcal{R}_0)\nabla\left[\frac{(-1)^k\tilde{U}^k(\mathcal{R})}{k!}\right]\cdot\nabla\tau_{n-k}(\mathcal{R}). \tag{A18}$$

with k is an integer in the interval $[1, n]$. We verify this conjecture with mathematical induction. Assume that Eq. (A18) is indeed satisfied in the large V limit. We perform integration

by parts and obtain

$$\tau_n(\mathcal{R}_0) \simeq \int \mathrm{d}\mathcal{R}\left[\frac{(-1)^k\tilde{U}^k(\mathcal{R})}{k!}\right]\nabla\cdot[G(\mathcal{R}|\mathcal{R}_0)\nabla\tau_{n-k}(\mathcal{R})],$$
$$= I_1^{(k)} + I_2^{(k)},$$

where

$$I_1^{(k)} = \int \mathrm{d}\mathcal{R}\left[\frac{(-1)^k\tilde{U}^k(\mathcal{R})}{k!}\right]\nabla G(\mathcal{R}|\mathcal{R}_0)\cdot\nabla\tau_{n-k}(\mathcal{R}), \tag{A19}$$

$$I_2^{(k)} = \int \mathrm{d}\mathcal{R}\left[\frac{(-1)^k\tilde{U}^k(\mathcal{R})}{k!}\right]G(\mathcal{R}|\mathcal{R}_0)\nabla^2\tau_{n-k}(\mathcal{R}). \tag{A20}$$

As is evident from similarity between I_1, I_2 and $I_1^{(k)}$, $I_2^{(k)}$ in Eqs. (A2), (A3), (A19), and (A20), $I_1^{(k)}$ is negligible in comparison to $I_2^{(k)}$. And, using Eq. (10), we can rewrite Eq. (A20) as

$$I_2^{(k)} = \int \mathrm{d}\mathcal{R}\, G(\mathcal{R}|\mathcal{R}_0)\left[\frac{(-1)^k\tilde{U}^k(\mathcal{R})}{k!}\right]\nabla\tilde{U}(\mathcal{R})\cdot\nabla\tau_{n-k-1}(\mathcal{R}),$$

$$= -\int \mathrm{d}\mathcal{R}\, G(\mathcal{R}|\mathcal{R}_0)\nabla\left[\frac{(-1)^{k+1}\tilde{U}^{k+1}(\mathcal{R})}{(k+1)!}\right]\cdot\nabla\tau_{n-k-1}(\mathcal{R}),$$

where we perform the integration by parts to obtain the last equality. Therefore, we conclude that if Eq. (A18) is satisfied for k, it is also satisfied for $k+1$. And, according to Eq. (11), the equation is satisfied for $k=1$, and thus Eq. (A18) holds for any k as long as $\tau_{n-k}(\mathcal{R})$ is defined. In particular, if $k=n$, we obtain

$$\tau_n(\mathcal{R}_0) \simeq -\int \mathrm{d}\mathcal{R}\, G(\mathcal{R}|\mathcal{R}_0)\nabla\left[\frac{(-1)^n\tilde{U}^n(\mathcal{R})}{n!}\right]\cdot\nabla\tau_0(\mathcal{R}), \tag{A21}$$

$$= \int \mathrm{d}\mathcal{R}\left[\frac{(-1)^n\tilde{U}^n(\mathcal{R})}{n!}\right]\nabla\cdot[G(\mathcal{R}|\mathcal{R}_0)\nabla\tau_0(\mathcal{R})]. \tag{A22}$$

By plugging this into Eq. (9), we obtain

$$\tau(\mathcal{R}_0) = \tau_0(\mathcal{R}_0) + \sum_{n=1}^{\infty}\int d\mathcal{R}\left[\frac{(-1)^n\tilde{U}^n(\mathcal{R})}{n!}\right]\nabla$$
$$\cdot[G(\mathcal{R}|\mathcal{R}_0)\nabla\tau_0(\mathcal{R})] + O(V^{-2}), \tag{A23}$$

$$= \tau_0(\mathcal{R}_0) + \int d\mathcal{R}\left(e^{-\beta U(\mathcal{R})}-1\right)\nabla$$
$$\cdot[G(\mathcal{R}|\mathcal{R}_0)\nabla\tau_0(\mathcal{R})] + O(V^{-2}), \tag{A24}$$

which reproduces Eq. (16).

APPENDIX B: THE LEADING-ORDER CORRECTION TO MEAN FIRST-PASSAGE TIMES

In this section, we derive the large volume limit asymptotic expression of the MFPT. We plug Eqs. (19) and (20) into Eq. (18) and obtain the correction term on the MFPT due to interparticle interactions as

$$\tau(\mathcal{R}_0) - \tau_0(\mathcal{R}_0) \simeq \int d\mathcal{R}\sum_{i<j} f_{ij}\nabla\cdot[G(\mathcal{R}_0|\mathcal{R})\nabla\tau_0(\mathcal{R})], \simeq -\frac{\Psi(\mathcal{R}_0)}{N\lambda_1}\int d\mathcal{R}\sum_{i<j} f_{ij}\nabla\cdot[\Psi(\mathcal{R})\nabla\tau_0(\mathcal{R})],$$
$$= \frac{\Psi(\mathcal{R}_0)}{N\lambda_1}\int d\mathcal{R}\sum_{i<j} f_{ij}\left[\frac{1}{D}\Psi(\mathcal{R}) - \nabla\Psi(\mathcal{R})\cdot\nabla\tau_0(\mathcal{R})\right],$$
$$= \frac{\Psi(\mathcal{R}_0)}{ND\lambda_1}\int d\mathcal{R}\sum_{i<j} f_{ij}\Psi(\mathcal{R}) - \frac{V^{N/2}\Psi(\mathcal{R}_0)}{N^2D\lambda_1^2}\int d\mathcal{R}\sum_{i<j} f_{ij}[\nabla\Psi(\mathcal{R})]^2,$$
$$\simeq \frac{\tau_0(\mathcal{R}_0)}{V^{N/2}}\int d\mathcal{R}\sum_{i<j} f_{ij}\Psi(\mathcal{R}) - \frac{\tau_0(\mathcal{R}_0)}{N\lambda_1}\int d\mathcal{R}\sum_{i<j} f_{ij}\sum_k\{\nabla_{\mathbf{r}_k}\Psi(\mathcal{R})\}^2.$$

Using the fact that all particles are identical, we can perform the sums above to get $\tau(\mathcal{R}_0) = \tau_0(\mathcal{R}_0)(1+\tau^{(1)}+\tau^{(2)}+\tau^{(3)})$ with

$$\tau^{(1)} \equiv \frac{N(N-1)}{2V^{N/2}}\int d\mathcal{R}\, f_{12}\Psi(\mathcal{R}), \tag{B1}$$

$$\tau^{(2)} \equiv -\frac{N(N-1)}{N\lambda_1}\int d\mathcal{R}\, f_{12}\{\nabla_{\mathbf{r}_1}\Psi(\mathcal{R})\}^2, \tag{B2}$$

$$\tau^{(3)} \equiv -\frac{N(N-1)(N-2)}{2N\lambda_1}\int d\mathcal{R}\, f_{12}\{\nabla_{\mathbf{r}_3}\Psi(\mathcal{R})\}^2. \tag{B3}$$

In what follows, we will simplify each term appearing above by following the procedure similar to Appendices. A 1 and A 2.

1. $\tau^{(1)}$

We first simplify $\tau^{(1)}$ as

$$\tau^{(1)} = \frac{N(N-1)}{2V^{N/2}}\left[\int d\mathbf{r}\,\psi_1(\mathbf{r})\right]^{N-2}$$
$$\times\int d\mathbf{r}_1 d\mathbf{r}_2\, f_{12}\psi_1(\mathbf{r}_1)\psi_1(\mathbf{r}_2),$$
$$\simeq \frac{N(N-1)}{2V}\int d\mathbf{r}_1 d\mathbf{r}_2\, f_{12}\psi_1(\mathbf{r}_1)\psi_1(\mathbf{r}_2), \tag{B4}$$

where we used the fact that the eigenfunction is almost uniform over the space at the large-volume (small-target) limit, $\psi_1(\mathbf{r}) \simeq 1/\sqrt{V}$.

2. $\tau^{(2)}$

The second contribution made by inter-searcher interaction, $\tau^{(2)}$ is given in Eq. (B1). We simplify it as

$$\tau^{(2)} = -\frac{N-1}{\lambda_1}\left[\int d\mathbf{r}\,\psi_1^2(\mathbf{r})\right]^{N-2} \times \int d\mathbf{r}_1 d\mathbf{r}_2\, f_{12}[\nabla_{\mathbf{r}_1}\psi_1(\mathbf{r}_1)]^2\psi_1^2(\mathbf{r}_2).$$

Further exploiting the normalization condition for the eigenfunction, $\int d\mathbf{r}\,\psi_1^2(\mathbf{r}) = 1$, we find $\tau^{(2)}$ as follows:

$$\tau^{(2)} = -\frac{N-1}{\lambda_1}\int d\mathbf{r}_1 d\mathbf{r}_2\, f_{12}[\nabla_{\mathbf{r}_1}\psi_1(\mathbf{r}_1)]^2\psi_1^2(\mathbf{r}_2). \quad \text{(B5)}$$

3. $\tau^{(3)}$

Similarly, the third contribution $\tau^{(3)}$ given in Eq. (B2) can be simplified as

$$\tau^{(3)} = -\frac{(N-1)(N-2)}{2\lambda_1}\int d\mathbf{r}_1 d\mathbf{r}_2\, f_{12}\psi_1^2(\mathbf{r}_1)\psi_1^2(\mathbf{r}_2) \times \int d\mathbf{r}_3\,[\nabla_{\mathbf{r}_3}\psi_1(\mathbf{r}_3)]^2.$$

Note that the integral over $\mathbf{r}_3$ leads to

$$\int d\mathbf{r}_3\,[\nabla_{\mathbf{r}_3}\psi_1(\mathbf{r}_3)]^2 = \oint d^{d-1}\mathbf{r}_3\,\hat{\mathbf{n}}\cdot[\psi_1(\mathbf{r}_3)\nabla_{\mathbf{r}_3}\psi_1(\mathbf{r}_3)] + \lambda_1\int d^d\mathbf{r}_3\,\psi_1^2(\mathbf{r}_3), = \lambda_1. \quad \text{(B6)}$$

Therefore, we have

$$\tau^{(3)} \simeq -\frac{(N-1)(N-2)}{2}\int d\mathbf{r}_1 d\mathbf{r}_2\, f_{12}\psi_1^2(\mathbf{r}_1)\psi_1^2(\mathbf{r}_2). \quad \text{(B7)}$$

As an interim summary, we conclude that the approximate search time of interacting searchers is

$$\tau(\mathcal{R}_0) \simeq \tau_0(\mathcal{R}_0)\{1+\tau^{(1)}+\tau^{(2)}+\tau^{(3)}\}, \quad \text{(B8)}$$

$$\simeq \tau_0(\mathcal{R}_0)\left\{1+\frac{N-1}{V}\int d\mathbf{r}_1 d\mathbf{r}_2\,[e^{-\beta v(|\mathbf{r}_1-\mathbf{r}_2|)}-1]F(\mathbf{r}_1,\mathbf{r}_2)\right\}. \quad \text{(B9)}$$

Here, combining Eqs. (B4), (B5), and (B7), we have defined $F(\mathbf{r}_1,\mathbf{r}_2)$ as

$$F(\mathbf{r}_1,\mathbf{r}_2) \equiv \frac{N}{2}\psi_1(\mathbf{r}_1)\psi_1(\mathbf{r}_2) - \frac{V}{\lambda_1}[\nabla_{\mathbf{r}_1}\psi_1(\mathbf{r}_1)]^2\psi_1^2(\mathbf{r}_2) - \frac{(N-2)V}{2}\psi_1^2(\mathbf{r}_1)\psi_1^2(\mathbf{r}_2). \quad \text{(B10)}$$

4. For short-ranged interactions

Let us now consider a case that the range of interparticle interactions under one's consideration, σ, is much shorter than the size of search domain $V^{1/d}$. In this case, one can evaluate the integral in (B9) analytically. First, we change variable $\mathbf{r}_1 - \mathbf{r}_2 = \mathbf{r}$ to get

$$\int d\mathbf{r}_1 d\mathbf{r}_2\,[e^{-\beta v(|\mathbf{r}_1-\mathbf{r}_2|)}-1]F(\mathbf{r}_1,\mathbf{r}_2) = \int d\mathbf{r}\,[e^{-\beta v(|\mathbf{r}|)}-1]\int d\mathbf{x}\,F(\mathbf{r}_1,\mathbf{r}_1+\mathbf{r}). \quad \text{(B11)}$$

Here, the upper limit of the integration over $|\mathbf{r}|$ is not a concern because the Mayer function is appreciable only for $|\mathbf{r}| < \sigma \ll V^{1/d}$. The function $F(\mathbf{r}_1,\mathbf{r}_1+\mathbf{r})$ can be expanded as $F(\mathbf{r}_1,\mathbf{r}_1+\mathbf{r}) = F(\mathbf{r}_1,\mathbf{r}_1) + \mathbf{r}\cdot[\nabla_{\mathbf{x}}F(\mathbf{r}_1,\mathbf{x})]_{\mathbf{x}=\mathbf{r}_1} + \cdots$. For short-ranged interactions, one can take only $F(\mathbf{r}_1,\mathbf{r}_1)$, neglecting the terms associated with $(\mathbf{r}\cdot\nabla_{\mathbf{x}})$. The neglected terms are roughly $\mathcal{O}(\sigma/V^{1/d})$ because the eigenfunction $\psi_1(\mathbf{r})$ composing the function F varies over the length scale of $V^{1/d}$. So we can replace $F(\mathbf{r}_1,\mathbf{r}_2)$ in (B9) with $F(\mathbf{r}_1,\mathbf{r}_1)$ and get

$$\tau(\mathcal{R})/\tau_0(\mathcal{R}) \simeq 1+\frac{N-1}{V}\int d\mathbf{r}\,[e^{-\beta v(|\mathbf{r}|)}-1]\int d\mathbf{r}_1\,F(\mathbf{r}_1,\mathbf{r}_1), \simeq 1-2\frac{N-1}{V}CB_2,$$

where B_2 is the second virial coefficient given by

$$B_2 = -\frac{1}{2}\int d\mathbf{x}\,[e^{-\beta v(|\mathbf{x}|)}-1],$$

and, according to Eq. (B10), C is determined by the eigenfunction integrals as

$$C = \int d\mathbf{r}\left[\frac{N}{2}\psi_1^2(\mathbf{r}) - \frac{V}{\lambda_1}[\nabla\psi_1(\mathbf{r})]^2\psi_1^2(\mathbf{r}) - \frac{(N-2)V}{2}\psi_1^4(\mathbf{r})\right].$$

Lastly, using Eqs. (A10) and (A11), we obtain $C = 2/3$, leading to the leading order correction to MFPT given in Eq. (21).

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[56] The effective diffusion coefficient is expressed in terms of the local osmotic pressure, Eq. (7.80) of [40]. Note that this result, $D(\rho) \propto d\Pi(\rho)/d\rho$, can be derived only after assuming an equilibrium (the osmotic pressure is defined by the equilibrium correlation function); for details, see Eqs. (7.67), (7.71), and sentences below the equations as well, of Ref. [40].
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