Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Materials for the paper "Diffusive escape through a narrow opening: new insights into a classic problem"¶¶

SM1 Numerical simulations

In this part of the Supplemental Materials we briefly discuss two numerical procedures used to check our theoretical predictions.

SM1.1 Numerical computation by a finite elements method

To verify the accuracy of the SCA, we solve the Poisson equation (2, 3) by using a finite elements method (FEM) implemented in Matlab PDEtool. This tool solves the following equation:

$$-\nabla(c\nabla u)+au=f, \tag{S1}$$

where c is a 2x2 matrix, and a and f are given functions.

In our case, we need to deal with the Laplace operator in radial or spherical coordinates. In two dimensions, the original equation (3) can be written in radial coordinates as

$$\frac{1}{r}\partial_r(re^{-U(r)}\partial_r)u+\frac{e^{-U(r)}}{r^2}\partial_\theta^2 u=-\frac{e^{-U(r)}}{D}, \tag{S2}$$

from which

$$-\begin{pmatrix}\partial_r\\ \partial_\theta\end{pmatrix}^\dagger c\begin{pmatrix}\partial_r\\ \partial_\theta\end{pmatrix}u=f, \tag{S3}$$

with $a=0$, $f=re^{-U(r)}/D$, and

$$c=\begin{pmatrix} re^{-U(r)} & 0\\ 0 & e^{-U(r)}/r\end{pmatrix}. \tag{S4}$$

In three dimensions, the Poisson equation (2) reads in spherical coordinates as

$$\frac{1}{r^2}\partial_r(r^2e^{-U(r)}\partial_r)u+\frac{e^{-U(r)}}{r^2}\frac{1}{\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta)u + \frac{e^{-U(r)}}{r^2\sin^2\theta}\partial_\varphi^2 u=-\frac{e^{-U(r)}}{D}. \tag{S5}$$

Since our solution does not depend on φ, the last term on the left-hand side can be omitted so that

$$-\begin{pmatrix}\partial_r\\ \partial_\theta\end{pmatrix}^\dagger c\begin{pmatrix}\partial_r\\ \partial_\theta\end{pmatrix}u=f, \tag{S6}$$

with $a=0$, $f=r^2e^{-U(r)}\sin\theta/D$, and

$$c=\begin{pmatrix} r^2e^{-U(r)}\sin\theta & 0\\ 0 & e^{-U(r)}\sin\theta\end{pmatrix}. \tag{S7}$$

We set the computational rectangular domain $V=[0,1]\times[0,\pi]$ with mixed boundary conditions (4), i.e., a zero flux condition for $\partial V\backslash\Gamma_0$, except for the segment $\Gamma_0=\{1\}\times[0,\varepsilon]$ representing the EW (see Fig. S1):

$$\begin{aligned}
\left(\partial_r u+\frac{k}{D}u\right)_{r=1}&=0 &&(\text{on }\Gamma_0),\\
(\partial_r u)_{r=1}&=0 &&(\text{on }\Gamma_1),\\
(\partial_r u)_{r=0}&=0 &&(\text{on }\Gamma_3),\\
(\partial_\theta u)_{\theta=0}&=0 &&(\text{on }\Gamma_4),\\
(\partial_\theta u)_{\theta=\pi}&=0 &&(\text{on }\Gamma_2).
\end{aligned} \tag{S8}$$

In Matlab, the generalised Neumann boundary condition has the form

$$\vec{n}\cdot(c\nabla u)+qu=g, \tag{S9}$$

where the matrix c is the same as in the PDE (S1). We set $g=0$ and

$$\begin{aligned}
q&=Re^{-U(R)}\kappa/D &&(\text{on }\Gamma_0),\\
q&=0 &&(\text{on }\Gamma_1\cup\Gamma_2\cup\Gamma_3\cup\Gamma_4)
\end{aligned} \tag{S10}$$

in two dimensions, and

$$\begin{aligned}
q&=R^2\sin\theta\; e^{-U(R)}\kappa/D &&(\text{on }\Gamma_0),\\
q&=0 &&(\text{on }\Gamma_1\cup\Gamma_2\cup\Gamma_3\cup\Gamma_4)
\end{aligned} \tag{S11}$$

in three dimensions. For fully reactive EW ($\kappa=\infty$), the Dirichlet boundary condition is imposed on Γ_0.

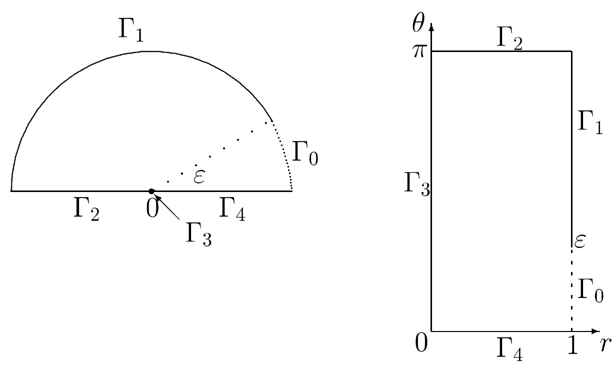

Fig. S1 The original domain (half-disc) and the associated computational domain (rectangle). Similar in 3D case.

SM1.2 Monte Carlo simulations

We also compute the distribution of first passage times to the EW by simulating diffusion trajectories which end up at the EW. In practice, we solve a Langevin equation by the following iterative procedure: after generating a uniformly distributed starting point $\mathbf{r}_0$, one re-iterates

$$\mathbf{r}_{n+1}=\mathbf{r}_n+D\delta\,\mathbf{f}(\mathbf{r}_n)+\sqrt{2D\delta}\;\xi_n\,, \tag{S12}$$

¶¶ Throughout these Supplementary Materials, we refer to the bibliography of the paper.

where δ is a one-step duration, $\mathbf{r}_n$ is the position after n steps, $\mathbf{f} = -\partial_r U(r)\mathbf{e}_r$ is the normalised applied force in the radial direction $\mathbf{e}_r$, and ξ is the normalised random thermal force. For instance, we have in two dimensions:

$$x_{n+1} = x_n + D\delta\ f(|\mathbf{r}_n|)\ x_n/|\mathbf{r}_n| + \sqrt{2D\delta}\ \xi_{x,n}\,,$$
$$y_{n+1} = y_n + D\delta\ f(|\mathbf{r}_n|)\ y_n/|\mathbf{r}_n| + \sqrt{2D\delta}\ \xi_{y,n}\,, \qquad \text{(S13)}$$

where $x_n/|\mathbf{r}_n|$ and $y_n/|\mathbf{r}_n|$ represent $\cos(\theta)$ and $\sin(\theta)$ in the projection of the radial force, and $\xi_{x,n}$, $\xi_{y,n}$ are independent normal variables with zero mean and unit variance.

At each step, one checks whether the new position (x_{n+1}, y_{n+1}) remains inside the disk: $x_{n+1}^2 + y_{n+1}^2 < R^2$. If this condition is not satisfied, the particle is considered as being on the boundary. If the particle hits the EW, the trajectory simulation is stopped and $n\delta$ is recorded as the generated exit time. Otherwise, the particle is reflected back and continues to diffuse. The Monte Carlo simulations in three dimensions are similar. Finally, the partial reactivity of the EW can be introduced by partial reflections[66,79].

SM2 Asymptotic behaviour of the series in (19) and (24)

We focus on the asymptotic behaviour of the infinite series $\mathscr{R}_\varepsilon^{(3)}$ and $\mathscr{R}_\varepsilon^{(2)}$, defined in (19) and (24), for potentials $U(r)$ which have a bounded first derivative for any $r \in (0,R)$. Our aims here are two-fold: first we establish the exact asymptotic expansions for these infinite series in the narrow escape limit $\varepsilon \to 0$, and second, we derive approximate explicit expressions for $\mathscr{R}_\varepsilon^{(3)}$ and $\mathscr{R}_\varepsilon^{(2)}$ which permit us to investigate their asymptotic behaviour in the limit $R|U'(R)| \to \infty$.

Our analysis is based on two complementary approaches. In the first approach we take advantage of the following observation. When $\varepsilon = 0$, there is no EW, and the MFET is infinite, whatever the potential is. Since $\mathscr{L}_U^{(d)}$ does not depend on ε, the divergence of the MFET as $\varepsilon \to 0$ should be ensured by the divergence of $\mathscr{R}_\varepsilon^{(d)}$. Suppose that we truncate the infinite series in (19) or (24) at some arbitrary $n = N^*$. Then, turning to the limit $\varepsilon \to 0$, we find that both $\mathscr{R}_\varepsilon^{(3)}$ and $\mathscr{R}_\varepsilon^{(2)}$ attain some constant values, which depend on the upper limit N^* of summation. As a consequence, these truncated sums should diverge as $N^* \to \infty$ while their small-ε behaviour is dominated by the terms with $n \to \infty$. One needs therefore to determine the asymptotic behaviour of $g_n(R)/g_n'(R)$ in this limit and to evaluate the corresponding small-ε asymptotics for $\mathscr{R}_\varepsilon^{(3)}$ and $\mathscr{R}_\varepsilon^{(2)}$. This will be done in the subsection SM2.1.

Next, in subsection SM2.2 we will pursue a different approach based on the assumption that, once we are interested in the behaviour of the ratio g_n/g_n' at $r = R$ only, we may approximate the coefficients in the differential equations (7) and (20), which are functions of r, by taking their values at the confining boundary. This will permit us to derive an explicit expression for $g_n(R)/g_n'(R)$ valid for arbitrary n, not necessarily large, and arbitrary $|U'(R)| < \infty$. This expression will be checked subsequently against an exact solution obtained for a triangular-well potential (see SM4 and SM5). We set out to show that an approximate expression for $g_n(R)/g_n'(R)$ and an exact result for such a choice of the potential agree very well already for quite modest values of n and the agreement becomes progressively better with an increase of $|U'(R)|$. On this basis, we also determine the small-ε, as well large-$RU'(R)$ asymptotic behaviour of $\mathscr{R}_\varepsilon^{(3)}$ and $\mathscr{R}_\varepsilon^{(2)}$, which agrees remarkably well with the expressions obtained within the first approach, and the exact solution derived for the particular case of a triangular-well potential.

SM2.1 Large-n asymptotics of $g_n(R)/g_n'(R)$ and the corresponding small-ε behaviour of the infinite series $\mathscr{R}_\varepsilon^{(3)}$ and $\mathscr{R}_\varepsilon^{(2)}$.

We introduce an auxiliary function $\psi = \psi_n(r) = g_n(r)/g_n'(r)$, which is the inverse of the logarithmic derivative of $g_n(r)$ and obeys, in virtue of (7) and (20), the following equations:

$$r^2\left(1-\psi'\right) + r\left(2 - rU'(r)\right)\psi - n(n+1)\psi^2 = 0 \qquad \text{(S14)}$$

for the 3D case, and

$$r^2\left(1-\psi'\right) + r\left(1 - rU'(r)\right)\psi - n^2\psi^2 = 0 \qquad \text{(S15)}$$

for the 2D case, respectively. We will seek the solutions of these non-linear Riccati-type differential equations in form of the asymptotic expansion in the inverse powers of n in the limit $n \to \infty$.

Supposing that $U'(r)$ does not diverge at any point within the domain, we find that the leading term of ψ in the limit $n \to \infty$ is given by $\psi \sim r/n$ for both 2D and 3D cases, which is completely *independent* of the potential $U(r)$. Pursuing this approach further, we make no other assumption to get the second term in this large-n expansion, while for the evaluation of the third term we stipulate that $|U''(r)| < \infty$. We have then for the 3D case

$$\psi = \frac{r}{n} - \frac{r^2U'(r)}{2n^2} + \frac{r^2\left(U'(r)\left(4 + rU'(r)\right) + 2\,rU''(r)\right)}{8n^3} + O\left(\frac{1}{n^4}\right), \qquad \text{(S16)}$$

and hence,

$$\frac{g_n(R)}{Rg_n'(R)} = \frac{1}{n} - \frac{RU'(R)}{2n^2} + \frac{RU'(R)\left(4 + RU'(R)\right) + 2R^2U''(R)}{8n^3} + O\left(\frac{1}{n^4}\right), \qquad \text{(S17)}$$

where the omitted terms decay in the leading order as $1/n^4$. Similarly, for the 2D case we find

$$\psi = \frac{r}{n} - \frac{r^2U'(r)}{2n^2} + \frac{r^2\left(U'(r)\left(2 + rU'(r)\right) + 2\,rU''(r)\right)}{8n^3} + O\left(\frac{1}{n^4}\right), \qquad \text{(S18)}$$

and hence,

$$\frac{g_n(R)}{Rg_n'(R)} = \frac{1}{n} - \frac{RU'(R)}{2n^2} + \frac{RU'(R)\,(2+RU'(R)) + 2R^2U''(R)}{8n^3} + + O\left(\frac{1}{n^4}\right). \tag{S19}$$

We observe that the asymptotic expansions (S17) and (S19) for the 3D and the 2D cases become different from each other only starting from the third term; first two terms are exactly the same. As it will be made clear below, we do not have to proceed further with this expansion and, as an actual fact, just two first terms will suffice us to determine the leading asymptotic behaviour of $\mathscr{R}_\varepsilon^{(3)}$ and just the first one will be enough to determine the analogous behaviour of $\mathscr{R}_\varepsilon^{(2)}$. In what follows, in SM4 and SM5 we will also check these expansions against the exact results obtained for the triangular-well potential, in which case the radial functions g_n and hence, the ratio $g_n(R)/g_n'(R)$ can be calculated exactly. We proceed to show that the asymptotic forms in (S17) and (S19) coincide with the exact asymptotic expansions at least for the first three terms.

Focusing first on the 3D case, we formally write

$$\frac{g_n(R)}{Rg_n'(R)} \equiv \frac{1}{n} - \frac{RU'(R)}{2n^2} + \left(\frac{g_n(R)}{Rg_n'(R)} - \frac{1}{n} + \frac{RU'(R)}{2n^2}\right), \tag{S20}$$

where the terms in brackets, in virtue of (S16) and (S17), decay as $1/n^3$ when $n \to \infty$. Inserting (S20) into (19), we have

$$\mathscr{R}_\varepsilon^{(3)} = \Sigma_1 - RU'(R)\Sigma_2 + \sum_{n=1}^{\infty}\left(\frac{g_n(R)}{Rg_n'(R)} - \frac{1}{n} + \frac{RU'(R)}{2n^2}\right)\frac{\phi_n^2(\varepsilon)}{(2n+1)}, \tag{S21}$$

where

$$\Sigma_1 = \sum_{n=1}^{\infty}\frac{\phi_n^2(\varepsilon)}{n(2n+1)}, \tag{S22}$$

$$\Sigma_2 = \frac{1}{2}\sum_{n=1}^{\infty}\frac{\phi_n^2(\varepsilon)}{n^2(2n+1)}, \tag{S23}$$

and $\phi_n(\varepsilon)$ is defined by (15).

Next, we find that in the limit $\varepsilon \to 0$,

$$\Sigma_1 = \frac{32}{3\pi}\varepsilon^{-1} + \ln(1/\varepsilon) - \frac{7}{4} + \ln 2 + O(\varepsilon), \tag{S24}$$

$$\Sigma_2 = \ln(1/\varepsilon) + \frac{1}{4} + \ln 2 + \frac{\pi^2}{12} + O(\varepsilon), \tag{S25}$$

$$\sum_{n=1}^{\infty}\left(\frac{g_n(R)}{Rg_n'(R)} - \frac{1}{n} + \frac{RU'(R)}{2n^2}\right)\frac{\phi_n^2(\varepsilon)}{2n+1} = O(1). \tag{S26}$$

Combining (S21) and (S24, S25, S26) renders our central result in (31) for the 3D case. The derivation of the asymptotic forms in (S24, S25) is straightforward but rather lengthy and we relegate it to the end of this subsection. Here we only briefly comment on the term in (S26). We have

$$\lim_{\varepsilon\to 0}\phi_n^2(\varepsilon) = (2n+1)^2, \tag{S27}$$

so that the sum in (S26) converges as $\varepsilon \to 0$ to

$$\sum_{n=1}^{\infty}\left(\frac{g_n(R)}{Rg_n'(R)} - \frac{1}{n} + \frac{RU'(R)}{2n^2}\right)(2n+1). \tag{S28}$$

In view of the discussion above and (S17), the terms in brackets decay as $1/n^3$, which implies that this series converges. In turn, it means that the expression in (S26) contributes in the limit $\varepsilon \to 0$ only to a constant, ε-independent term in the small-ε expansion of $\mathscr{R}_\varepsilon^{(3)}$.

For the 2D case we use only the first term in the expansion in (S16) to formally represent the ratio $g_n(R)/g_n'(R)$ as

$$\frac{g_n(R)}{Rg_n'(R)} \equiv \frac{1}{n} + \left(\frac{g_n(R)}{Rg_n'(R)} - \frac{1}{n}\right), \tag{S29}$$

where the terms in the brackets vanish as $1/n^2$. Then, inserting the latter identity into (24), we have the following expression for $\mathscr{R}_\varepsilon^{(2)}$:

$$\mathscr{R}_\varepsilon^{(2)} = 2\sum_{n=1}^{\infty}\frac{1}{n}\left(\frac{\sin(n\varepsilon)}{n\varepsilon}\right)^2 + 2\sum_{n=1}^{\infty}\left(\frac{\sin(n\varepsilon)}{n\varepsilon}\right)^2\left(\frac{g_n(R)}{Rg_n'(R)} - \frac{1}{n}\right). \tag{S30}$$

The first sum evidently diverges as $\varepsilon \to 0$, since

$$\lim_{\varepsilon\to 0}\left(\frac{\sin(n\varepsilon)}{n\varepsilon}\right) = 1 \quad \text{and} \quad \sum_{n=1}^{\infty}\frac{1}{n} = \infty. \tag{S31}$$

As a matter of fact, this sum can be calculated in an explicit form (see (47) in the main text) for an arbitrary ε. In the small-ε limit it is given by

$$2\sum_{n=1}^{\infty}\frac{1}{n}\left(\frac{\sin(n\varepsilon)}{n\varepsilon}\right)^2 = 2\ln(1/\varepsilon) + 3 - 2\ln 2 + O(\varepsilon^2). \tag{S32}$$

On the other hand, for the sum in the last line in (S30) we have

$$\lim_{\varepsilon\to 0}\sum_{n=1}^{\infty}\left(\frac{\sin(n\varepsilon)}{n\varepsilon}\right)^2\left(\frac{g_n(R)}{Rg_n'(R)} - \frac{1}{n}\right) = \sum_{n=1}^{\infty}\left(\frac{g_n(R)}{Rg_n'(R)} - \frac{1}{n}\right). \tag{S33}$$

Since the terms in brackets decay as $1/n^2$ according to (S19), we infer that the sum in (S33) converges, so that the second term in (S30) contributes only to the constant, ε-independent term in the small-ε expansion of $\mathscr{R}_\varepsilon^{(2)}$. Collecting (S30) to (S33) we arrive at the asymptotic expansion in (32).

Lastly, we outline the derivation of the asymptotic forms in (S24, S25). For this purpose, we represent the difference of two Legendre polynomials of orders $n-1$ and $n+1$ as

$$P_{n-1}(x) - P_{n+1}(x) = \frac{(2n+1)}{n(n+1)}(1-x^2)\frac{d}{dx}P_n(x). \tag{S34}$$

Using next the standard integral representation of the Legendre polynomials,

$$P_n(x) = \frac{1}{\pi}\int_0^{\pi} dz_1\, v_\varepsilon^n(z_1), \quad v_\varepsilon(z_1) = x + i\sqrt{1-x^2}\cos(z_1), \tag{S35}$$

we have

$$P_{n-1}(x)-P_{n+1}(x)=\frac{(2n+1)}{(n+1)}\ \frac{\sqrt{1-x^2}}{\pi}\int_0^{\pi} dz_1\,\mu_\varepsilon(z_1)\,\nu_\varepsilon^{n-1}(z_1)\,,$$

$$\mu_\varepsilon(z_1)=\sqrt{1-x^2}-ix\cos(z_1)\,. \tag{S36}$$

Plugging the latter representation into (S22), performing the summation over n, and setting $x=\cos\varepsilon$, we cast Σ_1 into the form of the following double integral:

$$\Sigma_1=\int_0^{\pi} dz_1\int_0^{\pi} dz_2\,\Phi_\varepsilon^{(1)}(z_1,z_2)\,, \tag{S37}$$

with

$$\Phi_\varepsilon^{(1)}(z_1,z_2)=\frac{1}{\pi^2}\left(\frac{1+x}{1-x}\right)\frac{\mu_\varepsilon(z_1)\,\mu_\varepsilon(z_2)}{\nu_\varepsilon^2(z_1)\nu_\varepsilon^2(z_2)}$$
$$\times\left(\big(1-\nu_\varepsilon(z_1)\nu_\varepsilon(z_2)\big)\ln\big(1-\nu_\varepsilon(z_1)\nu_\varepsilon(z_2)\big)+\mathrm{Li}_2\big(\nu_\varepsilon(z_1)\nu_\varepsilon(z_2)\big)\right), \tag{S38}$$

where $\mathrm{Li}_2(y)$ is the dilogarithm: $\mathrm{Li}_2(y)=\sum_{n=1}^{\infty}y^n/n^2$.

We focus next on the small-ε behaviour of $\Phi_\varepsilon^{(1)}(z_1,z_2)$. After straightforward but lengthy calculations, we find that in this limit $\Phi_\varepsilon^{(1)}(z_1,z_2)$ admits the following expansion

$$\Phi_\varepsilon^{(1)}(z_1,z_2)=B_1^{(1)}\varepsilon^{-2}+B_2^{(1)}\varepsilon^{-1}\ln(\varepsilon)+B_3^{(1)}\varepsilon^{-1}$$
$$+B_4^{(1)}\ln(\varepsilon)+B_5^{(1)}+O(\varepsilon)\,, \tag{S39}$$

where $B_j^{(1)}$ are functions of both z_1 and z_2:

$$B_1^{(1)}=-\frac{2}{3}\cos z_1\cos z_2\,,\quad B_2^{(1)}=\frac{8i}{\pi^2}\cos z_1\cos z_2\,(\cos z_1+\cos z_2)\,,$$
$$B_3^{(1)}=\frac{2i}{3\pi^2}\left(2\cos z_1\cos z_2\left[\pi^2-3-3i\pi+6\ln(\cos z_1+\cos z_2)\right]\right.$$
$$\left.-\pi^2\right)(\cos z_1+\cos z_2)\,,\ B_4^{(1)}=-\frac{2}{\pi^2}\left(\left(4-(\cos z_1-\cos z_2)^2\right)\right.$$
$$\left.\times\cos z_1\cos z_2+4(\cos z_1+\cos z_2)^2(1-2\cos z_1\cos z_2)\right), \tag{S40}$$

and

$$B_5^{(1)}=\frac{1}{9}\left(6-29\cos z_1\cos z_2+24\cos^2 z_1\cos^2 z_2\right.$$
$$\left.+6\,(3\cos z_1\cos z_2-2)\left(\cos^2 z_1+\cos^2 z_2\right)\right)$$
$$+\frac{1}{\pi^2}\Big[4(\cos z_1+\cos z_2)^2(1-2\cos z_1\cos z_2)$$
$$-\cos z_1\cos z_2\left(4+\cos^2 z_1+\cos^2 z_2+6\cos z_1\cos z_2\right)\Big]$$
$$+\frac{i}{\pi}\Big[\cos z_1\cos z_2\left(4-(\cos z_1-\cos z_2)^2\right)$$
$$+4(\cos z_1+\cos z_2)^2(1-2\cos z_1\cos z_2)\Big]$$
$$-\frac{2}{\pi^2}\Big\{\cos z_1\cos z_2\left(4-(\cos z_1-\cos z_2)^2\right)$$
$$+4(\cos z_1+\cos z_2)^2(1-2\cos z_1\cos z_2)\Big\}\ln(\cos z_1+\cos z_2)\,. \tag{S41}$$

Integrating $B_j^{(1)}$ over z_1 and z_2, we get

$$\int_0^{\pi}\int_0^{\pi}dz_1dz_2\,B_1^{(1)}=\int_0^{\pi}\int_0^{\pi}dz_1dz_2\,B_2^{(1)}=0\,,$$
$$\int_0^{\pi}\int_0^{\pi}dz_1dz_2\,B_3^{(1)}=\frac{32}{3\pi}\,,\qquad\int_0^{\pi}\int_0^{\pi}dz_1dz_2\,B_4^{(1)}=-1\,,$$
$$\int_0^{\pi}\int_0^{\pi}dz_1dz_2\,B_5^{(1)}=\ln 2-\frac{7}{4}\,. \tag{S42}$$

Collecting the expressions in (S42) we get the expansion in (S24). Note that the coefficient $32/(3\pi)$ in front of the leading term in (S24) was obtained earlier in [57].

Similarly, using (S36), we represent the infinite series Σ_2 in (S23) as

$$\Sigma_2=\int_0^{\pi}\int_0^{\pi}dz_1dz_2\,\Phi_\varepsilon^{(2)}(z_1,z_2), \tag{S43}$$

where

$$\Phi_\varepsilon^{(2)}(z_1,z_2)=\frac{1}{2\pi^2}\left(\frac{1+x}{1-x}\right)\frac{\mu_\varepsilon(z_1)\mu_\varepsilon(z_2)}{\nu_\varepsilon^2(z_1)\nu_\varepsilon^2(z_2)}$$
$$\times\left(\big(\nu_\varepsilon(z_1)\nu_\varepsilon(z_2)-1\big)\mathrm{Li}_2\big(\nu_\varepsilon(z_1)\nu_\varepsilon(z_2)\big)+\nu_\varepsilon(z_1)\nu_\varepsilon(z_2)\right), \tag{S44}$$

with $\nu_\varepsilon(z_{1,2})$ defined in (S35). The small-ε behaviour of $\Phi_\varepsilon^{(2)}(z_1,z_2)$ follows

$$\Phi_\varepsilon^{(2)}(z_1,z_2) = B_1^{(2)}\,\varepsilon^{-2} + B_3^{(2)}\,\varepsilon^{-1} + B_4^{(2)}\,\ln(\varepsilon) + B_5^{(2)} + O(\varepsilon)\,, \quad \text{(S45)}$$

where $B_1^{(2)}$, $B_3^{(2)}$, $B_4^{(2)}$ and $B_5^{(2)}$ are given explicitly by

$$B_1^{(2)} = -\frac{2}{\pi^2}\cos z_1 \cos z_2\,,\ B_3^{(2)} = -\frac{i}{3\pi^2}\left(6+(\pi^2-6)\cos z_1\cos z_2\right) \times (\cos z_1+\cos z_2)\,,\ B_4^{(2)} = -\frac{2}{\pi^2}\cos z_1\cos z_2\,(\cos z_1+\cos z_2)^2\,,$$

and

$$B_5^{(2)} = \frac{1}{3}\Bigg(\left(\cos^2 z_1+\cos^2 z_2\right)(1-2\cos z_1\cos z_2) + 3\cos z_1\cos z_2\,(1-\cos z_1\cos z_2)\Bigg) + \frac{1}{3\pi^2}\Bigg[6-6\left(\cos^2 z_1+\cos^2 z_2\right)(1-2\cos z_1\cos z_2) - 11\cos z_1\cos z_2 + 18\cos^2 z_1\cos^2 z_2\Bigg] + \frac{i}{\pi}\cos z_1\cos z_2\,(\cos z_1+\cos z_2)^2 - \frac{2}{\pi^2}\cos z_1\cos z_2\,(\cos z_1+\cos z_2)^2\ln(\cos z_1+\cos z_2)\,. \quad \text{(S46)}$$

Integrating $B_j^{(2)}$ over z_1 and z_2, we obtain

$$\int_0^\pi\int_0^\pi dz_1dz_2\,B_1^{(2)} = \int_0^\pi\int_0^\pi dz_1dz_2\,B_3^{(2)} = 0\,,$$
$$\int_0^\pi\int_0^\pi dz_1dz_2\,B_4^{(2)} = -1\,,$$
$$\int_0^\pi\int_0^\pi dz_1dz_2\,B_5^{(2)} = \frac{1}{4}+\ln 2+\frac{\pi^2}{12}\,. \quad \text{(S47)}$$

Collecting these results, we obtain the asymptotic expansion in (S25).

SM2.2 Approximation for $g_n(R)/g'_n(R)$ and its limiting behavior for sufficiently large $|U'(R)|$.

We pursue next a different approach for calculation of the logarithmic derivative of the radial functions at the boundary, and of the corresponding expressions for the infinite series $\mathscr{R}_\varepsilon^{(3)}$ and $\mathscr{R}_\varepsilon^{(2)}$. This approach is based on the assumption that, once we are only interested in the behaviour on the boundary only, we may replace the coefficients in the differential equations (7) and (20) by their values at the boundary. Such an approximation is legitimate, of course, only for the potentials for which $U'(R)$ exists. In doing so, we will be able to derive an explicit, albeit an approximate expression for $g_n(R)/g'_n(R)$ which is valid, in principle, for arbitrary n and arbitrary* $|U'(R)|<\infty$. This approximate expression will be subsequently checked against exact results obtained for the triangular-well potential (see SM4 and SM5) and the asymptotic forms in (S17) and (S19).

We turn to the differential equations (7) and (20) and replace the coefficients in these equations (which are functions of r) by their values at the boundary. This gives the following differential equations with constant coefficients:

$$g''_n + \left(\frac{2}{R} - U'(R)\right)g'_n - \frac{n(n+1)}{R^2}g_n = 0 \quad \text{(S48)}$$

and

$$g''_n + \left(\frac{1}{R} - U'(R)\right)g'_n - \frac{n^2}{R^2}g_n = 0 \quad \text{(S49)}$$

for the 3D and the 2D cases, respectively. Using the notation

$$\omega = RU'(R), \quad \text{(S50)}$$

we write down a general solution of (S48):

$$g_n = c_1\exp\left(\frac{r}{2R}\left((\omega-2)-\sqrt{(2n+1)^2+(\omega-2)^2-1}\right)\right) + c_2\exp\left(\frac{r}{2R}\left((\omega-2)+\sqrt{(2n+1)^2+(\omega-2)^2-1}\right)\right), \quad \text{(S51)}$$

where c_1 and c_2 are adjustable constants. We note that since $(2n+1)^2-1>0$ for any $n>0$, the expression under the square root is always positive. Further, differentiating (S51) and setting $r=R$, we get the following approximate expression for the inverse of the logarithmic derivative at the boundary:

$$\frac{g_n(R)}{Rg'_n(R)} \approx 2\left(\omega-2+\sqrt{(2n+1)^2+(\omega-2)^2-1} - \frac{2c_1\sqrt{(2n+1)^2+(\omega-2)^2-1}}{c_1+c_2\exp\left(\sqrt{(2n+1)^2+(\omega-2)^2-1}\right)}\right)^{-1}. \quad \text{(S52)}$$

We notice that the last term in brackets in (S52), which is the ratio of an algebraic and an exponential function, can be safely neglected because the exponential function becomes large when either (or both) n and/or $|\omega|$ are large. This yields the following approximation for the inverse logarithmic derivative, which is independent of the constants c_1 and c_2:

$$\frac{g_n(R)}{Rg'_n(R)} \approx \frac{2}{\omega-2+\sqrt{(2n+1)^2+(\omega-2)^2-1}} = \frac{\sqrt{(2n+1)^2+(\omega-2)^2-1}-\omega+2}{2n(n+1)}. \quad \text{(S53)}$$

The same arguments yield an analogous approximation for the 2D case:

$$\frac{g_n(R)}{Rg'_n(R)} \approx \frac{\sqrt{4n^2+(\omega-1)^2}-\omega+1}{2n^2}. \quad \text{(S54)}$$

In Figs. S3 and S5 in the following sections SM4 and SM5 we

* Note that the condition that $U'(R)$ is bounded does not prevent us to study the behaviour of $g_n(R)/g'_n(R)$ in the limit $|U'(R)|\to\infty$.

compare the expressions in (S53) and (S54) with the exact results for the ratio $g_n(R)/(Rg_n'(R))$ derived for the special case of a triangular-well potential in (50). We observe a fairly good agreement between the approximate forms in (S53) and (S54) and the exact results in (S107) and (S131) even for very modest values of n (say, for $n \geq 10$). For smaller n there are some apparent deviations which however become smaller the larger $|\omega|$ is.

We turn to the limit $n \to \infty$. We find that in this limit the expressions in (S53) and (S54) exhibit the following asymptotic behaviour

$$\frac{g_n(R)}{Rg_n'(R)} \approx \frac{1}{n} - \frac{\omega-1}{2n^2} + \frac{\omega^2-1}{8n^3} + O\left(\frac{1}{n^4}\right) \tag{S55}$$

and

$$\frac{g_n(R)}{Rg_n'(R)} \approx \frac{1}{n} - \frac{\omega-1}{2n^2} + \frac{\omega^2-2\omega+1}{8n^3} + O\left(\frac{1}{n^4}\right) \tag{S56}$$

for the 3D and the 2D cases, respectively. Comparing these expansions with the asymptotic forms in (S17) and (S19), we observe that they are identical in the leading terms for large $|\omega|$. This suggests, in turn, that the approximate expressions for the inverse of the logarithmic derivatives in (S53) and (S54) are reliable (as well as the assumptions underlying their derivation) for $|\omega|$ large enough.

Further, using (S53) and (S54), we evaluate approximate expressions for the infinite series $\mathscr{R}_\varepsilon^{(3)}$ and $\mathscr{R}_\varepsilon^{(2)}$, and the corresponding small-ε expansions. To this end, it is expedient to use an auxiliary integral identity

$$\sqrt{A^2+B^2} = A + B\int_0^\infty \frac{d\xi}{\xi} e^{-A\xi} J_1(B\xi)\,, \tag{S57}$$

where $J_1(\cdot)$ is the Bessel function. This identity is valid for A and B such that $|\mathrm{Im}B| < \mathrm{Re}A$.

2D case

We start with the 2D case, which is simpler than the 3D one, and set $A = 2n$ and $B = \omega - 1$. Such a choice evidently fulfils the condition of the applicability of the identity in (S57). We have then

$$\begin{aligned}\mathscr{R}_\varepsilon^{(2)} &\approx 2\sum_{n=1}^\infty \frac{\sin^2(n\varepsilon)}{n^3\,\varepsilon^2} - B\sum_{n=1}^\infty \frac{\sin^2(n\varepsilon)}{n^4\,\varepsilon^2} \\ &+ B\int_0^\infty \frac{d\xi}{\xi} J_1(B\xi)\sum_{n=1}^\infty \frac{\sin^2(n\varepsilon)}{n^4\,\varepsilon^2} e^{-2n\xi}\,,\end{aligned} \tag{S58}$$

where the symbol $\approx$ signifies that this expression is obtained via an approximate approach. The asymptotic small-ε behaviour of the first sum is given by (S32), while the second and the third terms converge to ε-independent constants :

$$\begin{aligned}\mathscr{R}_\varepsilon^{(2)} &\approx \underbrace{2\ln(1/\varepsilon) + 3 - 2\ln 2 + O(\varepsilon^2)}_{\text{first sum}} - \underbrace{B\frac{\pi^2}{6}}_{\text{second sum}} \\ &\underbrace{+ B\int_0^\infty \frac{d\xi}{\xi} J_1(B\xi)\mathrm{Li}_2(e^{-2\xi})}_{\text{third sum}}\,.\end{aligned} \tag{S59}$$

Since $J_1(z)$ is an odd function, $J_1(-z) = -J_1(z)$, the integral in the last line in (S59) is an even function of B, i.e., it depends only on $|B|$. For large $|B|$ (or large $|\omega|$), the major contribution to this integral comes from small values of ξ, $\xi \ll 1$, so that this integral is given approximately by

$$B\int_0^\infty \frac{d\xi}{\xi} J_1(B\xi)\mathrm{Li}_2(e^{-2\xi}) \approx |B|\frac{\pi^2}{6} + 2\ln|B| + O(1)\,, \tag{S60}$$

where the omitted terms $O(1)$ are B-independent constants. We therefore obtain

$$\mathscr{R}_\varepsilon^{(2)} \approx 2\ln(1/\varepsilon) + \frac{\pi^2}{6}R\big(|U'(R)| - U'(R)\big) + 2\ln(R|U'(R)|) + O(1)\,. \tag{S61}$$

We conclude that in the 2D case, the leading in the limit $\varepsilon \to 0$ term in $\mathscr{R}_\varepsilon^{(2)}$ is independent of the interaction potential and is identical to the result in (32) based on the large-n expansions. Remarkably, the second term in (S61) is non-zero for attractive potentials (negative $U'(R)$) only, and becomes identically equal to zero in case of repulsive potentials (positive $U'(R)$). As a matter of fact, this term provides the major contribution in the limit of infinitely strong attractive potentials. For instance, in the case of a triangular-well potential, one has $\mathscr{L}_U^{(2)} \sim 2/|\omega|$ from (55) for negative $U'(R)$ of very large amplitude, so that the MFET in the limit $\omega \to -\infty$ becomes

$$T_\varepsilon^{(2)} \simeq \left(\frac{r_0}{R}\right)^2 \frac{r_0^2}{8D} + \frac{\pi^2 R^2}{3D}\,. \tag{S62}$$

As discussed in the main text, the first term is the time for a particle started uniformly to reach the boundary (in presence of an infinitely strong attractive potential in the region $r_0 < r < R$), whereas the second term represents the MFPT from a uniform starting point on a circle of radius R to a point-like target ($\varepsilon = 0$).

3D case

In the 3D case we set $A = 2n+1$, which is real and positive, and $B = \sqrt{(\omega-2)^2-1}$. Note that the maximum imaginary value of B is 1, and it is less than the minimal value of $A = 3$, attained for $n = 1$, so that the identity in (S57) is valid for any n and ω. Using this identity, we can cast $\mathscr{R}_\varepsilon^{(3)}$ into the following form

$$\mathscr{R}_\varepsilon^{(3)} \approx -\frac{\omega-2}{2}\sum_{n=1}^\infty \frac{\phi_n^2(\varepsilon)}{n(n+1)(2n+1)} + \frac{1}{2}\sum_{n=1}^\infty \frac{\phi_n^2(\varepsilon)}{n(n+1)} + F_\varepsilon(B)\,, \tag{S63}$$

where

$$F_\varepsilon(B) = \frac{B}{2}\int_0^\infty \frac{d\xi}{\xi} e^{-\xi} J_1(B\xi)\sum_{n=1}^\infty \frac{\phi_n^2(\varepsilon)}{n(n+1)(2n+1)} e^{-2n\xi}\,. \tag{S64}$$

For the infinite series entering the first term on the right-hand-side of (S63) we have

$$\frac{1}{2}\sum_{n=1}^\infty \frac{\phi_n^2(\varepsilon)}{n(n+1)(2n+1)} = \Sigma_2 + \frac{1}{2}\sum_{k=1}^\infty (-1)^k \sum_{n=1}^\infty \frac{\phi_n^2(\varepsilon)}{n^{2+k}(2n+1)}\,, \tag{S65}$$

where Σ_2 and its asymptotic behaviour are defined in (S23) and (S25). Noticing that the second term on the right-hand side of (S65) converges to an ε-independent constant as $\varepsilon \to 0$, i.e.,

$$\lim_{\varepsilon\to 0}\sum_{k=1}^{\infty}(-1)^k\sum_{n=1}^{\infty}\frac{\phi_n^2(\varepsilon)}{n^{2+k}(2n+1)} = \sum_{k=1}^{\infty}(-1)^k\sum_{n=1}^{\infty}\frac{(2n+1)}{n^{2+k}} = -1-\frac{\pi^2}{6}\,, \tag{S66}$$

we infer that

$$\frac{1}{2}\sum_{n=1}^{\infty}\frac{\phi_n^2(\varepsilon)}{n(n+1)(2n+1)} = \ln(1/\varepsilon)+O(1)\,. \tag{S67}$$

The sum in the second term on the right-hand side of (S63) can be formally rewritten as

$$\begin{aligned}\frac{1}{2}\sum_{n=1}^{\infty}\frac{\phi_n^2(\varepsilon)}{n(n+1)} &= \sum_{n=1}^{\infty}\frac{\phi_n^2(\varepsilon)}{n(2n+1)}\left(1-\frac{1}{2(n+1)}\right)\\ &= \Sigma_1 - \frac{1}{2}\sum_{n=1}^{\infty}\frac{\phi_n^2(\varepsilon)}{n(n+1)(2n+1)}\,,\end{aligned} \tag{S68}$$

where Σ_1 and its asymptotic behaviour are defined in (S22) and (S24). Consequently, we have

$$\frac{1}{2}\sum_{n=1}^{\infty}\frac{\phi_n^2(\varepsilon)}{n(n+1)} = \frac{32}{3\pi}\varepsilon^{-1}+O(1)\,. \tag{S69}$$

Lastly, we consider the contribution in (S64). For large $|B|$, the major contribution to the integral comes from ξ close to 0. Since $\phi_n(\varepsilon)\to(2n+1)$ as $\varepsilon\to 0$, the sum would logarithmically diverge if both ε and ξ were set to 0. This simple observation suggests that this sum may exhibit a logarithmic dependence either on ε, or on ξ. In order to evaluate the contribution $F_\varepsilon(B)$, we adopt the summation technique used in the previous subsection. Recalling the integral representations in (S35, S36), we have

$$F_\varepsilon(B) = \frac{B}{2}\int_0^{\infty}\frac{d\xi}{\xi}J_1(B\xi)\,G_\varepsilon(\xi), \tag{S70}$$

where, explicitly,

$$G_\varepsilon(\xi) = e^{-\xi}\sum_{n=1}^{\infty}\frac{\phi_n^2(\varepsilon)\,e^{-2n\xi}}{n(n+1)(2n+1)} = \int_0^{\pi}dz_1\int_0^{\pi}dz_2\,\Phi_\varepsilon^{(3)}(z_1,z_2,\xi) \tag{S71}$$

and

$$\begin{aligned}\Phi_\varepsilon^{(3)}(z_1,z_2,\xi) &= \frac{e^{-\xi}}{\pi^2}\left(\frac{1+\cos\varepsilon}{1-\cos\varepsilon}\right)\mu_\varepsilon(z_1)\mu_\varepsilon(z_2)\\ &\times\sum_{n=1}^{\infty}\frac{2n+1}{n(n+1)^3}\left[\nu_\varepsilon(z_1)\nu_\varepsilon(z_2)\right]^{n-1}e^{-2n\xi}\,,\end{aligned} \tag{S72}$$

with $\mu_\varepsilon(z)$ and $\nu_\varepsilon(z)$ defined in (S35, S36). Denoting $\zeta = \nu_\varepsilon(z_1)\nu_\varepsilon(z_2)e^{-2\xi}$, we get

$$\begin{aligned}\Phi_\varepsilon^{(3)}(z_1,z_2,\xi) &= \frac{1}{\pi^2}\left(\frac{1+\cos\varepsilon}{1-\cos\varepsilon}\right)\mu_\varepsilon(z_1)\mu_\varepsilon(z_2)e^{-3\xi}\\ &\times\frac{\mathrm{Li}_3(\zeta)-\mathrm{Li}_2(\zeta)+(1-\zeta)\ln(1-\zeta)+\zeta}{\zeta^2}\,.\end{aligned} \tag{S73}$$

Now, we have two options, either to expand this function first in powers of ε and then in powers of ξ, or to expand it first in powers of ξ and then in powers of ε. These two options correspond to two possible orders of limits: $\varepsilon\to 0$ and $|B|\to\infty$.

(i) **Limit $\varepsilon\to 0$ for a fixed $|B|$.**
For a fixed $\xi>0$, we expand $\Phi_\varepsilon^{(3)}(z_1,z_2,\xi)$ in powers of ε to get

$$\begin{aligned}\Phi_\varepsilon^{(3)}(z_1,z_2,\xi) &= C_{-2}(z_1,z_2,\xi)\varepsilon^{-2}+C_{-1}(z_1,z_2,\xi)\varepsilon^{-1}\\ &+C_0(z_1,z_2,\xi)+O(\varepsilon).\end{aligned} \tag{S74}$$

Note that this expansion does not contain a term with logarithmical diverge as $\varepsilon\to 0$. Next, each coefficient $C_j(z_1,z_2,\xi)$ has to be expanded in powers of ξ. After integration over z_1 and z_2, the contributions from C_{-2} and C_{-1} vanish (as expected), and the leading terms are given by

$$\begin{aligned}F_0(B) &= \frac{B}{2}\int_0^{\infty}\frac{d\xi}{\xi}J_1(B\xi)\left[-2\ln\xi-2\ln 2-1+3\xi+O(\xi^2)\right]\\ &= |B|\ln|B|+|B|(\gamma-3/2)+O(1)\\ &= |\omega|\ln|\omega|+|\omega|(\gamma-3/2)+O(\ln|\omega|),\end{aligned} \tag{S75}$$

where $\gamma\approx 0.5772$ is the Euler-Mascheroni constant. Combining this contribution with (S67, S69), we obtain the small-ε asymptotic behaviour of $\mathscr{R}_\varepsilon^{(3)}$ for sufficiently large $|\omega|$:

$$\begin{aligned}\mathscr{R}_\varepsilon^{(3)} &\approx \frac{32}{3\pi}\varepsilon^{-1}-(\omega-2)\ln(1/\varepsilon)+\\ &+|\omega|\ln|\omega|+(\gamma-3/2)|\omega|+O(\ln|\omega|)\,.\end{aligned} \tag{S76}$$

We note that despite the fact that this small-ε asymptotics is formally valid for sufficiently large $|\omega|$, it predicts a spurious logarithmic divergence of the MFET in the limit $|\omega|\to\infty$. This divergence is clearly unphysical (a stronger attractive potential should reduce the MFET, instead of increasing it) and indicates that (S76) holds for large but bounded ω. Upon a more detailed analysis, we infer that (S76) is only applicable for $1\ll|\omega|\ll 1/\varepsilon$.

(ii) **Limit $|B|\to\infty$ for a fixed small ε.**
Expanding $\Phi_\varepsilon^{(3)}(z_1,z_2,\xi)$ in (S73) in powers of ξ, we have

$$\Phi_\varepsilon^{(3)}(z_1,z_2,\xi) = \Phi_\varepsilon^{(3),0}(z_1,z_2)+\xi\,\Phi_\varepsilon^{(3),1}(z_1,z_2)+O(\xi^2)\,, \tag{S77}$$

which yields, upon inserting the latter expansion into (S70),

$$F_\varepsilon(B) = \frac{1}{2}\int_0^{\pi}dz_1\int_0^{\pi}dz_2\left[|B|\,\Phi_\varepsilon^{(3),0}(z_1,z_2)+\Phi_\varepsilon^{(3),1}(z_1,z_2)\right]. \tag{S78}$$

Concentrating next on the narrow escape limit $\varepsilon\to 0$, we expand $\Phi_\varepsilon^{(3),0}(z_1,z_2)$ and $\Phi_\varepsilon^{(3),1}(z_1,z_2)$ in powers of ε to get

$$\begin{aligned}\Phi_\varepsilon^{(3),j}(z_1,z_2) &= B_1^{(3),j}(z_1,z_2)\,\varepsilon^{-2}+B_2^{(3),j}(z_1,z_2)\,\varepsilon^{-1}\ln(\varepsilon)\\ &+B_3^{(3),j}(z_1,z_2)\,\varepsilon^{-1}+B_4^{(3),j}(z_1,z_2)\ln(\varepsilon)+B_5^{(3),j}(z_1,z_2)+O(\varepsilon),\end{aligned} \tag{S79}$$

where $B_1^{(3),j}(z_1,z_2)$ with $j=0,1$ are given explicitly by

$$B_1^{(3),0} = -\frac{2\left(6\zeta(3)-\pi^2+6\right)}{3\pi^2}\cos z_1\cos z_2\,, \quad B_2^{(3),0}\equiv 0\,,$$

$$B_3^{(3),0} = \frac{2i}{3\pi^2}(\cos z_1+\cos z_2)\Big(3\left(4\zeta(3)-\pi^2+4\right)\cos z_1\cos z_2 - \left(6\zeta(3)-\pi^2+6\right)\Big)\,,$$

$$B_4^{(3),0} = -\frac{4}{\pi^2}\cos z_1\cos z_2\left(\cos z_1+\cos z_2\right)^2\,,$$

$$\begin{aligned} B_5^{(3),0} = {} & \frac{-4}{\pi^2}\cos z_1\cos z_2\left(\cos z_1+\cos z_2\right)^2\ln\left(\cos z_1+\cos z_2\right) \\ & + \frac{1}{9\pi^2}\Big(36+36\zeta(3)-6\pi^2+\left(144-33\pi^2+18\pi i+108\zeta(3)\right) \\ & \times \cos z_1\cos z_2\left(\cos^2 z_1+\cos^2 z_2\right) \\ & + \left(18\pi^2-72-72\zeta(3)\right)\left(\cos^2 z_1+\cos^2 z_2\right) \\ & + \left(47\pi^2-174-174\zeta(3)\right)\cos z_1\cos z_2 \\ & + \left(216-48\pi^2+36\pi i\right)\cos^2 z_1\cos^2 z_2\Big)\,, \end{aligned} \quad \text{(S80)}$$

and

$$B_1^{(3),1} = -\frac{2(2\zeta(3)-\pi^2+2)}{\pi^2}\cos z_1\cos z_2\,,$$

$$B_2^{(3),1} = -\frac{16i}{\pi^2}\cos z_1\cos z_2\left(\cos z_1+\cos z_2\right)\,,$$

$$\begin{aligned} B_3^{(3),1} = {} & -\frac{16i}{\pi^2}\cos z_1\cos z_2\left(\cos z_1+\cos z_2\right) \\ & \times\ln\left(\cos z_1+\cos z_2\right) + \frac{2i}{3\pi^2}\left(\cos z_1+\cos z_2\right) \\ & \times\Big(\cos z_1\cos z_2\left(12\zeta(3)+24-7\pi^2+12i\pi\right) \\ & -3\left(2\zeta(3)-\pi^2+2\right)\Big)\,, \end{aligned}$$

$$\begin{aligned} B_4^{(3),1} = {} & \frac{8}{\pi^2}\Big(\left(\cos^2 z_1+\cos^2 z_2\right)\left(2-5\cos z_1\cos z_2\right) \\ & +2\cos z_1\cos z_2\left(3-4\cos z_1\cos z_2\right)\Big)\,. \end{aligned} \quad \text{(S81)}$$

To find an explicit expression for $F_\varepsilon(B)$ in (S78), we now have to integrate all the coefficients $B_1^{(3),j}$ over z_1 and z_2. This can be done rather straightforwardly and we find that the double integrals

$$b_k^j = \frac{1}{2}\int_0^\pi\int_0^\pi dz_1\,dz_2\,B_k^{(3),j}(z_1,z_2)\,, \quad \text{(S82)}$$

are given explicitly by

$$b_1^0=b_2^0=b_3^0=0, \quad b_4^0=-1, \quad b_5^0=\ln 2-\frac{1}{4}\,, \quad \text{(S83)}$$

for $j=0$, and

$$b_1^1=b_2^1=b_4^1=0\,, \quad b_3^1=-\frac{32}{3\pi}\,, \quad \text{(S84)}$$

for $j=1$, respectively. Collecting these explicit expressions for the coefficients b_k^j, we get

$$F_\varepsilon(B) = |B|\,\ln(1/\varepsilon)+(\ln 2-1/4)\,|B|-\frac{32}{3\pi}\,\varepsilon^{-1}+O(1)\,. \quad \text{(S85)}$$

Note that the coefficient in front of the term which diverges as $1/\varepsilon$ is negative and is equal by the absolute value to the coefficient of the leading diverging term in (S67), so that these two terms cancel each other. Recalling next the definition of B for the 3D case, and combining (S78) with (S67, S69), we obtain the asymptotic behaviour of $\mathscr{R}_\varepsilon^{(3)}$ for very large $|\omega|$ and small fixed ε:

$$\mathscr{R}_\varepsilon^{(3)} \approx (|\omega|-\omega)\,\ln(1/\varepsilon)+(\ln 2-1/4)|\omega|+O(1)\,. \quad \text{(S86)}$$

Comparing the latter expression with (S76), we note that (S86) does not contain the term $|\omega|\ln|\omega|$ (that caused an unphysical divergence of the MFET in the limit $\omega\to-\infty$), and includes an extra term $(|\omega|-\omega)\ln(1/\varepsilon)$ so that the logarithmically diverging term in (S86) is twice larger than the one in (S76) in case of negative ω. We note that due to this additional numerical factor, the expression in (S86) reproduces correctly, in the limit $\omega\to-\infty$, the exact result obtained in[64] for the MFPT to the EW solely due to diffusion along the surface of the 3D spherical micro-domain. We also emphasise that the coefficient in front of $\ln(1/\varepsilon)$ is non-zero only for negative ω (attractive interactions), and vanishes for positive ω (repulsive interactions).

SM3 Systems without long-range interactions

We examine next the simplest case without long-range interactions, $U(r)\equiv 0$, so that a particle diffuses freely with a bounded micro-domain.

SM3.1 3D case

The general solution of equation (7) for the radial functions $g_n(r)$ reads

$$g_n(r) = c_1 r^n + c_2 r^{-n-1}. \quad \text{(S87)}$$

We set $c_1=1$ for convenience, and choose $c_2=0$ to ensure the regularity at the origin. Then, the particular solution $t_0(r)$ is

$$t_0(r) = \frac{R^2-r^2}{6D}, \quad \text{(S88)}$$

so that $t_0'(R)=-R/(3D)$. We therefore obtain

$$t(r,\theta) = \frac{R^2-r^2}{6D}+a_0-\frac{R^2}{3D}\sum_{n=1}^{\infty}\frac{\phi_n(\varepsilon)}{n}\left(\frac{r}{R}\right)^n P_n(\cos\theta), \quad \text{(S89)}$$

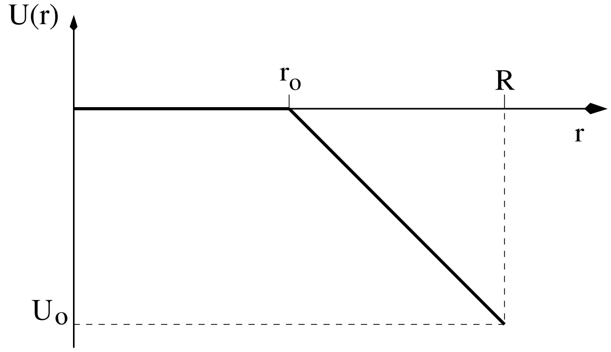

Fig. S2 A sketch of the triangular-well interaction potential in (50).

where the coefficient a_0 is fixed by the self-consistent condition in (18). This gives

$$a_0 = \frac{2R}{3\kappa(1-\cos\varepsilon)} + \frac{R^2 \mathscr{R}_\varepsilon^{(3)}}{3D}, \tag{S90}$$

with $\mathscr{R}_\varepsilon^{(3)}$ defined in (42). By integrating (S89) over the volume of the sphere, we find that the global MFET T_ε from a random location is given by (40).

We note finally that for a perfect EW (no barrier, $\kappa = \infty$), such that any arrival of the particle to the EW location will result in the escape from the sphere, the condition (17) reduces to

$$\int\limits_0^\varepsilon d\theta \sin\theta \; t(R,\theta) = 0. \tag{S91}$$

In other words, the original Dirichlet boundary condition at each point of the EW, $t(R,\theta) = 0$ for $0 \le \theta \le \varepsilon$, is replaced by a weaker condition requiring that the MFET vanishes on the EW *on average*. Hence, the condition (S91) implies that some values of $t(R,\theta)$ can become negative. As a consequence, the approximation is not expected to yield accurate results for the MFET with the starting point (r,θ) close to the EW. One can check numerically (not shown) that the approximation is nonetheless very accurate when the starting point is far from the EW. In general, the SCA is expected to be more accurate for small targets, as well as for weak reactivities κ.

SM3.2 2D case

In 2D case, the radial functions $g_n(r)$ are given by $g_n(r) = c_1 r^n + c_2 r^{-n} = r^n$, where we set $c_1 = 1$ and $c_2 = 0$. We also have

$$t_0(r) = \frac{R^2 - r^2}{4D}, \tag{S92}$$

from which $t_0'(R) = -R/(2D)$ follows. We therefore obtain

$$t(r,\theta) = \frac{R^2 - r^2}{4D} + a_0 - \frac{R^2}{D} \sum_{n=1}^{\infty} \frac{\sin(n\varepsilon)}{n^2 \varepsilon} (r/R)^n \cos(n\theta), \tag{S93}$$

with

$$a_0 = \frac{\pi R}{2\kappa\varepsilon} + \frac{R^2 \mathscr{R}_\varepsilon^{(2)}}{D}, \tag{S94}$$

and $\mathscr{R}_\varepsilon^{(2)}$ defined in (43). Integrating (S93) over the area of the circular micro-domain, we arrive at our result in (41).

Lastly, we note that the problem of finding the MFET through the fully reactive arc $(-\varepsilon,\varepsilon)$ of a disk, without LRI potential ($U(r) \equiv 0$) and without a barrier at the EW ($\kappa = \infty$) was solved analytically by Singer *et al.*[75] (see also[76,77]).

SM4 Triangular-well potential in 3D case

We now make a particular choice of the interaction potential between the diffusive particle and the boundary – a triangular-well radial potential defined in (50) (see Fig. S2). An advantage of such a choice is that i) it is simple but physically meaningful (see the discussion in[61]), ii) it permits to obtain an exact solution of the modified boundary-value problem and hence to check the accuracy of our predictions in (33) and (35), iii) it allows to verify our arguments behind the derivation of the asymptotic series in (S17) and (S19), and finally, iv) it helps to highlight some spectacular effects of the long-range particle-boundary interactions on the MFET.

SM4.1 Solution of the inhomogeneous problem (9).

First, we compute $t_0(r)$ by direct integration of the expression in (9) to get

$$t_0(r) = \begin{cases} \dfrac{r_0^2 - r^2}{6D} + H^{(3)}(\omega_0), & 0 \le r \le r_0, \\ H^{(3)}\left(\dfrac{\omega r}{R}\right), & r_0 < r \le R, \end{cases} \tag{S95}$$

where

$$H^{(3)}(z) = \frac{R^2}{D\omega^2} \Bigg[\left(\omega_0^3/3 + \omega_0^2 + 2\omega_0 + 2\right) e^{-\omega_0} \int\limits_z^\omega dx \frac{e^x}{x^2} - \omega(1-x_0) - \frac{2(1-x_0)}{\omega_0} + 2\ln x_0 \Bigg], \tag{S96}$$

with the dimensionless parameters

$$x_0 = \frac{r_0}{R}, \quad \omega = \frac{RU_0}{R-r_0} = \frac{U_0}{1-x_0}, \quad \omega_0 = \frac{r_0 U_0}{R-r_0} = x_0\omega.$$

Next, the derivative of $t_0(r)$ reads

$$t_0'(R) = \frac{R}{D\omega^3} \left(\omega^2 + 2\omega + 2 - \left(\omega_0^3/3 + \omega_0^2 + 2\omega_0 + 2\right) e^{\omega - \omega_0} \right). \tag{S97}$$

Integrating (S95), one finds the result in (57).

SM4.2 Radial functions $g_n(r)$

In order to solve (7), one finds solutions on each of the subintervals

$$g_n(r) = \begin{cases} A^- r^n + B^- r^{-n-1}, & 0 \le r \le r_0, \\ A^+ u_n\left(\dfrac{\omega r}{R}\right) + B^+ v_n\left(\dfrac{\omega r}{R}\right), & r_0 < r \le R, \end{cases} \tag{S98}$$

where $A^\pm$ and $B^\pm$ are unknown coefficients to be determined, and

$$\begin{aligned} u_n(z) &= z^n M(n,2n+2,z), \\ v_n(z) &= z^{-n-1} U(-n-1,-2n,z) \end{aligned} \tag{S99}$$

are two independent solutions in the presence of a triangular-well potential (50), $M(a,b,z)$ and $U(a,b,z)$ being Kummer's and Tricomi's confluent hypergeometric functions, respectively. The regularity of $g_n(r)$ at $r=0$ requires $B^-=0$. Requiring the continuity of $g_n(r)$ and of its derivative $g_n'(r)$ at $r=r_0$, one relates A^+ and B^+ to A^-:

$$\begin{aligned} A^- r_0^n &= A^+ u_n(\omega_0) + B^+ v_n(\omega_0), \\ nA^- R r_0^{n-1} &= A^+ \omega u_n'(\omega_0) + B^+ \omega v_n'(\omega_0). \end{aligned} \tag{S100}$$

These relations can be inverted to get

$$\begin{aligned} A^+ &= A^- \frac{\left(r_0^n v_n'(\omega_0) - nRr_0^{n-1} v_n(\omega_0)/\omega\right)}{u_n(\omega_0)v_n'(\omega_0) - v_n(\omega_0)u_n'(\omega_0)}, \\ B^+ &= A^- \frac{\left(-r_0^n u_n'(\omega_0) + nRr_0^{n-1} u_n(\omega_0)/\omega\right)}{u_n(\omega_0)v_n'(\omega_0) - v_n(\omega_0)u_n'(\omega_0)}. \end{aligned} \tag{S101}$$

The denominator in the latter expressions is the Wronskian of the solution, which can be calculated explicitly:

$$u_n(z)v_n'(z) - v_n(z)u_n'(z) = -\frac{(2n+1)!}{(n-1)!}\,\frac{e^z}{z^2}. \tag{S102}$$

Note that the Wronskian can be "absorbed" into a prefactor, which will then be factored out. We write then

$$g_n(r) = A^* \left[u_n\left(\frac{\omega r}{R}\right) - v_n\left(\frac{\omega r}{R}\right) w_n(\omega_0)\right], \tag{S103}$$

where

$$w_n(z) = \frac{zu_n'(z) - nu_n(z)}{zv_n'(z) - nv_n(z)}. \tag{S104}$$

We therefore obtain

$$\frac{g_n(R)}{Rg_n'(R)} = \frac{u_n(\omega) - v_n(\omega)\, w_n(\omega_0)}{\omega\, u_n'(\omega) - \omega\, v_n'(\omega)\, w_n(\omega_0)}. \tag{S105}$$

Next, using the relations

$$\begin{aligned} zu_n'(z) &= nz^n M(n+1,2n+2,z), \\ zv_n'(z) &= -\frac{n(n+1)}{z^{n+1}} U(-n,-2n,z), \end{aligned}$$

one can represent

$$\begin{aligned} zu_n'(z) - nu_n(z) &= nz^n \left[M(n+1,2n+2,z) - M(n,2n+2,z)\right] \\ &= \frac{nz^{n+1}}{2n+2} M(n+1,2n+3,z), \\ zv_n'(z) - nv_n(z) &= -nz^{-n-1}\left[(n+1)U(-n,-2n,z) + U(-n-1,-2n,z)\right] \\ &= -nz^{n+1} U(n+1,2n+3,z), \end{aligned}$$

so that

$$w_n(z) = -\frac{1}{2(n+1)}\,\frac{M(n+1,2n+3,z)}{U(n+1,2n+3,z)}. \tag{S106}$$

Taking together (S105) to (S106), we obtain

$$\begin{aligned} \frac{g_n(R)}{Rg_n'(R)} &= \frac{1}{n}\,\frac{M(n,2n+2,\omega)}{M(n+1,2n+2,\omega)} \left(1 - \frac{U(n,2n+2,\omega)}{M(n,2n+2,\omega)}\, w_n(\omega_0)\right) \\ &\times \left(1 + \frac{(n+1)U(n+1,2n+2,\omega)}{M(n+1,2n+2,\omega)}\, w_n(\omega_0)\right)^{-1}, \end{aligned} \tag{S107}$$

which is the desired exact expression for the ratio $g_n(R)/(Rg_n'(R))$ for the triangular-well potential.

For numerical computations, another representation in terms of the modified Bessel functions $I_{n+1/2}(z)$ and $K_{n+1/2}(z)$ can be convenient. Starting from the identities

$$\begin{aligned} M(n+1,2n+2,x) &= \Gamma(n+3/2)\left(\frac{4}{x}\right)^{n+1/2} e^{x/2} I_{n+1/2}(x/2), \\ U(n+1,2n+2,x) &= \frac{e^{x/2}}{\sqrt{\pi}x^{n+1/2}} K_{n+1/2}(x/2), \end{aligned} \tag{S108}$$

one can use the recurrence relations between Kummer's and Tricomi's functions to represent all the entries in (S107) in terms of $I_{n+1/2}(z)$ and $K_{n+1/2}(z)$. This gives

$$\begin{aligned} \frac{g_n(R)}{Rg_n'(R)} &= \frac{1}{n}\left(1 + \frac{\omega\, i_n(\omega)}{2(n+1)}\right)\left(1 + j_n(\omega,\omega r_0/R)\right)^{-1} \\ &\times \left(1 - j_n(\omega,\omega r_0/R)\,\frac{k_n(\omega) - 2\frac{n+1}{\omega}}{i_n(\omega) + 2\frac{n+1}{\omega}}\right), \end{aligned} \tag{S109}$$

with

$$\begin{aligned} i_n(z) &= \frac{I_{n+3/2}(z/2)}{I_{n+1/2}(z/2)} - 1, \quad k_n(z) = \frac{K_{n+3/2}(z/2)}{K_{n+1/2}(z/2)} + 1, \\ j_n(z,z_0) &= \frac{K_{n+1/2}(z/2)}{K_{n+3/2}(z_0/2)}\,\frac{I_{n+3/2}(z_0/2)}{I_{n+1/2}(z/2)}. \end{aligned} \tag{S110}$$

Before we proceed with the analysis of the asymptotic large-n behaviour of $g_n(R)/(Rg_n'(R))$, it might be expedient to note that in the particular case $r_0=0$, the expression in (S107) simplifies to give

$$\frac{g_n(R)}{Rg_n'(R)} = \frac{u_n(\omega)}{\omega\, u_n'(\omega)} = \frac{1}{n}\,\frac{M(n,2n+2,\omega)}{M(n+1,2n+2,\omega)}, \tag{S111}$$

which is just the first factor in (S107) since $w_n(0)$ appears to be equal identically to zero. In this particular case, we have

$$H^{(3)}(z) = \frac{1}{D\omega^2}\left[2\int_z^\omega dx \frac{e^x - x - 1}{x^2} - \omega(1-x_0)\right], \tag{S112}$$

so that the MFPT from a random location to any point on the boundary becomes

$$T_\pi^{(3)}(\kappa=\infty) = \frac{R^2}{D\omega^5}\left[2(e^\omega(\omega-1)+1) - \frac{3\omega^2+8\omega+12}{12}\omega^2\right]. \tag{S113}$$

Consequently, the MFPT to the EW from some fixed location has

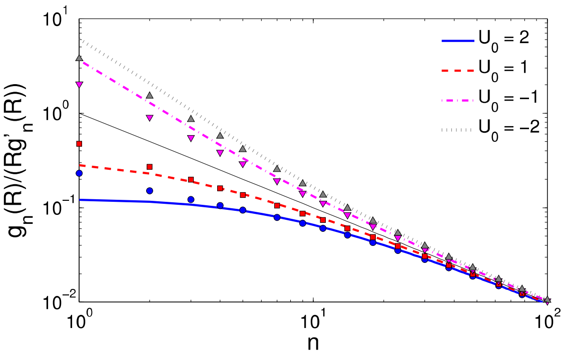

Fig. S3 The ratio $g_n(R)/(Rg'_n(R))$ vs the order n of the radial function for several values of U_0 with $r_0 = 0.8$ and $R = 1$. Comparison of the exact result in (S107) (symbols) and the approximate expression in (S53) (lines). Thin solid line is the $1/n$ asymptotics (solution of the problem with $U_0 \equiv 0$).

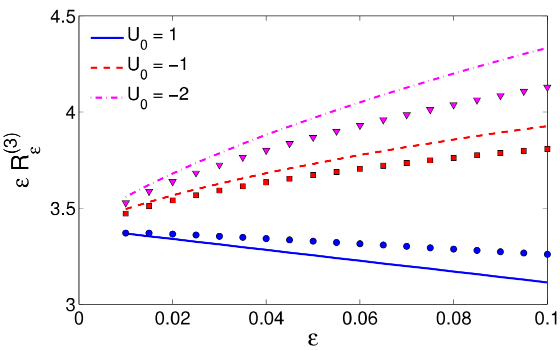

Fig. S4 Infinite series $\mathscr{R}_\varepsilon^{(3)}$, multiplied by ε, as a function of the angular size ε of the EW for $U_0 = 1$, $U_0 = -1$ and $U_0 = -2$ for $r_0 = 0$ and $R = 1$. Symbols represent the exact result obtained by numerical summation of (19) involving the expression in (S107), while curves show the asymptotic relation (31) without the last infinite sum.

the form:

$$t(r,\theta) = t_0(r) + a_0 + Rt_0'(R)\sum_{n=1}^{\infty} \frac{M\left(n, 2n+2, \dfrac{\omega r}{R}\right)(r/R)^n}{nM(n+1,2n+2,\omega)} \times \phi_n(\varepsilon)P_n(\cos(\theta)), \quad \text{(S114)}$$

where a_0 is given by (18) and, explicitly,

$$t_0'(R) = \frac{R}{D\omega^3}\left(\omega^2 + 2\omega + 2 - 2e^{\omega}\right). \quad \text{(S115)}$$

Consider next the behaviour of the inverse logarithmic derivative of the radial functions at the confining boundary in the limit $n \to \infty$ for arbitrary r_0. First, we find that the first factor in (S107) obeys

$$\frac{1}{n}\frac{M(n,2n+2,\omega)}{M(n+1,2n+2,\omega)} = \frac{1}{n} - \frac{\omega}{2n^2} + \frac{4\omega+\omega^2}{8n^3} + O\left(\frac{1}{n^4}\right). \quad \text{(S116)}$$

Second, we analyse the large-n behaviour of the second factor in (S107). Taking into account the definition of $w_n(z)$ in (S106), we observe that the correction term to unity has the form of a product of ratios of two Kummer's and Tricomi's functions with different arguments. The asymptotic large-n behaviour of the ratio of two Kummer's functions follows

$$\frac{M(n+1,2n+3,\omega_0)}{(n+1)M(n,2n+2,\omega)} = \exp\left(-\frac{\omega}{2}(1-x_0)\right) \times \left[\frac{1}{n} + \frac{\omega_0^2 - 4\omega_0 - (4-\omega)^2}{16n^2} + O\left(\frac{1}{n^3}\right)\right], \quad \text{(S117)}$$

i.e., is an expansion in the inverse powers of n. The ratio of two Tricomi's functions is given by

$$\frac{U(n,2n+2,\omega)}{U(n+1,2n+3,\omega_0)} = n\,\omega_0\,x_0^n \frac{\sum_{s=0}^{n+1}\binom{n+1}{s}\Gamma(n+s)/\omega^s}{\sum_{s=0}^{n+1}\binom{n+1}{s}\Gamma(n+s+1)/\omega_0^s}. \quad \text{(S118)}$$

Noticing that in the latter expression the major contribution to the sums in the numerator and the denominator stems from the terms with $s = n+1$, we infer that the leading behaviour of the ratio in (S118) in the limit $n \to \infty$ obeys

$$\frac{U(n,2n+2,\omega)}{U(n+1,2n+3,\omega_0)} \sim \frac{\omega_0\, n}{(2n+1)} x_0^{2n+1}, \quad \text{(S119)}$$

which means that the ratio of two Tricomi's functions vanishes *exponentially* fast with n as $n \to \infty$ for $x_0 < 1$ (i.e., $r_0 < R$). This implies, in turn, that the correction term to unity in the second factor in (S107) is exponentially small as $n \to \infty$ and hence, can be safely neglected.

Next, we consider the behaviour of the third factor in (S107) which is also a product of ratios of two Kummer's and Tricomi's functions. We have

$$\frac{M(n+1,2n+3,\omega_0)}{M(n+1,2n+2,\omega)} = \exp\left(-\frac{\omega}{2}(1-x_0)\right) \times \left[1 - \frac{4\omega_0 + \omega^2(1-x_0^2)}{16n} + O\left(\frac{1}{n^2}\right)\right] \quad \text{(S120)}$$

and

$$\frac{U(n+1,2n+2,\omega)}{U(n+1,2n+3,\omega_0)} = x_0^{n+1}\frac{\sum_{s=0}^{n}\binom{n}{s}\Gamma(n+1+s)/\omega^s}{\sum_{s=0}^{n+1}\binom{n+1}{s}\Gamma(n+1+s)/\omega_0^s}. \quad \text{(S121)}$$

Noticing that in the $n \to \infty$ limit the major contribution to the sums in the numerator and the denominator in the latter expression is provided by the terms with $s = n$, we find eventually that the leading behaviour of the ratio of two Tricomi's functions is defined by

$$\frac{U(n+1,2n+2,\omega)}{U(n+1,2n+3,\omega_0)} \sim \frac{\omega_0}{(2n+1)} x_0^{2n+1}. \quad \text{(S122)}$$

Therefore, due to the factor x_0^{2n+1}, which vanishes exponentially fast as $n \to \infty$, the third factor in (S107) appears to be exponentially close to 1 and can be safely neglected.

As a consequence, the leading asymptotic behaviour of $g_n(R)/(Rg_n'(R))$ in (S107) is entirely dominated by the first factor and hence, we have

$$\frac{g_n(R)}{Rg'_n(R)} = \frac{1}{n} - \frac{\omega}{2n^2} + \frac{4\omega+\omega^2}{8n^3} + O\left(\frac{1}{n^4}\right). \tag{S123}$$

The expansion in (S123) permits us to verify our general argument on the asymptotic behaviour of the ratio $g_n(R)/(Rg'_n(R))$ in the limit $n \to \infty$, presented in the beginning of SM2 (see (S17)). Recalling that $\omega = RU'(R) = U_0/(1-x_0)$ and that for such a potential $U''(R) = 0$, we observe a perfect coincidence of (S17), based on an intuitive (albeit quite plausible) argument, and the large-n expansion of the inverse of the logarithmic derivative, evaluated for an exactly solvable case of a triangular-well potential $U(r)$. Further, we note that the large-n behaviour of (S123) is dominated by the first factor, which is the solution for a particular case $r_0 = 0$. This implies, in turn, that in the large-n limit the dependence on r_0 is fully embodied in the dimensionless parameter ω.

Lastly, we compare the approximate expression (S53) for $g_n(R)/(Rg'_n(R))$ and the exact result in (S107) obtained for the triangular-well potential, see Fig. S3. We observe a fairly good agreement between the approximate formula (S53) and the exact result already for quite modest values of n, and notice that the agreement becomes even better for larger values of $R|U'(R)|$. Accordingly, our approximate small-ε expansion in (31) (without the infinite sum in the last line) and the exact result for $\mathscr{R}_\varepsilon^{(3)}$ agree well with each other, see Fig. S4. The smaller ε, the better agreement is.

SM5 Triangular-well potential in 2D case

SM5.1 Solution of the inhomogeneous problem (22)

Integrating Eq. (22), we get

$$t_0(r) = \begin{cases} \dfrac{r_0^2 - r^2}{4D} + H^{(2)}(\omega_0) & 0 \le r \le r_0, \\ H^{(2)}\left(\dfrac{\omega r}{R}\right) & r_0 < r \le R, \end{cases} \tag{S124}$$

where

$$H^{(2)}(z) = \frac{R^2}{D\omega^2}\Bigg[\left(\omega_0^2/2 + \omega_0 + 1\right)e^{-\omega_0}\int_z^{\omega} dx\,\frac{e^x}{x} - \omega(1-x_0) + \ln x_0\Bigg], \tag{S125}$$

Integrating (S124), one arrives at (63). One also gets

$$t'_0(R) = \frac{R}{D\omega^2}\left(\omega + 1 - \left(\omega_0^2/2 + \omega_0 + 1\right)e^{\omega-\omega_0}\right). \tag{S126}$$

SM5.2 Radial functions

In two dimensions, the solutions of (7) for a triangular-well potential read

$$\begin{aligned} u_n(z) &= z^n M(n, 2n+1, z), \\ v_n(z) &= z^{-n} U(-n, -2n+1, z). \end{aligned} \tag{S127}$$

Using the identities

$$\begin{aligned} zu'_n(z) &= nz^n M(n+1, 2n+1, z), \\ zv'_n(z) &= -n^2 z^{-n} U(-n+1, -2n+1, z), \end{aligned} \tag{S128}$$

one gets

$$\begin{aligned} zu'_n(z) - nu_n(z) &= \frac{nz^{n+1}}{2n+1} M(n+1, 2n+2, z), \\ zv'_n(z) - nv_n(z) &= -nz^{-n} U(-n, -2n, z), \end{aligned} \tag{S129}$$

so that $w_n(z)$ becomes

$$w_n(z) = \frac{zu'_n(z) - nu_n(z)}{zv'_n(z) - nv_n(z)} = -\frac{M(n+1, 2n+2, z)}{(2n+1)U(n+1, 2n+2, z)}. \tag{S130}$$

Combining these equations we obtain the following explicit expression for the inverse logarithmic derivative of the radial functions in the 2D case with the triangular-well potential:

$$\frac{g_n(R)}{Rg'_n(R)} = \frac{1}{n}\,\frac{M(n, 2n+1, \omega)}{M(n+1, 2n+1, \omega)}\left(1 - \frac{U(n, 2n+1, \omega)}{M(n, 2n+1, \omega)}\,w_n(\omega_0)\right) \times \left(1 + \frac{nU(n+1, 2n+1, \omega)}{M(n+1, 2n+1, \omega)}\,w_n(\omega_0)\right)^{-1}. \tag{S131}$$

As earlier in the 3D case, another representation can be obtained using (S108)

$$\frac{g_n(R)}{Rg'_n(R)} = \frac{1}{n}\,\frac{1 - i_n(\omega) + (1 + k_n(\omega))\,j_n(\omega, \omega_0)}{1 + i_n(\omega) + (1 - k_n(\omega))\,j_n(\omega, \omega_0)}, \tag{S132}$$

with

$$i_n(z) = \frac{I_{n+1/2}(z/2)}{I_{n-1/2}(z/2)}, \qquad k_n(z) = \frac{K_{n+1/2}(z/2)}{K_{n-1/2}(z/2)},$$

$$j_n(z, z_0) = \frac{K_{n-1/2}(z/2)}{K_{n+1/2}(z_0/2)}\,\frac{I_{n+1/2}(z_0/2)}{I_{n-1/2}(z/2)}. \tag{S133}$$

As in the 3D case, we consider first the solution in the particular case when $r_0 = 0$. One may readily observe that here $w_n(0) = 0$, which implies that (S131) attains a simpler form

$$\frac{g_n(R)}{Rg'_n(R)} = \frac{1}{n}\,\frac{M(n, 2n+1, \omega)}{M(n+1, 2n+1, \omega)}, \tag{S134}$$

which is again just the first factor in (S131).

Turning to the limit $n \to \infty$, we find that the first factor in (S131) obeys

$$\frac{1}{n}\,\frac{M(n, 2n+1, \omega)}{M(n+1, 2n+1, \omega)} = \frac{1}{n} - \frac{\omega}{2n^2} + \frac{2\omega+\omega^2}{8n^3} + O\left(\frac{1}{n^4}\right). \tag{S135}$$

Further, considering the second and the third factors on the right-hand side of (S131) we use a similar analysis as in the 3D case to find that their deviation from unity is exponentially small. This yields the following result for the behaviour of $g_n(R)/(Rg'_n(R))$ in the limit $n \to \infty$:

$$\frac{g_n(R)}{Rg'_n(R)} = \frac{1}{n} - \frac{\omega}{2n^2} + \frac{2\omega+\omega^2}{8n^3} + O\left(\frac{1}{n^4}\right). \tag{S136}$$

Recalling the definition of ω and noting that for the triangular-

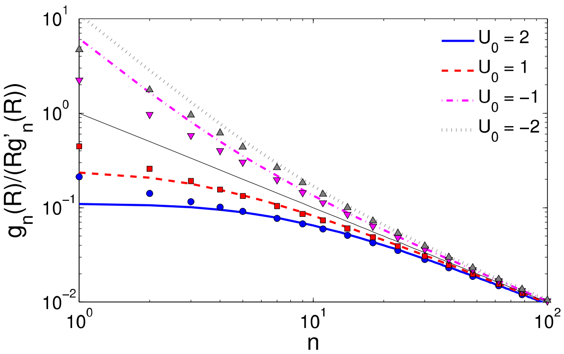

Fig. S5 The ratio $g_n(R)/(Rg'_n(R))$ vs the order n of the radial function for several values of U_0, with $r_0 = 0.8$ and $R = 1$. Comparison of the exact result in (S131) (symbols) and the approximate expression in (S54) (lines). Thin solid line is the $1/n$ asymptotics (solution for $U_0 \equiv 0$).

well potential $U''(R) = 0$, we again observe a perfect agreement between our expansion in (S19) and the exact result in (S136). We note as well that similarly to the 3D case, it appears that the large-n behaviour is dominated by the solution with $r_0 = 0$, which implies that the dependence on this parameter of the interaction potential is fully taken into account by the parameter ω.

Lastly, we compare the approximate expression (S54) for $g_n(R)/(Rg'_n(R))$ and the exact result in (S131) obtained for the triangular-well potential. We observe in Fig. S5 a fairly good agreement between the approximate formula (S54) and the exact result already for even smaller than in the 3D case values of n. The agreement becomes even better for larger values of $R|U'(R)|$.