Solitons in overdamped Brownian dynamics

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Solitons are commonly known as waves that propagate without dispersion. Here we show that they can occur for driven overdamped Brownian dynamics of hard spheres in periodic potentials at high densities. The solitons manifest themselves as periodic sequences of different assemblies of particles moving in the limit of zero noise, where transport of single particles is not possible. They give rise to particle currents at even low temperature that appear in band-like structures around certain hard-sphere diameters. At high temperatures, the band-like structures are washed out by the noise, but the particle transport is still dominated by the solitons. All these predicted features should occur in a broad class of periodic systems and are amenable to experimental tests.

Brownian motion occurs ubiquitously in many natural systems and is a relevant process in several technological applications. At high particle densities, its properties are strongly influenced by collective effects arising from many-body interactions. These effects become particularly pronounced for motion in channel-like structures, where the spatial confinement hinders particles to overtake each other. Examples of such single-file transport include particle motion through membranes [1], nanopores [2–6] and in nanofluidic devices [7–12], water permeation in nanomembranes [13–18], and catalytic processes in zeolites [19, 20]. Recent experiments on colloids driven by optical and magnetic fields allow to explore and investigate collective effects under well-controlled conditions [21–26].

Here we show that overdamped Brownian motion of hard spheres through periodic channel-like geometries has a puzzling behavior under external driving. This is reflected in a band-like structure of the particle current in dependence of the particle diameter \( \sigma \): only in small bands around certain \( \sigma \), particle transport is possible and the current is nonzero. We explain this behavior by well-defined deterministic motions of local excitations in the zero-noise limit. They represent propagating solitons of local density fluctuations. The solitons appear if \( \sigma \) lies in the bands and they govern the current behavior in the presence of noise also. At low noise, the band-like structure of the current is smeared out. At high noise, particle transport becomes possible for all \( \sigma \) but the magnitude of the current is still governed by the solitons. Changes of currents can be traced back to the solitons even for strong driving up to the critical tilting force, where potential barriers for particle motion disappear. We demonstrate these findings for a simple setup, which is amenable to direct experimental investigations.

The setup consists of a ring of 21 optical traps in a fluidic environment, where each trap is occupied by one particle, as illustrated in Fig. 1(a). A constant drag force tries to move the particles in clockwise direction, but there is no motion as the system is jammed. At some time instant, one well is removed, which leads to a “distorted particle configuration”, where a regular filling of each well by one particle is no longer possible, see Fig. 1(b). We consider the subsequent Brownian particle dynamics given by the Langevin equations

\[
\frac{dx_i}{dt} = \mu [f - U'(x_i)] + \sqrt{2D} \xi_i(t), \quad i = 1, \ldots, N+1, (1)
\]

FIG. 1. (a) Ring of \( (N + 1) = 21 \) optical traps filled with \( (N + 1) \) hard spheres with diameter \( \sigma \) in a fluid environment. The shades of red indicate the value of the optical potential. Areas marked in dark red (light red) correspond to potential minima (maxima). A drag force \( f \) tries to drive the particles in clockwise direction but the system is jammed and the particle positions fluctuate around the points of mechanical equilibria in the traps. (b) After removal of one trap (corresponding to an increase of the wavelength of the optical potential), particle transport becomes possible. (c) The resulting stationary current \( J(\sigma, f) \) shows peaks as a function of \( \sigma \) at \( \sigma_n = (n-1)/n \), \( n = 2, 3, \ldots \). Data are shown for \( f = 0.05 \) and noise strength \( D = 0.01 \). In the inset, two stochastic time evolutions of the instantaneous current are displayed for \( \sigma = 0.3, \sigma = 2/3 \) (purple curve) and \( \sigma = 0.62 \) (green curve). A moving average of the instantaneous current was taken for a time window of size \( 2.5 \times 10^5 \) to reduce the noise level.

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where \( U(x) = (U_1/2) \cos(2\pi x/\lambda) \) describes the periodic
optical potential, \( f \) is the constant drag force, \( \mu \) is the
particle mobility, \( D = k_B T \mu \) is the diffusion coefficient
with \( k_B T \) the thermal energy. The \( \xi_i(t) \) are Gaussian
white noise processes with zero mean and correlations
\( \langle \xi_i(t)\xi_j(t') \rangle = \delta_{ij}\delta(t - t') \). The distance between neigh-
bouring particles cannot be smaller than \( \sigma \) (hard-sphere
interaction) and the particles keep their order (single-
file motion). This system represents a minimal model for
studying Brownian single-file transport in periodic poten-
tials [26–29]. We set \( \mu = 1 \) in the following and choose
\( \lambda, \lambda^2/\mu U_1 \) and \( U_1 \) as units for length, time and energy,
respectively.

The hardcore interactions do not enter the equations
of motion (1) explicitly due to the singular form of the
hard-sphere potential. The interactions are taken into ac-
count by the constraint that neighboring particles must
have a distance larger than or equal to \( \sigma \). Our pro-
dure to generate particle trajectories is described in the
supplemental material (SM), see below.

Using this procedure, we determined currents in the
nonequilibrium steady state. This state forms after a
short transient time after the removal of one trap.
The instantaneous current is \( J(t; \sigma, f) = (N + 1)\dot{v}(t)/L \)
with \( \dot{v}(t) \) being the center of mass velocity, \( \dot{v}(t) =
[\sum_{j=1}^{N+1} dx_j(t)/dt]/(N+1) \). After averaging \( J(t; \sigma, f) \) over
time, we obtain the stationary current \( J(\sigma, f) \).

Figure 1(c) shows \( J(\sigma, f) \) as a function of \( \sigma \) for small
driving \( f = 0.05 \) and low noise \( D = 0.01 \) \( (k_B T / U_1 = \)
0.01), where a single particle would hardly surmount po-
tential barriers. For \( \sigma < 0.4 \) (not shown) the system
is indeed essentially jammed, i.e. there is no noticeable
current. However, \( J(\sigma, f) \) is not always negligibly small.
Besides nearly jammed states, phases of “running states”
occur, where significant particle transport is present. The
current shows peaks around maxima at particle diame-
ters

\[
\sigma_n = \frac{n-1}{n}, \quad n = 2, 3, \ldots , \tag{2}
\]

where the maxima \( J(\sigma_n, f = 0.05) \) in Fig. 1(c) increase
with increasing \( n \). Between the peak positions at \( \sigma_2 =
1/2 \) and \( \sigma_3 = 2/3 \), the current drops to small values. As
the distances between neighboring peaks become smaller
with increasing \( n \), the peaks overlap and the current
runs through minima with values significantly larger than
zero.

Figure 2 shows how the system changes between jammed and running states in dependence of \( \sigma \) and \( f \)
at two temperatures (or noise strengths \( D \)) in the regime
of weak driving (0 < \( f \) < 0.2). The jammed states refer
to regions, where \( J(\sigma, f) \) is vanishingly small (black ar-
eas in the figure), and the running states to regions with
noticeable \( J(\sigma, f) \), as indicated by the color coding (cf.
scale bar in the figure).

For low noise \( D = 0.01 \) [Fig. 2(a)], bands of running
states can be seen around the \( \sigma_n \) given in Eq. (2). When
increasing \( f \), the bands widen. We can furthermore iden-
tify lines of local maxima in the current, see the lines of
highest color brightness in Fig. 2(a). These lines appear
to be centered in stripes of the same color which form
a pattern in the upper right half of Fig. 2(a). For the
larger noise \( D = 0.1 \) [Fig. 2(b)], the bands around the \( \sigma_n \)
can no longer be seen but the stripe-like pattern is still
present.

How can we understand the occurrence of the alter-
ning phases of jammed and running states? Since we
obtain currents even for low noise, let us consider the
transport behavior in the limit of zero noise \( (D = 0) \). In
this case, the equations of motion (1) become determi-

cistic. Individual particles cannot surmount any barrier
and one may wonder, how particle transport is possible
without thermal activation. Collective effects must play
a role. They manifest themselves in the formation of n-
clusters, which consist of \( n \) mutually touching particles,
i.e., where the distance between nearest neighboring par-

icles equals \( \sigma \).

The effective potential \( U_n(x) = \sum_{j=1}^{n} U(x + (j-1)\sigma) \)
for an \( n \)-cluster to move in the cosine potential \( U(x) \) is

\[
U_n(x) = \frac{U_1}{2} \frac{\sin(n\pi\sigma)}{\sin(\pi\sigma)} \cos[2\pi x + (n-1)\pi\sigma]. \tag{3}
\]

It has the form as that for a single particle but with a
modified potential barrier \( U_1 \sin(n\pi\sigma)/\sin(\pi\sigma) \) that van-
ishes for the \( \sigma_n \) in Eq. (2). Accordingly, if \( n \) particles
of size \( \sigma_n \) would form a moving cluster, their collective
motion requires no thermal activation. This could be a
possible explanation for the occurrence of peaks in the
current at \( \sigma = \sigma_n \).

But can \( n \) particles remain attached? Actually, as we
show now, this not the case. The cluster dynamics is
more complex and given by certain conditions on the

FIG. 2. Current \( J(\sigma, f) \) as a function of \( \sigma \) and \( f \) in a color-
coded representation for different noise strengths (tempera-
tures) (a) \( D = 0.01 \) and (b) \( D = 0.1 \).
forces

\[ F_i = F(x_i) = f - U'(x_i) \]  

acting on the particles. Let us first consider a 2-cluster with particles at positions \( x_1 \) and \( x_2 = x_1 + \sigma \). If \( F_1 \) is positive and \( F_2 \) smaller than \( F_1 \), the two particles must move together, i.e. the 2-cluster moves as a whole. If \( F_1 \) is negative, one can draw an analogous conclusion, yielding the general condition \( F_1 \geq F_2 \) for the 2-cluster to move as a whole. If \( F_1 < F_2 \) by contrast, the particles detach.

For \( n \)-clusters with \( n > 2 \), the possibilities of movements become richer. For example, a 3-cluster has the \( 2^3 = 8 \) compositions \( \{111\}, \{2,1\}, \{1,2\}, \) and \( \{3\} \), which specify the possible movements: In the composition \( \{111\} \), all particles become detached. In \( \{2,1\} \), the first two particles move together, i.e. they form a subcluster, and the third particle detaches from the second. In \( \{1,2\} \), the last two particles move together as a subcluster and detach from the first, and in composition \( \{3\} \) all three particles keep in touch and the 3-cluster moves as a whole.

Considering a general composition \( \{m_1 \ldots m_s\} \) of a cluster of size \( n = \sum_{j=1}^{s} m_j \), the subclusters \( k \) of size \( n_k \) have the velocity \( \mu \bar{F}_k \) \((k = 1, \ldots, s)\), where \( \bar{F}_k \) is the mean force on the subcluster \( k \). As each subcluster must detach from its neighboring ones, one set of conditions for an \( n \)-cluster to move according to the composition \( \{m_1 \ldots m_s\} \) is

\[ \bar{F}_k < \bar{F}_{k+1}, \quad k = 1, \ldots, s - 1. \]  

This is the analogue to the situation of two particles considered above. In addition, particles within a subcluster must not detach, i.e. for all possible divisions of a subcluster into two sub-subclusters, the inequality \((5a)\) must be violated. This implies that for each subcluster \( k = 1, \ldots, s \) of size \( m_k \) in the composition \( \{m_1 \ldots m_s\} \), it must hold

\[ \frac{1}{\lambda} \sum_{j=1}^{i} F_{k,j} \geq \frac{1}{m_k - i} \sum_{j=i+1}^{m_k} F_{k,j}, \quad i = 1, \ldots, m_k - 1, \]

where \( F_{k,j} = F_l \) is the force on particle \( j \) in the \( k \)-th subcluster \((l = m_1 + m_2 + \ldots + m_{k-1} + j)\). Note that the conditions \((5a)\) and \((5b)\) are independent of the drag force \( f \). A more detailed derivation of them is given in SM.

Solving Eqs. (1) in the zero-noise limit subject to the conditions \((5a)\) and \((5b)\), we find specific types of soliton-like movements that occur for \( \sigma = \sigma_n \) and \( \sigma \) close to \( \sigma_n \) from Eq. (2) for larger \( f \). An example of such soliton is shown for \( \sigma = 0.51 \) and \( f = 0.2 \) in Fig. 3(a). At an initial time \( t_0 \), a 3-cluster starts moving, where its last particle is at a position of mechanical equilibrium, i.e. a minimum of the tilted potential \( U(x) - fx \). This 3-cluster moves until its first particle detaches at time \( t_1 \). After time \( t_1 \), the first particle relaxes to a position of mechanical equilibrium, and the 2-cluster continues moving, see the configuration at the time \( t_2 \) in Fig. 3(a). Finally, the 2-cluster attaches to the particle at the position of mechanical equilibrium right to it, leading to a new propagating 3-cluster at a time \( t_0 + \tau \). The process then repeats itself, meaning that the soliton motion is periodic with \( \tau \). After one period, the soliton has
moved by one wavelength, as indicated by the dashed lines in Fig. 3(a). Further examples of soliton propagation at weak driving are given in movie file 1 of the ancillary files to this manuscript. There we demonstrate also that the soliton propagation is essentially unaltered in the presence of weak thermal noise. The noise leads to a rattling of particle positions around the ones given by the deterministic time evolution.

In general, a soliton consists of a propagation composed of a periodic sequence of cluster movements. Analogous types of solitons occur close to all \( \sigma_n \): an \( n \)-cluster starts to move, followed by an \((n-1)\)-cluster until a period is finished. The emergence of these different types of \( n-(n-1) \)-solitons in dependence of \( \sigma \) and \( f \) is shown in Fig. 3(b). A band-like structure of the solitons occurs, which is reflecting the band-like structure of the current in the zero-noise limit shown in Fig. 3(c), as well as in the presence of weak noise in Fig. 2(a). The fact that the solitons give rise to currents for vanishing noise means that their motion does not require thermal activation. For the time intervals of a propagating \( n-(n-1) \)-soliton, where an \( n \)-cluster moves, we know from Eq. (3) that no potential barrier can stop the motion. When the \((n-1)\)-cluster moves, it always runs downhill the tilted potential.

The current generated by a soliton is \( J(\sigma,f) = \bar{\nu}_{\text{sol}}(\sigma,f)/L \), where \( \bar{\nu}_{\text{sol}}(\sigma,f) = \lambda/\tau(\sigma,f) \) is the mean velocity of a soliton. This velocity depends on the soliton type and can be calculated from the deterministic equation of motion, see SM.

For particle diameters \( \sigma = \sigma_n \), we can estimate the current \( J(\sigma_n,f) \) by assuming that an \( n \)-cluster is propagating the whole time. This is because during one period, the time intervals for motions of clusters of other sizes are generally much smaller than that of the \( n \)-cluster. For example, the soliton illustrated in Fig. 3(a) has \( \sigma \) close to \( \sigma_2 = 1/2 \) and the 2-cluster is moving most of the time. An \( n \)-cluster formed by particles of size \( \sigma_n \) does not need to surmount barriers \( U_n = 0 \) in Eq. (3). Accordingly, its particles propagate with velocity \( \mu f \). One period of the soliton covers the time, where the rightmost particle of the \( n \)-cluster starts to move and attaches to the next resting particle. This means that the rightmost particles moves a distance \( (\lambda - \sigma_n) \) during one period. We thus estimate \( \tau(\sigma_n,f) \approx (\lambda - \sigma_n)/\mu f \), yielding

\[
J(\sigma_n,f) = \frac{\bar{\nu}_{\text{sol}}(\sigma_n,f)}{L} = \frac{\lambda}{L\tau(\sigma_n,f)} \approx \frac{\mu f}{N(\lambda - \sigma_n)}.
\]

Revisiting the peaks in the current in Fig. 1(c) for low noise and \( f = 0.05 \), the estimate (6) yields \( J(\sigma_n,0.05) \approx 5 \times 10^{-3}, \ 7.5 \times 10^{-3}, \ 10^{-2} \) for \( n = 2, 3, 4, \ldots \) in good agreement with the simulated results.

The bands in Fig. 3(c) widen with increasing \( f \), because barriers become smaller and non-thermally activated motion of solitons becomes possible for particle sizes further away from the \( \sigma_n \). Movie file 2 in the ancillary files give examples for soliton motions at large \( f \).

Let us see, what happens if we consider stronger driving up to the critical tilting force \( f_c = \pi \), where there would be no barriers for a single particle, i.e. where \( F(x) \) in Eq. (4) starts to become positive for all \( x \). Figure 4(a) shows that for this larger range of driving forces a further type of \( n-(n-1)-(n+1) \)-soliton occurs involving clusters of size \((n-1), n, \) and \((n+1)\) \((n = 2, 3, \ldots)\). The regions of occurrence of these solitons separate those of the \( n-(n-1)\) and \((n+1)-n \)-solitons. They become smaller with decreasing \( f \) and terminate at the \( \sigma_n \) for \( f \to 0 \) (with extension zero). In fact, they are so narrow for small \( f \), that they cannot be resolved in Fig. 3(b). The time interval of the movement of the \((n-1)\)-cluster is practically negligible in comparison with the time intervals of the \( n \)-cluster motion, i.e. our estimate of the peak currents in Eq. (6) remains valid.

As long as \( f < f_c \), the current is still governed by the solitons. This is evident from the characteristic pattern of current values in Fig. 4(b). For \( f \lesssim 1.5 \), the isolines of constant currents in the \( \sigma-f \)-plane (dashed lines) follow closely the equation \( \mu f/N(\lambda - \sigma) = \text{const} \). This formula for isolines results when interpolating the peaks \( J(\sigma_n,f) \) in Eq. (6) by replacing \( \sigma_n \) with \( \sigma \). Analogous isolines can be drawn in Fig. 2, where we analyzed the impact of noise on the soliton-induced current. For overcritical tilting \( f > f_c \), isolines of constant current do not reflect soliton propagations, but are almost independent of \( \sigma \).

Already for a tilting slightly above the overcritical one, the current becomes close to that of independent particles (except for large \( \sigma \)).

In summary, we have shown that for driven overdamped Brownian motion through a periodic potential, particle transport in dense systems is possible although single particles cannot surmount the potential barriers.
The particle current is mediated by solitons, which are periodic sequences of particle clusters that propagate in the zero-noise limit. At weak driving force \( f \), solitons occur only for certain intervals of hard-sphere diameters centered around \( \sigma_n \) [Eq. (2)]. They lead to pronounced peaks in currents \( J(\sigma, f) \) as a function of \( \sigma \) for weak \( f \). In the \( \sigma-f \)-plane, the peaks correspond to bands that widen with increasing \( f \) and overlap each other at larger \( f \). Soliton-governed currents are observed up to the critical tilting force, beyond which single-particle motion becomes possible in the zero-noise limit. The behavior of the currents in the presence of noise (finite temperatures) is dominated by the soliton-induced transport. For weak noise (low temperatures), the band-like structure of the currents in the zero-noise limit remains visible. For larger noise (higher temperatures), the band-like structure is washed out, but the dependence of the current \( J(\sigma, f) \) on \( \sigma \) and \( f \) reflects the soliton dynamics.

The solitons always occur in a crowded system independent of the number of optical traps. If the filling factor \( N/M \) (\( N \) is number of particles, \( M \) number of traps) is smaller than one, they appear as rare events due to thermal fluctuations. In that case they have a finite lifetime, because they can annihilate with empty traps. Movie file 3 of SM demonstrates a short-lived soliton in a system of 19 particles and 20 traps. For filling factors \( N/M > 1 \), solitons could also occur as rare events, when \( \sigma \) is very different from \( \sigma_n \) given in Eq. (2) (black regions in Figs. 2-4). For particle sizes close to \( \sigma_n \), they are permanently present then. There are even other possible particle diameters for permanent soliton propagation in accordance with the conditions derived in SM. As an example, we show in movie file 4 of SM solitons for different numbers \( M \) of traps and particle number \( N = M + 1 \), and in movie file 5 a soliton for \( N = 22 \) particles and \( M = 20 \) traps.

For other types of periodic potentials than the sinusoidal one considered here, solitons will occur also. This is because the potential for a particle cluster has the same periodicity but its barriers can be much lower than that for a single particle, or even are vanishing. For an arbitrary periodic potential, conditions for an \( n \)-cluster to move barrier-free are derived in SM.

Traditionally, in systems with inertia, like the prominent Frenkel-Kontorova model [31], solitons are waves whose dispersion is suppressed by nonlinear effects. In our case, the solitons occur in the absence of inertia for fully overdamped dynamics, where the particles keep together in the clusters because the external forces are not able to separate them.

The general occurrence of solitons in overdamped Brownian dynamics suggests that they can be detected in different experimental setups in addition to the one sketched in Fig. 1. We expect them to play an important role in transport processes in crowded biological systems and microfluidic devices. In the latter case, in particular, noise is typically low and solitons can lead to significant enhancement of currents even at high density, where often jamming mitigates motion.

In our analysis here, we focused on hardcore interactions. For hard spheres with additional attractive interactions, cluster formations of particles will be easier, and solitons should occur for wider ranges of particle diameters at given temperature and forcing. An interesting question is, whether solitons can exist also in overdamped Brownian motion of particles with softcore repulsive interactions. Driven particle transport for such interactions can reflect features of hardcore systems [32], and we thus believe that periodic collective motions of localized particle assemblies are possible. These and other questions, e.g. on likewise soliton propagation in higher dimensions and for underdamped Brownian dynamics, open up promising perspectives for further research.

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Supplemental Material for
Solitons in overdamped Brownian dynamics
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In Sec. I of this Supplemental Material, we discuss how Brownian motion of hard spheres in an arbitrary external force field can be treated in the zero-noise limit. Conditions for barrier-free propagation of \( n \)-clusters in general periodic potentials are derived in Sec. II. Their meaning for the particle size is illustrated for a piecewise linear potential, and potentials represented by a finite number of Fourier coefficients. In Sec. III, we show how soliton velocities can be calculated analytically.

I. OVERDAMPED BROWNIAN MOTION OF HARD SPHERES IN THE ZERO-NOISE LIMIT

The overdamped Brownian motion of hard spheres in an arbitrary external force field \( f_{\text{ext}}(x) \) is described by the Langevin equations (1) in the main text. There, \( f_{\text{ext}}(x) = f - U'(x) \) with \( U(x) \) being the cosine potential. If a particle \( i \) is not in contact with other particles, its time-evolution in the zero-noise limit is

\[
\dot{x}_i = \frac{dx_i}{dt} = \mu f_{\text{ext}}(x_i),
\]

where we set \( \mu = 1 \) in the following.

For a particle in contact with other particles, we need to take into account interaction forces in Eq. (S1). An \( n \)-cluster is formed by \( n \) particles that are mutually in contact, but not in contact with other particles. Let \( x_1 \) be the coordinate of the first particle in the cluster, and \( x_i = x_1 + (i - 1)\sigma, \ i = 2, \ldots, n \) the coordinates of the other \((n-1)\) particles. We pose the following question: Under which conditions do particles \( i \) and \((i+1)\) in the \( n \)-cluster interact and what is the interaction force then? Knowing the answer to this question, we can include the respective interaction forces in Eq. (S1) to evolve the coordinates of particles in clusters.

The solution of the problem rests on the following properties:

(i) The interaction force \( f_{i,i+1} \) of particle \( i \) on particle \((i+1)\) in the \( n \)-cluster must be non-negative, \( f_{i,i+1} \geq 0 \).

(ii) The interaction forces obey Newton’s principle of action and reaction: The interaction force \( f_{i+1,i} \) of particle \((i+1)\) on particle \( i \) is \( f_{i+1,i} = -f_{i,i+1} \).

The equations of motions for the particles in the \( n \)-cluster are

\[
\dot{x}_1 = f_{1}^{\text{ext}} - f_{12} = f_{1}^{\text{tot}},
\]

\[
\dot{x}_i = f_{i}^{\text{ext}} + f_{i-1,i} - f_{i,i+1} = f_{i}^{\text{tot}}, \quad i = 2, \ldots, n-1,
\]

\[
\dot{x}_n = f_{n}^{\text{ext}} + f_{n-1,n} = f_{n}^{\text{tot}},
\]

where \( f_{i}^{\text{ext}} = f_{\text{ext}}(x_i) \) and \( f_{i}^{\text{tot}} \) is the total force acting on particle \( i \).
The $n$-cluster can move as a whole or fragment into separate subclusters, including 1-subclusters, i.e. single particles. There are $2^{n-1}$ possible compositions $\{m_1 \ldots m_s\}$, $1 \leq m_j \leq n$, $\sum_{j=1}^{s} m_j = n$, of the $n$-cluster by $m_j$-subclusters, $s = 1, \ldots, n$.

Let us consider an $m$-subcluster with particle coordinates $y_i$, $i = 1, \ldots, m$. For the subcluster $k$ in the composition $\{m_1 \ldots m_s\}$ of the $n$-cluster, $m = m_k$ and $y_i = x_i + (i-1)\sigma$ with $l = 1 + \sum_{j=1}^{k-1} m_j$. As the particles in the $m$-subcluster remain in contact, it must hold $\dot{y}_1 = \ldots = \dot{y}_m$. This is caused by the interaction forces between neighboring particles in the subcluster (unless the external forces acting on them are all equal). Because the interaction forces obey the principle of action and reaction, the subcluster velocity is given by the mean $\bar{f}_{\text{ext}}$ of the external forces acting on the particles, i.e. it holds

$$\dot{y}_1 = \ldots = \dot{y}_m = \bar{f}_{\text{ext}} = \frac{1}{m} (f_{1\text{ext}} + \ldots + f_{m\text{ext}}),$$  \hspace{1cm} (S3)

or $f_{j\text{tot}} = \bar{f}_{\text{ext}}$, $j = 1, \ldots, m$ [$f_{j\text{ext}} = f_{\text{ext}}(y_i)$ here]. Using the equations of motions for $\dot{y}_i$ in Eqs. (S2a)-(S2c) (for $n = m$ and $x_i$ replaced by $y_i$), we obtain $m$ linear equations for determining the $(m-1)$ interaction forces $f_{12}, f_{23}, \ldots, f_{m-1,m}$. Only $(m-1)$ of these equations are independent, since $\sum_{i=1}^{m} \dot{y}_i = m\bar{f}_{\text{ext}}$ does not depend on the interaction forces.

The system of linear equations has the solution

$$f_{i,i+1} = \sum_{j=1}^{i} f_{j\text{ext}} - i\bar{f}_{\text{ext}} = \frac{m-i}{m} \sum_{j=1}^{i} f_{j\text{ext}} - \frac{i}{m} \sum_{j=i+1}^{m} f_{j\text{ext}}, \quad i = 1, \ldots, m-1.$$  \hspace{1cm} (S4)

The interaction forces must be non-negative, which yields the conditions

$$\frac{1}{i} \sum_{j=1}^{i} f_{j\text{ext}} \geq \frac{1}{m-i} \sum_{j=i+1}^{m} f_{j\text{ext}}, \quad i = 1, \ldots, m-1,$$  \hspace{1cm} (S5)

for the considered $m$-subcluster to move without fragmentation. These conditions have a simple interpretation: the mean velocity of any group of particles on the left side of the subcluster must be larger than the mean velocity of the complimentary group of particles on the right side, i.e. no group of particles on the right side can outrun the group on the left side. Note that this is ensured by the inequalities (S5) irrespective of the sign of velocities (mean forces).

In addition, the considered subcluster must move independently from the other subclusters. This requires its velocity $\bar{f}_{\text{ext}}$ to be larger than the velocity $\bar{f}_{-\text{ext}}$ of its neighboring subcluster to the left, and to be smaller than the velocity $\bar{f}_{+\text{ext}}$ of its neighboring subcluster to the right,

$$\bar{f}_{-\text{ext}} < \bar{f}_{\text{ext}} < \bar{f}_{+\text{ext}}.$$  \hspace{1cm} (S6)

The conditions (S5) and (S6) on the external forces must be fulfilled between all subclusters in a composition $\{m_1 \ldots m_s\}$, $1 \leq m_j \leq n$. For the first and last subcluster of size $m_1$ and $m_s$, there is no condition with respect to a neighboring subcluster to the left and right, respectively.
In summary, we find that an $n$-cluster evolves into the composition $\{m_1 \ldots m_s\}$, if
\[
\bar{f}_k^{\text{ext}} = \frac{1}{m_k} \sum_{j=1}^{m_k} f_{k,j}^{\text{ext}} < \frac{1}{m_{k+1}} \sum_{j=1}^{m_{k+1}} f_{k+1,j}^{\text{ext}} = f_{k+1}^{\text{ext}}, \quad k = 1, \ldots, s - 1, \tag{S7a}
\]
\[
\frac{1}{m_k} \sum_{j=1}^{m_k} f_{k,j}^{\text{ext}} = \frac{1}{m_{k+1}} \sum_{j=1}^{m_{k+1}} f_{k+1,j}^{\text{ext}}, \quad i = 1, \ldots, m_k - 1, \quad k = 1, \ldots, s, \tag{S7b}
\]
where $f_{k,i}^{\text{ext}}$ is the external force on particle $i$ in the $k$-th subcluster [or the force $f_l^{\text{ext}}$ on particle $l$ in the $n$-cluster, where $l = i + \sum_{j=1}^{k-1} m_j$]. The conditions (S7a) and (S7b) correspond to the conditions (5a) and (5b) in the main text.

The inequalities (S7a) and (S7b) give in total $\sum_{k=1}^{s} (m_k - 1) + (s - 1) = (\sum_{k=1}^{s} m_k - 1) = n - 1$ conditions for a certain composition $\{m_1 \ldots m_s\}$ to occur. They are fulfilled only for one of the possible $2^{n-1}$ compositions. Given that composition, the time evolution of the particles in the $n$-cluster is uniquely determined.

We finally notice that this method of evolving hard-sphere systems can be applied also for overdamped Brownian dynamics in the presence of noise. One simply needs to consider the random forces mediated by the fluid as additional external forces. We have used already the corresponding simulation method when generating particle trajectories and compared it to existing schemes [1, 2]. Our simulation method can be extended to hard spheres with additional contact interaction and will be presented elsewhere [3].

II. BARRIER-FREE CLUSTER PROPAGATION IN PERIODIC POTENTIALS

Let $V(x)$ be a $\lambda$-periodic potential for single particles,
\[
V(x) = V(x + \lambda). \tag{S8}
\]
We are interested in the behavior of the corresponding potential $V_n(x)$ for $n$-clusters,
\[
V_n(x) = \sum_{j=1}^{n} V(x + (j - 1)\sigma). \tag{S9}
\]
This potential is also $\lambda$-periodic and can have significantly reduced or even vanishing barriers for certain particle diameters $\sigma$. For these $\sigma$ values, one would obtain barrier-free motion of an $n$-cluster composed of $n$ "glued" particles in mutual contact. If the external forces acting on the $n$-cluster satisfy inequalities (S7a) and (S7b) over an extended part of the period length $\lambda$, the cluster can give rise to a propagating soliton. We here derive conditions for the barrier-free motion of clusters. Following the choice of length unit in the main text, we set $\lambda = 1$.

The Fourier series expansion of the periodic potential is
\[
V(x) = \sum_{k=-\infty}^{\infty} c_k e^{2\pi i k x} = c_0 + 2 \text{Re} \left[ \sum_{k=1}^{\infty} c_k e^{2\pi i k x} \right], \tag{S10}
\]
where

$$c_k = \int_0^1 dx \, V(x) \, e^{-2\pi ikx}$$

are the Fourier coefficients. Inserting Eq. (S10) into Eq. (S9), we obtain the Fourier series of $V_n(x)$,

$$V_n(x) = n c_0 + 2 \Re \left[ \sum_{k=1}^{\infty} c_k e^{2\pi ikx} \sum_{j=1}^{n} e^{2\pi ikjx} \right] = n c_0 + 2 \Re \left[ \sum_{k=1}^{\infty} \frac{1 - e^{2\pi ikn\sigma}}{1 - e^{2\pi ik\sigma}} c_k e^{2\pi ikx} \right].$$

The potential becomes constant if the factor $(1 - e^{2\pi ikn\sigma})/(1 - e^{2\pi ik\sigma})$ is zero for all $k$. This is only possible, if $n\sigma$ is an integer, i.e. if the cluster length $n\sigma$ is an integer multiple of the wavelength. In that case, a cluster potential could be invariant with respect to the cluster position. Since $\sigma < 1$ [for $(N+1)$ particles and $N$ potential wells, $\sigma < N/(N+1)$], it follows that $V_n(x)$ can be constant only for diameters $\sigma$ equal to the rational numbers

$$\sigma_{m,n} = \frac{m}{n}, \quad m = 1,\ldots,n-1.$$  \hspace{1cm} (S13)

However, for the factor $(1 - e^{2\pi ikn\sigma})/(1 - e^{2\pi ik\sigma})$ to be zero, $k\sigma$ must not be an integer, because otherwise $(1 - e^{2\pi ikn\sigma})/(1 - e^{2\pi ik\sigma}) \to n \neq 0$ according to L’Hospital’s rule. This additional requirement of $k\sigma$ not being an integer, cannot be satisfied for all $k$ if $\sigma = \sigma_{m,n}$. It implies that the $c_k$ must be zero for those $k$, where $k\sigma_{k,n} = km/n$ is an integer.

To specify the corresponding values $k$ for a given $\sigma_{m,n}$ (given $m$ and $n$), we set $m = d(m,n)m'$ and $n = d(m,n)n'$, where $d(m,n)$ is the greatest common divisor of $m$ and $n$, and accordingly $m'$ and $n'$ are coprime. Then $km/n = km'/n'$ must be an integer, which implies that $k$ is an integer multiple of $n' = n/d(m,n)$. We therefore have to require

$$c_k = 0 \quad \text{for } k = j\frac{n}{d(m,n)}, \quad j = 1,2,\ldots$$  \hspace{1cm} (S14)

To summarize, for $V_n(x)$ to be constant, $\sigma$ has to be a rational number. If this rational number is $m/n$, then all $c_k$ must be zero for $k$ being an integer multiple of $d(m,n)$.

This sounds complicated, but the conditions can be satisfied for quite general periodic potentials. Let us first consider a case, where the periodic potential is represented by a finite number of Fourier coefficients, i.e. where only the first $k_{\text{max}}$ of the $c_k$ are nonzero ($c_k = 0$ for $k > k_{\text{max}}$). Then Eqs. (S14) are fulfilled if $n/d(m,n) > k_{\text{max}}$. This means that clusters of size $n$ formed by particles with diameter $\sigma_{m,n} = m/n$ move barrier-free if $n/d(m,n) > k_{\text{max}}$. In particular, since $d(n-1,n) = 1$, all $n$-clusters formed by particles with $\sigma = (n-1)/n$ move barrier-free for $n > k_{\text{max}}$.

For the cosine potential considered in the main text, $k_{\text{max}} = 1$, and Eqs. (S14) are satisfied for all $n$ and $m$, i.e. potential barriers for $n$-clusters vanish for all $\sigma = m/n$, $n = 2,3,\ldots$, and $m = 1,\ldots,n-1$. This is in agreement with Eq. (2) of the main text.

A further example is the asymmetric periodic potential

$$V(x) = 2 - \frac{1}{2} \sin(2\pi x) - \frac{1}{12} \sin(4\pi x)$$  \hspace{1cm} (S15)
often used in ratchet models [4, 5]. For this potential $k_{\text{max}} = 2$, and the nonzero Fourier coefficients are $c_0 = 2$, $c_1 = i/4$, and $c_2 = i/24$. Accordingly, all $n$-clusters formed by particles with diameter $m/n$ and with $n/d(m,n) > 2$ move barrier-free: 3-clusters if $\sigma = 1/3$ or $2/3$, 4-clusters if $\sigma = 1/4$ or $3/4$, etc. Note that for a 4-cluster formed by particles with diameter $2/4 = 1/2$, $d(m,n) = d(2,4) = 2$, $n/d(m,n) = 2$, i.e. for such a cluster the potential is not constant because $c_2 \neq 0$.

As an example for a periodic potential with an infinite number of nonzero Fourier coefficients, let us consider the periodically continued piecewise linear potential ($0 < x_0 < 1$)

$$ V(x) = \begin{cases} V_0 \frac{x}{x_0}, & 0 \leq x \leq x_0, \\ V_0 \frac{1-x}{1-x_0}, & x_0 \leq x \leq 1. \end{cases} \quad (S16) $$

The Fourier coefficients for this potential are

$$ c_k = -\frac{V_0}{4\pi^2 k^2} \frac{1 - e^{-2\pi i k x_0}}{x_0(1-x_0)}. \quad (S17) $$

Barrier-free motions of clusters can be obtained if $x_0$ is a rational number, $x_0 = q/p$ with $q, p \in \mathbb{N}$, with $q < p$ coprime. Clusters for which $V_n(x)$ is constant then are formed by an integer multiple of $p$ particles with diameter $q/n$, i.e. the possible $\sigma_{m,n}$ are given by $n = lp$ with $l \in \mathbb{N}$ and $m = q$. Since $x_0 = q/p = ml/n$, the Fourier coefficients $c_k$ with $k = jn/d(n,m)$ in Eq. (S17) indeed vanish:

$$ \exp(-2\pi i k x_0) = \exp\left(-2\pi i \frac{n}{d(m,n)} \frac{m}{n} l \right) = \exp\left(-2\pi i \frac{m}{d(m,n)} l \right) = 1. \quad (S18) $$

III. SOLITON VELOCITY AND SOLITON-INDUCED CURRENT

From the analysis of the deterministic motion in the zero-noise limit, we find the conditions (S7a), (S7b) on the external forces to yield solitons that are either of type $(n+1)$- or of type $n-(n-1)$-$(n+1)$. Knowing this, we can calculate the velocity of the solitons. This is exemplified here for the $(n+1)$-solitons.

Consider a state of an $(n+1)$-soliton, where an $(n+1)$-cluster is moving with particles having coordinates $x_0(t), x_0(t) + \sigma, \ldots, x_0(t) + n\sigma$. We fix the time origin by saying that the $(n+1)$-cluster started moving at time $t = 0$ at an initial position $x_0(0) = x_0^{\text{ini}}$. The propagation of the $(n+1)$-cluster terminates at a final position $x_0^{\text{fin}}$, when the first particle detaches from the $n$-particles to the right. According to the condition (S7a), this happens if

$$ f + \pi U_1 \sin(2\pi x_0^{\text{fin}}) = f + \frac{\pi U_1}{n} \sum_{k=1}^{n} \sin[2\pi(x_0^{\text{fin}} + k\sigma)] = f + \frac{\pi U_1 \sin(n\pi \sigma)}{n \sin(\pi \sigma)} \sin \left[ 2\pi \left( x_0^{\text{fin}} + \frac{n+1}{2} \sigma \right) \right], $$

yielding

$$ \sin(2\pi x_0^{\text{fin}}) = \frac{\sin(n\pi \sigma)}{n \sin(\pi \sigma)} \sin \left[ 2\pi \left( x_0^{\text{fin}} + \frac{n+1}{2} \sigma \right) \right]. \quad (S18) $$
One solution of this equation is
\[ x_{\text{fin}}^0 = \frac{1}{2} + \frac{1}{2\pi} \arccot \left| \frac{n \sin(\pi \sigma)}{\sin(\pi n \sigma) \sin[\pi (n+1)\sigma]} \right| \cot[\pi (n+1)\sigma]. \] (S19)

Any \( x_{\text{fin}}^0 + m, m = 0, \ldots, (N-1) \), is a solution also, i.e. when the distance of the position from \( x_{\text{fin}}^0 \) equals an integer multiple of the wavelength.

The final position of the \((n+1)\)-cluster gives the initial position \( x_{\text{ini}}^1 \) for the \(n\)-cluster,
\[ x_{\text{ini}}^1 = x_{\text{fin}}^0 + \sigma. \] (S20)

The motion of the \(n\)-cluster terminates at a position \( x_{\text{fin}}^1 \), when it attaches to the next (nearly) resting particle in the system. Then the motion of a new \((n+1)\)-cluster starts, with a position \( x_0^1 \) of its first particle equal to \( x_{\text{fin}}^1 \), because the soliton motion is periodically repeating itself after one wavelength. Accordingly,
\[ x_{\text{fin}}^1 = x_{\text{fin}}^0 + 1, \] (S21)

where \( x_{\text{fin}}^0 \) is a position of a resting particle, i.e. any position
\[ x_{\text{rest}}^m = \frac{1}{2} + \frac{1}{2\pi} \arcsin \left( \frac{f}{\pi U_1} \right) + m, \quad m = 0, \ldots, N-1. \] (S22)

of mechanical equilibrium in the tilted potential \([U(x) - fx]\). We choose \( m = 0 \), i.e.
\[ x_{\text{ini}}^0 = x_{\text{ini}}^1 = \frac{1}{2} + \frac{1}{2\pi} \arcsin \left( \frac{f}{\pi U_1} \right). \] (S23)

The velocities \( v_n \) and \( v_{n+1} \) of the \(n\) and \((n+1)\)-cluster are given by the mobility \( \mu = 1 \) times the mean forces \( \bar{F}_n \) and \( \bar{F}_{n+1} \) acting on the cluster. These mean forces are \((k = n, n+1)\)
\[ \bar{F}_k(x) = \frac{1}{k} \sum_{i=0}^{k-1} F(x_i) = \frac{1}{k} \sum_{i=0}^{k-1} (f + \pi U_1 \sin[2\pi (x + i\sigma)]) = f + \frac{\pi U_1 \sin(\pi k \sigma)}{k} \frac{\sin[\pi (2x + (k-1)\sigma)]}{\sin(\pi \sigma)}. \] (S24)

The times \( \tau_n \) and \( \tau_{n+1} \) for the motion of the \(n\) and \((n+1)\)-cluster in the intervals \([x_{\text{ini}}^1, x_{\text{fin}}^0]\) and \([x_{\text{ini}}^0, x_{\text{fin}}^1]\) then are
\[ \tau_n = \int_{x_{\text{ini}}^1}^{x_{\text{fin}}^0} \frac{dx}{\bar{F}_n(x)}, \] (S25a)
\[ \tau_{n+1} = \int_{x_{\text{ini}}^0}^{x_{\text{fin}}^1} \frac{dx}{\bar{F}_{n+1}(x)}. \] (S25b)

The time period of the soliton is \( \tau = \tau_n + \tau_{n+1} \) and its mean velocity \( \bar{v}_{\text{sol}} = 1/\tau \). The current generated by the soliton
FIG. S1. Analytically calculated soliton-induced current [Eq. (S26)] as a function of particle diameter $\sigma$ in comparison with simulated data for $f = 0.05$. The dotted line refers to an interpolation of the peak currents given in Eq. (6) of the main text.

is

$$J = \frac{\tilde{v}_{\text{sol}}}{L} = \frac{1}{L(\tau_n + \tau_{n+1})}.$$  

(S26)

This analytical result for the current is in excellent agreement with simulated data, see Fig. S1.

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