Supplementary Information

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1 Parameterization of a neighbourhood of $\Omega_\alpha$

We provide a brief argument for the following statement made in the main text: given a regular point $x \in \Omega_\alpha$, there exists a differentiable parameterization of a neighbourhood $N(x) \subset \mathbb{R}^3$ of the form $y \times \{y_\alpha_i\}_{i=1}^m$, with $y \in \mathbb{R}^{3n-m}$, such that $\nabla y \cdot \nabla y_\alpha_i = 0$ on $\Omega_\alpha$.

Recall that a regular point $x \in \Omega_\alpha$ is a point such that the Jacobian of the transformation $x \rightarrow (y_\alpha_1(x), \ldots, y_\alpha_m(x))$ has rank $m$. If $x$ is regular then it has a neighbourhood $N_\alpha(x) \subset \Omega_\alpha$ that is a differentiable manifold with co-dimension $m$ $(1, 2)$, so there exists a parameterization near $x$ by $y \in \mathbb{R}^{3n-m}$; let the associated mapping be $z : \mathbb{R}^{3n-m} \rightarrow \Omega_\alpha$.

Given some point $x' \in \Omega_\alpha'$ (not necessarily on $\Omega_\alpha$), we define a mapping $x' \rightarrow (y_\alpha_i, y)$ as $(y_\alpha_i(x'), y(x'))$, where $y(x')$ is found from the limit of the gradient flow map, i.e. $y(x') = z^{-1}(\lim_{t \rightarrow \infty} \phi(t))$ where $\phi$ solves $\frac{d\phi}{dt} = -\nabla \sum_i U(y_\alpha_i(\phi))$, $\phi(0) = x'$. (We abbreviate $y_\alpha_i$ to mean the full list of constraint variables.) Results from (3) (see also (4)) show that this map exists and is smooth enough in a neighbourhood $\subset \Omega$ of $x \in \Omega_\alpha$, provided $\Omega_\alpha$ is regular and $U(y)$ is sufficiently smooth. Since the mapping $x' \rightarrow (y_\alpha_i, y)$ has full rank at $x \in \Omega$, it does also in a neighbourhood $N(x) \subset \Omega$ and so by the Inverse Function Theorem it is invertible. The orthogonality at $\Omega_\alpha$ follows because this is a level set of the constraints.

Note that while this provides the required parameterization in a neighbourhood of $x \in \Omega_\alpha$, we have not shown that it extends to the set $\Omega_\alpha'$ (see equation (7) in main text). This is not a problem for the asymptotic calculations, as these remain valid if $\Omega_\alpha'$ is replaced with an atlas of local parameterizations $N(x)$, patched together with a partition of unity – the asymptotics only require the local behaviour near $y_\alpha_i = 0$ and are not sensitive to the cutoffs at $r_c$.

2 Quotient space metric and equations

In this section we give more details about the quotient space and metric structure on it, and show how these arise naturally from our equations. Although these facts are well-known in Riemannian geometry $(2, 5)$ and well-used in chemistry and mechanics $(6; 7; 8)$, we have not found a reference dealing succinctly with our particular context so we collect the relevant facts and demonstrations here.

The manifold structure on the quotient space Recall that we defined the quotient space associated with a manifold $\Omega_\alpha$ to be $\Omega_\alpha^Q = \Omega_\alpha / G$, where the $G = SE(3)$ is the Special Euclidean group, i.e. the group of rotations and translations of a cluster. Then $\Omega_\alpha^Q$ is a smooth manifold if the Lie group $G$ acts properly and freely on $\Omega_\alpha$ ($(6)$, Prop. 4.1.23 p.266, $(5)$). To act properly is a compactness condition and it can be checked that it is satisfied for $SE(3)$. To act freely mean
that the only element \( g \in G \) such that \( g \cdot x = x \) is the identity. This is the case provided there is no cluster in \( \Omega_\alpha \) such that the spheres all lie on a line; for floppy manifolds with up to two bonds broken this is true when \( n \geq 5 \).

The orbit of a cluster \( x \) is the set of points of the form \( g \cdot x \) for \( g \in G \), and is written as \([x]\). Each orbit is identified as an element in \( \Omega_\alpha^Q \) by the canonical projection

\[
\pi : \Omega_\alpha \to \Omega_\alpha / G := \{ [x] : x \in \Omega_\alpha \}. \tag{S1}
\]

This projection shows how to map the tangent spaces to each other, via the pushforward map. Let \( T_\alpha(x), T_\alpha^Q([x]) \) be the tangent spaces at \( x \in \Omega_\alpha \), \([x] \in \Omega_\alpha^Q \) respectively. The tangent vectors map as follows: if \( c(t) \in \Omega_\alpha \) is a curve such that \( c(0) = x \), then the tangent vector \( c'(0) \in T_\alpha(x) \) maps to the tangent vector \( \frac{d}{dt} \pi(c(t))|_{t=0} \in T_\alpha^Q([x]) \). Note that tangent vectors can also be identified as derivations, which we will write as \( \partial_t \).

**Metric on the quotient space** The group \( G \) acts isometrically on \( \Omega_\alpha \), which means it respects the inner product \( \langle \cdot, \cdot \rangle_{\alpha} \) on the manifold: given \( t_1, t_2 \in T_\alpha(x) \), the inner product satisfies \( \langle t_1, t_2 \rangle_{\alpha} = \langle g \cdot t_1, g \cdot t_2 \rangle_{\alpha} \) for all \( g \in G \). Therefore one can construct a metric on the quotient manifold that is compatible with the projection (making the projection a Riemannian submersion), and this metric is unique (5).

To specify the metric we decompose \( T_\alpha(x) \) into the vertical subspace \( T_\alpha^v(x) \), containing the directions tangent to the action of \( G \), and the horizontal subspace \( T_\alpha^h(x) \), its orthogonal complement. Therefore \( T_\alpha(x) = T_\alpha^v(x) \oplus T_\alpha^h(x) \).

Let \( P_\alpha : T_\alpha \to T_\alpha^h \) the orthogonal projection operator (we omit the argument \( x \) for succinctness.) Let \([t]\) denote an element of \( T_\alpha^Q \) that has representative \( t \in T_\alpha \). The metric \( g_\alpha \) on the quotient space \( \Omega_\alpha^Q \) is computed from the metric \( g_\alpha \) on \( \Omega_\alpha \) as

\[
\langle [t_1], [t_2] \rangle_{g_\alpha^Q} = \langle P_\alpha t_1, P_\alpha t_2 \rangle_{g_\alpha}.
\tag{S2}
\]

**Fokker-Planck equations on the quotient space** Next we show how this differential structure arises naturally as a result of our manipulations to the Fokker-Planck equation.

Consider a point \( x_0 \in \Omega_\alpha \), and let us parameterize a neighbourhood on \( \Omega_\alpha \) in such a way that at \( x_0 \), the directions tangent to infinitesimal rotations and translations are orthogonal to the remaining variables. This can be done with the standard Euler angles. Let

\[
R_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix}, \quad R_y(\theta) = \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix}, \quad R_z(\theta) = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]

be the matrices for rotation of a point about the \( x, y, z \) axes respectively, with block-diagonal versions appropriate to a cluster of \( n \) particles \( R_x(\theta), R_y(\theta), R_z(\theta) \). These are obtained as, for example,

\[
R_x(\theta) = \begin{pmatrix} R_x(\theta) \\ & \ddots \\ & & R_z(\theta) \end{pmatrix}
\]

with \( n \) copies along the diagonal and zeros everywhere else, and similarly for the other matrices.

Let

\[
T(\mu_1, \mu_2, \mu_3) = (\mu_1, \mu_2, \mu_3, \mu_1, \mu_2, \mu_3)^T
\]
be a vector representing translations. Let \( \phi(y) : \mathbb{R}^p \to \mathbb{R}^{3n} \) parameterize the remaining directions with \( \phi(0) = x_0 \), so that a neighbourhood of \( x_0 \) on \( \Omega_\alpha \) can be parameterized with variables \((\theta_x, \theta_y, \theta_z, \nu_1, \nu_2, \mu_3)\) as

\[
x = R_z(\theta_z)R_y(\theta_y)R_x(\theta_x)\phi(y) + T(\mu_1, \mu_2, \mu_3).
\]  

(S3)

We can choose \( \phi(y) \) so that it is orthogonal to infinitesimal rotations and translations at \( x_0 \): this means that we require \( \frac{\partial \phi}{\partial y_k} \bigg|_{y=0} \cdot \left( \frac{\partial R_x}{\partial \theta_x} \bigg|_{\theta_x=0} x_0 \right) = 0 \), for each \( y_k \) and each rotation matrix; the condition for translations is satisfied if the center of mass of \( x_0 \) is at the origin.

The metric tensor on \( \Omega_\alpha \) is \( g_{\alpha} = J^T J \) where \( J \) is the Jacobian of the transformation \((\theta_x, \theta_y, \theta_z, \nu_1, \nu_2, \mu_3, y) \to x \). This has a simple block diagonal structure at \( x_0 \):

\[
g_{\alpha}(x_0) = \begin{pmatrix} \bar{g}_\alpha & 0 & 0 \\ 0 & I_3 & 0 \\ 0 & 0 & I_3 \end{pmatrix}, \quad \text{where} \quad I = \begin{pmatrix} \sum_i y_i^2 + z_i^2 - \sum_i x_i y_i & -\sum_i x_i z_i & -\sum_i x_i z_i \\ -\sum_i x_i y_i & \sum_i x_i^2 + z_i^2 - \sum_i y_i z_i & -\sum_i y_i z_i \\ -\sum_i x_i z_i & -\sum_i y_i z_i & \sum_i x_i^2 + y_i^2 \end{pmatrix}.
\]  

(S4)

Here \( \bar{g}_\alpha \) is the \( p \times p \) contribution from the \( y \)-variables, \( I_3 \) is the \( 3 \times 3 \) identity matrix, and \( I \) is the moment of inertia tensor, which assumes the configuration is written as \( x = (x_1, y_1, z_1, \ldots, x_n, y_n, z_n) \).

We will write its determinant as \( I^2(x_0) \equiv \det(I) \).

Therefore the Fokker-Planck equation on \( \Omega_\alpha \) after integrating over the fast variables has the following form at \( x_0 \):

\[
\partial_t (\kappa^{m} h \alpha p) = \frac{1}{\sqrt{|g_\alpha|}} \partial_t \left( \sqrt{|g_\alpha|} \kappa^{m} h \alpha g^{ij} \partial_j p \right) + \sum_{\beta \to \alpha} j_\beta \cdot \hat{n}^\beta \alpha
\]

\[
= \frac{1}{\sqrt{|g_\alpha|} I^2} \partial_u \left( \sqrt{|g_\alpha|} I^2 \kappa^{m} h \alpha \bar{g}^{uv} \partial_v p \right) + \frac{1}{\sqrt{|g_\alpha|} I^2} \partial_\alpha \left( \sqrt{|g_\alpha|} I^2 \kappa^{m} h \alpha \bar{g}^{ab} \partial_b \bar{p} \right) + \sum_{\beta \to \alpha} j_\beta \cdot \hat{n}^\beta \alpha.
\]  

(S5)

Here \( g_{ij} \), \( g_{uv} \) are the elements of \( g_\alpha \), \( \bar{g}_\alpha \) respectively, \( a, b \) index the rotational and translational variables, and we have substituted (S4) in the second equation. We will not deal with the flux explicitly as this comes from the same manipulations on the higher-dimensional manifolds.

Integrating (S5) over orbits gets rid of the second term on the RHS, by Stokes’ theorem, so we are left with

\[
\partial_t (\kappa^{m} h \alpha I \bar{p}) = \frac{1}{\sqrt{|g_\alpha|}} \partial_u \left( \sqrt{|g_\alpha|} \kappa^{m} h \alpha I \bar{g}^{uv} \partial_v \bar{p} \right) + \sum_{\beta \to \alpha} j_\beta \cdot \hat{n}^\beta \alpha.
\]  

(S6)

where \( \bar{p} \) is the integrated value of \( p \) on an orbit (this is \( C \bar{p} \) if \( p \) is constant on the orbit, where the constant \( C \) does not depend on \( x_0 \).) Because this does not depend on the location along the orbit of a point, we can identify it with a function on the quotient space as \( \bar{p}(x, t) = \tilde{p}^Q([x], t) \).

For the same reason we can identify tangent vectors via the canonical projection as \( \partial_u \bar{p} = \partial_u \tilde{p}^Q \).

The metric \( \bar{g}_{uv} \) has the same elements as the quotient metric \( \bar{g}_{[u][v]} \) because it only involves tangent vectors in the horizontal subspace, and it is independent of the representative \( x_0 \) that we chose for \([x_0]\) because \( G \) acts isometrically.

After identifying functions, tangent vectors, and the metric in (S6) with their projections in the quotient space, we obtain equation (20) in the main text.
Representing the quotient space  To parameterize the quotient manifold it is convenient to map it to a space that has an explicit representation. For our numerical implementation we store the edge-lengths of all the particles (we call this “bond-distance” space.) This representation actually forms the quotient space with reflections as well, so it is only diffeomorphic to $\Omega_\alpha^Q$ if $\Omega_\alpha$ does not contain a cluster where all of the particles lie in a plane.

An alternate parameterization would be to constrain one vertex to be at the origin, one vertex to lie on the $x$-axis, and one vertex to lie on the $xy$-plane. This would embed $\Omega_\alpha^Q$ in $\Omega_\alpha$.

Given a parameterization of the quotient manifold in some space $B$ with canonical projection $\pi$, the tangent vectors and metric can be computed from the pushforward map (S1) via numerical differentiation. That is, given a point $[x] \in B$ with representative $x \in \Omega_\alpha$ where this is two-dimensional, we compute the two unit tangent vectors $t_1, t_2 \in T_\alpha(x)$ that are perpendicular to the infinitesimal rotations and translations. This is easy to do from the null space of the matrix $M$ defined in section 4.1. We take small steps in each of these directions to obtain points $x_1 = x + \Delta s t_1$, $x_2 = x + \Delta s t_2$, project to $B$, and obtain first-order estimates of the quotient tangent directions as $[t_1] = (\pi(x_1) - x)/\Delta s$, $[t_2] = (\pi(x_2) - x)/\Delta s$. These have lengths 1 and inner product $\langle t_1, t_2 \rangle_{g_\alpha}$, which defines the metric on $B$.

We use a first-order scheme to find the distance between two nearby points $[x_1], [x_2]$ in $B$. We find the separation vector $v = [x_1] - [x_2]$, project this onto the tangent space at $[x_1]$ and find the length of this projection. We repeat at the tangent space to $[x_2]$ and average the lengths.

Note that parameterizing the quotient manifold as a subset of $\Omega_\alpha$ would imply slightly different numerical algorithms. For example, to find the distance between two nearby points, one would simply project the separation vector $v$ onto the horizontal tangent space at $x_1$, $x_2$ (these representatives can be chosen equal to $[x_1], [x_2]$) – this might be more efficient than the bond-distance space method.

3 Adjoint equations

In this section we compute the backward Fokker-Planck equation associated with equation (20). We could derive this using the same asymptotic procedure on the backward equation associated with equation (2), however we prefer to demonstrate how to convert between the forward and backward sticky equations directly. We only outline the arguments here, leaving several steps to the reader.

Recall that the backward equation describes the evolution of $u(x, t)$, the expected value of some function $g(x)$ that starts with a unit mass at $x$ and is subsequently stirred by the probability dynamics. \footnote{If we were to construct a stochastic process $X_t$ with Fokker-Planck equation (20) and with initial condition $X_0 = x$, then we would be able to write $u(x, t) = \mathbb{E}_x(X_t)$. Unfortunately we are only aware of such constructions for processes that have singular measures on manifolds of co-dimension 1 (9), and not processes that are sticky on manifolds of several different dimensions simultaneously, so we focus instead on the PDE interpretation.} This is obtained from the transition probability measure $P_x(dy, t)$ as

$$ u(x, t) = \int_{\Omega} P_x(dy, t) g(y) = \int_{\Omega} p(x, y, t) g(y) d\rho(y) $$

(S7)

where the transition probability has initial condition $P_x(y, 0) = \sum_\alpha \delta_\alpha(y - x)$ and we have used the fact that it has a density $p(x, y, t)$ with respect to the equilibrium measure $d\rho(y)$ (see equation (24)). Note this implies $p(x, y, 0) = \sum_\alpha \delta_\alpha(y - x)/\kappa_\alpha$. 

\[ \int_{\Omega} P_x(dy, t) g(y) = \int_{\Omega} p(x, y, t) g(y) d\rho(y) \]
We suppose that $P_x$ satisfies the Chapman-Kolmogorov equation as this property holds for the original probability measure $p' dx$ from which it derives:

$$\int_{z\in \Omega} P_x(dz, t-s) P_z(dy, s) = P_x(dy, t). \quad (S8)$$

This allows us to write

$$u(x, t) = \int_{\Omega} P_x(dz, t-s) u(z, s) = \int_{\Omega} p_x(z, t-s) u(z, s) d\rho(z). \quad (S9)$$

We can now obtain an evolution equation for $u$. Applying $\partial_t$ to (S9) and using equation (24) gives

$$\frac{\partial u}{\partial t} = \int_{\Omega} p_t d\rho(y) = \int_{\Omega} (\text{div grad } p) u d\rho(y)$$

$$= \int_{\Omega} p \text{ (div grad } u) + \sum_i \int_{\Omega_i} u (\text{grad } p \cdot \hat{n}) - p \text{ (grad } u \cdot \hat{n}) + \kappa_i u \text{ div grad } p.$$

Here \{\Omega_i\} is the set of manifolds of co-dimension 1 that form the boundary of the full space $\Omega$, $\kappa_i$ are the sticky factors along these manifolds, $\text{div}$, $\text{grad}$ denote differential operators on $\Omega$ and $\text{div}_i$, $\text{grad}_i$ will denote those on $\Omega_i$. $\hat{n}$ denotes a generic outward normal to the appropriate manifold, and integration is with respect to the volume element appropriate for each manifold. We now substitute for $\text{grad } p \cdot \hat{n}$ using the forward sticky equations to obtain

$$\frac{\partial u}{\partial t} = \int_{\Omega} p \text{ (div grad } u) + \sum_i \int_{\Omega_i} u (\text{div}_i \kappa_i \text{ grad}_i p - \kappa_i \text{ div grad } p)$$

$$- p \text{ grad } u \cdot \hat{n} + \kappa_i u \text{ div grad } p$$

$$= \int_{\Omega} p \text{ (div grad } u) + \sum_i \int_{\Omega_i} p (\text{div}_i \kappa_i \text{ grad}_i u - \text{grad } u \cdot \hat{n})$$

$$+ \sum_j \int_{\Omega_j} \sum_{i \rightarrow j} \kappa_i (u \text{ grad}_i p \cdot \hat{n}^{(ij)} - p \text{ grad}_i u \cdot \hat{n}^{(ij)}) \quad (S10)$$

Here \{\Omega_j\} is the set of manifolds of co-dimension 2, forming the boundaries of the manifolds $\Omega_i$; the sum in the final term is over all manifolds $\Omega_i$ that have $\Omega_j$ as a boundary, and $\hat{n}^{(ij)}$ is the outward normal vector from $\Omega_i$ at $\Omega_j$.

Evaluating (S10) at $s = t$ gives the backward sticky equations

$$\partial_t u = \text{div grad } u \quad \text{ in } \Omega$$

$$\kappa_i \partial_t u = \text{div}_i \kappa_i \text{ grad}_i u - \nabla u \cdot \hat{n} \quad \text{ in } \Omega_i \quad (S11)$$

$$\partial_t u = \text{(boundary terms)} \quad \text{ in } \Omega_j$$

We stop at the first two terms; the interested reader can show that evaluating the boundary terms leads to the expected equations on the lower-dimensional manifolds. This set of equations is identical to the forward equations, so the system is self-adjoint.


4 Parameterizing the manifolds

In this section we outline the method we used to parameterize the quotient manifolds $\Omega_Q^\alpha$ describing clusters of hard spheres with up to 2 bonds broken. The method can be broken down into two separate sets of algorithms. The first algorithm generates points on the manifold, by taking linear steps along the tangent directions and projecting back down to the manifold. This is sufficient to calculate the 1-dimensional manifolds. The second algorithm links up the points with bars to form a simplex on which calculations can be performed, and is required for 2- and higher-dimensional manifolds.

4.1 1-dimensional manifolds

Consider first the 1-dimensional manifolds. We take steps along the manifold as follows: given a point $x_0 \in \Omega_\alpha$, a set of bond-distance constraints $\{y_k\}_{k=1}^m$, and a basis $\{t_i\}_{i=1}^6$ for the part of the tangent space at $x_0$ parallel to rotational and translational motions, we form a matrix

$$M = (\nabla y_1, \ldots, \nabla y_m, t_1, \ldots, t_6)^T$$

and compute the null space of $M$. When $x_0$ is a regular point on the manifold, this null space contains a single vector $v$ lying in the tangent space of $\Omega_\alpha(x_0)$, so we take a step in that direction as $x_1 = x_0 + (\Delta s)v$. Because $v$ is orthogonal to translations and rotations, the length of our step in the quotient metric is $||x_1 - x_0||_Q^\alpha = \Delta s + O(\Delta s^2)$.

This step pushes us slightly off the manifold, so we project back down to it by finding a set of Lagrange multipliers $\lambda_k$ so that the projected point $x_1' = x_1 + \sum_k \lambda_k \nabla y_k(x_1)$ lies on the manifold, i.e. we solve the nonlinear system of equations $y_k(x_1 + \sum_k \lambda_k \nabla y_k(x_1)) = 0$ (10). This is easily done using Newton’s method as we are typically very close to the manifold.

Beginning with a rigid cluster $x_0$ with an associated set of bond constraints, we break a bond by deleting one of the constraints, and perform the steps above until another bond is formed. This provides an ordered set of points in the quotient manifold, along with distances between them – this is a “line”.

4.2 2-dimensional manifolds

Computing the 2-dimensional manifolds is more involved; here are the steps we followed.

**Compute the boundaries** First, we compute the boundaries of the manifold. To compute a 2-dimensional manifold $\Omega_Q^\alpha$ with constraint list $y_1(x), \ldots, y_n(x)$, we start with a corner point $x_0 \in \Omega_Q^\alpha$ with two extra constraints $y_{i_1}(x), y_{i_2}(x)$. Deleting one of these, say $y_{i_1}$, we walk along the 1-dimensional manifold (as in the previous section) until another bond is formed, corresponding say to constraint $y_{i_2}$. We add this to our constraint list, delete the next extraneous constraint $y_{i_2}$, and repeat. We continue in this way, deleting one extraneous constraint at each corner, until we reach the original corner $x_0$. This gives us the boundary of $\Omega_Q^\alpha$, including corners.

**Generate points in the interior** Second, we generate a collection of points in the interior. Beginning with every point on the boundary, we generate lines in the interior by holding all constraints fixed except the one that takes us off the boundary, and walk in this direction until we exit the manifold. We throw away points that are too close in some metric to existing points to avoid generating too many points.
Triangulate the points Third, we triangulate the points. Many typical algorithms will not work here because our surface is not embedded in $\mathbb{R}^3$, so we adopt an algorithm proposed by by (11) (see also (12)) that works as follows.

1. Map the boundary to a fixed convex polygon in $\mathbb{R}^2$.

2. Map the interior points to the interior of that region in $\mathbb{R}^2$, by letting each interior point be a convex combination of its neighbouring points. More specifically: let $x_1, \ldots, x_n$ be the set of interior points, and let $N_i$ be a neighbourhood of an interior point $x_i$. Given a set of strictly positive weights $\lambda_{ij}$ such that $\sum_{x_j \in N_i} \lambda_{ij} = 1$, find parameter points $u_1, \ldots, u_n \in \mathbb{R}^2$ that solve the linear system of equations

$$u_i = \sum_{x_j \in N_i} \lambda_{ij} u_j, \quad i = 1, \ldots, n.$$ 

Each $u_i$ is contained in the convex hull of its neighbours, so it will be in the interior of the region defined in step (1) (11).

3. Triangulate the parameter points in $\mathbb{R}^2$ (we use a Delauney triangulation.) This lifts back to a triangulation of the manifold.

To implement this, we choose the boundary region so that the corners lie on a circle with a fixed radius, and the line segments joining them lie on arcs of circles whose lengths are approximately the same as the lines they are parameterizing. Points along these arcs are placed so the inter-point distance in the plane is proportional to the distance in the quotient metric between the points. The quality of the triangulation will depend on the choice of boundary region, and we find better qualities as the angles at the corners more closely represent the angles on the manifold.

Choosing the neighbourhood $N_i$ is a balance between sampling many points to get a smoother parameterization, and choosing fewer points so the manifold is roughly linear in the neighbourhood and does not contain any folds or other external branches of the manifold. We choose the neighbourhood to be the $k$ nearest points along the manifold, where a range of roughly $8 \leq k \leq 15$ works well for the step sizes we use, but $k$ will increase as step size decreases.

There are many ways to choose the weights; the most straightforward is for them to be the same, but almost as straightforward is for them to be inversely proportional to distance in some metric. For rapid but still good quality results we use the metric in bond-distance space – this takes the list of pairwise bond distances and computes the Euclidean distance between the vectors.

Improve the triangulation Finally, we improve the quality of the triangulation by letting the triangle sides be springs and evolving the points on the manifold with the spring forces, re-triangulating when necessary. Springs are chosen to be slightly longer than the average distance between points so the points want to spread out and fill the whole space. When a point hits a boundary it is absorbed, and is subsequently constrained to move along the boundary. This algorithm was introduced by (13) for a triangulation of the Euclidean plane, and we adapt it by replacing the length in the plane with the distance metric in the quotient manifold. In practice, we typically use bond-space distance instead as this is faster to compute and still gives a good quality triangulation.
Integration on the manifolds. To compute quantities integrated over the manifolds, such as for the partition functions $z_{\text{geom}}^{\alpha}$, we used finite elements on the simplex with standard piecewise linear elements. The sides of the triangles must be calculated in the quotient space metric.

4.3 Remarks

Topology. The calculations above require that the 2-dimensional manifolds be topologically equivalent to a disc. Because we have obtained smooth parameterizations, we are confident that this is true for all the floppy manifolds under consideration. Alternatively, one could show this from a collection of points using Betti numbers (14), for example.

This points to an interesting question in discrete geometry – under what conditions is the topology of floppy manifolds a polygon? One has to rule out surfaces of higher genus and non-orientable surfaces, among other things. We expect this can be shown for low-dimensional manifolds and small $n$, but larger $p$ or $n$ may be more complicated.

Numerical parameters and convergence. For the calculations reported in the text we used a step size of $\Delta s = 0.01$ to calculate the one-dimensional manifolds, and $\Delta s = 0.05$ to generate points on the boundary and interior of the 2-dimensional manifolds. When generating points we threw away points that were closer than $0.5 \Delta s$ in bond-distance space to already-generated points. We typically ran the triangulation step 3 times before re-triangulating, using a step size of $\Delta t = 0.1$ and an internal pressure parameter of 1.2 (see (13)), although a small selection of manifolds had to be re-triangulated after each spring step. We ran the triangulation until the area of the manifold, computed in bond-distance space, changed less than $\Delta s/20$ after 3 consecutive re-triangulations.

We checked for convergence in two ways: by calculating the manifolds using a coarser resolution ($\Delta s = 0.1$ for the 2-dimensional manifolds, $\Delta s = 0.05$ for the 1-dimensional manifolds), and by running the triangulation algorithm for longer, until the minimum triangle quality ($q = 2r_{in}/r_{out}$, the ratio between (twice) the radius of the largest inscribed circle and the smallest circumscribed circle, see e.g. (15)) was greater than 0.2. Both tests allowed us to conclude that our calculated ratios $Z_2/Z_1$, $Z_1$, $Z_0$ are correct to $\pm 0.05$, $\pm 0.01$ respectively (although we have not reported this many decimal points for the latter).

5 Simulations

We have performed Brownian dynamics simulations of interacting particles to test our asymptotic calculations. We solve equation (2) with $D = \beta = 1$ using a forward Euler timestep. For the potential we started with a Morse potential with maximum depth $E$ at $r = 1$ and range parameter $\rho$; this takes the form $U(r) = Ee^{-\rho(r-1)}(e^{-\rho(r-1)} - 2)$. The hard-core part for $r < 1$ was modelled with a parabolic potential of the form $U(r) = \frac{1}{2}m^2U''(1)(r-1)^2 - E$ for some number $m$; we choose $m = 2$. This constrains the time step to be $\Delta t \ll (m^2U''(1))^{-1}$ and we typically choose a factor of 6–8 less. The sticky factor, accounting for the parabolic part, is $\kappa = \frac{m+1}{m} \frac{e^{E\rho^2}}{\sqrt{2E\rho^2}} \sqrt{\frac{\pi}{2}}$.

The whole potential was truncated at $r_c = 1 + 4/\rho$, by adding a linear term to keep the force continuous at $r_c$, as $U_{\text{trunc}}(r) = U(r) - U(r_c) + U'(r_c)(r - r_c)$ for $r < r_c$, and $U_{\text{trunc}}(r) = 0$ otherwise. This modifies the sticky parameter to

$$\kappa = \frac{m+1}{m} \frac{\exp(E - U(r_c) - U'(r_c)(1 - r_c))}{\sqrt{2E\rho^2}} \frac{\sqrt{\pi}}{\sqrt{2}}$$ 

(S12)
We began with an initial condition drawn from the equilibrium distribution of rigid modes, and ran several copies of the simulation for a very long time. At time increments of $1 \times 10^{-2}$ we checked to see which floppy mode the cluster occupied by forming its adjacency matrix, computing the number of bonds, and if this number was $\geq 3n - 6 - 2$, finding the adjacency matrix in our list of floppy modes to which it was topologically equivalent. This allows us to compute the occupation probabilities of each floppy mode.

To form the adjacency matrix, we said particles were bonded when they were at a distance of less than $1 + 2/\rho$; this is the range beyond which the force is negligible. (Choosing a bond distance of $1 + 1/\rho$ gave results that were inconsistent with the asymptotics.) We used the Matlab function `graphisomorphism.m` to determine topological equivalencies.

We also kept track of transitions between rigid clusters, by recording the times and mode numbers at which the system first hits a rigid state that occupies a separate part of configuration space than the previous rigid state. This is easily done by checking whether or not the current adjacency matrix of a rigid mode is identical to the adjacency matrix of the previous rigid mode.

Figure S1 shows the simulated probabilities versus theoretically computed probabilities of each floppy mode for $n = 7, 8$, for simulations using a Morse potential with the same parameters as in the text (Figure 7): $E = 8.5$, $\rho = 30$, $dt = 2 \times 10^{-6}$. This implies the sticky parameter is $\kappa = 16$. Again, there is excellent agreement.

Figure S2 plots the elements of the transition count matrix for $n = 6, 7, 8$ from simulations, versus two theoretical calculations. The blue markers come from the leading-order asymptotic approximation, computed from equation (29). The magenta markers come simply restricting the dynamics to the network of points and lines, which gives geometric rates of $(Z_0 + \kappa^{-1}Z_1)^{-1} \sum_k Q_k^{-1}$ – these are the blue rates multiplied by $1/(1 + \kappa^{-1}Z_1/Z_0)$, so are asymptotically equivalent, but uniformly smaller. These rates do a better job of predicting the simulated rates for this value of the range parameter.

To calculate rates for $n = 7, 8$ we have grouped the 0-dimensional modes that are very close together into one mode (these are modes $\{1, 4\}$ for $n = 7$, modes $\{1, 2, 3, 4\}$ for $n = 8$). The rate from a mode in this group to a mode not in the group is the sum of the rates out of each mode in a group, and the rates within a group are ignored. We were able to make a distinction between modes in a group only by using a range parameter of $\rho = 150$ (not shown).

Table S1 shows the ratios $Z_{p+1}/Z_p$ extracted from the simulations. These are uniformly smaller than the theoretically computed values, but approach the theory as the range of the potential decreases. This is because the simulations use an excess bond length that is finite rather than infinitesimal, so some clusters are counted as being on $p$-dimensional manifolds, when in the limit they would be on $p + 1$-dimensional manifolds. One could potentially correct for this if one had no knowledge of the potential, but wanted to use these measurements to estimate the sticky parameter.

### 6 Data

We provide details for the floppy modes for $n = 6$. Details for $n = 7, 8$ are available upon request.

Table S2 reports the following quantities for each mode: the volume $S \equiv \int_{\Omega} 1$, mean geometrical sticky parameter $\bar{h} \equiv (\int_{\Omega} h)/S$, mean rotational contribution $\bar{I} \equiv (\int_{\Omega} I)/S$, multiplicity $n_\alpha$ (divided by a constant). Each of the integrals is over a single manifold in the set of isomorphic manifolds, and the average for rigid modes is simply the point value. For floppy modes we also report the corners, in the order they occur as one travels around the boundary.
Figure S1: Simulated versus theoretical probabilities of floppy modes, for $n = 7$ (top), $n = 8$ (bottom), for a Morse potential with range parameter $\rho = 30$. The running time of each simulation varied and is given in the title.

Figure S2: Elements of the count matrix for $n = 6, 7, 8$ (left, middle, right).
Table S1: Ratios extracted from simulations with different range and sticky parameters. These were computed as (time in $p$ + 1-dimensional modes) / (time in $p$-dimensional modes) / $\kappa$, where $\kappa$ is computed using (S12). Parameters were (A) $dt = 2e^6$, $E = 8.5$, $\rho = 30$ ($\kappa = 16$), (B) $dt = 8e^{-7}$, $E = 10$, $\rho = 50$ ($\kappa = 31$), (C) $dt = 2.5e^{-7}$, $E = 10.6$, $\rho = 150$ ($\kappa = 22$).

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<th>$n_\alpha$</th>
<th>$z_\alpha$</th>
<th>corners</th>
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Table S2: Free energy data for each mode, $n = 6$. 

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<th>$Z_1/Z_0$</th>
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Figure S3: Vibrational contribution to the free energy $-\log h(x)$ along selected 1-dimensional manifolds (blue line). Markers indicate the transition state computed in (16) for a potential with finite width.

Figure S4 provides a way to identify the individual modes. It shows the rigid clusters with particles numbered. The table indicates how to reach each floppy mode by starting with a given rigid structure and breaking selected bonds. In most cases there are multiple ways to reach each floppy structure and every possible bond combination that does so is listed.

Figure S3 plots the transition states computed in (16) along each of the identified 1-dimensional floppy manifolds.

References


Figure S4: Rigid clusters for $n = 6$. Left, Mode 1 (polytetrahedron), Right, Mode 2 (octahedron). The table below shows which bonds to break to reach each floppy mode.

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