INTERACTING MANY-PARTICLE SYSTEMS OF DIFFERENT PARTICLE TYPES CONVERGE TO A SORTED STATE

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Abstract. We consider a model class of interacting many-particle systems consisting of different types of particles defined by a gradient flow. The corresponding potential expresses attractive and repulsive interactions between particles of the same type and different types, respectively. The introduced system converges by self-organized pattern formation to a sorted state where particles of the same type share a common position and those of different types are separated from each other. This is proved in the sense that we show that the property of being sorted is asymptotically stable and all other states are unstable. The models are motivated from physics, chemistry, and biology, and the principal investigations can be useful for many systems with interacting particles or agents. The models match particularly well a system in neuroscience, namely the axonal pathfinding and sorting in the olfactory system of vertebrates.

Key words. many-particle systems, gradient flows, stability, self-organization, pattern formation, neuroscience, olfactory system

AMS subject classifications. 37N25, 37C75, 82C22, 82C44, 92C15, 92C20

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1. Introduction. Many physical, chemical, and biological systems consist of an ensemble of interacting particles, species, or agents which is segregated into groups whose members have specific properties and fulfill certain functions. This can range from a microscopic level—for example, biomolecular units such as membrane proteins involved in cell signaling or phase separation of liquids—to a macroscopic level, comprising among others social populations and multibody systems. Depending on the system considered, interactions between agents within one group or between agents of different groups can affect, for example, the activity of the agents, resulting in an increase or a decrease of the activity, or the interactions may cause a change of affinity for a certain binding molecule. Further important examples are interactions influencing the acceleration and the velocity of moving particles. These interactions may also vary with time or with the configuration of the system.

There exists a broad literature on the topic of interacting many-particle systems. In statistical physics, equilibrium properties of ensembles are the quantities of interest (see, e.g., [27, 28]). Nonequilibrium situations and increased order can be observed in nature and comprise pattern formation due to self-organization in complex physical, chemical, and biological systems. Examples in physics can be found in [14, 15, 16, 33, 57], and those in chemical systems in [2, 9, 26, 32, 37, 42, 48, 49]. Well-known examples in biology are models for bacteria like myxobacteria [3, 41, 50, 51, 52]; cell sorting, a

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morphogenetic phenomenon which is the key to the ability of diverse cells to segregate
to form organized tissues and organs \[11, 44\]; ant colonies \[7, 13, 34, 35\]; and swarm
formation \[8, 10, 56\]. Other interdisciplinary applications range from pedestrian mod-
els \[17, 18, 19\] to distributed robotics \[1, 12, 31, 36, 47, 54\]. One major focus of research
is, for example, the relationship between stochastic many-particle models and approx-
imating macroscopic description by partial differential equations \[38, 39, 40\]. In all
these given examples there is the common interest to find out whether the system is
able to self-organize, i.e., whether in some sense ordered states with a certain structure
emerge. The mathematical description of these structures can be more or less difficult.
In many cases a mode expansion with, e.g., Fourier modes turns out to be extremely
useful, as often just a small number of modes have to be considered to approximate
the systems with high accuracy (see, e.g., \[15, 16, 37\]). In the framework of linear sta-
bility analysis, the stability of the structures can then be determined by investigating
the stability of stationary solutions of the time-dependent mode coefficients. It has
to be mentioned that the stationary solutions are at fixed positions, which allows us
to use standard linear stability analysis. Often, it is possible to show a specific type
of behavior by utilizing, e.g., monotonicity of the vector fields \[20, 21, 22, 23, 24, 46\].
This standard linear stability analysis is not possible in the case investigated in the
present paper because the equilibrium positions of our system depend on the initial
values, and we are interested in the stability of certain sorting properties.

An impressive example of a self-organization process with emergence of a sorted
state can be observed in a field of biology, namely in physiology: In the olfactory
system of vertebrates which governs the sense of smell, a sorting process of great
complexity takes place. With numerous olfactory receptor neurons, animals detect
the various odorants of their surroundings (for example, a mouse has a few million
olfactory receptor neurons). They are located in the olfactory epithelium, a tissue
covered with mucus located above the nose. Long extensions of these neurons, called
axons, connect the olfactory epithelium with the olfactory bulb, a part of the brain
where the incoming signals are preprocessed before they are transmitted to the cor-
tex. The olfactory receptor neurons consist of groups of different types (about 1000
different types in the olfactory system of a mouse \[6\]), and the members of these types
are randomly distributed on the olfactory epithelium \[43, 53, 55\]. Growing towards
the bulb, the axons of the olfactory receptor neurons sort in such a way that the axons
representing the same receptor type converge onto the same site in the bulb. These
convergence sites are called glomeruli \[4, 5, 30, 45\]. That is, in summary, an initially
completely intermingled state in the olfactory system changes into a sorted state. It
should be stressed that the positions of the glomeruli, i.e., of the sorted groups, are
not fixed but depend on the initial positions of the receptor neurons in the olfactory
epithelium. The fact that the positions of the sorted groups are not fixed requires
a new approach to analyzing the sorted states of a mathematical model which can
reproduce this phenomenon.

In the present paper, a large system of interacting motile particles that can move
spatially in \(\mathbb{R}^2\) is studied, which respects the situation in the olfactory system if the
third dimension, i.e., the direction in which all axons are growing monotonously, is
identified with time. Nevertheless, it should be possible to extend our results to \(\mathbb{R}^N\).

The ensemble consists of particles belonging to groups of different types. The par-
ticles of different groups represent the axons of different receptor types. It is assumed
that, at the beginning, the positions of the particles are disordered, i.e., unsorted;
that is, particles of different type can be located next to each other. We focus on
the question of whether under certain conditions a self-organizing process can occur
during which the positions of the particles change from an initially totally intermingled, i.e., unsorted, state to a state of positions ordered by types. It is assumed that the interactions between two particles belonging to the same group are attractive, resulting in a decrease of the distance between them. Between particles belonging to different groups, repulsive interactions are assumed, resulting in an increase of the distance between them. Our results show that under certain conditions the considered model system reproduces the expected self-organization, i.e., the convergence to a sorted state. It has to be emphasized that the positions of particles ordered by types, constituting a sorted state, are not fixed but depend on initial positions of the particles. This prevents the application of standard procedures of linear stability analysis, namely the computations of fixed points and the linearization of the vector field around them. Instead, we show the stability of the property of being sorted. We say that a state displays the property of being sorted if particles representing different types are separated from each other by a certain distance, and particles of the same type either share the same position or are out of range of each other. Such states we also call semisorted states. To analyze the property of being sorted, we introduce a sorting score that measures for the semisorted states how many particles of the same type do not share the same position. It is shown that semisorted states are the only stable configurations. Furthermore, we show that the sorting score decreases only if the system is disturbed, which means that the sorting becomes better. With this tool we are able to show that the property of being sorted is asymptotically stable, and that all other states are unstable.

The paper is organized as follows. First, in the next section, the model is defined, and in section 3, we state our main result, which is proven in sections 3.1 and 3.2 and summarized in section 3.3. In section 4, two examples are given, while section 5 concludes the paper.

2. The model class considered. For the model class considered, which has the potential to generate the described sorting behavior, the following assumptions are made: It is assumed that there exist interactions between all particles, being effective over a certain distance. To bring particles of one group together, interactions between particles of the same group are assumed to be attractive. On the other hand, the positions of the different groups shall be separated at the end of the process; hence interactions between particles belonging to different groups are assumed to be repulsive.

The ensemble of $n = \sum_{k=1}^{m} n_k$ particles is divided into $m$ subgroups of size $n_k$ with $k \in \{1, \ldots, m\}$, each representing a certain type or character. No volume is assumed for the particles; i.e., they don’t exclude themselves spatially and can sit on top of each other.

The motion of one particle with position $x \in \mathbb{R}^N$ in a central interaction field that is induced by another particle can be described by
\[
\dot{x} = -V'(\|x\|) \frac{x}{\|x\|},
\]
with a sufficiently smooth potential function $V: \mathbb{R} \to \mathbb{R}$ and the Euclidean norm $\|\cdot\|$. We will later mainly focus on the case $N = 2$. Here, the prime is used to denote the derivative with respect to the distance, i.e., $V'(d) = \partial_d V(d)$, where $d = \|x\|$. For $\|x\| > 0$

\begin{align}
V'(\|x\|) > 0 \quad & \text{if the interaction field is attractive,} \\
V'(\|x\|) < 0 \quad & \text{if the interaction field is repulsive.}
\end{align}
Hereby, \( \|x\| \) describes the distance of the considered particle to the position of the other particle inducing the central interaction field which is shifted to the origin.

No external force field is assumed in our model which could direct all particles from group \( k \) to a point \( p_k \) for all \( k \); it is rather assumed that each particle generates a field of abstract interactions which all the other particles can sense. This will potentially induce the particles to self-organize and to converge to a sorted state. These interactions are to be effective only along the difference vector; hence, the interaction \( f_{ij} \) sensed by particle \( i \) regarding particle \( j \) is written as

\[
(2.3) \\
\quad f_{ij} = -V_{ij}'(d_{ij}) \frac{x_i - x_j}{d_{ij}} \quad \forall i \neq j
\]

and \( f_{ii} = 0 \). Hereby, the Euclidean distance \( d_{ij} \) between the positions of particle \( i \) and particle \( j \) is used, i.e.,

\[
\quad d_{ij} = \|x_i - x_j\| = \langle x_i - x_j, x_i - x_j \rangle^{\frac{1}{2}} = d(x_i, x_j).
\]

Then, the second part on the right-hand side of (2.3) is the normalized direction vector connecting position \( x_i \) and position \( x_j \). \( V_{ij} \) is a potential function with property (2.1) if particle \( i \) and particle \( j \) belong to the same group, and with property (2.2) if they belong to different groups. In the following, a potential function with property (2.1), i.e., an attractive potential, is denoted by \( V_+ \), and a potential function with property (2.2), i.e., a repulsive potential, is denoted by \( V_- \).

More specifically we require \( V_- : (0, \infty) \to \mathbb{R} \) to be \( C^2 \), and \( V_+ : [0, \infty) \to \mathbb{R} \) to be extendable to a \( C^2 \) function on an interval \( (-\epsilon, \infty) \ni 0 \), for some \( \epsilon > 0 \), such that

\[
(2.4) \\
\quad V_+(0) = 0 \quad \text{and} \\
(2.5) \\
\quad V_+''(0) > 0.
\]

Furthermore, we assume that the potentials have finite ranges:

\[
\quad r_+ := \sup\{r > 0| V_+'(r) \neq 0\} < \infty \quad \text{and} \quad r_- := \sup\{r > 0| V_-'(r) \neq 0\} < \infty.
\]

The reason for this assumption is that finite ranges are more realistic in biological systems. A repulsive potential with finite range avoids causing particles of different type to continue moving away from each other, as they would do otherwise. In summary, the derivatives of the potential function fulfill with the finite ranges above

\[
(2.6) \\
\quad V_+'(\|x\|) > 0 \quad \text{for} \quad 0 < \|x\| < r_+, \\
(2.7) \\
\quad V_-'(\|x\|) < 0 \quad \text{for} \quad 0 < \|x\| < r_-.
\]

For convenience, we will assume later that

\[
(2.8) \\
\quad V_+(0) = 0, \\
(2.9) \\
\quad \inf_{r > 0} V_-(r) = 0.
\]

These will be the standing assumptions on the interaction potentials throughout the paper. Please refer to section 4 for examples of the interaction potentials and for corresponding plots in Figures 4.1, 4.2, 4.4, and 4.5 for illustration.
To simplify the notation when referring to the different groups of particles, the following sets are introduced:

\[ I = \{1, \ldots, n\}, \text{ the set of all particles}, \]

\[ I_k \subseteq I, \text{ the set of particles of type } k, \quad \bigcup_{k=1}^{m} I_k = I, I_k \cap I_{k'} = \emptyset \quad \forall k \neq k'. \]

We will let \( n_k := |I_k| \) denote the number of particles of type \( k \), and also use \( \tau : I \to \{1, \ldots, m\} \) to denote the function which maps a particle index to the type this particle belongs to.

Summation of all interactions acting on a particle \( i \) yields the equation of motion of this particle:

\[ \dot{x}_i = \sum_{j=1}^{n} f_{ij} = \sum_{j=1, j \neq i}^{n} -V'_{ij}(d_{ij}) \frac{x_i - x_j}{d_{ij}}. \]

Hence, the ODE system for all particles can be written as

(2.10) \[ \dot{x} = F(x), \]

where \( x = (x_1, \ldots, x_n)^T \in \mathbb{R}^N \) and

\[ x(0) = (x_1(0), \ldots, x_n(0))^T \in \mathbb{R}^N \setminus \mathcal{T} \quad \text{with} \]

\[ \mathcal{T} := \{ x \in \mathbb{R}^N | \exists i, j \text{ with } \tau(i) \neq \tau(j) \text{ and } x_i = x_j \} \]

being the set of states where repulsive particles are on top of each other. The right-hand side is \( F = (F_1, \ldots, F_n)^T \in C^1(\mathbb{R}^N \setminus \mathcal{T}, \mathbb{R}^N) \) with components \( F_i = \sum_{j=1, j \neq i}^{n} -V'_{ij}(d_{ij}) \frac{x_i - x_j}{d_{ij}}. \)

Using the notation introduced above, \( F_i \) for (2.10) can be written as

(2.11) \[ F_i = \sum_{j \in I_{\tau(i)}} -V'_{ij}(d_{ij}) \frac{x_i - x_j}{d_{ij}} + \sum_{j' \in I \setminus I_{\tau(i)}} -V'_{ij'}(d_{ij'}) \frac{x_i - x_j'}{d_{ij'}}. \]

In general we assume that

(2.12) \[ \lim_{r \to 0} V_-(r) = \infty, \]

but bounded potentials could be considered as well if one takes care of the initial energy of the system to avoid having repulsive particles going through each other.

To summarize, we assume the dynamical system model (2.10) with (2.11) and that the attractive potentials satisfy (2.4), (2.5), (2.6), (2.8) and the repulsive potentials fulfill (2.7), (2.9), (2.12).

It is important to remark that introducing the total energy

(2.13) \[ E(x) := \frac{1}{2} \sum_{i,j=1}^{n} V_{ij}(d_{ij}) \]

and using \( \nabla d_{ij} = \frac{\partial d_{ij}}{\partial x_i} = \frac{x_i - x_j}{d_{ij}} \) for the \( i \)th \( N \)-dimensional component, we can also write (2.10) as

(2.14) \[ \dot{x} = -\nabla E(x), \]

where \( \nabla \) is the usual gradient on \( \mathbb{R}^N \).

In the following, we restrict our analysis to the case \( N = 2 \), but most results are also true without any changes for higher dimensions.
3. Proof of the convergence to a sorted state. In this section we turn to the question of whether our model is able to reproduce the desired property of a self-organized transition from an unsorted into a sorted state where particles of the same type share a common position and particles of different types are separated from each other.

Under certain technical conditions on the interaction potentials given later in Theorem 3.8 we are able to prove that the system converges to a sorted state, which is the main result of the present paper. First, we formulate the main result in general words.

**Theorem 3.1 (main result, nontechnical).** The solution of the many-particle system (2.10) with arbitrary initial conditions (where particles of different type are not on top of each other) converges for large times to a completely sorted or so-called semisorted state where particles of different type are spatially separated from each other and several clusters of particles of the same type could coexist. These clusters of particles of the same type could merge due to a perturbation of the system but could not split up into further subclusters, which means that the grade of sorting can only improve.

The key point of our results is to prove convergence to a sorted state by using a characterization by a so-called sorting score rather than by specific positions of the particles, as they will vary for each sorted state depending on initial conditions.

The proof of convergence is carried out in the following steps. First note that we can restrict our analysis to stationary solutions, as the $\omega$-limit set of a solution to (2.10) consists only of stationary points. This is due to the fact that (2.10) is a gradient descent flow (see (2.14) and, e.g., [25]) and trajectories are bounded because of finite interaction ranges. In the second step we show that the property of being sorted is asymptotically stable, i.e., that the considered particle system converges to completely sorted or semisorted states where particles of different type are separated from each other and several clusters of particles of the same type could coexist. By defining the sorting score, we prove that such clusters consisting of particles of the same type could merge due to a perturbation of the system but could not split up into further subclusters. In other words, with the sorting score we show that the grade of sorting can only improve. This is done in section 3.1. In the third and last step, which can be found in section 3.2, we show that every unsorted stationary point of (2.10) is unstable. Section 3.3 collects all our results and summarizes them in Theorem 3.9, which is a more technical reformulation of Theorem 3.1.

3.1. Stability of sorted states. This section provides the details on the stability part of Theorem 3.1.

**Definition 3.2.** Define a sorted group to be a subset $G \subset I_k$ such that

$$d(x_i, x_j) = 0 \quad \forall i, j \in G,$$

and such that $G$ is maximal with respect to this property. A state $x \in \mathbb{R}^{2n}$ is said to be semisorted if

$$d(x_i, x_j) \geq r_+ \quad \text{if } i, j \in I_k \text{ belong to different sorted groups},$$

i.e., particles of the same type belonging to different sorted groups are separated by a distance of at least $r_+$, and

$$d(x_i, x_j) \geq r_- \quad \text{if } \tau(i) \neq \tau(j),$$

i.e., particles of different type are separated by a distance of at least $r_-$. 


We also define the sorting score $\sigma(x)$ of a semisorted state to be

$$
\sigma(x) = \sum_{k=1}^{m} \sum_{i,j \in I_k} (1 - \delta(x_i, x_j)),
$$

where $\delta(x, y) = 1$ if $x = y$ and $\delta(x, y) = 0$ if $x \neq y$. A state which is not semisorted is called unsorted.

With this definition we get for a semisorted state $x \in \mathbb{R}^{2n}$ a partition of each index set $I_k = \bigcup_{i=1}^{g_k} G_k^i$ and thus a partition of the total index set $I = \bigcup_{k=1}^{m} \bigcup_{i=1}^{g_k} G_k^i$, where $g_k$ is the number of sorted groups for particles of type $k$. It follows that $\sigma(x) = 0$ for the best possible sorting. Therefore, a completely sorted state is defined as a semisorted state with $\sigma(x) = 0$. The maximum of $\sigma(x)$ is reached for a state where each group consists of exactly one particle. Combinatorically, for each type, the term

$$
\sum_{i,j \in I_k} (1 - \delta(x_i, x_j))
$$

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$$
\sum_{i,j \in I_k} (1 - \delta(x_i, x_j))
$$

in the definition of $\sigma$ is proportional to the mean distance of a point configuration, where $n_k$ points are distributed on a subset of $n_k$ points in a metric space where all distances are equal.

For convenience we have assumed in section 2 that $V_+(0) = 0$ and $\inf_{r > 0} V_-(r) = 0$. The latter is due to the finite interaction ranges equivalent to $V_-(r) = 0$ for $r \geq r_-$. We will write $V_{\max} := \sup_{r > 0} V_+(r)$, which is equal to $V_+(r)$ for $r \geq r_+$. Then the minimum of the total energy, defined in (2.13), reached at a completely sorted state is $\min_{x \in \mathbb{R}^{2n}} E(x) = 0$. We will use

$$
\mathcal{S} := E^{-1}(0) := \{x \in \mathbb{R}^{2n} | E(x) = 0\}
$$

to denote the set of completely sorted states.

**Lemma 3.3.** The total energy $E(x)$ of a semisorted state is strictly increasing as a function of the sorting score; in fact, for semisorted states $x, y \in \mathbb{R}^{2n}$,

$$
\sigma(x) > \sigma(y) \implies E(x) \geq E(y) + V_{\max}.
$$

**Proof.** Since $V_+(0) = 0$ and $\inf_{r > 0} V_-(r) = 0$, the total energy in a semisorted state is proportional by a factor of $V_{\max}$ to the number of pairs of particles of the same type that are separated by a distance of at least $r_+$. The sorting score $\sigma(x) > \sigma(y)$ means that the number of such pairs is greater in the state $x$ than in $y$. It can also be observed that in a semisorted state the total energy is proportional by a factor of $\frac{1}{2} V_{\max}$ to the sorting score. □

**Proposition 3.4.** If every unsorted state is unstable, then sorting is asymptotically stable in the sense that for each semisorted state $x$ there is some neighborhood $U_x$ around $x$ such that for each solution $y(t)$ with $y(0) \in U_x$ the only possible stable equilibrium $y^*$ in the $\omega$-limit set of $y(t)$ is a semisorted state with at least as good sorting as $x$:

$$
\sigma(y^*) \leq \sigma(x).
$$

**Proof.** Take $U_x$ to be $E^{-1}([0, E(x) + V_{\max}))$. Then Lemma 3.3 applies. □

This description is used to capture the situation where different sorted groups of particles of the same type merge after a perturbation and end up in a state with a better sorting score.

**Theorem 3.5.** The property of being a completely sorted state, i.e., $y$ semisorted and $\sigma(y) = 0$, is asymptotically stable in the sense that there is some neighborhood $U$ of $\mathcal{S}$ such that the $\omega$-limit set of any solution $x(t)$ with $x(0) \in U$ is in $\mathcal{S}$. Furthermore,
the neighborhood $U$ can be selected so that, for any solution starting in $U$, the size function of a type of particles

\begin{equation}
L_{k}(x(t)) := \sum_{i \in I_{k}} \|x_{i} - \bar{x}_{k}\|^2
\end{equation}

is strictly decreasing towards zero for every $k \in \{1, \ldots, m\}$. Here $\bar{x}_{k} = \frac{1}{n_{k}} \sum_{i \in I_{k}} x_{i}$ denotes the center of mass of the particles of type $k$.

This means that a perturbed completely sorted state will converge to the set of completely sorted states again in such a way that the geometric size (3.2) of each group is constantly decreasing.

Proof. For each $I_{k}$ we consider the time derivative of the size function $L_{k}(x(t))$ which is used as a Lyapunov function in a similar way as in [29]:

\begin{equation}
\frac{d}{dt} L_{k}(x(t)) = 2 \sum_{i \in I_{k}} \langle x_{i} - \bar{x}_{k}, \dot{x}_{i} - \dot{\bar{x}}_{k} \rangle
\end{equation}

\begin{align}
&= \frac{2}{n_{k}^{2}} \sum_{i,l,m \in I_{k}} \langle x_{i} - x_{l}, \dot{x}_{i} - \dot{x}_{m} \rangle \\
&= \frac{1}{n_{k}} \sum_{i,l \in I_{k}} \langle x_{i} - x_{l}, \dot{x}_{i} - \dot{x}_{l} \rangle \\
&= \frac{1}{n_{k}} \sum_{i,l \in I_{k}, j \in I} \langle x_{i} - x_{l}, f_{ij} - f_{ij} \rangle \\
&= \frac{1}{n_{k}} \left( \sum_{i,l,j \in I_{k}} \langle x_{i} - x_{l}, f_{ij} \rangle + \sum_{i,l,j \in I_{k}, l \notin I_{k}} \langle x_{i} - x_{l}, f_{ij} - f_{ij} \rangle \right) \\
&= \frac{1}{n_{k}} \left( \sum_{i,l,j \in I_{k}} \langle x_{i} - x_{l}, f_{ij} \rangle + \sum_{i,l,j \in I_{k}} \langle x_{i} - x_{l}, f_{ij} \rangle + \sum_{i,l,j \in I_{k}, l \notin I_{k}} \langle x_{i} - x_{l}, f_{ij} - f_{ij} \rangle \right) \\
&= \sum_{i,l \in I_{k}} \langle x_{i} - x_{l}, f_{il} \rangle + \frac{1}{n_{k}} \sum_{i,l \in I_{k}, j \in I \setminus I_{k}} \langle x_{i} - x_{l}, f_{ij} - f_{ij} \rangle \\
&= \sum_{i,l \in I_{k}} \left( x_{i} - x_{l} - V'_{i}(d_{il}) \frac{x_{i} - x_{l}}{d_{il}} \right) \\
&\quad + \frac{1}{n_{k}} \sum_{i,l \in I_{k}, j \in I \setminus I_{k}} \left( x_{i} - x_{l} - V'_{ij}(d_{ij}) \frac{x_{i} - x_{j}}{d_{ij}} + V'_{ij}(d_{ij}) \frac{x_{i} - x_{j}}{d_{ij}} \right) \\
&= \sum_{i,l \in I_{k}} -V'_{i}(d_{il})d_{il} + \frac{1}{n_{k}} \sum_{i,l \in I_{k}, j \in I \setminus I_{k}} \left( x_{i} - x_{l} - V'_{ij}(d_{ij}) \frac{x_{i} - x_{j}}{d_{ij}} + V'_{ij}(d_{ij}) \frac{x_{i} - x_{j}}{d_{ij}} \right). \tag{d}
\end{align}

Here, we used

\[
\sum_{i,l,m} \langle x_{i} - x_{l}, g_{im} \rangle \quad \text{with} \quad g_{im} = -g_{mi}
\]

\[
= \sum_{i,l,m} \langle x_{i}, g_{im} \rangle - \sum_{i,l,m} \langle x_{l}, g_{im} \rangle
\]
\begin{align*}
&= \sum_{l} \left( \sum_{i,m} (x_{i}, g_{im}) \right) - \sum_{l} \left( x_{l} \sum_{i,m} g_{im} \right) \\
&= \frac{\eta_{k}}{2} \sum_{i,m} \left( (x_{i}, g_{im}) + (x_{m}, g_{mi}) \right) + 0 \\
&= \frac{\eta_{k}}{2} \sum_{i,m} \langle x_{i} - x_{m}, g_{im} \rangle
\end{align*}

for (3.3a) and (3.3c).

We would like to remark that (3.3b) shows that the size function \( L_k \) is equal to 
\[ \frac{1}{n_k} \sum_{i,j} \| x_i - x_j \|^2. \]

We will now determine the sign of (3.3d). Due to the assumption \( V'_+ \geq 0 \), the first term in (3.3d) is clearly nonpositive and bounded in absolute value from below by

\begin{equation}
\left| \sum_{i,j \in I_k} -V'_+(d_{ij}) d_{ij} \right| \geq V'_+(r_{k_1}^{\max}) r_{k_1}^{\max} = V''_+(\xi_k)(r_{k_1}^{\max})^2
\end{equation}

for some \( \xi_k \in (0, r_{k_1}^{\max}) \) using the mean value theorem, since we have assumed that \( V_+ \) is \( C^2 \) close to 0. Here we are interested in small

\[ r_{k_1}^{\max} := \max_{i,j \in I_k} d_{ij}. \]

For \( j \in I \setminus I_k \) let \( \nu_j(x) := \frac{x - x_j}{\| d(x, x_j) \|} \) denote the direction vector field pointing away from \( x_j \). The second term in (3.3d) can be bounded in absolute value from above by

\begin{align*}
\frac{1}{n_k} \left| \sum_{i,j \in I_k, j \in I \setminus I_k} \langle x_i - x_l, -V'_+(d_{ij}) \nu_j(x_i) + V'_+(d_{ij}) \nu_j(x_l) \rangle \right| \\
\leq \frac{1}{n_k} \sum_{i,j \in I_k, j \in I \setminus I_k} r_{k_1}^{\max} \| -V'_+(d_{ij}) \nu_j(x_i) + V'_+(d_{ij}) (\nu_j(x_i) + D\nu_j |_{x_i}(x_l - x_i) + O(d_{ij}^2)) \| \\
\leq \frac{1}{n_k} \sum_{i,j \in I_k, j \in I \setminus I_k} r_{k_1}^{\max} \left( |V'_+(d_{ij})| - |V'_+(d_{ij})| \right) \\
&\quad + |V'_+(d_{ij})| \left( \| D\nu_j |_{x_i}(x_l - x_i) \| + O((r_{k_1}^{\max})^2) \right).
\end{align*}

Clearly, we can put a bound on the operator norm of the derivative \( D\nu_j |_{x_i} \) of \( \nu_j \) evaluated at \( x_i \) by a lower bound on \( d(x_i, x_j) \). Such a lower bound on distances between repulsive particles can be provided by an upper bound on the total energy; if \( E(x) < \varepsilon \), then for \( \tau(i) \neq \tau(j) \) one obtains \( d_{ij} > r_\varepsilon - \delta \) for some \( \delta > 0 \). Choosing \( \varepsilon \) small enough will then force \( \delta \) to be small. This uniform lower bound on the distances \( d_{ij} > R = r_\varepsilon - \delta \) for different types of particles then provides an \( \alpha(R) > 0 \) such that

\[ \| D\nu_j |_{x_i}(x_l - x_i) \| \leq \alpha(R) \| x_l - x_i \| \leq \alpha(R)r_{k_1}^{\max}. \]

The uniform lower bound for \( d_{ij} \) also provides an upper bound for

\[ A(x) := \max_{i,j \in I, \tau(i) \neq \tau(j)} |V'_+(d_{ij})| \]

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since $V'_-(r_-) = 0$. Also we can estimate $|V'_j(d_{ij}) - V'_j(d_{ij})|$ as
\[ |V'_j(d_{ij}) - V'_j(d_{ij})| = |V''(\zeta_{ij})(d_{ij} - d_{ij})| \leq |V''(\zeta_{ij})| r_{k}^{\max} \]
for some $\zeta_{ij}$ between $d_{ij}$ and $d_{ij}$ since $V_-$ is $C^2$. All in all, we can bound (3.5) by
\[ \frac{1}{n_k} \sum_{i \in I_k, j \in I \setminus I_k} (|V''(\zeta_{ij})| + A(x)\alpha(R))(r_{k}^{\max})^2 + O((r_{k}^{\max})^3). \]

Just as $A(x)$ is bounded above by a lower bound on $d_{ij}$, $\tau(i) \neq \tau(j)$, then so is $|V''(\zeta_{ij})|$, since $V''_-(r_-) = 0$ and $V_-$ is $C^2$, so we can make the coefficient to $(r_{k}^{\max})^2$ arbitrarily small. Since $V'''(0) > 0$ it follows from (3.4) that for sufficiently small energy $E(x)$ and sufficiently small $r_{k}^{\max} > 0$, the first term in (3.3d) will dominate and $\frac{d}{dt}L_k(x(t)) < 0$.

The maximal distance in a group $r_{k}^{\max}$ can also be controlled in terms of the energy; clearly a sufficiently small upper bound on $E(x)$ forces an upper bound on $r_{k}^{\max}$ for each $k$, since $V(x)$ is monotonically increasing for small $r$.

In summary, there exists a $\delta_1 > 0$ such that there is a neighborhood $U$ with sufficiently small energy
\[ S \subset U := E^{-1}([0, \delta_1]) \]
which is positively invariant under the flow since the energy is decreasing, and such that for each $k \in \{1, \ldots, m\}$, $\frac{d}{dt}L_k(x(t)) < 0$ for any solution in $U$ with $L_k(x(t)) > 0$.

By finiteness of ranges, any solution $x(t)$ is bounded and thus has an $\omega$-limit set. In the case of bounded repulsive potentials, this is also true if the initial energy is sufficiently low. An $\omega$-limit of a solution to a gradient flow system must be a critical point; cf., e.g., [25]. It then follows from the discussion of the time derivative of $L_k(x(t))$ that the $\omega$-limit set of a solution starting in $U$ must be a critical point in $E$, and hence of (2.10), with $L_k(z) = 0$ for each $k \in \{1, \ldots, m\}$. However, such a state can clearly be a critical point only if all the sorted groups are out of range, i.e., $z \in S = E^{-1}(0)$.

\[ \Box \]

**3.2. Instability of unsorted states.** In the following we will prove a result on the instability of unsorted states, under specific conditions on the potentials.

For a fixed $q \in \mathbb{R}^2$, the Hessian of a function of the type $\phi : p \mapsto V(d(p, q))$, is considered as a quadratic form,
\[ \text{hess}_p (v, v) = V''(r) \langle v, \nabla r \rangle^2 + \frac{V'(r)}{r} \langle \dot{v}, \nabla r \rangle^2. \]

Here $v$ is a vector in $\mathbb{R}^2$, $\dot{v}$ is the counterclockwise rotation of $v$ by an angle of $\frac{\pi}{2}$ (i.e., $iv$, when considering $\mathbb{R}^2$ as $\mathbb{C}$), and we use $\nabla r = \frac{d}{d(p, q)}$. We also introduce the shorthand notation $r = d(p, q) = \langle p - q, p - q \rangle^{\frac{1}{2}}$ and $\nabla r = \frac{d}{d(p, q)}$ for the direction vector from $q$ to $p$.

The Laplacian of $\phi$ is then
\[ \Delta \phi(p) = \text{trace hess}_p (v, v) = V''(r) + \frac{1}{r}V'(r), \]
again with $r = d(p, q)$.

For the interaction between two particles $x_i, x_j \in \mathbb{R}^2$ we will use
\[ \text{hess}_{x_i, x_j}^{i,j} \]
to denote the Hessian of the function \( x_i \mapsto V_{ij}(d_{ij}) \), where \( d_{ij} = d(x_i, x_j) \) and \( V_{ij} \) is either \( V \) or \( V^* \).

Notice that \( \text{hess}^{i,j}_{x_i,x_j} = \text{hess}^{j,i}_{x_j,x_i} \).

To simplify notation, we use the convention \( \text{hess}^{i,j}_{x_i,x_j} = 0 \) and also write \( \Delta V_{ij}(d_{ij}) = V''_{ij}(d_{ij}) + \frac{1}{d_{ij}} V'_i(d_{ij}) \) for the Laplacian of the function \( x_i \mapsto V_{ij}(d_{ij}) \), since this depends only on the distance \( d_{ij} \).

We will consider a perturbation vector \( v = \sum_{i=1}^n v_i = (w_1, w_2, \ldots, w_n) \in \mathbb{R}^{2n} \), decomposed such that

\[
v_i = (0, 0, \ldots, w_i, 0, \ldots, 0)
\]

is the perturbation of the \( i \)th particle. That is, each two-dimensional coordinate of \( v_i \) is zero except for the \( i \)th coordinate, which is \( w_i \in \mathbb{R}^2 \).

The Hessian of the energy \( E(x) := \frac{1}{2} \sum_{i,j=1}^n V_{ij}(d_{ij}) \) is then as a quadratic form on \( \mathbb{R}^{2n} \)

\[
\text{hess}^E_x(v, v) = \text{hess}^E_x \left( \sum_{i=1}^n v_i, \sum_{i=1}^n v_i \right) = \sum_{i,j=1}^n \text{hess}^E_x(v_i, v_j).
\]

One can verify that, with the notation introduced in (3.7), we can write this as

\[
(3.8) \quad \sum_{i,j=1}^n \text{hess}^E_x(v_i, v_j) = \sum_{i,j=1}^n \text{hess}^{i,j}_{x_i,x_j}(w_i, w_i) - \sum_{i,j=1}^n \text{hess}^{i,j}_{x_i,x_j}(w_i, w_j)
\]

\[
(3.9) \quad = \frac{1}{2} \sum_{i,j=1}^n \text{hess}^{i,j}_{x_i,x_j}(w_i - w_j, w_i - w_j),
\]

where \( w_i := \pi_i(v_i) \) is the nonzero component of \( v_i \). The first term in (3.8) corresponds to the \( 2 \times 2 \)-block diagonal terms \( \left[ \frac{\partial^2 E_x}{\partial x_k \partial x_l} \right]_{k,l=1,\ldots,2} \) of the matrix representation of the Hessian. Formula (3.9) reflects the translation invariance of the energy; moving points \( x_i, x_j \) with velocity vectors \( w_i, w_j \) is like moving one of the points with velocity vector \( w_i - w_j \).

We will denote the convex hull of a set \( X \subseteq \mathbb{R}^2 \) by \( \text{hull}(X) \). The following simple lemma is fundamental.

**Lemma 3.6.** Let \( f : (0, \infty) \to \mathbb{R} \) be a smooth injective function, and let \( X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^2 \) be a finite configuration of points. Define \( V(p) := \sum_{i=1}^n f(d(p, x_i)) \). Then for \( p \notin X \) the line through \( p \) with direction \( \nabla V(p) \) intersects the convex hull of \( X \).

**Proof.** We have

\[
(3.10) \quad \nabla V(p) = \sum_{i=1}^n f'(d(p, x_i)) \frac{p - x_i}{d(p, x_i)}.
\]

Let \( x_i, x_j \) be such that the angle \( \cos^{-1} \left( \langle \frac{x_i - p}{d(p, x_i)}, \frac{x_j - p}{d(p, x_j)} \rangle \right) \) is maximal. Then clearly, since \( f' \) will have the same sign everywhere, each term in (3.10) points into the same half of the closed cone spanned by the direction vectors \( \frac{x_i - p}{d(p, x_i)} \) and \( \frac{x_j - p}{d(p, x_j)} \). Thus the sum \( \nabla V(p) \) points into this half cone, and the line through \( p \) with direction vector \( \nabla V(p) \) must intersect \( \text{hull}(X) \). Note that the line between \( x_i \) and \( x_j \) is contained in \( \text{hull}(X) \). \( \square \)
**LEMMA 3.7.** Let a finite set $X \subset \mathbb{R}^2$ of cardinality $n$ consist of $m$ disjoint subsets, $X = \bigcup_{i=1}^{m} X_i$, and suppose that the distance between each pair of these subsets satisfies $d(X_i, X_j) \geq r$. There is an $\alpha_n \in (0, 1]$, depending on $n$, such that

$$\max_{i=1,\ldots,m} \left\{ \max_{x \in X_i} d(x, \text{hull}(X \setminus X_i)) \right\} \geq \alpha_n r.$$  

**Proof.** Let $Y = \partial \text{hull}(X) \cap X$; i.e., $Y$ consists of the extremal points of the convex hull of $X$. Then $Y$ is the set of vertices of a convex $n_1$-gon, with $n_1 \leq n$.

Choose an orientation of the boundary of the $n_1$-gon spanned by $Y$, via an ordering of the vertices, and let $\alpha_i$ be the turning angle at the vertex $x_i$, $i = 1, \ldots, n_1$, i.e., the angle between exterior normals to the edges meeting at $x_i$. Then $\sum_{i=1}^{n_1} \alpha_i = 2\pi$. Thus either $\alpha_i = \frac{2\pi}{n_1}$, $i = 1, \ldots, n_1$, or

$$\max_{i=1,\ldots,n_1} \alpha_i > \frac{2\pi}{n_1}.$$  

Let $x_i \in Y \cap X_i$ be a vertex of maximal turning angle $\alpha_i > \frac{2\pi}{n_1} \geq \frac{2\pi}{n}$.  

Now, either the point closest to $x_i$ in $\text{hull}(X \setminus X_i)$ is a vertex, in which case the distance is at least $r$, or the closest point is on an edge between two vertices $x_k, x_l \in X \setminus X_i$. In the latter case, $d(x_i, \text{hull}(X \setminus X_i))$ is the altitude from $x_i$ in the triangle with vertices $x_i, x_k, x_l$. The edges emanating from $x_i$ have length at least $r$, and the interior angle $\beta_i$ at $x_i$ is at most

$$\beta_i \leq \pi - \alpha_i \leq \pi - \frac{2\pi}{n} = \pi \left(1 - \frac{2}{n}\right).$$  

By elementary trigonometry, we observe that

$$\alpha_n = \cos \left(\frac{\pi}{2} \left(1 - \frac{2}{n}\right)\right)$$  

will satisfy the requirement. \qed

Figure 3.1 illustrates the geometric significance of the number $\alpha_n$ in Lemma 3.7. As is seen from the proof, the “worst-case scenario” for obtaining the desired bound is when all points are located as the vertices of a regular $n$-gon. The number $\alpha_n$ is then given as the altitude from a vertex (onto the convex hull of the other vertices) in a regular $n$-gon. Figure 3.1 shows this situation—here eight particles, divided into two subgroups of four particles, are located as the vertices of a regular 8-gon.

**THEOREM 3.8.** Consider a dynamical system of $n$ particles of $m$ different types in $\mathbb{R}^2$, as described above, given by

$$\dot{x} = -\nabla E(x),$$  

where $E(x) := \frac{1}{2} \sum_{i,j=1}^{n} V_{ij}(d_{ij})$. Suppose that there exists a radius $r_1 > 0$ such that

$$\Delta V_-(r) = V_n''(r) + \frac{1}{r} V'_n(r) < -\left(\max_{k \in \{1,\ldots,m\}} (n_k - 1)(n - n_k)\right) \left(\sup_{s > 0} \Delta V_-(s)\right)$$  

for $r < r_1$, and such that the range of $V_+$ is small compared to $r_1$, specifically:

$$\frac{\alpha_n r_1}{r_+} > \max_{k \in \{1,\ldots,m\}} n_k.$$  

Then the only possible stable critical points are semisorted states.
Fig. 3.1. Illustration of Lemma 3.7 in the situation where we have two disjoint groups of particles.

Proof. The idea of the proof is to show that stability of an equilibrium forces particles of different types to be separated by at least a distance of $r_1$. We can then apply Lemma 3.7 to find a particle such that its distance to the convex hull of the particles of different type is at least $\alpha_n r_1$. Finally, we will use the condition on the ratio between the range $r_1 + r_+$ and $r_1$ to show that we have not got enough particles to support such an equilibrium when the repulsive interactions are still in range.

Now suppose that $x \in \mathbb{R}^{2n}$ is an equilibrium configuration. If there is a perturbation vector $v \in \mathbb{R}^{2n}$ such that

$$hess_x E(v, v) < 0,$$

then $x$ is not a local minimum of $E$ and $x$ is an unstable equilibrium; cf., e.g., [25]. Assume that some particles of different types, say $x_\alpha, x_\beta$, have distance $d_{\alpha \beta} < r_1$, $\tau(\alpha) := k_1 \neq \tau(\beta) := k_2$. We can choose a perturbation vector

$$v_w = (w_1, w_2, \ldots, w_n) \in \mathbb{R}^{2n}$$

such that $w_i = w$ for $i \in I_{k_1}$ and $w_i = 0$ otherwise. This corresponds to a translation of the particles of type $k_1$. The only nonvanishing terms of the Hessian of the energy with this perturbation are the terms involving only the type $k_1$ particles and then the repulsive interactions with the other groups of particles. Using expression (3.9), we get

$$hess_x E(v_w, v_w) = \frac{1}{2} \sum_{i,j=1}^{n} hess^{ij}_{x_i,x_j} (w_i - w_j, w_i - w_j)$$

$$= \sum_{i \leq n_{k_1}, j \geq n_{k_2} + 1} hess^{ij}_{x_i,x_j} (w, w),$$

since $w_i = w$ for $i \in I_{k_1}$ and 0 otherwise. Thus, by the translation invariance of the system, the Hessian of the attractive interactions between the type $k_1$ particles is vanishing with such a perturbation.
If we take the mean over all \( w \in S^1 \subset \mathbb{R}^2 \), we obtain

\[
(3.14) \quad \frac{1}{2\pi} \int_{S^1} \text{hess}_x^E(v_w, v_w)dw = \sum_{i \leq n_{k_1}, j \geq n_{k_2} + 1} \frac{1}{2} \text{trace}\left(\text{hess}_{x_i(x_j)}^{ij}\right) = \frac{1}{2} \sum_{i \leq n_{k_1}, j \geq n_{k_1} + 1} \Delta V_{-}(d_{ij}).
\]

By assumption, one of the terms in the sum, \( \Delta V_{-}(d_{\alpha\beta}) \), is so large negative that it dominates a possible positive contribution not greater than

\[
(n_{k_1} - 1)(n - n_{k_1}) \sup_{r > 0} \Delta V_{-}(r).
\]

It follows that the expression (3.14) is negative, and hence there will be some directions \( w \in S^1 \) for which \( \text{hess}_x^E(v_w, v_w) < 0 \). Thus the equilibrium is unstable.

So, if \( x \) is a stable equilibrium, groups of particles of different types must be separated by a distance of \( r_1 \). Now consider the subset \( J \subseteq I \) consisting of indices of particles where some repulsive interaction is in range, i.e., \( J := \{ i \in I | \exists j : \tau(i) \neq \tau(j), \quad d(x_i, x_j) < r_+ \} \). If \( J \neq \emptyset \), it follows that there exists a particle, say \( x_\alpha, \alpha \in I_k \cap J \), whose distance to hull(\( \bigcup_{l \in J \setminus l_k} \{ x_i \}) \) is at least \( \alpha r_1 \). Let \( p \in \text{hull}(\bigcup_{l \in J \setminus l_k} \{ x_i \}) \) be the point which is closest to \( x_\alpha \), let

\[
v = \frac{x_\alpha - p}{\| x_\alpha - p \|} \in S^1
\]

be the direction vector from \( p \) to \( x_\alpha \), and let \( L \) be the line orthogonal to \( v \) through \( p \). Then \( d(x_\alpha, L) \geq \alpha r_1 \) and \( L \) divides \( \mathbb{R}^2 \) into two open half planes, one of them, say \( H_1 \), containing \( x_\alpha \), and the closure of another one, \( H_2 \), containing hull(\( \bigcup_{l \in J \setminus l_k} \{ x_l \} \)).

Since the repulsive interaction determined by the particles \( \bigcup_{l \in J \setminus l_k} \{ x_l \} \) is directed away from hull(\( \bigcup_{l \in J \setminus l_k} \{ x_l \} \)) outside the convex hull, it is now clear that for any point \( q \in H_1 \) the total repulsion \( F_{-}(q) = \sum_{j \in J \setminus l_k} -V'(d(q, x_j)) \frac{q-x_j}{\|q-x_j\|} \) has a positive projection onto \( v \), \( \langle v, F_{-}(q) \rangle > 0 \), whenever \( F_{-}(q) \) is nonzero.

Now, for any point \( x_i \in \bigcup_{l \in I_k \cap J} \{ x_l \} \cap H_1 \), where the repulsive interactions are in range, there must be another point \( x_j \in \bigcup_{l \in I_k} \{ x_l \} \cap H_1 \) such that \( d(x_i, x_j) < r_+ \); otherwise the attractive interaction on \( x_i \) cannot cancel out the repulsive interaction on \( x_i \). Suppose that there is some \( x_i \in \bigcup_{l \in I_k} \{ x_l \} \cap H_1 \setminus B(L, r_+) \) such that \( d(x_i, L) \) is minimal and such that some attractive interaction is in range, where \( B(L, r_+) \) denotes an \( r_+ \)-neighborhood of \( L \). Then, clearly, the attractive interaction on \( x_i \) would have a positive projection onto \( v \), and thus the attractive and a possible repulsive interaction on \( x_i \) could not cancel out. It follows that we have a sequence of points of type \( k = \tau(\alpha) \), with separation less than \( r_+ \), extending from \( x_\alpha \) to an \( r_+ \)-neighborhood of \( L \). But this is impossible by the criterion on the maximum number of particles of the same type.

We have now excluded stable critical points, where repulsive interactions are in range. Clearly the only other possibility is then a semisorted state. \( \square \)

Remark. The bound on the ratio of the ranges \( r_1, r_+ \) used in the theorem is not optimal. It is definitely possible to obtain better bounds depending on the type number tuple \( (n_1, \ldots, n_k) \).

This provides the final details to prove our main result stated in Theorem 3.1 and given in more detail in the following in Theorem 3.9.
3.3. The main theorem and summary of the results. The above achievements allow us to reformulate the main result already given in Theorem 3.1, now with more technical details.

**Theorem 3.9 (technical version of Theorem 3.1).** The \( \omega \)-limit set of a solution of (2.10) consists only of stationary points. Under the assumptions on the interaction potentials given in Theorem 3.8, every unsorted stationary point of (2.10) is unstable. Furthermore, the property of being sorted is asymptotically stable in the sense that for each semisorted state \( x \) there is some neighborhood \( U_x \) around \( x \) such that for each solution \( x(t) \) with \( x(0) \in U_x \) the only possible stable equilibrium \( y \) in the \( \omega \)-limit set of \( x(t) \) is a semisorted state with at least as good sorting as \( x \):

\[
\sigma(y) \leq \sigma(x),
\]

where \( \sigma \) is the sorting score defined in (3.1).

This implies immediately that a completely sorted state, i.e., \( x \) semisorted and \( \sigma(x) = 0 \), is asymptotically stable.

4. Examples. In this section we give two sets of examples for the potential functions \( V_-(r) \) and \( V_+(r) \). The first one fulfills the conditions under which Theorem 3.1 holds. The second one violates these conditions to demonstrate that the sorting properties are very robust with respect to the technical assumptions. We consider a specific case with 60 particles divided into four groups of size \( n_k = 15 \), but the example can easily be adapted to other particle numbers as well.

4.1. Potentials fulfilling the assumptions needed for the proof. Consider the repulsive potential

\[
V_-(r) = \begin{cases} 
- \log\left(\frac{r}{\pi} + \arctan(\log(r))\right) + a_1, & r < r_-, \\
-a_2 \exp\left(-a_3 \frac{(r-r_-)^4}{4}\right) + a_2, & r_- \leq r \leq r_-, \\
0, & r > r_. \end{cases}
\]

We choose \( r_- := 100 \) and solve for the other constants to ensure that the function is \( C^2 \). This results in the following approximate values:

\[
a_1 \approx 1.0681501107543880397,
\]

\[
a_2 \approx 2.058632061311512352 \cdot 10^{-2},
\]

\[
a_3 \approx 2.398238886527602273 \cdot 10^{-7}.
\]

The Laplacian \( \Delta V_-(r) = V_-'(r) + \frac{1}{r} V_''(r) \) fulfills

\[
\sup_{r > 0} \Delta V_-(r) \approx 0.40566728618254025807,
\]

and if we choose \( r_1 \leq 0.13 \), we have

\[
\Delta V_-(r) < -0.41(n_k - 1)(n - n_k) 
\]

for \( r \leq r_1 \)

with \( n = 60 \) and \( n_k = 15 \), which ensures that (3.12) of Theorem 3.8 is fulfilled. The graph of \( V_-(r) \) can be seen in Figure 4.1.

Consider furthermore the attractive potential

\[
V_+(r) = \begin{cases} 
 b_1 r^2, & r < r_2, \\
 b_2 \exp\left(-b_3 \frac{(r-r_2)^4}{4}\right) + b_4, & r_2 \leq r < r_+, \\
 V_{\text{max}} = \text{const.}, & r \geq r_+.
\end{cases}
\]
Here $b_1$ is a parameter used to vary the strength of the attraction. If we solve the $C^2$ conditions for the other constants, we get

$$b_2 = \frac{2(r_+ - r_2)r_2^2b_1}{\exp(-\frac{2r_2 + r_+}{4r_2})(2r_2 + r_+)};$$

$$b_3 = \frac{2r_2 + r_+}{r_2(r_2 - r_+)^3},$$

$$b_4 = b_1r_2^2 - b_2 \exp \left(-b_3 \frac{(r_2 - r_+)^4}{4}\right).$$

We choose the parameters as follows:

$$b_1 = 10^{11},$$

$$r_+ = \cos \left(\frac{\pi}{2} \left(1 - \frac{2}{n}\right)\right) \frac{r_1}{n_k} - 10^{-7},$$

$$r_2 = \frac{r_+}{2}.$$

The choice of $r_+$ ensures that condition (3.13) is fulfilled. The graph of $V_+(r)$ can be seen in Figure 4.2.

In Figure 4.3, a simulation with 60 particles, divided into four groups of the same size, can be seen. After sorting has taken place, the sorted groups will converge to the sorted equilibrium where repulsive interactions are out of range.

**4.2. Potentials violating the assumptions needed for the proof.** The sorting properties are very robust with respect to the technical assumptions (3.12) and (3.13) which are made throughout the paper and under which Theorem 3.1 holds. To demonstrate this we will give a second example of a system showing self-organized sorting with potentials violating these assumptions.
Fig. 4.2. Attractive potential $V_+(r)$ (see (4.2)).

Fig. 4.3. Simulation with 60 particles, divided into four groups of the same size. Particles of the same type are plotted in the same color. Potential functions (4.1) and (4.2) are used as described above. The initial values of the particles are random positions in $[0, 10^{-5}] \times [0, 10^{-5}]$. The simulation clearly visualizes the convergence to a sorted state.

A simple choice for the repulsive potential is

$$V_-(r) = a/r,$$

where the parameter

$$a = 1.0 \cdot 10^{-16}$$
was chosen for the numerical simulation. The graph of $V_-(r)$ is plotted in Figure 4.4.

The attractive potential was chosen as

\begin{equation}
V_+(r) = b_1/(1 + \exp(-b_2(r^2 - b_3)))
\end{equation}

with parameters

\begin{align*}
b_1 &= 1.0, \\
b_2 &= 1.0 \cdot 10^2, \\
b_3 &= 1.0 \cdot 10^{-2}.
\end{align*}

This potential has some sigmoidal shape with zero derivative for $r = 0$. The graph of $V_+(r)$ is shown in Figure 4.5.
For both the repulsive and the attractive potential, the conditions of finite ranges are only approximately fulfilled, as the derivative of the potential function gets arbitrarily close to zero from a certain range onwards.

A simulation result with the total number of particles $n = 60$ and the size of the subgroups $n_k = 15$, using the potential functions (4.3) and (4.5) which violate the assumptions (3.12) and (3.13), is shown in Figure 4.6. This demonstrates that the sorting properties are not sensitive to a particular choice of the attractive and repulsive potentials as long as a reasonable choice is made for the ranges. This suggests that the presented self-organized sorting should be observable also in particle systems of application areas where the particular shape of the repulsive and the attractive potential varies.

5. Summary and discussion. This paper demonstrates that complex sorting of particles of different types can be obtained by a simple model based on attraction between particles of the same type and repulsion between particles of different types. The desired results for the model based on a gradient flow are obtained by specific conditions on the interaction potentials. This was done by using Lyapunov functions and instability arguments via the Hessian of the energy.

The stability part of our main result already works for a very large class of potentials, and it might be possible to generalize also the instability results to a larger class of potentials (which include, e.g., Lennard-Jones potentials) and to extend the findings to higher spatial dimensions.

The sorting score of the final state of the system certainly depends on the ratio of the diameter of the initial positions to the range and also on the relative magnitude...
of the interactions between the particles.

The sorting properties of the particles were demonstrated and visualized also with numerical simulations for two different examples representing cases where the assumptions of our proof were fulfilled as well as violated. The latter case shows nevertheless sorting which demonstrates how robust the self-organized sorting is with respect to variations in the particle interactions.

In order to get a more realistic model for the axonal pathfinding in the olfactory system, several further features would have to be included, like limited lifetime of axons or geometric constraints from the olfactory system. Until today, the experimental findings in the field of olfactory mapping still cannot determine the detailed interactions between axons of the same type and between those of different types. The results of the present paper contribute to the process of understanding this system in more detail by showing that sorting is indeed possible just by assuming particle interactions where the sorting emerges as self-organization and no “supervised” guidance mechanism is needed.

Even though a simplified model has been used for the olfactory system, our results reproduce well the experimental findings of sorted axon species and demonstrate nicely how complex behavior like sorting can emerge from simple model assumptions.

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REFERENCES


