Stripe, gossamer, and glassy phases in systems with strong nonpairwise interactions

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We study structure formation in systems of classical particles in two dimensions with long-range attractive short-range repulsive two-body interactions and repulsive three-body interactions. Stripe, gossamer, and glass phases are found as a result of nonpairwise interaction.

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I. INTRODUCTION

The problem of stripe and cluster formation is important in a wide range of physical systems, ranging from soft matter [1–3] to hard condensed matter [4,5] and magnets [6], to name a few. A case of stripe formation which has been especially widely investigated is systems of particles with competing multiscale two-body interactions. In the context of superconductivity, a multiscale long-range attractive short-range repulsive interaction is possible between vortices in multicomponent type-1.5 superconductors [7] (for a review see Ref. [8]). The recent experimental claims of stripe and gossamer phases of vortex matter in superconductors [9–11] prompted theoretical investigations of whether or not such structure formation of vortex matter in multiband superconductors is possible (see, e.g., Refs. [12–15]).

Intervortex potentials with short-range repulsive long-range attractive pairwise interaction only allow formation of simple clusters in equilibrium situations. In Ref. [12] the question was raised if, in principle, stripe phases can occur as a result of nonpairwise intervortex forces. The calculated three-body intervortex forces in type-1.5 superconductors are repulsive [12,16] and can certainly be sufficiently strong to result in stripe formation for kinetic and entropic reasons. However, since accurate calculations of intervortex many-body forces in field theory is highly computationally demanding, they have been investigated in only a small number of cases.

Here we ask the following more general question: what kind of unconventional ordering patterns can occur in systems with repulsive nonpairwise interactions? Previous studies of the structural effects of nonpairwise interactions have shown that for a short-range attractive, long-range repulsive pairwise interaction, an attractive or repulsive nonpairwise interaction had little effect for the ranges studied [17]. In Ref. [18] it was reported that repulsive pairwise and attractive nonpairwise interactions have been found to cause clustering of particles under certain conditions. The works [19,20] simulated driven crystal phases in two-dimensional systems with three-body forces. We investigate a model of point particles, with long-range attractive short-range repulsive two-body interaction, and repulsive three-body interaction. We will investigate the structure formation of such a system by tuning the relative strength of the two- and three-body interactions, as well as temperature and particle density. We will demonstrate that the system possesses a rich variety of pattern formation such as stripe, gossamer, and glassy phases.

II. MODEL

Consider particles interacting with a pairwise potential which is repulsive at short particle separation and attractive at longer separation, such that there is a preferred separation between two particles. In the case of three particles with such a pairwise interaction, the ground-state configuration will occur when the particles form an equilateral triangle, with a line constituting an energetically excited state. In the case of many particles, the tendency of three particles to form a triangle will favor a hexagonal symmetry of the structure formation. In this paper we will begin by considering how the ground state of three particles is changed by adding a repulsive nonpairwise interaction upon the two-body interaction and we will then show how the nonpairwise interaction affects the structure formation in systems of many particles. As we will see, the ground state of three particles will for a sufficiently strong three-body repulsion, be that of a straight line instead of a triangular configuration, a tendency which will cause a variety of structural phases in systems of many particles.

The total interaction potential energy $U(\boldsymbol{X})$ of N classical point particles with two-body and three-body interactions in the state $\boldsymbol{X} = \{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N\}$, is in general given by

$$U(\boldsymbol{X}) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} u_{2\mathrm{B}}(\boldsymbol{r}_i, \boldsymbol{r}_j) + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \sum_{k=j+1}^{N} u_{3\mathrm{B}}(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}_k), \tag{1}$$

where $u_{2\mathrm{B}}$ corresponds to the pairwise two-body interaction (which we take to be long-range attractive and short-range repulsive) and $u_{3\mathrm{B}}$ corresponds to the nonpairwise three-body interaction (taken to be purely repulsive). We model the pairwise interaction $u_{2\mathrm{B}}$ of two particles i, j as a sum of Gaussians:

$$\frac{u_{2\mathrm{B}}(r_{ij})}{\varepsilon_{2\mathrm{B}}} = e^{-ar_{ij}^2} - be^{-c(r_{ij}-d)^2}, \tag{2}$$

where $\varepsilon_{2\mathrm{B}}$ is a parameter that determines the strength of the interaction, and $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$ is the distance between particles i and j.

The three-body interaction potential of three particles i, j, k is modeled by

$$\frac{u_{3\mathrm{B}}(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}_k)}{\varepsilon_{3\mathrm{B}}} = f(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}_k) + f(\boldsymbol{r}_j, \boldsymbol{r}_i, \boldsymbol{r}_k) + f(\boldsymbol{r}_k, \boldsymbol{r}_i, \boldsymbol{r}_j), \tag{3}$$

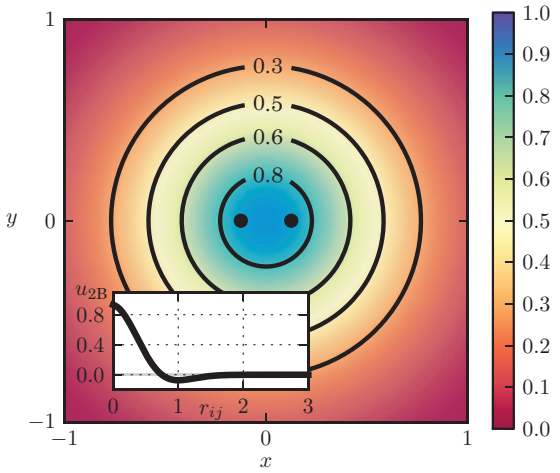

FIG. 1. (Color online) Depiction of the model studied. The contour plot is of the three-body interaction energy experienced by a particle with position $\boldsymbol{r} = (x,y)$ by two other particles fixed at positions $\boldsymbol{r}_1 = (-0.125,0)$, $\boldsymbol{r}_2 = (0.125,0)$ (indicated by black dots), i.e., a plot of $f(\boldsymbol{r},\boldsymbol{r}_1,\boldsymbol{r}_2)$ with f defined in Eq. (4). The model parameters are $\varepsilon_{3B} = 1.0$, $\alpha = 2.0$, $w = 0.8$. The inset shows the two-body interaction potential (2) against particle separation with $\varepsilon_{2B} = 1.0$, $a = 3.0$, $b = 0.2$, $c = 3.0$, and $d = 0.60$.

where the function f is a two-dimensional Gaussian:

$$f(\boldsymbol{r}_i,\boldsymbol{r}_j,\boldsymbol{r}_k) = e^{-\alpha[(x_i-R_x)^2+(y_i-R_y)^2]-\ell^2/w^2}, \tag{4}$$

where $\boldsymbol{R} = (R_x,R_y) = (\boldsymbol{r}_j + \boldsymbol{r}_k)/2$ is the center of mass of the pair (j,k), $\ell = |\boldsymbol{r}_j - \boldsymbol{r}_k|$ is the distance between the particles (j,k), and α, w are model parameters which characterize the range of the interaction. In Fig. 1 we plot the potentials for a set of parameters that will, unless otherwise stated, be used throughout this article. These potentials have a quite similar form as multiband intervortex potentials in type-1.5 superconductors [12,16].

III. SIMULATION METHOD

We investigate structure formation of the system by using the Metropolis Monte Carlo (MC) algorithm [21] with parallel tempering [22,23]. Our system is considered to be a fixed number of N particles inside an $L \times L$ box so that the density $\rho = N/L^2$. We impose periodic boundary conditions by the minimum image convention [24]. We take a MC trial move to be a displacement of a randomly chosen particle by a randomly chosen distance in a random direction.

In order to quantitatively assess the tendency of the system to form a stripe phase, we define the parameter

$$\Psi_S = \left| -1 + \frac{1}{N}\sum_{i=1}^{N}\left|\sum_{j=1}^{2}\exp(i2\phi_{ij})\right|\right|, \tag{5}$$

where the sum in j runs over the two nearest neighbors of particle i, and ϕ_{ij} is the angle of the line joining the particles, with respect to an arbitrary axis. The parameter is constructed such that it is unity if three particles form a straight line and vanishes if the particles form an equilateral triangle. For many particles, Ψ_S is unity if they form several straight lines, or close to unity if they form curved and/or intersecting lines.

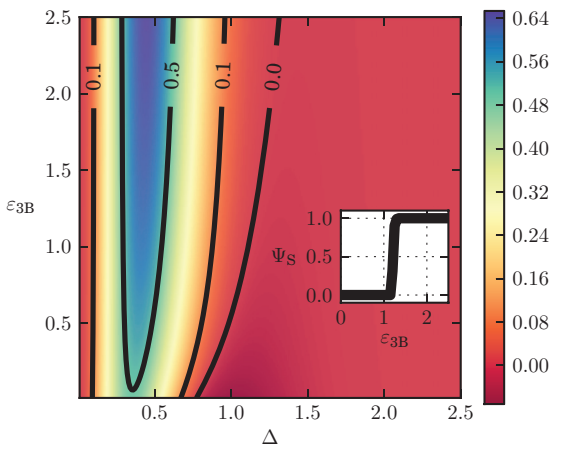

FIG. 2. (Color online) The existence of a stripe phase for $N = 3$. Displayed is the difference ΔE of an equilateral triangle of side Δ and a straight equidistant line with spacing Δ, as a function of Δ and ε_{3B}. In the region to the left, where $\Delta E > 0$, the three-body repulsion is sufficiently strong to cause the system to energetically favor a line over a triangle. The inset confirms this by showing the ground-state value of Ψ_S versus ε_{3B} obtained from MC simulations with three particles, where the ground state is obtained by slow cooling.

IV. RESULTS

We begin by considering the simplest relevant case of a particle triplet, $N = 3$, and demonstrate that, at a certain critical strength of the three-body interaction, it becomes energetically favorable for the particles to align in a straight equidistant line rather than an equilateral triangle. We compare the two cases by computing the total interaction energy of an equilateral triangle with sides Δ, as well as for a straight equidistant line with spacing Δ. We plot the difference $\Delta E = (E_{\text{triangle}} - E_{\text{line}})/(\varepsilon_{2B} + \varepsilon_{2B})$ as a function of particle spacing Δ and ε_{3B}, shown in Fig. 2. As is seen, there is a region in which the line configuration is energetically favorable, which is also confirmed with the MC simulation shown in the inset of Fig. 2. As can be checked from Eq. (5), for $N = 3$ the parameter Ψ_S is exactly unity for a straight line, and exactly zero for the case of an equilateral triangle. In the MC simulation three particles were given random initial positions and their ground-state configuration was determined by slowly cooling the system to $T = 0$. The ground-state value of Ψ_S is then calculated from the final $T = 0$ configuration. For each ε_{3B}, the cooling simulation was repeated several times from which the average Ψ_S was computed.

We now proceed to consider larger systems and the effect of the strength of the three-body interaction. MC simulation snapshots for several values of ε_{3B} are shown in Fig. 3 where the same transition into a stripe phase as in the three-particle case of Fig. 2 is seen [see Fig 3(e)]. As one increases ε_{3B} from zero, at first the main effect is to increase the mean nearest-neighbor distance of the particles [see inset in Fig. 3(a)], amounting to only a quantitative and not qualitative difference in the structure formation, as the preferred number of nearest neighbors of a given particle is still six. For the values $\varepsilon_{3B} = 0.0, 1.0$ [Figs. 3(a) and 3(b)], the two-body interaction dominates and enforces a hexagonal symmetry. However, when ε_{3B} surpasses a critical value predicted by the results

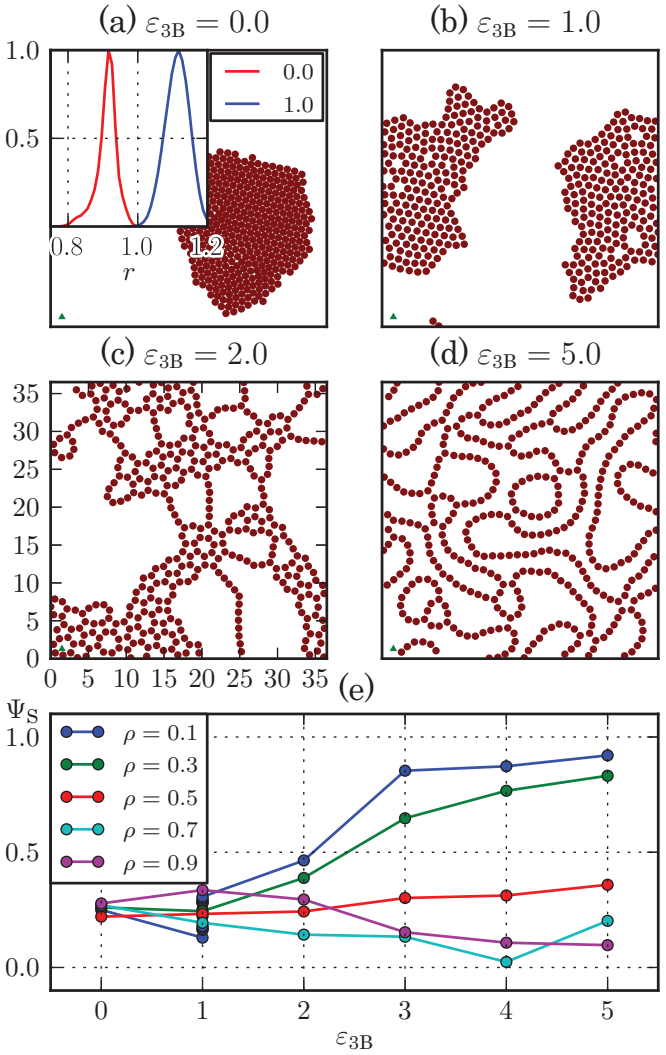

FIG. 3. (Color online) By increasing the three-body interaction strength ε_{3B}, various phases are induced in systems of many particles. Displayed in panels (a)–(d) are structure formation for increasing ε_{3B} at constant density $\rho = 0.3$ with $N = 400$. Panel (e) shows how Ψ_S depends on the strength of the three-body interaction for various densities. The inset of (a) shows normalized distributions of nearest-neighbor distances for the cases $\varepsilon_{3B} = 0.0$ and $\varepsilon_{3B} = 1.0$. For comparison, the green triangle in the lower-left corner of panels (a)–(d) has side equal to the minimum separation of the two-body potential.

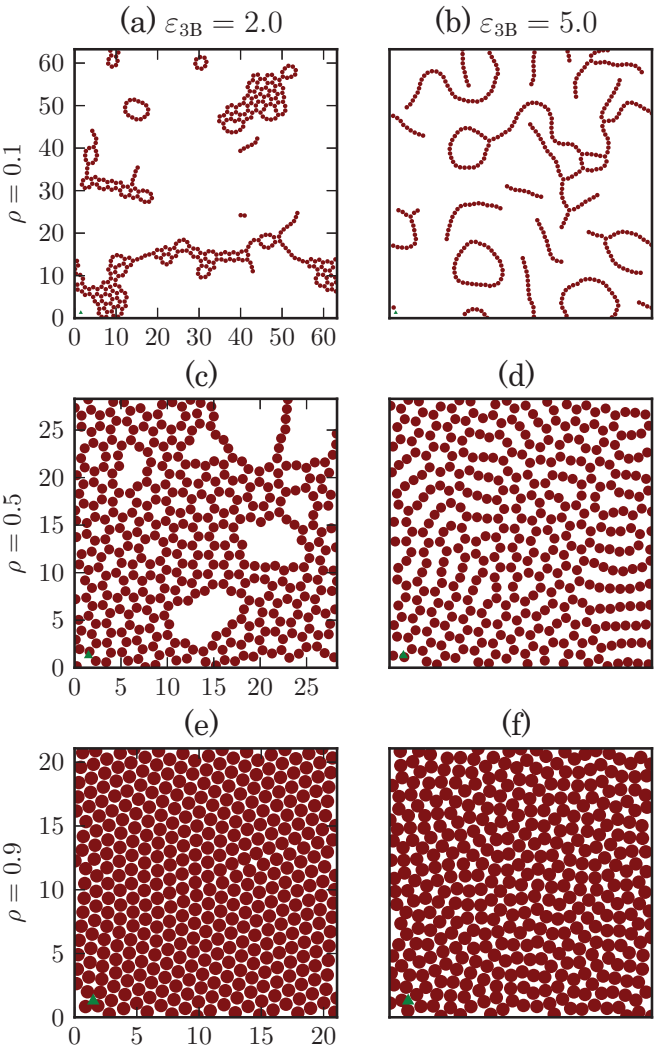

FIG. 4. (Color online) By increasing density for the case of competing two-body and three-body interactions (left column) and a dominating three-body interaction (right column), various structural phases are obtained. Here $N = 400$.

of Fig. 2, there is a qualitative change as the system will first form a gossamer structure for $\varepsilon_{3B} = 2.0$ [Fig. 3(c)], where the system prefers particle bonds with only three nearest neighbors due to a competition of the two- and three-body interactions. Further increasing the nonpairwise repulsion to $\varepsilon_{3B} = 5.0$ [Fig. 3(d)], a filamentary stripe structure formation appears as the system prefers having only two nearest neighbors due to a domination of the three-body interaction. We also note in Fig. 3(e) that the stripe phase can only arise at low densities where there is room for the particles to spread into their filamentary structures.

Consider now the effects of increasing density for the cases $\varepsilon_{3B} = 2.0$ [where there is competition between the two-body interaction and the three-body interaction; see Fig. 3(c)], and $\varepsilon_{3B} = 5.0$ [where the three-body interaction dominates; see Fig. 3(d)]. Results are given in Fig. 4. For the case $\varepsilon_{3B} = 2.0$ (left column) the gossamer-like clusters will, when increasing density, be pushed together into a hexagonal lattice. For the case $\varepsilon_{3B} = 5.0$ (right column) the filamentary stripe structures will first be squeezed into a gossamer structure, where the pressure forces some particles to accept having three nearest neighbors rather than the preferred value of two. Further increasing the density enhances this frustration and creates a disordered state—a tendency we will investigate in the next paragraph.

By comparing Figs. 4(e) and 4(f), it is evident that at high densities a relatively weak three-body repulsion yields a symmetric lattice and a strong three-body interaction a structurally disordered state. This suggests that a strong nonpairwise repulsion creates a glassy phase at high densities in the sense that the system is very unlikely to find its ground state during a fast cooling [25]. We investigate this by performing long simulations with parallel tempering to find a structurally

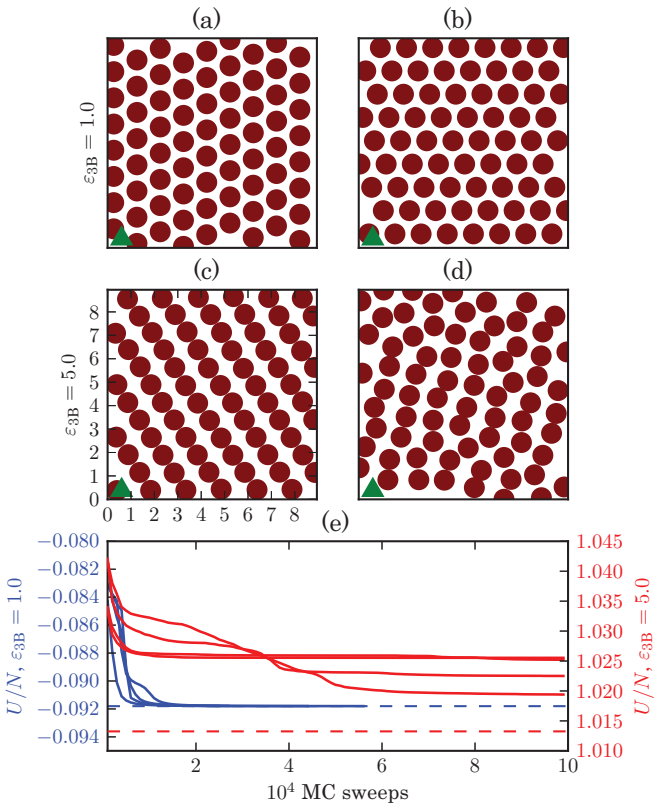

FIG. 5. (Color online) A glassy phase occurs for a strong three-body repulsion at high density. Here $\rho = 0.9$ with $N = 72$. Panels (a) and (b) show configurations for $\varepsilon_{3B} = 1.0$ obtained by parallel tempering and fast cooling, respectively. Panels (c) and (d) are for $\varepsilon_{3B} = 5.0$. Panel (e) shows the evolution of the total internal energy per particle during four fast-cooling simulations for each system, with ground-state energies obtained by parallel tempering shown with dashed lines.

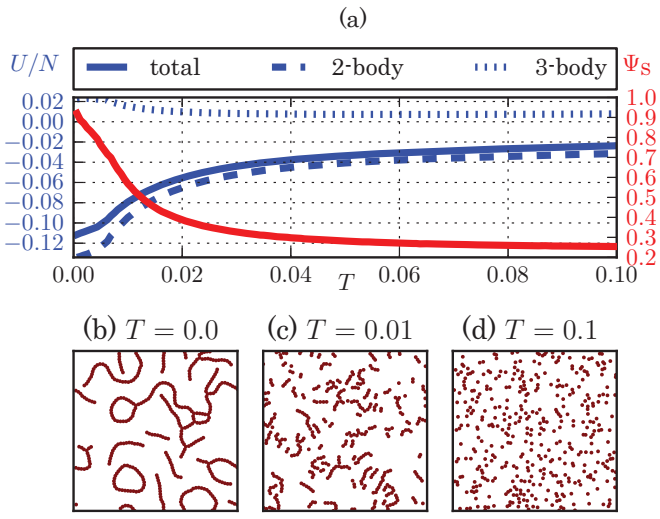

FIG. 6. (Color online) Thermal effects of the stripe phase. Here $\varepsilon_{3B} = 5.0$, $\rho = 0.1$ with $N = 400$. Displayed in panel (a) are the thermally averaged total internal energy U per particle N (with two- and three-body contributions as dashed and dotted lines, respectively) and Ψ_S against temperature T. The lower panels are three snapshots of the system in the low-, intermediate-, and high-temperature phases.

symmetric ground state and compare with states obtained from a $T = 0$ MC simulation from a random initial configuration (which we consider to be a fast cooling). Results are given in Fig. 5. As seen in Fig. 5(e), the system converges to the ground state in the case of fast cooling for $\varepsilon_{3B} = 1.0$, indicating a nonglassy system. However, for $\varepsilon_{3B} = 5.0$, fast cooling simulations consistently fail to produce the ground state. Thus a glassy phase occurs for strong nonpairwise repulsion at high densities, as the particles experience frustration preventing them to find their ground state, which enforces disorder in the structure formation of the system.

Next, we consider melting properties of the stripe phase where the system is dilute and has strong three-body interactions. As seen in Fig. 6, the system undergoes a melting transition as temperature is increased, associated with the loss of stripe ordering quantified by Ψ_S. When increasing temperature, individual particles can dissociate from their stripes, causing the chains to be broken and shorter on average,

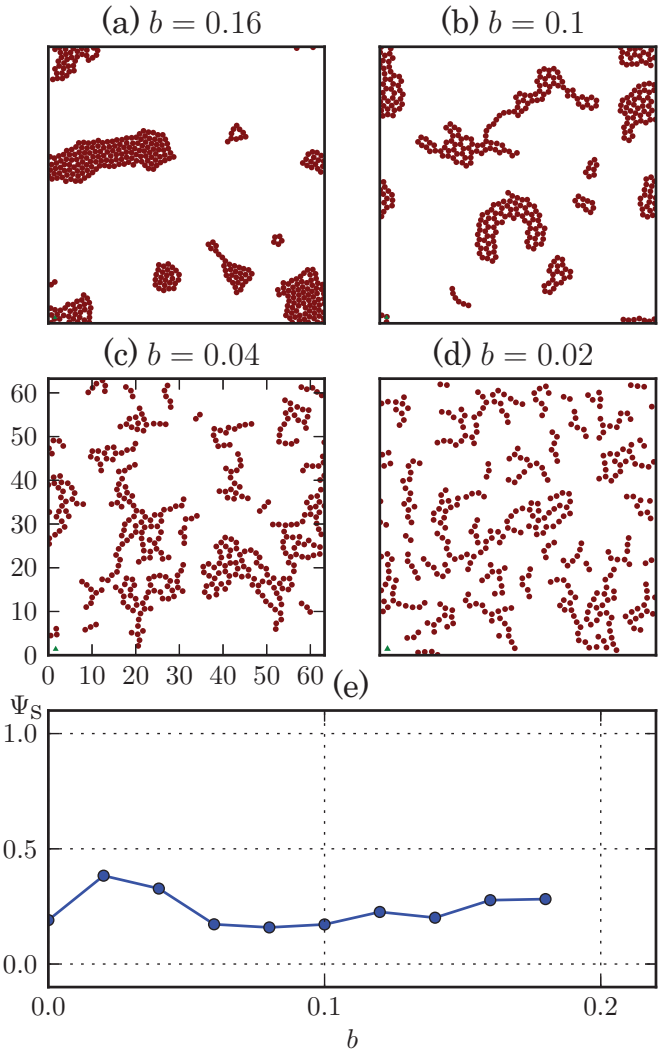

FIG. 7. (Color online) Decreasing the two-body minimum by decreasing the parameter b does not induce a clear stripe phase for the parameters studied. Panels (a)–(d) show structure formation for $\rho = 0.1$, $N = 400$, $\varepsilon_{3B} = 1.0$, when decreasing b. Panel (e) shows how Ψ_S depends on b.

as seen in Fig. 6(c), a process which continues until the system is melted [see Fig. 6(d)]. In the melted phase the three-body contribution to the total interaction energy diminishes and almost vanishes [see Fig. 6(a)].

Finally, rather than varying the strength of the three-body interaction ε_{3B} we consider decreasing the depth of the minimum of the two-body potential characterized by the parameter b in Eq. (2), while keeping the strength of the three-body interaction constant. Results are given in Fig. 7. Decreasing the minimum b amounts to a weaker long-range attraction of the particles and can change the structure formation by creating voids, as seen in Fig. 7(b), or stripe-like tendencies as seen in Figs. 7(b), 7(c), and 7(d). However, no clear stripe phase [compare with Fig. 4(b)] with a significantly high value of Ψ_S occurs, as seen in Fig. 7(e). In the stripe phase, the two-body interaction is what binds the particles in the chains, which means that, as the long-range attraction of the two-body interaction weakens, the particles in the chains become less tightly bound, which in turn counteracts the tendency of the three-body interaction to cause a stripe phase.

V. CONCLUSIONS

In conclusion, we have demonstrated that for a system of classical particles in two dimensions with a two-body short-range repulsive long-range attractive interaction favoring clustering with hexagonal symmetry, an additional repulsive three-body interaction can significantly alter the structure formation. The form of the potentials which we investigated is inspired by the form of interaction between vortices in type-1.5 superconductors. For weak three-body repulsions, the difference is only quantitative as the mean nearest-neighbor separation of the particles becomes larger, but a sufficiently strong three-body repulsion can cause a qualitative change as the system enters new phases. In the stripe phase, the ground state of a triplet is a straight equidistant line rather than an equilateral triangle; a tendency which can be quantified by the parameter Ψ_S defined in Eq. (5). When varying the relative strengths of the pairwise and nonpairwise potentials, three phases are found: one where the pairwise interaction dominates which yields hexagonal symmetry in the structure formation, one where the nonpairwise interaction dominates which yields a stripe phase, and one phase where there is competition between the pairwise and nonpairwise interactions, which yields a phase of gossamer structure formation. At high densities, a strong nonpairwise interaction causes glassy behavior of the system as the particles experience frustration and will not easily find their ground state.

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