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Dynamics and Directional Locking of Colloids on Quasicrystalline Substrates

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ABSTRACT

Recently it has been shown that novel colloidal orderings can occur on fivefold and sevenfold quasicrystalline substrates created with optical arrays. Using numerical simulations we examine the types of dynamical phases that arise for colloidal and other types of particles driven over quasicrystalline substrates. We find that even though the substrate has no translational order, directional locking effects can occur in which the particles lock to certain orientational symmetry directions of the substrate as the applied drive is rotated. We also find dynamical commensuration effects where the magnitude of the locking undergoes oscillations as a function of the ratio of the number of particles to the number of pinning sites. We also find that the dynamical structures formed by the particles are markedly different for different driving directions and include disordered states, partially ordered triangular lattices, and anisotropic Archimedean type ordering. The Archimedean type ordering was previously observed experimentally for particles on quasiperiodic substrates in the absence of a drive. We find that the dynamic locking is much more pronounced for fivefold substrates than for sevenfold substrates. We also discuss how our results relate to the dynamical ordering observed in vortices and colloids driven over periodic and random substrates.

Keywords: Colloid, optical traps, quasicrystalline

1. INTRODUCTION

Quasicrystals are interesting structures that have no translational ordering but still possess orientational ordering.[1,2] One of the best known examples is the fivefold Penrose tiling such as that shown in Fig. 1. Recently it was experimentally demonstrated for charged colloidal particles interacting with fivefold quasicrystalline substrates that a number of interesting ordering transitions can occur.[3–5] For strong substrates the colloids simply adopt the quasicrystalline ordering of the substrate. For weak substrates, the repulsive interactions between the colloids dominate and the colloids form a weakly pinned triangular lattice. At intermediate substrate strength the colloids form a novel Archimedean type structure where a tessellation of the colloid positions reveals a combination of triangular and square tiles. The Archimedean tiling has a quasi-one dimensional structure that can be aligned along any one of the five orientational ordering directions of the quasicrystalline array. Studies with sevenfold coordinated substrates generally produce quasicrystalline or partially disordered colloidal configurations.[6] There have also been several studies examining vortices in type-II superconductors with quasicrystalline arrays of pinning sites.[7,8] Vortices in superconductors have several similarities to charged colloids in that they repel each another and form a triangular lattice in the absence of a substrate. In the vortex system, a series of commensuration effects were observed as a function of vortex density.[7,8] Commensuration effects have been predicted and observed for vortex systems with square or triangular pinning arrays, when the effectiveness of the pinning is enhanced at magnetic fields where the number of vortices is an integer multiple or rational ratio of the number of pinning sites.[9–11] For a quasicrystalline pinning array, commensurate effects occur at integer matching fields; however, strong matching effects were also observed at fillings corresponding to the golden mean or rational fractions of the golden mean.[7,8]

Here we examine the dynamical structures that form when colloids and other particles are driven over fivefold and sevenfold quasicrystalline substrates. When vortices are driven over periodic square or triangular substrates, a rich variety of distinct dynamical phases are possible.[12–16] It would be interesting to see whether particles driven over quasicrystalline arrays exhibit similar dynamical effects or whether the dynamics would more strongly

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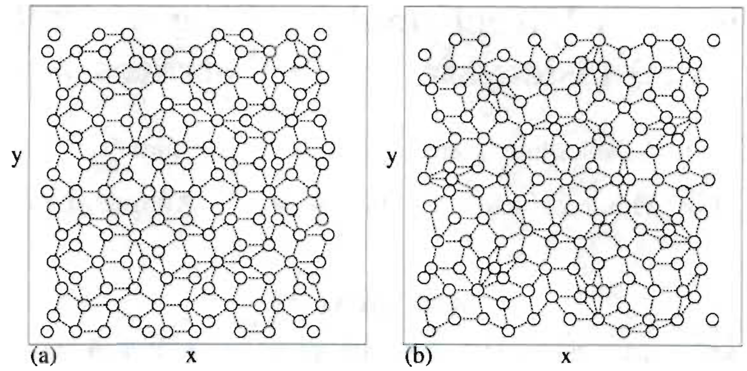

Figure 1. Locations of the pinning sites for (a) a fivefold coordinated substrate and (b) a sevenfold coordinated substrate.

resemble those of particles driven over random substrates due to the lack of translational order in the quasicrystalline substrates. One effect observed on periodic substrates is directional locking of driven particles when the direction of the external drive is rotated with respect to the substrate.[17–25] In the absence of a substrate the particles simply move in the direction of the external force; however, on a periodic substrate the particles lock to certain substrate symmetry directions. This locking occurs for a range of external drive angles so that a plot of the average velocity versus drive angle contains a series of steps corresponding to the locked motion. For a square array, locking occurs for $\theta = \tan^{-1}(m/n)$, with m and n integers. The steps appear at $(m, n) = (0, 1)$ or 0°, (1,1) or 45°, (1,2) or 22.5°, and so forth.[17,18] The largest steps correspond to the smallest values of m and n. Directional locking was initially proposed for vortices moving over square and triangular pinning arrays where a series of steps with a devil's staircase structure was predicted.[17] A similar series of steps was also predicted for a triangular pinning array at $\theta = \tan^{-1}(\sqrt{3}m/(2n+1))$, with m and n integers. Here the most prominent lockings occur at 0°, 30°, and 60°.[17] In the initial work on vortices it was proposed that directional locking should occur generally in other systems including colloids moving over optical trap arrays. Directional locking was later observed experimentally for colloids moving over a square array of optical traps when the trap array was rotated with respect to the external drive direction.[18] Since then, there have been a wide range of studies of directional locking in colloidal systems. One application of the effect is in particle separation, where a lateral separation can be achieved when one species of colloid locks to a symmetry direction of the substrate but the other species moves in the direction of the external drive.[19–21,23,24]

Directional locking effects can occur in the single or non-interacting particle limit; however, when interactions are present it was shown in the initial vortex work that a variety of novel dynamical structures occur such as disordered phases between the locking directions, square lattices, triangular lattices, and distorted lattices.[17] An open question is whether directional locking can arise for particles moving over quasicrystalline substrates. It might be expected that since there is no translational order in the substrate, the particle dynamics would resemble that of particles driven over random substrates; however, since the directional locking is related to the orientational order of the substrate, it may be possible that directional locking could arise even for quasicrystalline substrates. When interacting particles are driven over quasicrystalline substrates, they may form a dynamically ordered phase. This phase could resemble the smectic state observed for particles moving over random substrates, or it could be similar to the dynamically ordered states found in the directionally locked states for particles moving over periodic substrates.

2. COMPUTATIONAL MODEL

We consider a two-dimensional system with periodic boundary conditions in the x and y-directions. The sample contains N_p pinning sites placed in a fivefold or sevenfold quasicrystalline pattern as illustrated in Fig. 1. We add N particles to the system, where we specifically consider charged colloids and vortices in type-II superconductors.

The motion of particle i is obtained by integrating the following overdamped equation of motion:

$$\eta \frac{d\mathbf{R}_i}{dt} = \mathbf{F}_i^{cc} + \mathbf{F}_i^{p} + \mathbf{F}^{ext} + \mathbf{F}_i^{T}. \quad (1)$$

Here $\eta = 1$ is a phenomenological damping term. The first term is the particle-particle interaction force. For the colloidal system it has the form $\mathbf{F}_i^{cc} = -\sum_{i\neq j}^{N} \nabla V(R_{ij})\hat{\mathbf{R}}$ with $V(R_{ij}) = (E_0/R_{ij})e^{-\kappa R_{ij}}$. Here $E_0 = Z^{*2}/4\pi\epsilon\epsilon_0$, where ϵ is the solvent dielectric constant, Z^* is the effective colloid charge, and $1/\kappa$ is the screening length. The pinning sites are modeled as attractive parabolic potentials of radius R_p with a maximum pinning force of F_p, with $\mathbf{F}_i^p = \sum_{k=1}^{N_p}(F_p R_{ik}^{(p)}/R_p)\Theta(R_p - R_{ik}^{(p)})\hat{\mathbf{R}}_{ik}^p$. Here Θ is the Heaviside step function, $R_k^{(p)}$ is the location of pinning site k, $R_{ik}^{(p)} = |\mathbf{R}_i - \mathbf{R}_k^{(p)}|$, and $\hat{\mathbf{R}}_{ik}^{(p)} = (\mathbf{R}_i - \mathbf{R}_k^{(p)})/R_{ik}^{(p)}$. The initial particle configurations are obtained by simulated annealing from a high temperature molten state. The thermal Langevin kicks used during the simulated annealing $\mathbf{F}_i^T$ have the properties $\langle F_i^T\rangle = 0$ and $\langle F_i^T(t)F_j^T(t')\rangle = 2\eta k_B T\delta_{ij}\delta(t-t')$ where k_B is the Boltzmann constant. After the annealing an external drive is applied at a varied angle,

$$\mathbf{F}^{ext} = A\sin(\theta(t))\hat{\mathbf{x}} + A\cos(\theta(t))\hat{\mathbf{y}}. \quad (2)$$

Here the force amplitude is A, $\theta = \omega t$, and ω is the frequency of the rotation which we set very small so as to avoid any transient effects. We set $A/F_p = 1.081$ so the particles do not remain pinned. We measure the velocity response in the x and y directions, $\langle V_x\rangle = N_v^{-1}\sum_{i=1}^{N_v}\mathbf{v}\cdot\hat{\mathbf{x}}$ and $\langle V_y\rangle = N_v^{-1}\sum_{i=1}^{N_v}\mathbf{v}\cdot\hat{\mathbf{y}}$. We use the same simulation method for the vortex system where the vortex-vortex interaction force has the form $F_i^{vv} = \sum_{j\neq i}^{N_v} f_0 K_1(R_{ij}/\lambda)\hat{\mathbf{R}}_{ik}$ where K_1 is the modified Bessel function, $f_0 = \phi_0^2/(2\pi\mu_0\lambda^3)$, and $\phi_0 = h/2e$ is the flux quantum. In superconductors, artificial pinning sites are generally made with nanoholes or magnetic dots; however, for vortices in Bose-Einstein condensates, pinning sites can be made with optical traps.[26]

3. DIRECTIONAL LOCKING AND ORDERING TRANSITIONS ON A DECAGONAL SUBSTRATE

In Fig. 2(a) we plot the velocity response in the y-direction as the drive is gradually rotated counterclockwise away from the x direction for a fivefold coordinated substrate. Figure 2(a) is for the colloidal case with $N/N_p = 2.9$ and $F_p = 0.75$. Here $\langle V_y\rangle$ versus θ shows a series of steps which are indicative of directional locking. For a fivefold substrate the most prominent lockings occur at integer multiples of $\theta = 360°/10 = 36°$ marked as $0/1, 1/1, 2/1$ and so forth. Additionally, smaller steps appear at rational fractional ratios of these steps including $3/2$, $5/2$, $1/4$, $3/4$, and $5/4$, as highlighted in the figure. In Fig. 2(b) we plot the corresponding fraction of sixfold coordinated particles P_6 versus θ. For a lattice with perfect triangular order, $P_6 = 1.0$. We find a series of peaks in P_6 with the most prominent steps centered at the $1/1$, $2/1$ and $0/1$ lockings where the system has $P_6 \approx 0.78$. There is also a series of smaller peaks at the fractional locking steps. This result indicates that the structure of the system changes in the different locking regions. A closeup of the $(1,1)$ step from Fig. 2 is illustrated in Fig. 3. Here there is a clear plateau in $\langle V_y\rangle$ on the locking step indicating that the particle is moving along a fixed direction even when the external force is not aligned in this direction. We note that in the absence of a substrate $\langle V_y\rangle$ versus θ would follow a smooth sinusoidal curve. In Fig. 4 we plot $\langle V_y\rangle$ and P_6 versus θ for vortices moving over a decagonal pinning array with $N/N_p = 3.225$. Here a set of steps appears that is similar to those found in the colloidal system, with the most prominent steps falling at $0/1, 1/1$, and $2/1$. There are also smaller steps at the fractional lockings. The velocity steps are accompanied by a series of peaks in P_6 with the most prominent peaks appearing at integer multiples of 36°. This result shows that it is possible for directional locking to occur on quasicrystalline substrates and that the results are general to a variety of different systems.

We next consider the nature of the ordered and disordered moving structures on and near the locking steps. In Fig. 5 we illustrate the Delaunay triangulation of the vortex system from Fig. 4 on the $(0,1)$ step [Fig. 5(a)], the $(1,1)$ step [Fig. 5(c)], and just above the $(1,1)$ step where the system is not locked [Fig. 5(e)]. Square tiles are marked in a darker color (red) and triangular tiles are marked in a lighter color (white). On the locking steps, all of the square tiles are aligned in the same direction, along 0° for the $(0,1)$ step and along 36° for the $(1,1,)$ step. The square tiles also generally form one-dimensional rows. The triangular tiles are aligned in the same direction and also form one-dimensional rows. On the locking steps the system contains a mixture

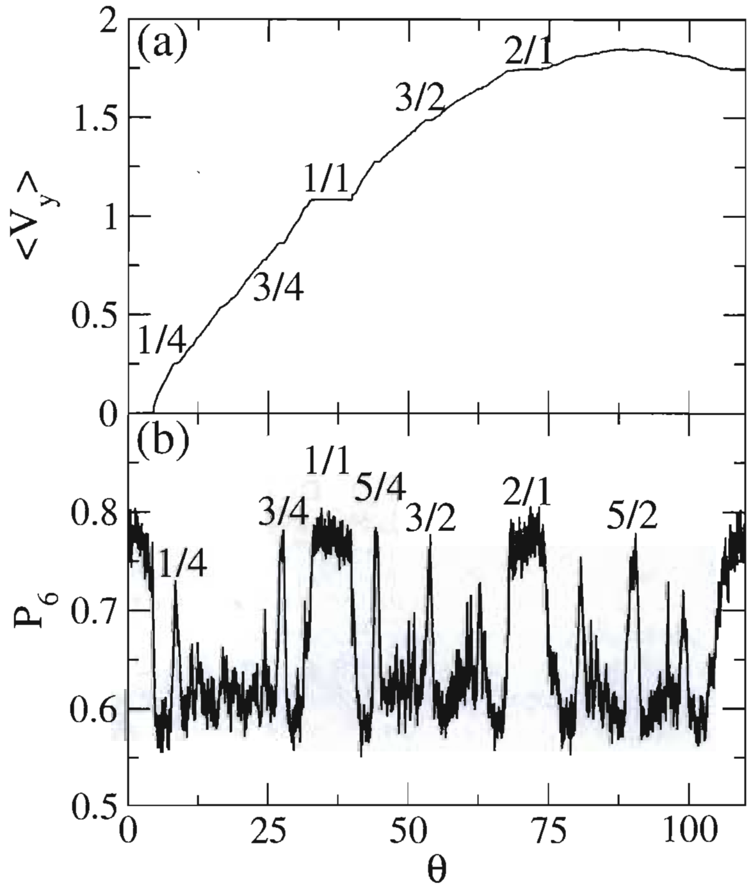

Figure 2. (a) The average velocity response $\langle V_y \rangle$ vs θ for colloids driven over a fivefold coordinated substrate with $N/N_p = 2.9$ and $F_p = 0.75$. (b) The corresponding fraction of sixfold coordinated particles P_6 vs θ. For a decagonal substrate, directional locking occurs at integer multiples of $\theta = 360/10 = 36°$, corresponding to the steps marked 1/1 and 2/1. There are additional steps that correspond to rational fractional ratios of the x and y drives.

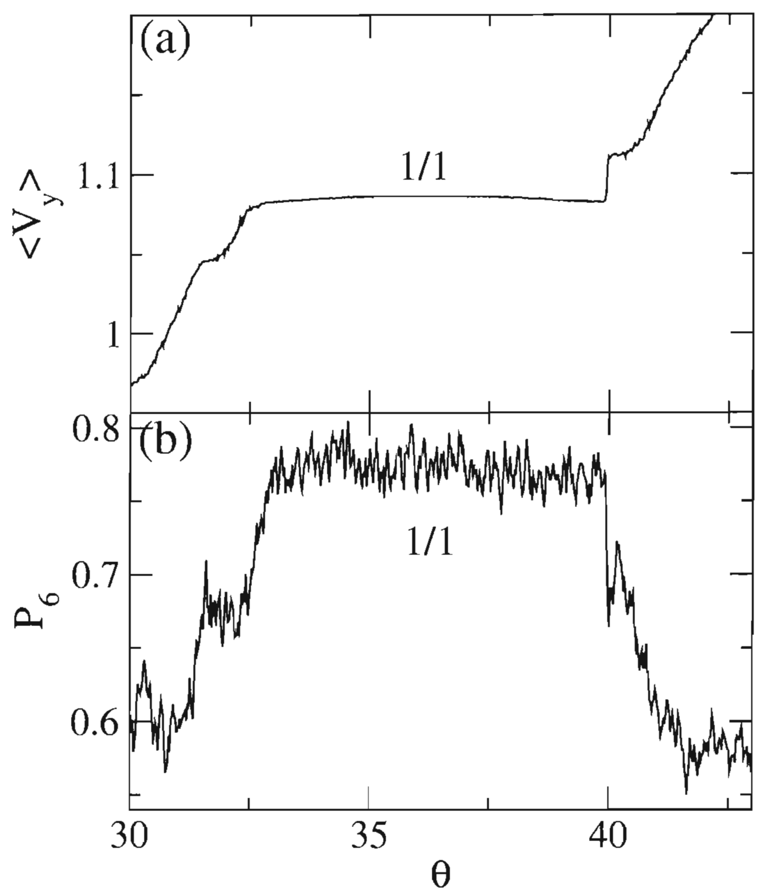

Figure 3. (a) A closeup of $\langle V_y \rangle$ vs θ on the 1/1 step from Fig. 2(a). (b) The corresponding P_6 vs θ. This shows more clearly that the system becomes ordered on the locking step.

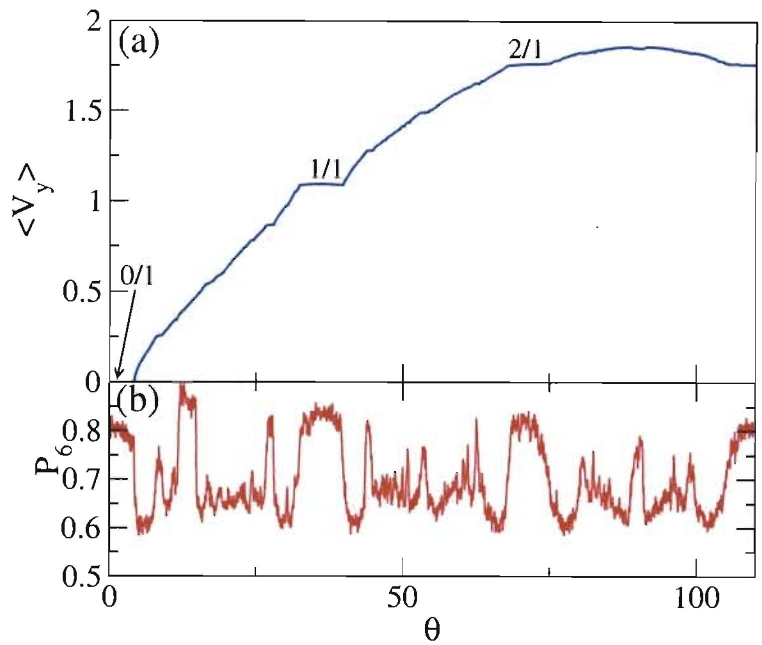

Figure 4. (a) The average velocity $\langle V_y \rangle$ vs θ for vortices moving over a decagonal pinning array with $N/N_p = 3.225$. (b) The corresponding P_6 vs θ. The same directional locking and dynamic ordering observed for the colloids occurs for the vortex system.

of square and triangular tiles which we call a dynamic Archimedean tiling. In the absence of an applied drive, we note that the particles adopt a quasicrystalline structure and do not form an Archimedean tiling. When a drive is applied, the effectiveness of the pinning is reduced and the particles form an Archimedean tiling that is similar to the tiling found in static experiments for colloids on decagonal substrates.[3–5] We always observe the formation of this type of Archimedean tiling along the integer locking directions for both the colloid and vortex systems provided that the pinning is significantly strong. For weaker pinning the system forms an almost completely triangular ordering similar to that observed in experiments with weak substrates.[3,4] The dynamical Archimedean tiling appears oriented only along integer multiples of 36°. This is the same behavior observed in the static experiments, where Archimedean tilings were also oriented only along integer multiples of 36°. In the static system, sometimes multiple orientations would appear in different regions of the sample separated by grain boundaries. In our system the orientation of the Archimedean tiling is always the same throughout the entire sample due to the symmetry breaking induced by the applied driving force. In the unlocked regimes away from the velocity steps, the square and triangular tilings are no longer aligned and the structure is strongly disordered. To better quantify the ordering we also examine the structure factor $S(k)$. In Fig. 5(b) we plot $S(k)$ for the $(0,1)$ step illustrated in Fig. 5(a), showing the appearance of a smectic structure with two prominent peaks. There are also weaker peaks corresponding to the square and triangular ordering of the two sets of tiles. A similar structure appears in Fig. 5(d) for the $(1,1)$ state from Fig. 5(c), while in Fig. 5(f), $S(k)$ for the non-step region in Fig. 5(e) has a ring type structure indicative of liquid ordering. The colloidal system shows orderings similar to those illustrated in Fig. 5 both on and off of the locking steps. We note that these structures can change as a function of filling. Strong locking steps occur for $2 < N_v/N_p < 4.5$ and for $N_v/N_p < 1/2$, while the locking steps are very weak near $N_v/N_p = 1.61$. Near $N_v/N = 1.61$ the orderings along the steps are mostly square rather than Archimedean.

4. DIRECTIONAL LOCKING ON TETRADECAGONAL SUBSTRATES

We next consider the case for a tetradecagonal or sevenfold coordinated substrate. In Fig. 6(a) we plot $\langle V_y \rangle$ versus θ and in Fig. 6(b) we plot the corresponding P_6 versus θ for a colloidal system with $N/N_p = 2.9$. In

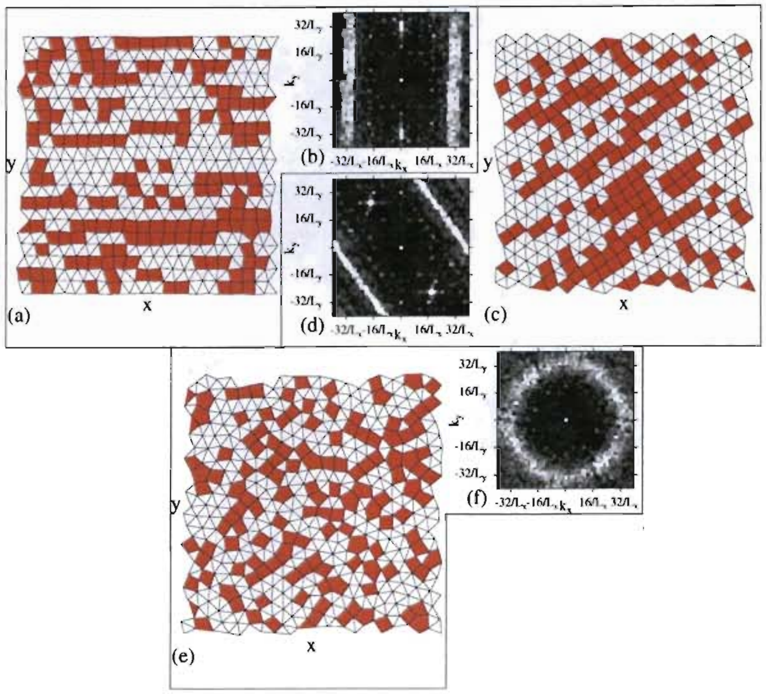

Figure 5. The Delaunay triangulation of the particles from the system in Fig. 4. The square tiles are dark colored (red) and the triangular tiles are light colored (white). (a) On the 0/1 locking step the particles form a dynamic Archimedean tiling with rows of squares and triangles aligned in the x direction. (b) The structure factor $S(k)$ for the system in (a) has a smectic structure. (c) A similar structure appears on the 1/1 locking step but is aligned along 36°. (d) $S(k)$ for the 1/1 locking shows a tilted smectic structure. (e) Just above the 1/1 locking step in an unlocked regime, the system is disordered and there is no alignment of the tiles. (f) $S(k)$ for the non-locking region in (c) has a ring type structure indicative of a liquid ordering.

this case, locking steps occur at integer multiples of $\theta = 360/14 = 25.71°$, with the largest locking steps at 0/1, 1/1, 2/1, 3/1, and 4/1. In general the locking steps for the tetradecagonal substrates are much smaller than those for the decagonal substrates. We find some smaller steps near the fractional ratios of 1/4, 3/4, 5/4, and 11/4. At the integer locking steps there are also peaks in P_6. Along the locking steps the structure of the moving system does not have the Archimedean type ordering observed for the decagonal substrate; instead, the ordering is more consistent with a moving smectic phase composed of sixfold coordinated particles moving along one-dimensional channels separated by aligned dislocations. In the nonlocking regions, the particle structure is disordered and a ring feature appears in $S(k)$. The magnitude of the steps also depends on the filling of the system. In Fig. 7(a) we plot $\langle V_y \rangle$ versus θ for vortices on a tetradecagonal substrate at $N/N_p = 3.9$ while Fig. 7(b) shows the corresponding P_6 versus θ. Here steps appear only at integer multiples of 25.71°. In Fig. 8(a,b) we plot $\langle V_y \rangle$ and P_6 versus θ for the same system at a lower filling of $N/N_p = 2.96$. In this case the integer locking steps are smaller; however, there are now clear fractional matching steps, as indicated by the peaks in P_6.

5. SUMMARY

We have investigated the dynamics of colloids and vortices moving over fivefold and sevenfold quasicrystalline substrates. When the system is driven with a slowly rotating external drive, it exhibits directional locking similar to that observed for periodic substrates. For decagonal arrays the locking occurs along the orientationally ordered directions of the quasicrystalline substrate at angles that are integer multiples of 36°. There are also smaller locking effects at fractional ratios of the locking angles. For sevenfold coordinated substrates, the directional locking occurs along seven angles which are integer multiples of 25.7°. In general the locking steps are more pronounced for the decagonal substrates than for the tetradecagonal substrates. On the locking steps the system

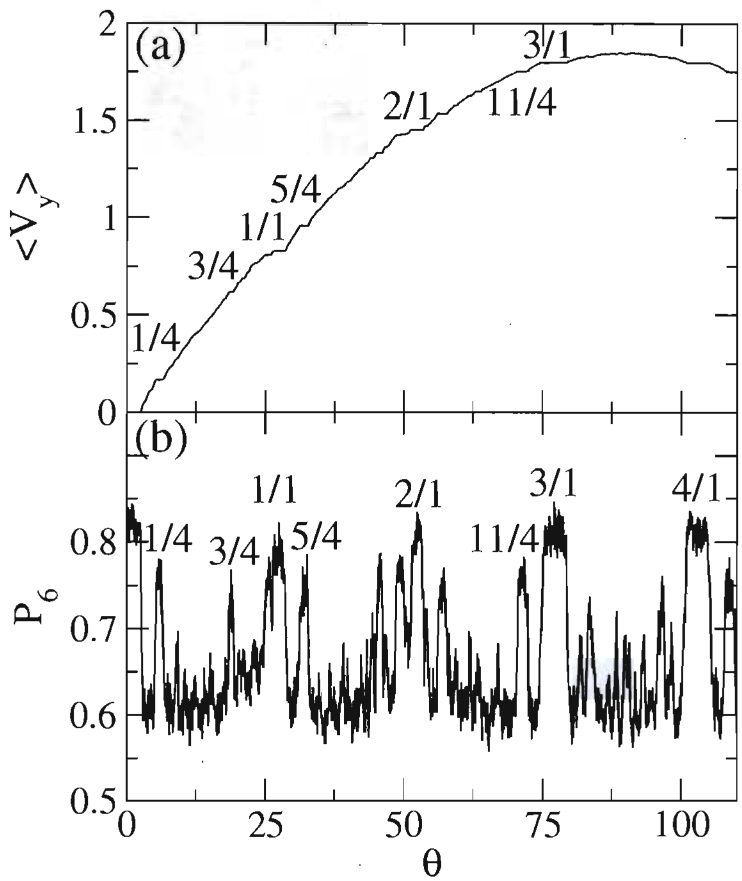

Figure 6. $\langle V_y \rangle$ vs θ for colloids moving over a tetradecagonal array. Here the prominent lockings occur at integer multiples of $\theta = 360/14 = 25.71°$. These steps are marked 1/1, 2/1, 3/1, and 4/1. There are also smaller steps that correspond to rational fractional ratios of the integer multiple steps. (b) The corresponding P_6 vs θ indicates that along the directional locking steps the system is more ordered.

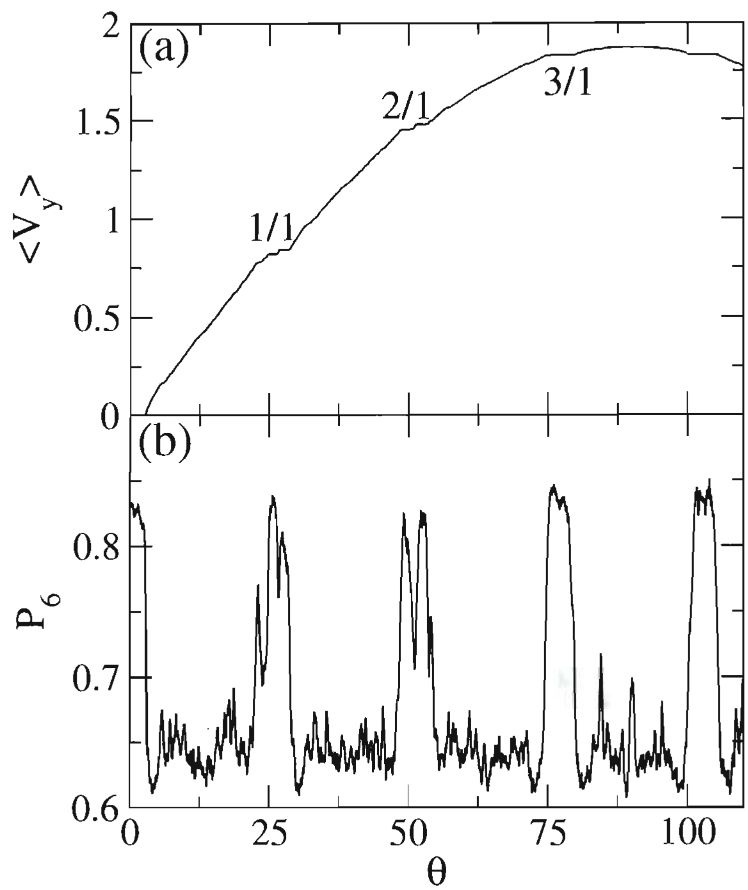

Figure 7. $\langle V_y \rangle$ vs θ for a vortex system driven over a tetradecagonal substrate at $N/N_p = 3.9$. We find a similar set of locking phases as in the colloid system of Fig. 6; however, only the integer locking steps occur. (b) The corresponding P_6 vs θ.

can undergo a transition from a disordered to an ordered phase. In the ordered phase the particles move in one-dimensional channels that have a dynamic Archimedean structure on the decagonal substrates. In this case a Delaunay triangulation of the particle positions reveals a series of aligned rows of square and triangular tiles. This dynamical Archimedean ordering is similar to the Archimedean type tiling found for non-driven colloids on decagonal substrates. When the ratio of the number of particles to the number of substrate minima is varied, the width of the locking steps can also vary. When the locking steps are weakest, the particles form moving square lattices along the locked steps. Our results show that directional locking effects can arise on substrates possessing only orientational order but no translational order. In the future it would be interesting to investigate dynamical locking for other types of systems such as attracting or aggregating particles. In this case the particles may form clump like structures in the dynamically locked regimes and may break up when driven along the nonlocking directions. It would also be interesting to examine the noise fluctuations in both the locking and nonlocking regimes.

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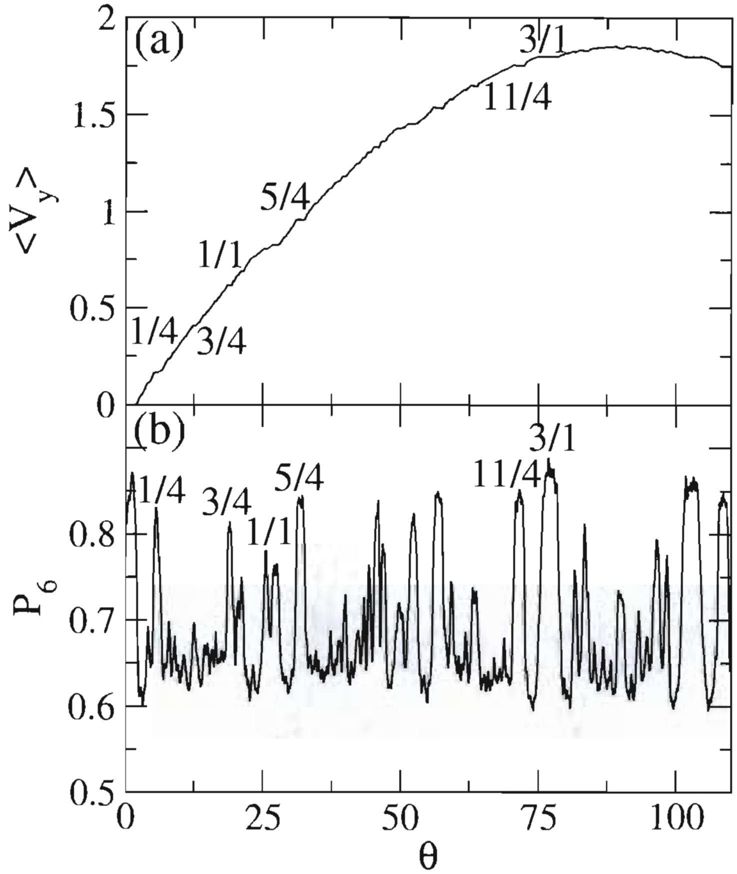

Figure 8. $\langle V_y \rangle$ vs θ for a vortex system driven over a tetradecagonal substrate at $N/N_p = 2.96$. (b) The corresponding P_6 vs θ. In this case fractional locking steps occur.

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