Nonexistence of motility induced phase separation transition in one dimension

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We introduce and study a model of hardcore particles obeying run-and-tumble dynamics on a one-dimensional lattice, where particles run in either +ve or -ve x-direction with an effective speed v and tumble (change their direction of motion) with a constant rate ω. We show that the coarse-grained dynamics of the system can be mapped to a beads-in-urn model called misanthrope process where particles are identified as urns and vacancies as beads that hop to a neighbouring urn situated in the direction opposite to the current. The hop rate is same as the magnitude of the particle current;we calculate it analytically for two particle system and show that it does not satisfy the criteria required for a phase separation transition. Nonexistence of phase separation in this model, where tumbling dynamics is rather restricted, necessarily imply that motility induced phase separation transition can not occur in other models in one dimension with unconditional tumbling.

An important class of nonequilibrium systems is that of active matter systems (AMS)[1] where the individual constituents are self-propelled; instances of such systems include bird flocks[2], bacterial colonies[3], photophoretic colloidal suspensions[4] and actin filaments[5] etc. They exhibit a number or interesting features like large number fluctuations[1], clustering and pattern formation[4]. A major area of interest in the study of AMS has been the so-called *motility-induced phase separation* (MIPS)[6–13] which refers to spatially separated high and low density regimes. Such aggregation or clustering of particles has been observed experimentally in many active matter systems[4]. The relevance of such aggregation process has also been proposed as a mechanism of formation bacterial biofilms[3], which are sources of infection.

Occurrence of MIPS relies on an argument that effective velocity of active particles decrease in crowded or high density regions formed either by explicit dependence of local density or merely by exclusion. Naturally such a slowing down of movement further increases the density of particles and gives rise to a feedback loop allowing the stable high density (liquid-like) regions to form and coexist with a low density (gas-like) phase elsewhere. MIPS has been widely investigated in simulations and apparent separation has been observed. Theoretical investigations of this phenomenon have thus far concentrated on continuum models[8–11] where motility parameters, such as particle flux or velocity are characterized as functions of the coarse-grained local density[6,7]. Lattice models of active particles have been studied in one and two dimensions numerically[14] with run and tumble particles (RTPs). RTPs move at a fixed speed in the direction of their current orientation (a *run*) until they *tumble* and change their orientation. In one dimension (1D), the two orientations (say, $\pm$) are usually referred to as the internal degrees of the particle (*spin*), which flips with a certain rate. Analytical studies of these lattice models are limited. Recently Slowman et. al.[15,16] have obtained an exact solution for *two* RTPs which exhibits certain jamming induced attraction between the particles of the opposite spins, indicating possibility of a phase separated state for many particle systems. Dandekar et. al.[17] found a mean-field solution of RTPs in 1D which is a good approximation when tumbling rate is large.

An element of surprise in the formation of a phase separated state *without* any explicit attractive interaction has added excitement to the study of MIPS and raised questions about the stability of such states in 1D even though fluctuating hydrodynamic equations have predicted them[6,7]. Recent works have added to the doubt by showing that MIPS phase transition in 2D belongs to the Ising universality class[18] which does not have a counterpart in one dimension. In this Letter we argue and show explicitly, using 1D lattice models of RTPs, that indeed MIPS transition can not occur in 1D; the inhomogeneous states observed in numerical simulations and in hydrodynamic models are only long lived transient states.

First we introduce a generic model of hardcore RTPs in 1D with a restricted tumbling and show that its coarse-grained dynamics can be mapped to a beads-in-urn model, namely a misanthrope process[19], where beads hop to their neighbouring urn situated in the opposite direction of the particle current, with a rate same as the magnitude of current. The functional form of hop rate is determined from the exact steady state results of the model with only two RTPs. To determine if MIPS transition is possible, we use the following criterion. If a system of hardcore particles phase separates as its density ρ crosses a threshold ρ^* then the maximum density at which it remains homogeneous is ρ^*. Since systems with homogeneous density are well described in the grand canonical ensemble (GCE) by a unique chemical potential μ (or fugacity $z = e^{\mu}$), we argue that phase separation transition is possible in a system when its density in GCE attains a maximum value $\rho^* = \mathrm{Max}[\rho(z)]$ which is less than unity (the density of a fully occupied lattice). Nonexistence of MIPS transition in restricted tumbling model would imply that the same can not occur in any other RTP model in 1D where tumbling occurs more frequently.

The restricted tumbling model: We introduce a generic

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model of RTPs on a one dimensional periodic lattice with sites labeled by $i = 1, 2, \ldots L$, where particles follow a dynamics,

$$+0 \underset{q_+}{\overset{p_+}{\rightleftharpoons}} 0+; \quad -0 \underset{q_-}{\overset{p_-}{\rightleftharpoons}} 0-; \quad +\pm \underset{\omega_-}{\overset{\omega_+}{\rightleftharpoons}} -\pm\,. \qquad (1)$$

where $\tau_i = \pm$ corresponds to presence of a particle at site i, running in +ve or −ve x -direction, and $\tau_i = 0$ represents a vacant site. The forward (backward) moving rates of RTPs are given by $p_\pm$ and $q_\pm$ respectively and tumbling of direction occurs with rates $\omega_\pm$. The effective velocity at which particles move is proportional to $(p_\pm - q_\pm)$. To make a correspondence of this restricted tumbling model (RTM) with the usual continuum models studied in 1D, we must ensure that the RTPs move along their spin (±) directions with same speed[20], i.e., $p_+ - q_+ = v = q_- - p_-$. We will also take $\omega_+ = \omega = \omega_-$, unless specified otherwise.

A special case of RTM with $p_+ = \alpha = q_-, p_- = 0 = q_+$ and unrestricted tumbling dynamics, $+ \underset{\omega}{\overset{\omega}{\rightleftharpoons}} -$ was studied earlier[15] and an exact steady state solution was obtained for a system of two RTPs. It turned out that these two particles experience an effective attractive interaction in the steady sate when their spins are opposite; it is envisaged that this attraction might be the source of MIPS states observed in corresponding hydrodynamic models. In comparison to this model, in Eq. (1) we have dropped one of the transition rates $+0 \underset{\omega}{\overset{\omega}{\rightleftharpoons}} -0$; as a consequence, particles do not tumble if they are not assisted by a right neighbour. This restriction helps us getting an approximate steady state of the system without tampering the main aim: the proposition that a stable MIPS state *can not* be sustained in 1D. Since frequent tumbling of particles help the system to clear jamming, a proof of nonexistence of MIPS in RTM necessarily guarantees its nonexistence in any other model that has more liberal tumbling dynamics.

Mapping to beads-in-urn model: The microscopic configurations of RTM model $\{\tau_i\}$ can be viewed as urns containing beads –each particle is an urn that contains beads which are uninterrupted sequence of 0s (vacancies) to the right of the particle (as described in Fig. 1(a)). The spin ± of the particle is termed as the internal degree of the urn. Thus we have a beads-in-urn model of N urns indexed by $k = 1, 2, \ldots N$, each carrying an internal degree $\sigma_k = \pm$ and $m_k = 0, 1, 2 \ldots$ beads. The dynamics (1) now translates to hopping of a bead from urn k to $k+1$ $(k-1)$ with rate $q_{\sigma_{k+1}}$ (p_{σ_k}), and flipping of internal degree of an urn from $\sigma_k \to -\sigma_k$ with rate $\omega_{\sigma_k}\delta_{m_k,0}$. The total number of beads $\sum_{k=1}^{N} m_k = L - N \equiv M$ is conserved by the dynamics. Like particle density $\rho = \frac{N}{L}$, the bead density $\eta = \frac{M}{N} = \frac{1-\rho}{\rho}$ is also conserved.

The mapping of RTM to beads-in-urn model is exact but we could not solve for its steady-state. For our purpose, i.e., to know if the maximum particle density in GCE is less than unity, it is enough to look at a coarse-grained picture of the model where internal degrees of

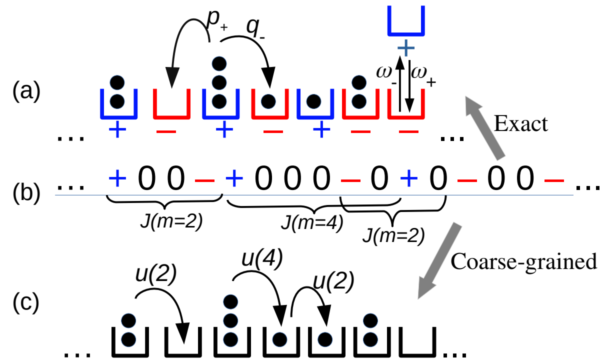

FIG. 1. Mapping lattice model of RTPs to an urn model (misanthrope process) where hop rate of a particle from one urn to the next depends on the total particles present in the departure and the arrival urn. The current $J(m)$ that passes through two consecutive domain having in total m vacant sites, plays the role of hop rate $u(m)$.

the urns do not play any role. In the coarse-grained picture we aim at finding the average particle current $J(m)$ that flows across a domain of size m, irrespective of its internal degree σ_k, which is then interpreted as an effective hop rate of beads moving to a neighbouring urn (situated along the direction opposite to the particle current). Since in the exact mapping of RTP model and urn model (Fig 1(a)) the hop rate dependn on the internal degree of both the arrival and the departure urns, we expect that in the coarse-grained picture too the hop rate $u(m_k, m_{k+1})$ depends on the number of particles in the departure site k and the arrival site $k+1$. Its functional form can be calculated from the exact steady state current $J(m) \equiv u(m = m_k + m_{k+1})$ carried by the beads in a system of two urns and m beads (demonstrated in Fig. 1(c)). Such coarse-grained descriptions are reliable and have helped researchers[21] earlier to establish impossibility of phase separation transition in certain lattice models[22] where rigorous numerical simulations have exhibited apparent phase separated states. It also helped in predicting *true* phase separation transition in many other models[21,23,24].

Two urns: To calculate the current $J(M)$ that flows through two consecutive domains of total size M, we consider a system of length $L = M + 2$, having exactly two particles, which is same as two urns containing M beads in total. In this case, the steady state probabilities $P(\{\sigma_k m_k\})$ of configurations $\{\sigma_k m_k\}$ can be calculated using matrix product ansatz[25] extended to urn models in Ref.[26],

$$P(\{\sigma_k m_k\}) = \frac{1}{Q_M} Tr[\prod_{k=1}^{N} X_{\sigma_k}(m_k)] \quad \text{with}$$
$$Q_M = \sum_{\{\sigma_k\}} \sum_{\{m_k\}} Tr[\prod_{k=1}^{N} X_{\sigma_k}(m_k)] \delta\left(\sum_{k=1}^{N} m_k - M\right), (2)$$

where the δ-function ensures the conservation of the total number of beads in N urns.

The matrix functions $X_{\sigma_k}(m_k)$ that represents an urn k of type σ_k containing m_k particles must satisfy the steady state condition $\frac{dP}{dt} = \mathcal{M}P = 0$ with Markov matrix $\mathcal{M}$ corresponding to the dynamics described in Fig 1(a). This condition for any configuration $\{\sigma_k m_k\}$ can be expressed as $\sum_{k=1}^{N} \mathrm{Tr}[H_k^R + H_k^T] = 0$ where H_k^R and H_k^T correspond to the run and the tumble dynamics occurring at urn k respectively,

$$\begin{aligned} H_k^R &= -(p_{\sigma_k} + q_{\sigma_{k+1}})X_{\sigma_{k-1}}(m_{k-1})X_{\sigma_k}(m_k)X_{\sigma_{k+1}}(m_{k+1}) \\ &\quad + q_{\sigma_k} X_{\sigma_{k-1}}(m_{k-1}+1)X_{\sigma_k}(m_k-1)X_{\sigma_{k+1}}(m_{k+1}) \\ &\quad + p_{\sigma_{k+1}} X_{\sigma_{k-1}}(m_{k-1})X_{\sigma_k}(m_k-1)X_{\sigma_{k+1}}(m_{k+1}+1), \\ \text{and} \quad H_k^T &= \omega[X_{-\sigma_k}(0) - X_{\sigma_k}(0)]X_{\sigma_{k+1}}(m_{k+1}). \end{aligned} \tag{3}$$

We now introduce some suitable choice of auxiliary matrices $\tilde{X}_{\sigma_k,\sigma_{k+1}}(m_k, m_{k+1})$, yet to be determined along with $X_{\sigma_k}(m_k)$, so that both $\sum_k H_k^R$ and $\sum_k H_k^T$ vanish; one such cancellation scheme for H_k^R is,

$$\begin{aligned} H_k^R &= \tilde{X}_{\sigma_{k-1},\sigma_k}(m_{k-1}, m_k)X_{\sigma_{k+1}}(m_{k+1}) \\ &\quad - X_{\sigma_{k-1}}(m_{k-1})\tilde{X}_{\sigma_k,\sigma_{k+1}}(m_k, m_{k+1}). \end{aligned} \tag{4}$$

We find that a choice $\tilde{X}_{\sigma,\sigma'}(m,n) = h_{\sigma,\sigma'} X_\sigma(m) X_{\sigma'}(n)$ with some scalar parameter $h_{\sigma,\sigma'}$ does satisfy the steady state condition with 2×2 matrices

$$X_+(m) = \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}, X_-(m) = \gamma^m \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}, \tag{5}$$

where $\gamma = \frac{p_+ + q_-}{p_- + q_+}$, $h_{\sigma,-\sigma} = 0$, and

$$h_{\sigma,\sigma} = \begin{cases} q_\sigma(1-\gamma^\sigma) & m > 0, n > 0 \\ 0 & \text{else.} \end{cases} \tag{6}$$

We need not bother about the condition $\sum_k \mathrm{Tr}[H_k^T] = 0$, because the individual terms in the sum vanishes, as $X_\sigma(0)X_{\sigma'}(m) = X_{\sigma'}(m)$ for all σ, σ', m. The only troubling part on the way of exact solution is Eq. (6) that requires $h_{\sigma,\sigma}$ to vanish for some values of m, n. This condition forces $h_{\sigma,\sigma}$ to depend explicitly on m, n and a consistent solution can not be obtained for generic rates; one can, however, obtain an approximate steady state (discussed in later part of this article). This difficulty, however, does not arise when $q_\sigma(1-\gamma^\sigma) = 0$. In this case, i.e., when $\gamma = 1$, or $q_\pm = 0$ or both, the steady state written in matrix product form is exact. But neither of these cases constitutes the scenario of MIPS (as all particles move, effectively, in the same direction).

We proceed with $N = 2$, where again, matrices (5) provide an exact matrix product steady state for all $p_\sigma, q_\sigma, \omega_\sigma$. This is because, our cancellation scheme (3) puts constraints on the product of three consecutive matrices which are irrelevant when $N = 2$ (we can then set $h_{\sigma,\sigma'} = 0$). The steady state probabilities are then,

$$P_{\sigma_1\sigma_2}(m) = \frac{Tr[X_{\sigma_1}(m)X_{\sigma_2}(M-m)]}{\sum_{\sigma_1,\sigma_2}\sum_{m=0}^{M} Tr[X_{\sigma_1}(m)X_{\sigma_2}(M-m)]}.$$

where m is number of beads in the 1st urn. Explicitly, $P_{++}(m) = 1/Q_M$, $P_{--}(m) = \gamma^M/Q_M$ and $P_{-+}(m) = \gamma^m/Q_M = P_{+-}(M-m)$. The magnitude of current carried by the beads is same as the total current carried by $+$ and $-$ particles and its average value is,

$$J(M) = \sum_{\sigma_1,\sigma_2,m} P_{\sigma_1\sigma_2}(m)(p_{\sigma_1} - q_{\sigma_2}).$$

For large M, taking $\gamma^M \to 0(\infty)$ when $\gamma < 1$ ($\gamma > 1$),

$$J(M) = M\frac{1-\gamma}{M+c}; c = \begin{cases} 1 + \frac{2}{1-\gamma} & \gamma \le 1 \\ 1 + \frac{2}{1-\gamma^{-1}} & \gamma > 1 \end{cases} \tag{7}$$

Here we have used $p_\pm = q_\mp$, a condition required for RTPs to have a well defined continuum limit.

As we have argued earlier, in the coarse-grained model of many urns, $J(M)$ serves as the hop-rate: a single bead hops from k to $(k+1)$-th urn with rate $u(m_k, m_{k+1}) \equiv u(m_k + m_{k+1}) = J(m_k + m_{k+1})$. This urn model is a specific example of misanthrope process[19] that can be solved exactly; its steady state is factorized $P(\{m_k\}) \sim \prod_{k=1}^{N} f(m_k)$ with $f(m) = \prod_{n=1}^{m} \frac{u(1,n-1)}{u(n,0)} = 1$. In the grand canonical ensemble where both $N, M = \sum_{k=1}^{N} m_k$ vary keeping L fixed, the partition function is

$$Z(z,y) = \sum_{N=0}^{\infty} z^N F(y)^N = \frac{1}{1 - zF(y)} \tag{8}$$

where $F(y) = \sum_m f(m)y^m = \frac{1}{1-y}$. Here, z, y are the fugacities associated with N, M respectively so that, $\langle N \rangle = z\frac{\partial}{\partial z}\ln Z(z,y)$ and $\langle M \rangle = y\frac{\partial}{\partial y}\ln Z(z,y)$. We set $L = \langle N \rangle + \langle M \rangle$ to obtain $z = \frac{L}{(1+L)F(y) + yF'(y)}$ and

$$\rho(y) \equiv \frac{\langle N \rangle}{L} = \frac{F(y)}{F(y) + yF'(y)} = 1 - y. \tag{9}$$

The maximum value of density in the GCE is then $\rho^* = 1$ (obtained when $y \to 0$) and thus the system remains homogeneous and *can not* phase separate (following the criterion we discussed) for any particle density $0 \le \rho \le 1$.

The above argument is based on the coarse-grained picture where the main assumption is that hop rate $u(m,n)$ depends on the total number of particles present in the departure and the arrival urns. The actual form of $u(.)$ is unimportant in obtaining the result $\rho^* = 1$, but we would like to check from the Monte Carlo simulations of the model if the functional form given by Eq. (7) is indeed valid. In fact, for $\gamma < 1$, we expect from Eq. (7) $u(m)^{-1}$ to be a linear function of m^{-1} with y-intercept $(1-\gamma)^{-1}$ and slope $\frac{3-\gamma}{(1-\gamma)^2}$. To calculate the same from simulations, first we calculate $F_r(m+n), F_l(m+n)$, the number of times particles move to right or left in a large time interval, when the arrival and departure box has exactly m and n beads respectively (internal degree of urns are ignored). Also we keep track of $F(m+n)$, the number

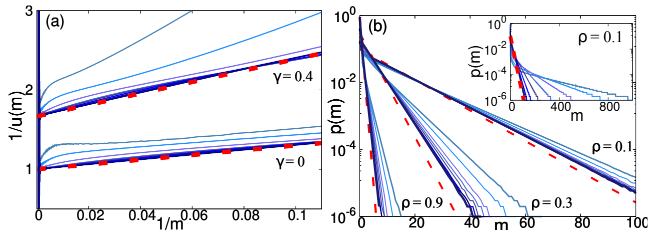

FIG. 2. (a) Hop rate $u(m)^{-1}$ obtained from numerical simulations (solid line) for $\gamma = 0, 0.4$ and $\omega \in (0.005, 1)$ are compared with Eq. (7) (dashed line) when $\rho = 0.02$. All the curves approach the asymptotic value $(1-\gamma)^{-1}$ linearly as predicted. (b) Marginal distribution $p(m)$ of the separation m (distance between consecutive particles) are compared for $\gamma = 0$ and $\rho = 0.1, 0.3, 0.9$ in semi-log scale. Solid lines (results from simulations for $\omega \in (0.2, 10)$) are shown along with dashed lines, $\rho(1-\rho)^m$ obtained from coarse-grained description of the model. The inset shows the same for $\rho = 0.1$ but smaller $\omega \in (0.003, 1)$. In all cases $p(m)$ shows exponential behaviour; but for small ω, the correlation length is substantially larger than the predicted value $1/|\ln(1-\rho)|$. Here, $p_+ = \gamma = q_-$, $p_- = 1 = q_+$, $L = 10^4$. In each case, statistical averaging is done for more than 10^7 samples.

of jump-events attempted during that interval. Clearly, $u(m,n) = (F_r(m+n) - F_l(m+n))/F(m+n)$. In Fig. 2(a) we plot $u(m)^{-1}$ versus m^{-1} for $\gamma = 0, 0.4, \rho = 0.02$ and $\omega = 0.003$ to 1; in all cases, $u(m)^{-1}$ is found to be linear for large m with y- intercept approaching $(1-\gamma)^{-1}$, which is the asymptotic value of the current obtained from exact solution of the two-urn system. Their slopes, however, differ a bit. Further, in Fig. 2(b) we plot the marginal distribution $p(m)$ of number beads m for $\gamma = 0, \rho = 0.1, 0.3, 0.9$, ω varying in the range (0.2 to 10). The dashed line corresponds to the theoretical curve obtained from the coarse-grained picture, $p(m) \sim y^m f(m) = y^m$, where $y = 1-\rho$, and thus, the correlation length is $\xi = 1/|\ln(1-\rho)|$. For all cases shown Fig. 2(b), $p(m)$ exhibits an exponential distribution, closer to the theoretical prediction for large ω. As $\omega \to 0$ the exponential feature remains persistent but the correlation length increases substantially. This is also expected as ergodicity is broken at $\omega = 0$, where the system falls into an absorbing state.

In summary, the coarse-grained picture turns out to be a good description of the RTP model as the $p(m)$ decays exponentially for large m as predicted; although the correlation length differs substantially for small tumbling rates. But an exponential form of $p(m)$ is enough to assure that, in GCE, the fugacity can be tuned appropriately to obtain any desired particle density ρ and thus, the system remains homogeneous for any $0 < \rho < 1, w > 0$ and $\gamma \geq 0$. It is also indicative that any other RTP model where tumbling occurs more frequently can not undergo a MIPS transition.

Approximate solution: Another approach to study the possibility of MIPS transition in this RTP model is to extend the matrix product state given by Eq. (5) to many

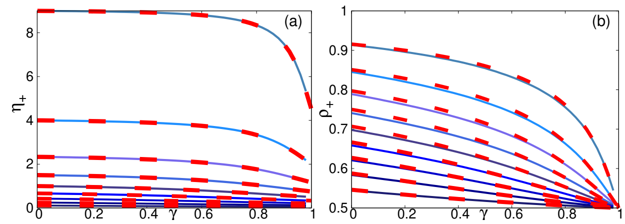

FIG. 3. (a) η_+, the density of beads in + urn and (b) ρ_+, the fraction of + urns are shown as a function of γ for different $\rho = 0.1$ to 0.9 (top to bottom). Data from Monte Carlo simulations (solid lines), averaged over 10^7 samples are compared with Eqs. (10) (dashed line). Other parameters are $L = 10^3$, $p_+ = \gamma = q_-$, $p_- = 1 = q_+$ and $\omega = 1$.

urns. It would have been an exact solution if $h_{\sigma,\sigma}$ in Eq. (6) were not forced to vanish for some cases. Ignoring this fact one may take $h_{\sigma,\sigma} = q_\sigma(1-\gamma^\sigma) \quad \forall m,n \geq 0$ to get an approximate steady state solution for small $q_\pm$ when $\gamma \simeq 1$, which corresponds to small velocity limit of the RTP model. The grand canonical partition function $Z(z,y)$ is given by Eq. (8), with fugacities z, y associated with N, M, and

$$F(y) = \sum_{\sigma=\pm}\sum_{m=0}^{\infty} y^m Tr[X_\sigma(m)] = \frac{1}{1-y} + \frac{1}{1-\gamma y}.$$

The density of the system is now (similar to Eq. (9)),

$$\rho(y) = \frac{F(y)}{F(y) + yF'(y)} = \frac{(1-y)(1-\gamma y)(2-y-\gamma y)}{(1-\gamma y)^2 + (1-y)^2}$$

Clearly, the maximum density that can be achieved in GCE by tuning y is $\rho^* = 1$ (when $y = 0$) and thus, following the criterion we discussed earlier, this RTP model *can not* undergo a phase separation transition.

To justify that it is indeed a good approximation, we calculate the steady state average of η_+, the density of beads in + urns and ρ_+, the fraction of urns having internal degree +,

$$\eta_+ = \frac{1}{N}\sum_{k=1}^{N} m_k \delta_{\sigma_k,+}; \qquad \rho_+ = \frac{1}{N}\sum_{k=1}^{N}\delta_{\sigma_k,+}, \qquad (10)$$

and plot it in Fig. 3 as a function of γ (dashed lines), for different ρ in the range (0.1, 0.9), along with those obtained from the Monte Carlo simulations of the model (solid lines). They match quite well for all $\gamma < 1$. Thus the approximate solution describes the RTP model very well and also indicates nonexistence of MIPS transition in 1D. This is consistent with recent results[18] that MIPS transition in 2D belongs to the magnetic transition in Ising models, a transition which is also absent in 1D.

One possible way to generate a *true* phase separated state in 1D is to use severely reduced tumbling rate, say $\omega \sim \frac{1}{L}$, so that it can not win over the run-dynamics in the thermodynamic limit. In fact, recently Kourbane-Houssene et. al.[27] have introduced a RTP model where the difference of run-rates (or effective velocity) is proportional to $\frac{1}{L}$ and the tumbling rate is proportional to $\frac{1}{L^2}$ and have shown using an exact coarse-grained hydrodynamic description that the homogeneous phase in 1D is not stable in certain regimes of density and rates. Another way would be to bias the tumbling rates strongly, say $\omega_+ \gg \omega_-$. In this case a phase separation transition occurs[28] when $q_\pm = 0$, where the dynamics of RTM reduces to that of a two species exclusion process[29]. Its extension to small $q_\pm \simeq 0$, is a RTP model (having a good continuum limit) and it is reasonable to assume that the phase separation features may also survive there. Yet another possibility is to introduce defects - recent studies[30] have shown that a jammed phase does exist in RTM like models with defects. More investigation is required in all these directions to confirm if RTP models in 1D can phase separate.

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