Model of overdamped motion of interacting magnetic vortices through narrow superconducting channels

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(Received 28 August 2009; published 28 September 2009)

The microscopic description of several physical systems can be successfully accomplished in terms of the overdamped flow approximation. It is under this broad framework that we investigate the flow of interacting particles in overdamped motion through narrow and irregular channels. By direct comparison with results from molecular dynamics simulations, we show that the behavior of the overdamped system is fully compatible with a continuum coarse-grained model, described in terms of a nonlinear diffusion equation. Remarkably, our results reveal that even in such cases where only a few layers of particles move through the channel, it is possible to obtain a consistent description for the density profiles from the continuum model. Moreover, we demonstrate the general validity of our theoretical approach with results from extensive numerical simulations of different model systems, including the propagation of vortices in superconducting substrates, the movement of pedestrians through corridors, and the flow of colloidal particles in pores.

DOI: 10.1103/PhysRevB.80.104513 PACS number(s): 74.78.Na, 45.70.Vn, 74.25.Qt

I. INTRODUCTION

A great deal of attention has been directed to the dynamics of interacting particles in confined geometries.1 Important examples of such systems are colloidal suspensions,2 charge density waves,3 ion channels,4 vortex dynamics in superconductors,5 and pedestrian traffic.6 These systems exhibit a remarkable variety of complex behaviors depending on particular conditions.7,8 Although many of the phenomena observed in such systems are related to the discrete nature of their constituents, a general macroscopic description could help model and predict the dynamics of large systems comprising many interacting particles. Under this framework, a continuum formulation based on a coarse-grained description of the motion of overdamped particles has been proposed in previous studies.9,10

It is the aim of the present study to investigate the flow of interacting particles undergoing overdamped motion through narrow and irregular channels. In particular, we focus on the situation where there is an obstacle to the flow, being either an energy barrier or a constriction in the channel. Surprisingly, we observe that even in such confined geometries, the continuum approach can successfully describe the density profiles obtained from direct molecular dynamics simulations of distinct physical systems, including the propagation of vortices, colloidal particles and flow of pedestrians in narrow channels.

II. MODEL FORMULATION

Our theoretical approach is initially tested for flow of vortices through a superconducting substrate, although it is generally valid for any overdamped system. We therefore consider the following equation of motion:12–15

$$\eta \dot{\mathbf{v}}_i = F^{pp}_i + F^{\text{ext}}_i + F^I_i,$$

where $F^{pp}_i$ represents the particle-particle interaction, $F^{\text{ext}}_i$ is the external force acting on every particle, and $F^I_i$ is the thermal interaction. In the case of vortex lines, the effective viscosity $\eta$ can be expressed in terms of material parameters, namely, $\eta = \Phi_0^2 d/2\pi \xi^2 \rho_N$, where $d$ is the sample thickness, $\xi$ is the coherence length, $\rho_N$ is the resistivity in the normal state, and $\Phi_0 = h/2e$ is the quantum of magnetic flux. The particle-particle interaction is given by $F^{pp}_i = \sum_{j \neq i} \eta_f K_i(r_{ij}/\lambda) \hat{r}_{ij}$,16–19 where $\hat{r}_{ij} = (r_i - r_j)/|r_i - r_j|$ is the unitary vector in the direction of the axis from vortex $j$ to vortex $i$, $K_i(r_{ij}/\lambda)$ is the modified Bessel function, $f_0 = \Phi_0^2 d/2\pi \mu_0 \lambda^3$ is the force strength, and $\lambda$ is the London penetration length.

For completeness, we present here the reasoning behind the formulation of the continuum model.9,10 We start from the continuity equation for the local density of particles, $\partial \rho / \partial t = - \nabla \cdot \mathbf{J} + k_B T \nabla^2 \rho$, where $\mathbf{J} = \rho \mathbf{v}$ is the particle current, $\mathbf{v}$ is the local average velocity, and the second term on the right accounts for thermal diffusion. As expressed in Eq. (1), we should expect this velocity to depend on the drive from the external force and the particle-particle interaction. It has been shown10 that the particle-particle interaction can be associated with the local density gradient as $\langle F^{\text{ext}} \rangle = a \nabla \rho$, where the parameter $a$ can be deduced from the microscopic particle-particle interaction as $a = 1/2 \int d^2 r \mathbf{F}(\mathbf{r}) \cdot \mathbf{r}$, which gives $a = d \Phi_0^2 / \mu_0 = 2\pi f_0 \lambda^3$ for the case of vortices.10 This expression, however, is valid only at relatively large density values, $\rho > \Phi_0/\lambda^2$, and when the density gradient varies slowly $\nabla^2 \rho < \Phi_0/\lambda^4$. Considering all these assumptions, we can now rewrite the continuity equation as

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} = \nabla \cdot [\rho(a \nabla \rho - \mathbf{F})] + k_B T \nabla^2 \rho(\mathbf{r}, t),$$

where we have reduced the notation by dropping the superscript of the external force.

In narrow channels, and neglecting shear effects with the channel walls, the velocity profile is weakly dependent of the transversal coordinate, unless close to geometrical
obstacles. This fact allows us to adopt a simpler quasi-one-dimensional version of the transport model. Under steady-state conditions and neglecting thermal fluctuations, Eq. (2) reduces to

\[ \rho \left( a \frac{d}{dx} \rho - F \right) = J, \tag{3} \]

where the conservation of the number of particles imposes the particle current \( J \) to be constant.

### III. Results

The first numerical experiment we perform is a finite narrow box closed in all four directions in which vortexes are pushed by an external force \( F \) against one of the lateral walls. In our idealized model, we treat the interaction with the channel walls as purely repulsive. Shear stress with the walls and bulk interactions with pinning centers are not included in our model system. In a closed box steady flux is not possible, \( J = 0 \), and the solution of Eq. (3) is a linear profile, \( \rho(x) = F/a(x-x_0) \), with \( x_0 \) being the position where the density vanishes, \( \rho(x_0) = 0 \). In order to test the assumptions of our model, we perform molecular dynamics simulations for different values of \( N, F, \) and \( L \) until the system reaches mechanical equilibrium. Here, we estimate the density profile \( \rho(x) \) as the local magnetic field averaged over time and normalized by the quantum of flux \( \Phi_0 \). From the slope of this profile (see Fig. 1), we can directly calculate the transport parameter \( a \). As shown in Fig. 2, our results indicate that the behavior of \( a \) can be approximately described by a single curve expressing its dependence on \( L \) alone, over a broad range of \( N \) and \( F \) values.

It is important to mention that, strictly speaking, the theoretical prediction \( a = 2 \pi f_0 \lambda^3 / \Phi_0 \) (the dashed line in Fig. 2) should be only valid for unconstrained systems. In a confined channel, if the width of the channel is of the order of the characteristic length \( \lambda \), the local density becomes somewhat smaller than the number of particles per unit of area. Such a discrepancy can be explained by the fact that vortices cannot leave the channel, while part of the magnetic field propagates out. This is equivalent to introducing an effective cross section for vortex transport that is greater than the width of the channel, therefore leading to an estimate of \( a \) that is larger than the value predicted theoretically.

We now try to extrapolate our findings from the static \( (J=0) \) to the dynamical case \( (J \neq 0) \). Our objective is to test if the values of \( a \) obtained from the static case can be used to describe particle flow driven by an external force through a long narrow channel and across an obstacle in the form of a potential jump \( \Delta U \) as shown in Fig. 3.

In our simulations, we model this with a force given by \( F' = \Delta U / \delta \), where \( \delta \) is the width of the region where the potential varies. The potential jump \( \Delta U \) is given in units of \( f_0 \lambda \), the force is given in units of \( f_0 \), and the length in units of \( \lambda \). We adopt \( \delta = 0.1 \lambda \), but the results become independent of

![FIG. 2. (Color online) Variation in the parameter \( a \) against the width of the channel \( L \). In order to obtain these results, we perform simulations in a confined system, as shown in Fig. 1, for several different conditions. The effective value of the parameter \( a \) is then obtained from the slope of the (linear) density profile. As the channel gets narrower, we observe deviations from the theoretical value, \( a = 2 \pi f_0 \lambda^3 / \Phi_0 \). The solid line indicates the least-squares fit to the points of the function \( a(L) = [2 \pi + c \exp(-bL)](f_0 \lambda^3 / \Phi_0) \), with \( c = 2.74 \) and \( b = 0.19 \). The parameter \( a \) is given in units of \( f_0 \lambda^3 / \Phi_0 \), and \( L \) in units of \( \lambda \).](https://doi.org/10.1103/PhysRevB.80.104513)
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\[ \rho(x) = \frac{J}{F} \left\{ 1 + W[F(x)] \right\}, \]  

(4)

where \( f(x) = \exp(-1 + \rho_0 F/J + F^2/aJx) \) is the analytical solution Eq. (3). The best fit shown as the dashed red lines, follows closely the simulations data in all four cases.

\[ \Delta U = 0.2, 0.6, 0.28, \text{ and } 6.0, \] respectively. Moreover, the values for the current \( J \) obtained from the adjustment agree with the values obtained from the molecular dynamics up to the second decimal digit. The results obtained with this procedure, show in Fig. 5, are compared with the molecular dynamics simulation. Expectedly, it provides a superior description for \( \rho(x) \) than the numerical solution of Eq. (3) in the absence of free parameters to fit (see Fig. 4), particularly for large values of \( \Delta U \). Moreover, the best values for the current density \( J \) are in good agreement with the values obtained from molecular dynamics simulations. The discrepancy observed in the results presented in Figs. 4(c) and 4(d) when compared to those shown in Figs. 5(c) and 5(d), can be attributed to the fact that the boundary conditions at the barrier interface are affected by the discrete nature of the particle system.

As an alternative approach to show the consistency between continuum model and molecular dynamics simulations, we can also solve analytically Eq. (3) separately for each section of the channel, before and after the obstacle, and account for the effect of the obstacle explicitly in the boundary conditions. In this case, the external force \( F \), transversal section \( L \), and current \( J \), are constant in each section and the solution of Eq. (3) is given by:

\[ \rho(x) = \frac{J}{F} \left\{ 1 + W[F(x)] \right\}, \]  

(4)

where \( f(x) = \exp(-1 + \rho_0 F/J + F^2/aJx) \) is the analytical solution Eq. (3). The best fit shown as the dashed red lines, follows closely the simulations data in all four cases.

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Next, we apply our coarse-grained approach to a narrow channel with a bottleneck, as shown in Fig. 6.

As before, we use molecular dynamics simulation to generate the density profiles, but now the general solution Eq. (4) is applied together with the continuity constraints at the channel junctions, \( J_1L_1 = J_2L_2 \) and \( L_1\int_0^1 \rho_1(x)dx + L_2\int_{X_2}^1 \rho_2(x)dx = N \), where the indexes 1 and 2 correspond to the narrower and wider sections of the system, respectively. We emphasize here that the effective values for the parameter \( a \) used for each section are independently obtained from the numerical simulations with a closed box (see Fig. 2). Both the density profile from molecular dynamics and the best fit to the data of Eq. (4) are shown in Fig. 7. The excellent agreement substantiates the validity of our conceptual approach with a quasi-one-dimensional model, even in this case where the width of the channel is not constant. Note that, with this geometry, the external applied force produces a local increase in the particle density in the constricted region. This gives a way to control the local magnetic field density in superconductors with a transversal electric current.
As shown in the inset of Fig. 7, the agreement between simulations and continuum model is rather impressive for this system. Our continuum approach to particle flow can also be applied to the transport of charged colloidal particles. These systems are usually modeled by an interaction potential in the Yukawa’s form:

\[ V_{ij} = \frac{-\kappa r_{ij}}{r_{ij}} f_0 \lambda^2, \]

where we have used \( \kappa = 0.8 \) for the screening parameter. The density profiles for a system of particles interacting via Eq. (6) and passing through an obstacle barrier is shown in Fig. 8. As before the density profile can be suitably adjusted by using Eq. (3), further confirming the validity and broad-range applicability of the continuum description to model the collective motion of particles undergoing overdamped dynamics in confined and irregular channels.

IV. CONCLUSIONS

In summary, we investigated the general problem of flow of interacting particles in overdamped motion through confined geometries. Regardless of the complex geometries and boundary conditions involved, we have shown the remarkable fact that the microscopic behavior of the overdamped system is fully compatible with a continuum coarse-grained model, described in terms of a nonlinear diffusion equation. We corroborated the general validity of our theoretical approach with results for three distinct physical systems. Our results show that the quantity \( a \), which parameterizes the effective strength of the interaction between the particles, needs to be adjusted to account for the confined geometry. We observed that for certain conditions, where the force acting on the particles varies rapidly over short distances, the theoretical predictions deviate from the results obtained for the discrete system of particles. However, it was possible to show that these deviations may be accounted for by finding the proper boundary conditions in the interface region where the external force varies. As an extension for future work, we will apply Eq. (2) to describe the behavior of more complex systems, including, for instance, stress with the walls, interactions with pinning centers, or substrates whose geometries are networks of interconnected channels as observed, for instance, in the rivers of elastic flow of interacting particles.

ACKNOWLEDGMENTS

We thank CNPq, CAPES, FUNCAP, FACEPE, and FINEP for financial support.
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19. This is the adequate expression for vortex interaction in bulk form. For the thin film case, one should use the appropriate expression. Nevertheless, as we show in the body of the article, the results are independent of the form of the interaction, as long as it is repulsive and short-ranged.