Simultaneous effect of an external magnetic field and gas-induced friction on the caging of particles in two-dimensional Yukawa systems

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1 INTRODUCTION

Strongly coupled plasmas are characterized by a pair-interaction potential energy that dominates the average kinetic energy of the particles.[1] Systems with this property appear in a wide variety of physical systems, as well in various laboratory settings, and can be described by the “one-component plasma” (OCP) model, which considers explicitly only a single type of charged species and assumes an inter-particle potential that accounts for the presence and effects of the other type(s) of species. The non-polarizable form of the interaction potential is the Coulomb type, while the polarizable form is the Yukawa type; the corresponding systems are, respectively, quoted as Coulomb-OCP and Yukawa-OCP (YOCP). This latter type represents an important model system for dusty plasmas, for example, Refs. [2–5]. In the simulations of these systems, the background plasma environment is accounted for by the screening of the Coulomb potential. Moreover, the presence of the gaseous environment may be taken into account by using the Langevin simulation approach,[6–9] where two additional terms are incorporated into the equation of motion. One of the terms represents a friction by a homogeneous background, while the other term adds momentum to the particles in form of random kicks that change the direction of the motion. The action of these two terms can be balanced to reach a desired system temperature. In several studies, a simplified approach, which neglects the presence of the gaseous background, has been used to study the properties of idealized (frictionless) Yukawa liquids. This latter approach is justified for describing experiments conducted at very low pressures. The presence/absence of friction can significantly influence some of the properties of the systems, for example, the lifetime of collective excitations.

The possibility of the presence of an external magnetic field has opened a new area of dusty plasma research. Interesting new effects (like the appearance of ordered structures) have been observed in the experiments,[10–12] which, however, are closely related to the influence of the magnetic field on the discharge plasma that embeds the dust suspension itself. The reason for
this is that due to the specific charge-to-mass ratios, the electrons and ions become very strongly magnetized before any effect on the dust particles sets on. Understanding the effects observed experimentally is difficult because of the very demanding computational needs—simulation of dusty plasma experiments with strong magnetic fields is certainly an emerging area\textsuperscript{[13]}. To overcome the problem of the magnetization of the discharge plasma, another approach, based on the equivalence of the (magnetic) Lorentz force and the Coriolis force experienced in a rotating frame of reference, was advised in Refs. \textsuperscript{[14, 15]}. Implementation of this method and a successful identification of magnetoplasmons in a “quasi-magnetized” rotating dusty plasma were reported by Hartmann et al.\textsuperscript{[16]}

Most of the computational studies have, meanwhile, concentrated on idealized systems, where the dust particles experience the effect of the magnetic field, whereas the surrounding medium is left unperturbed by this field. Many of the properties of such idealized systems have been studied by many-body (typically Molecular Dynamics) simulations. Collective excitations have been explored in Refs. \textsuperscript{[17, 18]}; the effect of the magnetic field on the diffusion was analysed in Refs. \textsuperscript{[19, 20]}, while heat transport was addressed by Ott et al.\textsuperscript{[21]}

Many of the properties of the strongly coupled complex plasmas are strongly related to one of its outstanding features, the quasi-localization of the particles in these systems\textsuperscript{[22]}; the particles oscillate in the local wells of the potential surface, which changes due to the diffusion of the particles on a timescale that can be significantly longer as compared with the timescale of oscillations. A mathematical framework based on tracking the surroundings of individual particles has been developed by Rabani et al.\textsuperscript{[23]}; the duration of the localization can be quantified by means of the so-called “cage correlation functions”. The effect of a static uniform external magnetic field on the cage correlation functions in frictionless two-dimensional Yukawa systems has been investigated by Dzhumagulova et al.\textsuperscript{[24]} while the effect of the friction force, induced by the presence of the buffer gas, has been addressed by Dzhumagulova et al.\textsuperscript{[25]} Here, our aim is to study the simultaneous effect of the magnetic field and the friction on the cage correlation functions. The interplay of these two effects is an open question that can only be answered by a systematic parametric study due to the inherent non-linearity of the system under investigation. Our studies are based on Langevin dynamics (LD) simulation into which a proper description of the movement of the particles under the influence of an external magnetic field is incorporated.\textsuperscript{[26–28]}

Our numerical integration scheme of the particles’ equations of motion follows the approach of Ref. \textsuperscript{[29]}, which takes into account the external magnetic field in the expansion of positions and velocities in the Taylor series. In Ref. \textsuperscript{[30]}, we introduced the friction force into the Velocity Verlet scheme, which is used in the present simulations. The scheme has been verified via comparisons of the cage correlation functions obtained in the limiting cases, when the friction force or the Lorentz force tends to be zero.

The model and the computational methods are described in Section 2, while the results are presented in Section 3. A brief summary is given in Section 4.

2 | MODEL AND COMPUTATIONAL METHOD

We adopt the following form for the potential that results from the mutual interaction of the particles and the screening property of the surrounding plasma environment:

$$\phi(r) = \frac{Q}{4\pi\varepsilon_0} \exp(-r/\lambda_D),$$

where $Q$ is the charge of the particles, and $\lambda_D$ is the screening (Debye) length.

We study a two-dimensional (2D) system; the particles move in the $(x, y)$ plane, and the magnetic field is assumed to be homogeneous and directed perpendicularly to the layer of the particles, that is, $\mathbf{B} = (0, 0, B)$. The equation of motion of the particles (given here for particle $i$) is

$$m\ddot{\mathbf{r}}_i(t) = \sum_{i\neq j} F_{ij}(r_{ij}) + Q[\mathbf{v}_i \times \mathbf{B}] - \nu m\mathbf{v}_i(t) + \mathbf{F}_{Br},$$

where the first term on the right side gives the sum of inter-particle interaction forces (to be computed for $(i, j)$ particle pairs that are separated by a distance $r_{ij}$), the second is the Lorentz force, and the third term represents the friction force (proportional to the particle velocity, $\nu$ is the friction coefficient of the dust particles in the background gaseous environment), while the fourth term represents an additional randomly fluctuating “Brownian” force that models the random kicks of the gas atoms on the dust particles.

The ratio of the inter-particle potential energy to the thermal energy is expressed by the coupling parameter

$$\Gamma = \frac{Q^2}{4\pi\varepsilon_0 a k_B T},$$
where $T$ is temperature, and $a = (1/\pi n)^{1/2}$ is the 2D Wigner–Seitz radius, with $n$ being the areal number density of the particles. We introduce the screening parameter $\kappa = a/\lambda_D$. The strength of the magnetic field is expressed in terms of

$$\beta = \Omega/\omega_p,$$

(4)

where $\omega_p = \sqrt{nQ^2/2e\omega_m}$ is the nominal 2D plasma frequency, and $\Omega$ is the cyclotron frequency. The strength of the friction is defined by the dimensionless parameter

$$\theta = \nu/\omega_p.$$  

(5)

So, the system is fully characterized by four parameters: $\Gamma$, $\kappa$, $\beta$, and $\theta$.

We apply the Langevin Dynamics (LD) simulation method to describe the motion of the particles governed by the equation of motion given above. To integrate this equation, a new numerical scheme based on the Taylor expansion of the particle acceleration and velocity, followed by the correct choice of all the terms that are not higher than $O((\Delta t)^2)$, is used, in which the time step does not depend on the magnitude of the magnetic field. This scheme was obtained by applying the technique developed by Spreiter and Walter, but takes into account the friction force. We obtained the following equations for the positions and velocities of the particles without taking into account $\mathbf{F}_{Br}$ (which can be added subsequently):

$$r_i(t + \Delta t) = r_i(t) - \frac{1}{(\Omega^2 + v^2)}[(v v_i(t) + \Omega v_i(t))(\exp(-v\Delta t) \cos(\Omega\Delta t) - 1)
+ (v v_i(t) - \Omega v_i(t))\exp(-v\Delta t) \sin(\Omega\Delta t)]
+ \frac{1}{(\Omega^2 + v^2)^2}[C(\Omega\Delta t)(v^2 - \Omega^2)\Delta^2_i(t) + 2v\Omega\Delta^2_i(t)]
+ S(\Omega\Delta t)(v^2 - \Omega^2)\Delta^2_i(t) - 2v\Omega^2\Delta^2_i(t)]$$  

(6)

$r_i(t + \Delta t)$ can be obtained from (6) by replacing $x \rightarrow y$ and $\Omega \rightarrow -\Omega$. Here, $\sigma$ is the part of the acceleration that does not depend on the velocities, and, furthermore,

$$S(\Omega\Delta t) \equiv \exp(-v\Delta t) \sin(\Omega\Delta t) - \Omega\Delta t$$  

(7)

and

$$C(\Omega\Delta t) \equiv \exp(-v\Delta t) \cos(\Omega\Delta t) - 1 + v\Delta t.$$  

(8)

The velocity components are given as:

$$v_i(t + \Delta t) = \exp(-v\Delta t)(v_i(t) \cos(\Omega\Delta t) + v_i(t) \sin(\Omega\Delta t))
+ \frac{1}{\Omega^2 + v^2}[\exp(-v\Delta t)(\Omega \sin(\Omega\Delta t) - v \cos(\Omega\Delta t))\Delta^2_i(t) + v\Omega\Delta^2_i(t)]
- \exp(-v\Delta t)(\Omega \cos(\Omega\Delta t) + v \sin(\Omega\Delta t))\Delta^2_i(t) + \Omega \Delta^2_i(t)]
+ \frac{1}{(\Omega^2 + v^2)^2}[[\exp(-v\Delta t)((v^2 - \Omega^2) \cos(\Omega\Delta t) - 2v\Omega \sin(\Omega\Delta t))
+ (\Omega^2 - v^2) + (\Omega^2 + v^2)v\Delta t] \frac{d}{dt}\Delta^2_i(t) + \{\exp(-v\Delta t)((v^2 - \Omega^2) \sin(\Omega\Delta t)
+ 2v\Omega \cos(\Omega\Delta t)) - 2v\Omega + (\Omega^2 + v^2)v\Delta t] \frac{d}{dt}\Delta^2_i(t)]$$  

(9)

$v_i(t + \Delta t)$ can be obtained from (9) by replacing $x \rightarrow y$ and $\Omega \rightarrow -\Omega$.

We investigate the localization of the particles characterized by the cage correlation function by using the method of Ref. [23], which allows the tracking of the changes in the surroundings of individual particles. We use a generalized neighbour list $\ell_i$, for particle $i$, $\ell_i = \{f_{i,1}, f_{i,2}, ..., f_{i,N}\}$. ($f_{i,i}$ is excluded from the neighbour list, i.e. only “real” neighbours are taken into account.) Due to the underlying sixfold symmetry of the system considered here, we always search for the six closest neighbours of the particles, and the f-s corresponding to these particles are set to a value 1, while all other f-s are set to 0.

The similarity between the surroundings of the particles at $t = 0$ and $t > 0$ is measured by the list correlation function (defined as the normalized scalar product of the list correlation functions at times $t$ and 0):

$$C_{\ell}(t) = \frac{\langle \ell_i(t) \cdot \ell_i(0) \rangle}{\langle \ell_i(0)^2 \rangle},$$  

(10)

where $\langle \cdot \rangle$ denotes averaging over particles and initial times. Obviously, $C_{\ell}(t = 0) = 1$, and $C_{\ell}(t)$ is a monotonically decaying function.

The number of particles that have left the original cage of particle $i$ at time $t$ can be determined as

$$N_i^{out}(t) = \ell_i(0)^2 - \ell_i(t)^2.$$

(11)
FIGURE 1  Cage correlation functions for $\Gamma = 20$ and $\kappa = 2$ for (a) $\beta = 0.5$ and (b) $\beta = 1$ for a wide range of the friction coefficient $\theta$. The legend shown in (a) also holds for panel (b). The inset in (b) zooms to the region where the correlation functions cross the $C_{\text{cage}} = 0.1$ line (at times that correspond to the caging time). Panels (c) and (d) show the same functions with semi-logarithmic scales to allow a better observation of the long-time behaviour.

Here, the first term gives the number of particles around particle $i$ at $t = 0$, which equals to six in our case. The second term gives the number of “original” particles that remained in the surrounding after time $t$. The cage correlation function $C_{\text{cage}}(t)$ is obtained by averaging the function $\Theta(c - N_{\text{out}}^i)$ over particles and initial times, that is,

$$C_{\text{cage}}(t) = \langle \Theta(c - N_{\text{out}}^i(0,t)) \rangle,$$

where $\Theta$ is the Heaviside function. We compute the cage correlation functions for $c = 3$, and take the definition of the “caging time” introduced by Donkó et al.\cite{31} according to which $t_{\text{cage}}$ is defined as the time when $C_{\text{cage}}$ decays to a value 0.1.

The number of simulated particles is fixed at $N = 1000$ that move within a quadratic simulation box. The positions of the particles are chosen randomly at the initialization of the simulations, and their velocities are sampled from a Maxwellian distribution with a temperature that corresponds to the value of specified $\Gamma$. During the initial phase of the simulations, the system is thermalized, but thermostation is stopped before the data collection phase starts.

3 | RESULTS

Below, we present the results of our simulations obtained for the cage correlation functions under the conditions of the simultaneous presence of the external magnetic field and the friction imposed by the background gaseous environment. In order to use the same numerical scheme throughout our work, we had to use finite values of the magnetic field and the friction coefficient. The field-free and/or frictionless cases are approximated by using very small values of these coefficients ($10^{-6}$–$10^{-5}$) in the simulations. The results obtained this way approximate the “true” $\beta = 0$ and/or $\theta = 0$ results well within the statistical noise of the results. Nonetheless, at the presentation of the results, we give the precise (low) values of these coefficients used in the respective simulations.

Figure 1a shows the $C_{\text{cage}}^3(t)$ functions obtained at fixed system parameters $\kappa = 2$ and $\Gamma = 20$ at a magnetic field $\beta = 0.5$, with the friction coefficient $\theta$ scanned over the domain between $10^{-5}$ (representing a case with vanishing friction) and 0.5
The effect of a changing strength of magnetic field on the cage correlation functions is presented in Figure 2 for $\Gamma = 20$ and $\kappa = 2$, for the $\theta = 0.1$ (panel (a)), and $\theta = 0.5$ (panel (b)) values of the friction coefficient. The correlation functions increase monotonically with increasing $\beta$ in both cases, and a stronger influence is found at the lower value of friction (panel (a)). (These data are also shown in semi-logarithmic representation in the panels (c) and (d) of Figure 2.)
FIGURE 3  Dependence of the caging time on the friction parameter $\theta$ at given values of $\beta$ in the highly magnetized domain. Note the non-monotonic dependence of $T_{cage}$ on $\theta$ for the $\beta > 0$ cases. The dashed horizontal lines correspond to $T_{cage}$ at $\theta = 0$.

(b) Values of the friction coefficient at the minimum of the caging time and at the crossing with the horizontal lines (at $\theta > 0$) in panel (a). (c) Caging time as a function of the normalized magnetic field strength for selected values of the friction coefficient.

($\theta_{cross}$) where the effect of magnetic field and friction “compensate each other”, that is, when $T_{cage}$ becomes the same again as at $\beta = 0$, both increase with increasing magnetic field. These dependences are displayed in Figure 3b. Both dependences appear to be nearly linear; the minimum occurs at $\theta_{min} \approx 0.13\beta$, while the crossing is found at $\theta_{cross} \approx 0.26\beta$. The dependence of the caging time as a function of $\beta$ is found to be monotonic for any fixed value of the friction coefficient, as can be seen in Figure 3c.

The interplay of the magnetic field and the friction is non-trivial. Both mechanisms, when acting alone, are known to increase the caging time. The magnetic field results in this by forcing the particles to move on circular trajectories. When the Larmor radius is smaller than the inter-particle separation, diffusive motion across the field lines is significantly hindered, and the caging time is enlarged.\(^{24}\) The effect of friction on the caging time is similar\(^{25}\) but results from a different physical mechanism. As explained earlier, the presence of the gaseous environment is modelled via a damping mechanism by the background (as a continuum) and by a random (“Brownian”) force that emulates random kicks by gas particles. The first of these slows down the particle motion, while the second increases the energy of the particle but randomizes its direction of velocity. The inverse of the frequency $\nu$ (related to the friction coefficient as $\theta = \nu/\omega_p$) can be viewed as the timescale for the change of the direction of velocity.

Figures 4 and 5 show typical particle trajectory segments for various parameter settings. Figure 4 displays these for vanishing magnetic field ($\beta = 10^{-6}$), while in Figure 5, the magnetic field is fixed at $\beta = 1.5$. The four panels of both figures correspond to increasing values of the friction coefficient. The length of recording is $\omega_p T = 200$ for all cases. (Moreover, $\Gamma = 20$ and $\kappa = 2$, as before.)

The trajectory seen in Figure 4a for vanishing friction is smooth, and deflections of the velocity are due to inter-particle “collisions”. When friction is introduced, the nature of the motion is changed, and more frequent changes of direction of motion are apparent already in Figure 4b, which correspond to $\theta = 0.2$. With further increasing friction, these “breaks” become even more frequent, and the particle tends to execute a random walk, which is, however, guided by the neighbouring particles—note the decreasing size of the coordinate domains within which the particle is located during the (constant) time of recording. This is the reason of an increasing caging time with increasing $\theta$.

Figures 5a displays the trajectory of a single particle for $\beta = 1.5$ at vanishing friction. The trajectory consists of smooth “loops” due to the cyclotron motion of the particle combined with diffusion and interaction with the other particles. Such a
strong magnetic field significantly enhances the localization of the particle. When the friction is introduced (see Figure 5b, for which θ = 0.2), the circular trajectories (i.e. the loops) are still well visible; however, they are distorted by the random changes of the velocity due to effect of friction. This way, the confining effect of the magnetic field is decreased. At further increased friction (distorted) loops are only visible for parts of the trajectory, as seen in Figure 5c for θ = 0.6, while they almost completely disappear in Figure 5d, which shows the highly damped case of θ = 1. In the latter case, the localization by friction prevails. The case shown in panel (b) corresponds to the minimum of the caging time as a function of θ (see Figure 3a). For this case, θ = 0.2, which corresponds to a “friction” frequency ν = 0.2ωp. The time scale of the motion over one loop, T, for this highly magnetized (Ω ≫ ωp) case is ΩT = βωpT ∼ 2π, from which νT ≈ θ(2π/β) ≈ 0.83, i.e. the timescale of the change of the direction of motion is approximately the same as the cyclotron period. We suspect that this is the effect that partially destroys the efficiency of the confinement of the particles by the magnetic field. When the number of collisions per loop doubles (recall that θcross ≃ 2θmin), the positive effect of the friction on the localization starts to dominate.

4 | SUMMARY

In this paper, we have investigated the simultaneous effect of friction induced by the gas environment, as well as a homogeneous external magnetic field, on the quasi-localization of dust particles in a 2D layer. The system has been described by LD simulation. We have found that, when acting alone, both an increasing friction coefficient and an increasing strength of the magnetic field enhance the caging of the particles, as quantified by the cage correlation functions. When present simultaneously, however, a non-trivial interplay of the two effects was observed. For a fixed magnetic field (β > 0), the increasing friction was found to first decrease the caging time and then to increase it beyond a certain value of the friction coefficient that depends on the magnetic field strength. A qualitative explanation was given for these observations based on the analysis of the peculiarities of the trajectories of individual particles; however, a more detailed, quantitative understanding of the effect calls for further studies that include the analysis of the velocity autocorrelation function of the particles.
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