# Dynamics of two-dimensional one-component and binary Yukawa systems in a magnetic field

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We consider two-dimensional Yukawa systems in a perpendicular magnetic field. Computer simulations of both one-component and binary systems are used to explore the equilibrium particle dynamics in the fluid state. The mobility is found to scale with the inverse of the magnetic field strength (Bohm diffusion), for strong fields ($\omega_c/\omega_p \gtrsim 1$). For bidisperse mixtures, the magnetic field dependence of the long-time mobility depends on the particle species, providing an external control of their mobility ratio. At large magnetic fields, the highly charged particles are almost immobilized by the magnetic field and form a porous matrix of obstacles for the mobile low-charge particles.

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## I. INTRODUCTION

Transport properties in liquids are relevant for various applications ranging from solvation of tablets [1] and the penetration of salt ions into fresh river water [2] to imbibition problems [3]. Hence, there is a need for a basic understanding of particle diffusion on the most fundamental level of the individual particles. The particle trajectories, as governed by Newton's equation of motion with the interparticle forces, are the natural starting point to understand and predict the transport properties [4]. Already in equilibrium this is still a nontrivial problem of classical statistical mechanics.

Yukawa systems are a quintessential model of softly interacting systems and are used to study, e.g., complex plasmas [5–7], colloidal suspensions [8], the warm dense matter state [9], or the interior of white dwarf stars [10]. Further, in the limit of vanishing screening, this model reduces to Coulomb systems, such as ions in Paul traps; e.g., Refs. [11,12]. Typically, the interaction between the particles in these systems is strong and repulsive, so that, at high densities, the system can exhibit both fluid and solid phases [13]. In this paper, we study the particle dynamics of a two-dimensional Yukawa liquid which is exposed to an external magnetic field of strength $B$.

Although the presence of a magnetic field does not alter the equilibrium static properties, such as phase transitions, the dynamics is strongly affected [14]. Due to the Lorentz force, the charged particles exhibit a circular motion [15–17] which is expected to slow down the particle migration. Therefore the magnetic field opens the fascinating possibility of changing the dynamical properties of the system externally without preparing a new experiment with different particles. The magnetic field might, however, change other aspects of the experiment, such as the plasma parameters in complex plasma experiments, which in turn influence details of the interaction between the particles (screening); see below.

Some aspects of the dynamics of a one-component plasma in a magnetic field have been considered in previous studies [5,14,16,18–21]. In particular, the motion of few-particle clusters in magnetic fields has been analyzed by both experiments and simulation [15,17,22–24]. The dynamics of three-dimensional ionic binary mixtures has also been under investigation in early as well as recent research [25–28], with a particular focus on astrophysical plasmas and those encountered in inertial confinement fusion. A recent work by Kalman *et al.* focuses on the description of the collective excitation of waves in two-dimensional binary Yukawa systems [29]. Binary Yukawa systems have also been studied in the context of white dwarfs where liquid and crystalline ionic mixtures are expected to exist [10], whereas binary Coulomb systems were observed in ion trap experiments [12].

Here, we focus on two-dimensional systems and explore the long-time dynamics by computer simulations. We confirm the $1/B$ scaling of the long-time diffusion coefficient for strong magnetic fields [16] for the two-dimensional system. We moreover consider binary systems composed of high-charge and low-charge particles [30–32]. Our motivation to study a binary system comes from the fact that the magnetic field affects the dynamics of the particle species differently. Thereby, the individual particle dynamics can be steered externally via the magnetic field. One important parameter is the mobility ratio of the two species, which governs the mutual diffusion and is one key parameter for the nature of the kinetic glass transition in mixtures [33–35]. This ratio is typically fixed by the mass ratio [36] and the interactions [37] and can therefore not be easily tuned. Here we show that this ratio can be controlled by an external magnetic field insofar as the high-charge particles are more strongly immobilized than the low-charge particles. For large magnetic fields, it is even conceivable that the high-charge particles are almost immobilized while the low-charge particles are still mobile. This opens the way to realizing a porous model matrix in two dimensions. Recently a similar matrix has been created by adsorbing colloidal particles onto a substrate [38]. Our approach, however, is more flexible as everything can be controlled externally.

This paper is organized as follows: In Sec. II we describe our model of complex plasmas in a magnetic field. In Sec. III we describe results for the one-component case. Binary mixtures are then considered in Sec. IV. Finally, we conclude in Sec. V.

## II. MODEL

We consider one-component systems and charge-asymmetric binary mixtures of uniform mass $m$, charge ratio

 

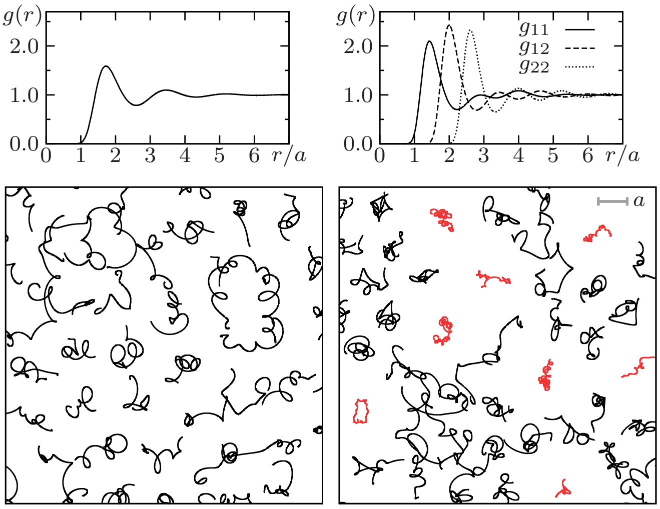


FIG. 1. (Color online) Pair distribution functions and particle trajectories during time $\omega_p t = 30$ at $\Gamma = 30$, $\beta = 0.5$. Left: One-component system. Right: Binary mixture with $Q_r = 4$ and $n_r = 1/3$. The highly charged particles are shown in red (gray).

$Q_r = q_2/q_1$, and density ratio $n_r = n_2/n_1$, where the numeric indices label the particles species. The particles are situated in a two-dimensional quadratic simulation box of side length $L$, giving rise to partial densities $n_{1,2} = N_{1,2}/L^2$, and interact via a screened Coulomb interaction with screening length $\lambda$,

$$V_{ij}(\mathbf{r}_i,\mathbf{r}_j) = \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|}\exp(-|\mathbf{r}_i - \mathbf{r}_j|/\lambda). \quad (1)$$

In addition, we consider the influence of an external magnetic field $B$ perpendicular to the particle plane, giving rise to the cyclotron frequency $\omega_{c,1,2} = |q_{1,2}|B/(mc)$ ($c$ is the speed of light).

The system is fully described by a set of five parameters: $Q_r$, $n_r$, $\kappa$, $\Gamma$, and $\beta$. Here, the screening strength is defined as $\kappa = a/\lambda$ with the Wigner-Seitz radius $a = [\pi(n_1 + n_2)]^{-1/2}$, $\Gamma = \Gamma_1 = Q_1^2/(ak_BT)$ ($T$ is the temperature), and $\beta = \beta_1 = \beta_2 = \omega_{c,1,2}/\omega_{p,1,2}$, where $\omega_{p,1,2} = (2q_{1,2}^2/(a^3m))^{1/2}$ is the nominal Coulomb plasma frequency. In the following, we normalize lengths by $a$ and times by the inverse of $\omega_p \doteq \omega_{p,1}$.

Our investigations are carried out by molecular dynamics simulation for $N = 16\,320$ particles and encompass a measurement time of $\omega_p t = 100\,000$ which is preceded by an equilibration period. The simulation is carried out in the microcanonical ensemble at $\kappa = 1$; typical trajectory snapshots are shown in Fig. 1. Notice the familiar circular paths induced by the magnetic field and the different mobility of the particle species in the binary system. An external magnetic field does not influence the equilibrium structure of one-component systems or binary mixtures (by the Bohr–van Leeuwen theorem). The charge ratio, on the other hand, has a strong influence on the structure as quantified by the pair distribution function $g_{\alpha\beta}(r)$; see the upper graphs in Fig. 1. In the binary mixture, the lightly charged particles exhibit a smaller correlation gap at small distances and a lower peak height, indicating a smaller degree of correlation in this subsystem. The highly charged subsystem is considerably more correlated [see $g_{22}(r)$ in Fig. 1], and the cross correlation between the particles species [$g_{12}(r)$] falls in between.

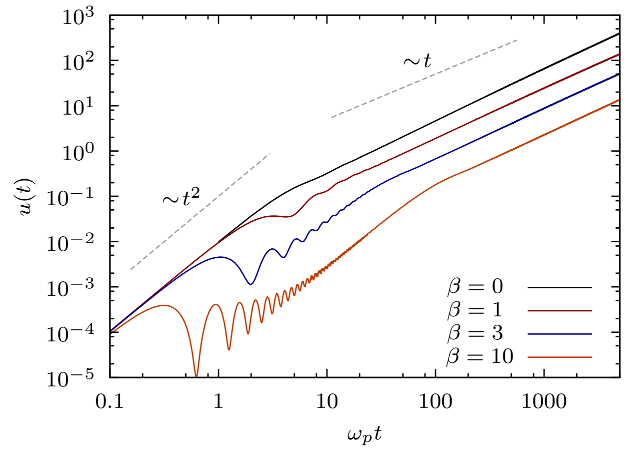


FIG. 2. (Color online) MSD of a one-component system with $\Gamma = 100$ at different magnetic field strengths. The straight lines indicate linear and quadratic growth. The order of the curves is the same as in the key.

The study of the dynamics of the system is undertaken by calculating the mean-squared displacement (MSD) $u(t)$ defined as

$$u(t) = \langle|\mathbf{r}_i(t + t_0) - \mathbf{r}_i(t_0)|^2\rangle_{i,t_0}, \quad (2)$$

where the averaging is over all particles and all starting times $t_0$. According to classical transport theory, the diffusion coefficient follows as

$$D = \tfrac{1}{4}\lim_{t\to\infty}\tfrac{u(t)}{t}. \quad (3)$$

Since the existence of Fickian diffusion is doubtful for strongly coupled two-dimensional Yukawa systems [39,40], we evaluate Eq. (3) at a fixed time instant $t\omega_p = 4850$ and denote it $D^*$, keeping in mind that this measure of the mobility should not be identified with the long-time diffusion coefficient.

## III. ONE-COMPONENT SYSTEM

Before investigating the binary system, we first establish the general diffusion trends in a magnetized, one-component two-dimensional (2D) Yukawa system [41]. The behavior of the MSD in such a system at $\Gamma = 100$ is shown in Fig. 2 for different magnetic field strengths. For $\beta = 0$, the ballistic regime with a quadratic increase at small times is followed by a quasidiffusive regime in which the MSD grows almost linearly with time. With increasing magnetic field, the signature of the circular paths is visible in the MSD curves as an oscillatory growth. The localization of individual particles at high magnetic field values gives rise to an additional regime at very small time delays during which the MSD is subdiffusive, i.e, during which $u(t)$ grows less than linearly with time.

The scaling of the diffusivity $D^*$ as a function of the magnetic field strength is of central interest with regard to the dynamics of the system. This scaling is shown in Fig. 3. For small values of $\beta$, the rapidity of the diffusive motion is unaffected, regardless of the coupling constant $\Gamma$. Only

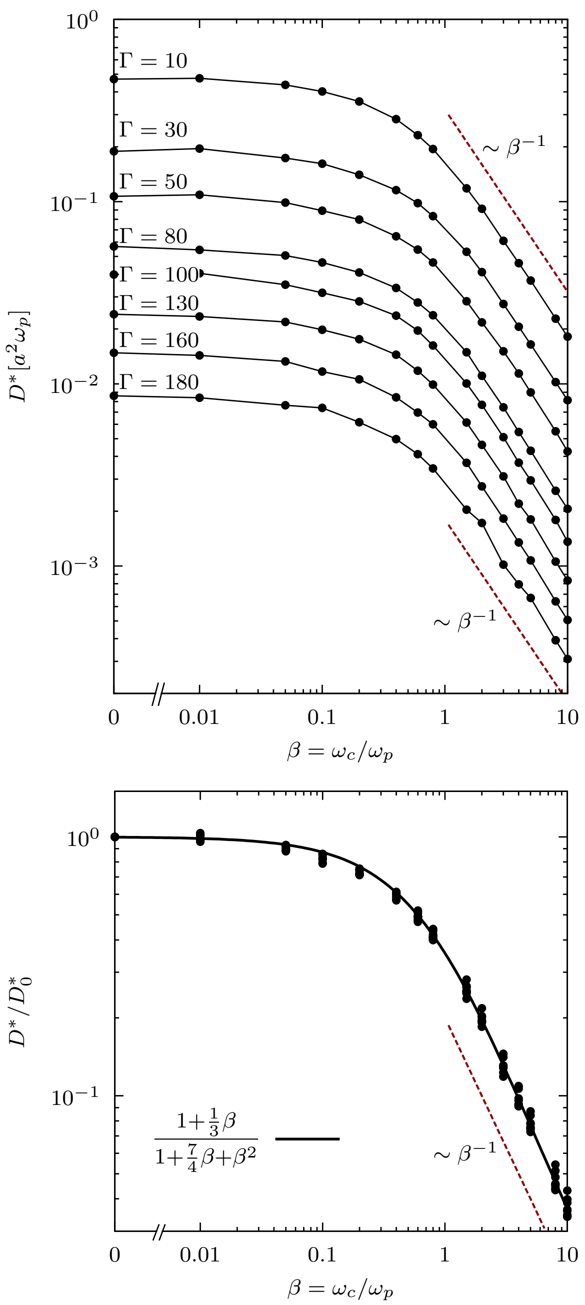


FIG. 3. (Color online) Top: $D^*$ as a function of $\beta$ for values of $\Gamma$ as indicated in the figure. The dotted lines show a decay $\beta^{-1}$ as a guide for the eye. Bottom: $D^*$ normalized by the field-free value $D_0^* = D^*(0)$. The normalized values fall on a universal curve for all values of $\Gamma$.

when magnetic field effects become important at $\beta \gtrsim 0.1$ does $D^*$ begin to decay. At $\beta \approx 1$, the scaling becomes the familiar Bohm type diffusion, $D^* \propto 1/\beta$ [45]. This is the same behavior that was found in the diffusion *perpendicular* to the field in strongly coupled three-dimensional one-component plasmas (OCPs) [16].

The functional form of the $D^*(\beta)$ dependence is quite insensitive to $\Gamma$, as demonstrated in the lower graph of Fig. 3. This is in contrast with the corresponding behavior of a three-dimensional OCP [16] which shows a clear $\Gamma$ dependence in both field-parallel and -perpendicular diffusion.

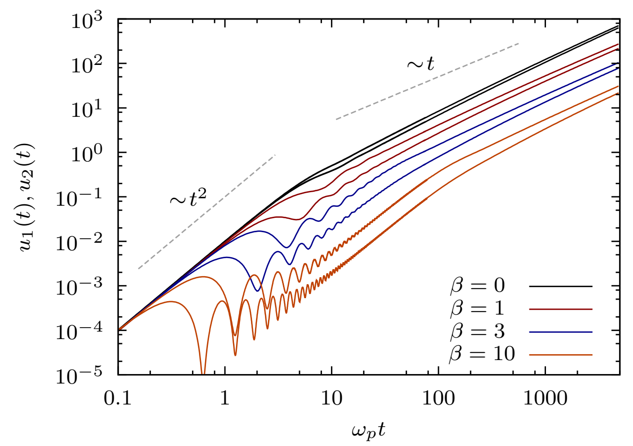


FIG. 4. (Color online) MSD of a binary system with $n_r = 1$, $Q_r = 0.5$, and $\Gamma = 100$ at different magnetic field strengths. The lower of each pair of curves corresponds to the more highly charged particles. The straight lines indicate linear and quadratic growth. The order of the curves is the same as in the key.

The reason for the more complex behavior in 3D systems is the mutual interference between the two diffusion directions (mediated by the strong coupling between the particles), which is absent in 2D systems.

## IV. BINARY SYSTEM

In this section, we expand on the previous investigation and consider charge-asymmetric binary Yukawa systems with a repulsive interaction. The density ratio is fixed to $n_r = 1$, i.e., $N_1 = N_2$, while the charge ratio $Q_r$ and the magnetic field strength $\beta$ are varied.

Figure 4 shows the MSD of such a binary system at $Q_r = 0.5$ and different magnetization; for each value of $\beta$, there are two curves, reflecting the two particle species. Evidently, the particles carrying a lower charge are more mobile, regardless

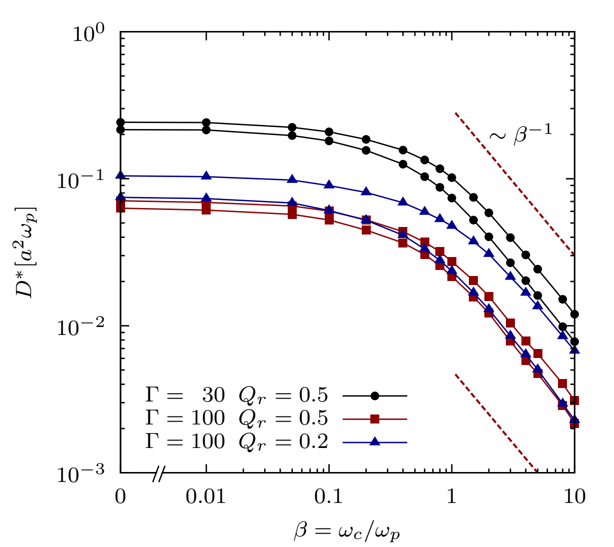


FIG. 5. (Color online) $D^*$ as a function of $\beta$ for binary systems with charge ratio $Q_r = 0.5$ and $Q_r = 0.2$. The lower one of each pair of curves corresponds to the more highly charged species. The dotted lines show a decay $\beta^{-1}$ as a guide for the eye.

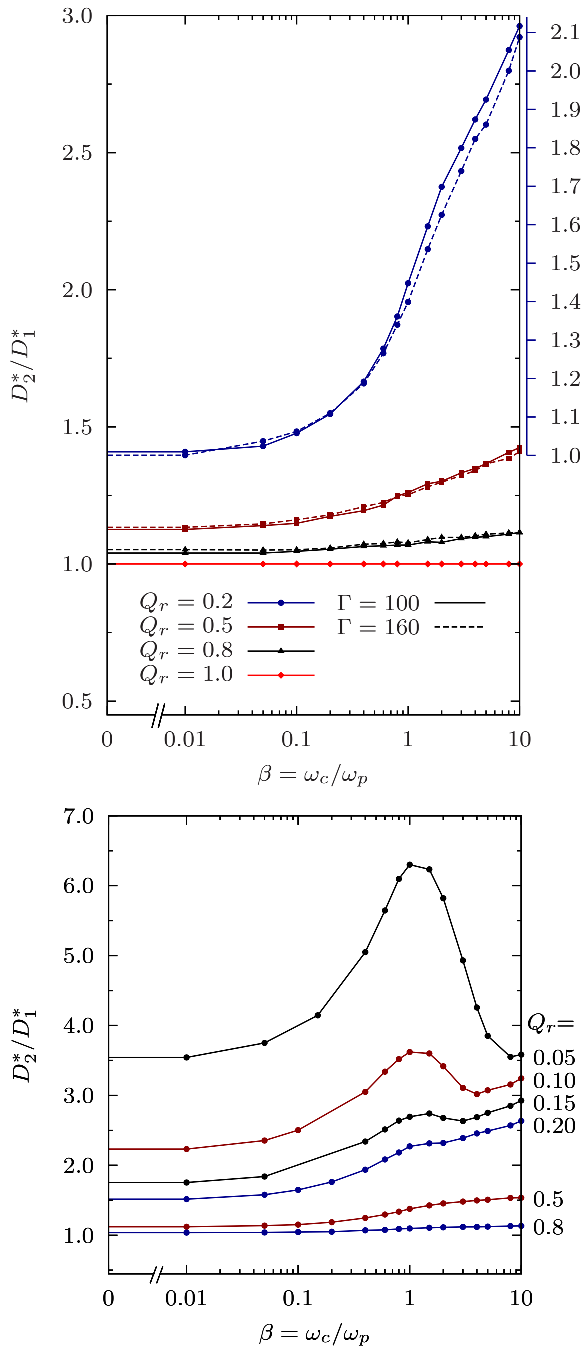


FIG. 6. (Color online) Ratio $D_2^*/D_1^*$ for $\Gamma = 100,160$ (top) and $\Gamma = 30$ (bottom) at different charge ratios $Q_r$ as a function of $\beta$. The right axis in the top graph shows the relative change for $Q_r = 0.2, \Gamma = 100$, normalized to $\beta = 0$.

of the magnetic field strength. For increasing $\beta$, however, the disparity in mobility between the two species grows steadily, as evidenced by the increasing gap between the two MSD curves when going from zero magnetic field to $\beta = 10$.

More data are presented in Fig. 5, which shows $D^*$ as a function of $\beta$ for two values of $Q_r$. The functional form of the data is comparable to that in the one-component case considered in the previous section and is well described by Bohmian diffusion for both species for $\beta \gtrsim 1$. A closer look, however, reveals that the response of the less highly charged (more mobile) species is shifted to higher values of $\beta$ which results in an increase in the mobility ratio between the two species.

In the upper graph of Fig. 6, this is demonstrated for strong coupling $\Gamma = 100,160$, by plotting the ratio $D_2^*/D_1^*$. While a modest charge ratio of $Q_r = 0.8$ results only in a small variation of this ratio, the influence of the magnetic field grows with decreasing $Q_r$, so that at $Q_r = 0.2$, the magnetic field alone can be used to manipulate the mobility ratio by a factor of 2 for $\beta = 10$ (see the right-hand scale in Fig. 6). Since the mobility ratio plays a crucial role during the glass transition, this effect can be leveraged to investigate the conditions for glass formation in one and the same system by controlling the mobility ratio by the external magnetic field.

The relatively simple dependence of $D_2^*/D_1^*$ on $\beta$ for strongly coupled plasmas shown in the upper part of Fig. 6 has to be contrasted with the more intricate behavior of the same ratio for $\Gamma = 30$ (lower graph in Fig. 6). Here, a highly nonmonotonic dependence of the ratio $D_2^*/D_1^*$ is observed, which becomes more strongly pronounced for more disparate charge ratios. The strong growth of $D_2^*/D_1^*$, which is undisturbed at large values of $\Gamma$, is suppressed at magnetic field strengths surpassing $\beta \approx 1$, leading to the formation of a pronounced peak at this value of $\beta$.

The microscopic reason for the suppression at large magnetic fields lies in the reduced mobility of the lightly charged species and is elucidated by considering the ratio $\Delta = r_{L,2}/\sqrt{n_1}$ of two length scales: the Larmor radius $r_{L,2}$ of the lightly charged species and the average nearest-neighbor distance $\sqrt{n_1}$ of the highly charged species. For small values of $\Delta$ (large magnetic fields), a lightly charged particle will perform many gyrations before colliding with a highly charged particle. For very large values of $\Delta$, its trajectory is only weakly influenced by the magnetic field before a collision occurs. At $\Delta = 1/4$, however, the trajectory leads, at thermal velocity of the particle, to a collision with one of the highly charged particles, effectively preventing the diffusion of the lightly charged particle (see the schematic in Fig. 7). This

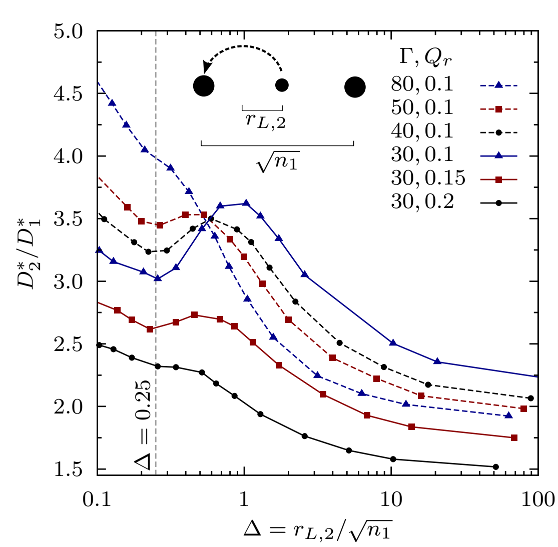


FIG. 7. (Color online) Ratio $D_2^*/D_1^*$ as a function of $\Delta = r_{L,2}/\sqrt{n_1}$. Note that small values of $\Delta$ correspond to large magnetic fields, and vice versa.

results in a reduction of $D_2^*/D_1^*$ at $\Delta = 1/4$. We have tested this simple geometric reason by plotting data for the mobility ratio as a function of the geometric parameter $\Delta$; see Fig. 7 (notice that $r_{L,2}$ is a function of both $\Gamma$ and $Q_r$). In fact, a resonant dip in the mobility ratio is formed around $\Delta = 1/4$, supporting the underlying picture. This geometric resonance effect persists across different parameter regimes, but becomes less pronounced as $Q_r$ or $\Gamma$ is increased, since an increased particle coupling leads to stronger caging effects.

## V. CONCLUSION

In conclusion, we have explored the dynamics of charged particles with Yukawa interaction in a layer exposed to a perpendicular magnetic field which allows for an additional external control of the particle transport. Our results, when extended to three dimensions, are of relevance to white dwarf stars in which binary ionic mixtures are exposed to a magnetic field; see, e.g., Ref. [10]. Another application is to binary mixtures of ions in Paul traps [11,12].

Further, our simulation results can be verified in dusty plasma experiments. One possibility is to use a rotating plasma which exactly mimics the effect of a magnetic field on the heavy dust component(s) [15,17] without disturbing the light plasma components, as was confirmed in recent experiments on two-dimensional plasmas [15,46]. The extension to two dust components appears to be straightforward. An experimental realization of an unmagnetized binary system was recently reported [47], where it was confirmed that the particle interaction of this system is of the Yukawa type and that the vertical separation of the two species can be much smaller than the horizontal interparticle distance [48]. The second possibility consists in using strong magnets that are now available in several laboratories [49]. However, the interesting range of magnetizations, $\beta \gtrsim 1$, can be reached only with submicron particles, which, in fact, have recently attracted great interest [50]. These systems do not allow for a direct optical diagnostics and, therefore, rely strongly on simulation results. The present results are expected to be a valuable starting point, whereas for a quantitative comparison, obviously, the effect of the magnetic field on the electrons and ions, will also have to be incorporated [51,52].

We have demonstrated that the mobility in two-dimensional Yukawa systems adheres to the same $1/B$ Bohm scaling as in three-dimensional systems. In contrast to three-dimensional systems, however, the functional form of the scaling is largely independent of the coupling $\Gamma$, indicating a decoupling of magnetic and interaction effects.

Our main focus has been on the response of a charge-asymmetric binary mixture to an external magnetic field. Since the two subsystems are affected differently by the magnetic field, the mobility ratio between them can be controlled by the strength of the magnetic field. For less strongly coupled systems and high charge asymmetry, we have found that the circular trajectories of the lightly charged particles can be in resonance with the positional configuration of the highly charged particles, which leads to a distinct reduction of the mobility of the former. This is an interesting realization of a porous model matrix in a fluid system.

For future studies, as regards binary systems, a systematic understanding of the two-dimensional glass transition in binary mixtures lies ahead, where the magnetic field is exploited as a steering wheel to change the mobility ratio between the particle species. Moreover, it is known that the crystallization process out of an undercooled melt depends sensitively on the mobility ratio in binary systems [53] such that the magnetic field can be used to tune crystal nucleation in mixtures [54–57].

## ACKNOWLEDGMENTS

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