Contrib. Plasma Phys. **49**, No. 10, 760 – 764 (2009) / **DOI** 10.1002/ctpp.200910089

Anomalous and Fickian Diffusion in Two-Dimensional Dusty Plasmas

T. Ott and **M. Bonitz***

Christian-Albrechts-Universität zu Kiel, Institut für Theoretische Physik und Astrophysik, Leibnizstraße 15, 24098 Kiel, Germany

Received 05 November 2009, accepted 11 November 2009
Published online 16 December 2009

Key words Strongly-coupled plasmas, dusty or complex plasmas.
PACS 52.27.Gr, 52.27.Lw, 82.70.Dd, 66.10.cg

We provide an overview on diffusion in frictionless two-dimensional Yukawa liquids as a model for dusty plasmas. Results are obtained for the combined influence of temperature and screening length on the character of diffusion, i.e., on the value of the diffusion exponent at long times.

1 Introduction

The possibility of directly observing the motion of interacting charged particles is the primary reason for the interest in dusty plasmas in the last decades [1]. In dusty plasmas, micron-sized particles are a fourth constituent in a plasma discharge, besides neutrals, ions and electrons. Under typical experimental conditions, these dust particles become negatively charged due to the influx of electrons and interact via a Debye-screened Coulomb interaction. Because of their high mass, high charge and large size, it is possible to track them on comfortable spatio-temporal scales. When compared to other trackable systems of interacting particles, such as charged colloids, another advantage of dusty plasmas is the relatively low damping of the particles' motion which is mainly due to neutral drag.

A particularly interesting setup of dusty plasmas are quasi-two-dimensional layers of particles, because they allow the experimental study of systems with lowered dimensionality. Such systems have been found to exhibit a number of anomalies, and among those is an anomalous diffusion behaviour. It has been predicted [2] that motion can never be diffusive in two-dimensional systems. Early computer simulations of excluded-volume hard-disk systems by Alder and Wainwright showed a slowly decaying tail of the momentum autocorrelation function which makes the calculation of a diffusion coefficient by means of the Green-Kubo formulas impossible [3]. Recent simulations have indicated a slightly faster decay [4]. In such anomalously diffusive systems, the mean-squared displacement does not increase linearly with time but instead proportional to some power α of time, where $\alpha > 1$.

A number of groups have performed measurements of the mean-squared displacement in quasi-two-dimensional dusty plasma setups [5–13]. These measurements include overdamped vertically aligned strings of particles [5–8] as well underdamped monolayers of single dust particles [9–11]. Most systems were reported to show non-diffusive behaviour at least on intermediate time-scales and in some cases over the full range of time observed. One notable exception is the underdamped monolayer examined by Nunomura *et al.* in which no anomalous diffusion was found [11].

These experiments have instigated computer simulations in recent years in which dusty plasmas were modelled by interacting Yukawa-systems. The intent of these simulations was to examine the diffusion process in two-dimensional [9, 14–18] as well as in quasi-two-dimensional [19, 20] systems and to answer the question whether motion in such arrangements is diffusive (Fickian) or anomalously diffusive.

In these simulations, diffusion was found to be normal for high temperatures and near the ordering transition [14, 16] and anomalous in-between [15, 16], giving rise to a non-monotonic temperature dependence of α

* Corresponding author: E-mail: bonitz@physik.uni-kiel.de

for two-dimensional monolayers. Friction-induced subdiffusion was also observed [17]. The dependence on the interaction range has been a topic of controversy [17, 18]. For extended quasi-two-dimensional systems, a slow vanishing of superdiffusion was found for increasingly broader systems [20]. Earlier simulations [21, 22] of strongly damped Yukawa fluids had shown normal diffusion.

In this contribution, we aim to give a unified overview of the combined temperature/interaction-range dependence of the diffusion exponent α in frictionless Yukawa fluids.

2 Normal and Anomalous Diffusion

Gauging the nature of the diffusion is commonly done by inspection of two quantities, the velocity autocorrelation function (VACF) $C_v(t)$ and the mean-squared displacement (MSD) $u_r(t)$. The VACF is defined as $C_v(t) = \langle \vec{v}(t) \cdot \vec{v}(0) \rangle$, assuming stationarity in time. From $C_v(t)$, the diffusion coefficient D can be calculated according to the following prescription [23]:

$$D = \frac{1}{N_d} \int_0^\infty C_v(t) dt, \tag{1}$$

where N_d is the number of dimensions. If $C_v(t)$ decays too slowly for the integral in Eq. (1) to converge, motion is ascribed to anomalous diffusion.

The MSD is calculated from the particles displacement relative to an arbitrary starting time, $u_r(t) = \langle |\vec{r}(t) - \vec{r}(0)|^2 \rangle$, and the diffusion coefficient can be calculated as

$$D = \lim_{t \to \infty} \frac{1}{2N_d} \frac{u_r(t)}{t}. \tag{2}$$

If $u_r(t)$ does not grow linearly with time at long times, D is not time-independent and diffusion is anomalous. A common parametrization of $u_r(t)$ is

$$u_r(t) = C \cdot t^\alpha, \tag{3}$$

where C is a constant and α is the *diffusion exponent*. The value of α is used to classify motion as diffusive ($\alpha = 1$), ballistic ($\alpha = 2$), and sub- or superdiffusive ($\alpha < 1$ or $\alpha > 1$), i.e., anomalous.

We will concentrate on the MSD and the diffusion exponent as indicator for anomalous diffusion in the following. This is motivated by the fact that it is both easier to measure experimentally and provides a clearer picture when compared to the VACF in most cases.

3 Simulation details

We model the interaction of the dust grains in the plasma by a Yukawa interaction [24], so that the full Hamilton function is given by

$$H(\vec{p}, \vec{r}) = \sum_i^N \frac{\vec{p}_i^2}{2m_i} + \sum_{i<j}^N \frac{Q^2}{4\pi\varepsilon_0} \frac{\exp\left(-r_{ij}/\lambda_D\right)}{r_{ij}}, \tag{4}$$

where N is the particle number, m is the particle mass, Q is the charge and $r_{ij} = |\vec{r}_i - \vec{r}_j|$. Instead of the screening length λ_D, in the following we use $\kappa = a_{ws}/\lambda_D$, where $a_{ws} = (n\pi)^{-1/2}$ with the areal density n, to indicate the interaction range. The Coulomb coupling parameter is given by $\Gamma = (Q^2/4\pi\varepsilon_0) \times (1/a_{ws}k_BT)$.

For the simulations, we use $N = 20.000$ particles subject to periodic boundary conditions in a two-dimensional square box. The equations of motion are integrated using the Swope algorithm [25]. In the initial phase of the simulation, the system is thermalized by constant rescaling of the velocities to yield the desired temperature. After this equilibration, the system is advanced without further equilibration, i.e., in the microcanonical NVE-ensemble. Data acquisition is done once every plasma period, where the plasma frequency is $\omega_p = (Q^2/2\pi\varepsilon_0 m a_{ws}^3)^{1/2}$. A κ-dependent cut-off is used in calculating the forces and the results are checked against variation of this cut-off to ensure the validity of this approximation. This allows for a favorable scaling of $\mathcal{O}(N)$ of the simulation costs.

After the completion of a specific run, the positional data is post-processed to compute the MSD. Due to the stationarity and ergodicity of the equilibrated system, we use each different timestep as an independent starting point $\vec{r}(0)$ for the calculation of the MSD and average over all particles to improve statistics. This is possible because diffusion is a single-particle quantity, as opposed to other transport coefficients such as the viscosity and the thermal conductivity [23].

4 Results and Discussion

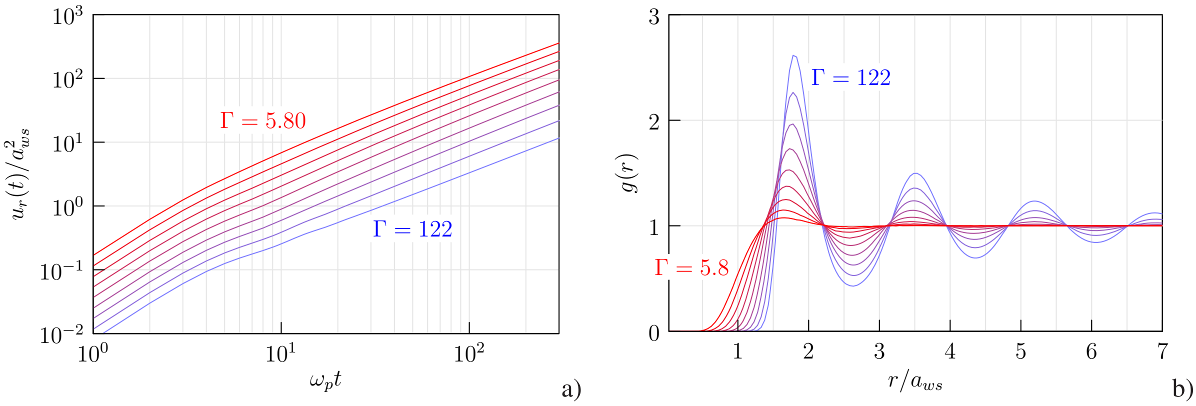

Fig. 1 **a**) The MSD $u_r(t)$ as a function of time and **b**) the pair distribution function $g(r)$ for fixed interaction range $\kappa = 1$ and different values of the Coulomb coupling Γ. Subsequent curves differ in Γ by factors of 1.46. (Online colour: www.cppjournal.org)

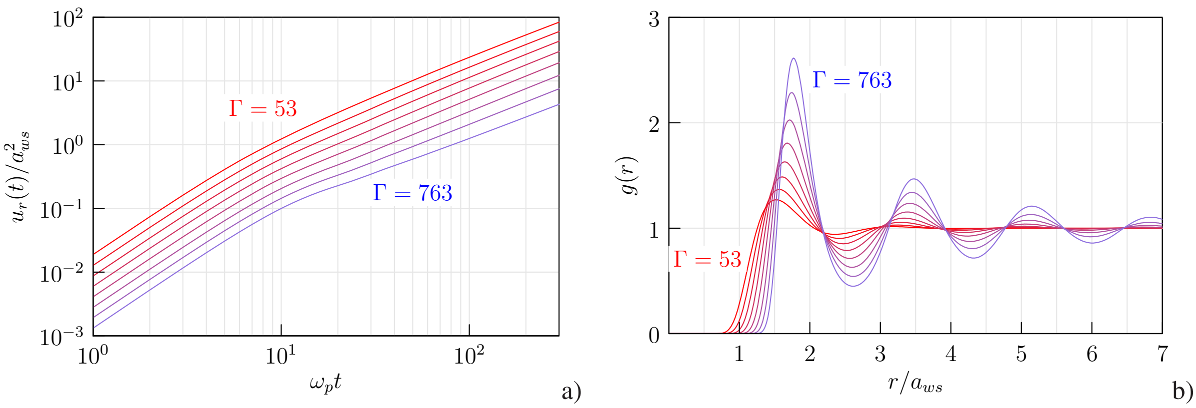

Fig. 2 Same as Fig. 1, but for $\kappa = 3$. (Online colour: www.cppjournal.org)

In Figs. 1a and 2a, we show the course of $u_r(t)$ over time for fixed interaction ranges $\kappa = 1.0$ and 3.0 in a double-logarithmic representation. Both systems exhibit essentially the same behaviour: At small time-scales, the particles move ballistically, as indicated by a slope (in the double-logarithmic plot) of $\alpha = 2$. After having suffered collisions with other particles, the particles' migration is slowed down, $\alpha < 2$. After the transition phase, during which some particles still move undisturbed while others have already undergone considerable momentum transfer in collisions, all particles eventually, on longer time-scales, exhibit near-diffusive motion, $\alpha \approx 1$. The free ballistic motion is more prolonged for $\kappa = 3$ due to the smaller range of the interaction which decreases the scattering cross-section.

Figs. 1a and 2a also compromise the Γ-dependence of the MSD. Cooler liquids (blue curves, high Γ) show significantly smaller mean-squared displacements than hotter liquids (red curves, small Γ) and additionally exhibit small oscillatory modulations at intermediate time-scales due to increased local order resulting in caged motion of individual particles. This is evident from the pair distribution functions $g(r)$ [23] depicted in Figs. 1b and 2b, where strong modulations for cool liquids indicate an increase in next-neighbour correlations. The liquid character of the systems is evident from the exponential decay of the envelope of $g(r)$.

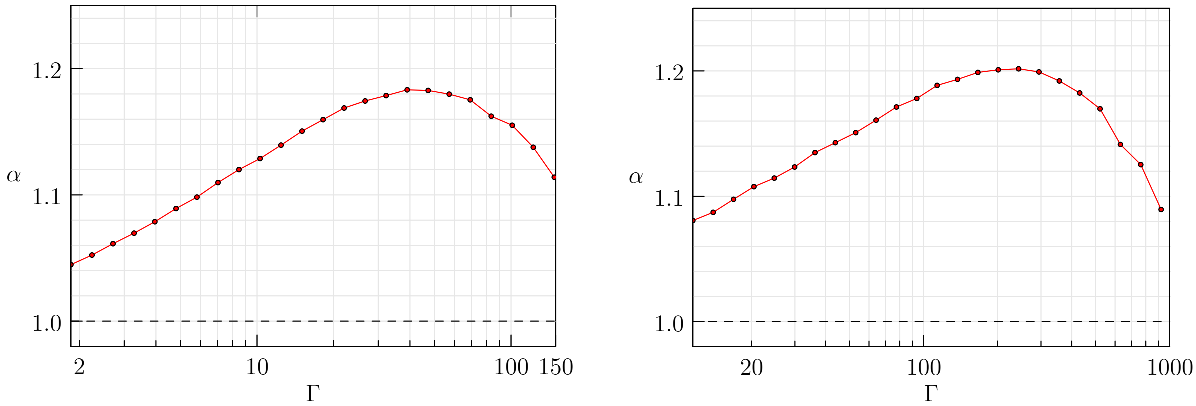

Fig. 3 The diffusion exponent α as a function of the coupling parameter for **left:** $\kappa = 1$ and **right:** $\kappa = 3$. Notice the different scalings of the Γ-axis.

To deduce the diffusion exponent from the MSD curves according to Eq. (3), we choose a range $\omega_p t \in [200, 320]$ and read off the slope of $\log(u_r(\log(t))$ during this time. The results are depicted in Figs. 3a and b. Again, the two systems behave very similar. The Γ-dependence of α is non-monotonic with a pronounced maximum at intermediate couplings. At very low coupling (high kinetic energy), the system shows only slight superdiffusion with α being very close to one. At this coupling, the system is largely dominated by binary collisions and the local order is very low (cf. Figs. 1b and 2b). This small degree of correlation apparently diminishes the strength of superdiffusion. On the other end of the Γ-scale, at very high couplings and close to the disordering transition, the particles experience long trapping times in local cages which again reduces superdiffusive motion. In the region in-between these two limiting cases, superdiffusion is most pronounced. This suggests that collective effects which are mediated by the strong coupling are at least partly responsible for the observed anomalous behaviour of two-dimensional diffusion in Yukawa liquids and dusty plasmas.

Results for the Γ-dependence have been obtained for $\kappa = 0.56$ earlier by Liu and Goree [15], and while their numerical values for α differ considerably from ours, the general properties of the dependence are similar. The differing values of α may be attributed to a different prescription for extracting α.

The strong resemblance of Figs. 3a and b suggests an universal behaviour of the anomalous diffusion exponent. To compare the two systems with different interaction range κ, in Fig. 4 we depict α as a function of the relative coupling $\Gamma^{\mathrm{rel}} = \Gamma/\Gamma_c(\kappa)$, where Γ_c is the κ-dependent coupling at which crystallization occurs. It is apparent that this scaling results in a close, but not complete universality of the $\alpha - \Gamma^{\mathrm{rel}}$-relation which still exhibits a small κ-modulation.

To examine this κ-modulation more closely, in Fig. 4, we also show the corresponding data for $\kappa = 2$. Three regimes can be identified: For $\Gamma^{\mathrm{rel}} < 0.4$, α grows with increasing κ, while for $\Gamma^{\mathrm{rel}} > 0.4$, the opposite is true. In a narrow region close to the maximum of the $\alpha(\Gamma^{\mathrm{rel}})$-curves, α is nearly independent of κ. The decreased collision cross-section of high-κ liquids allows for an enhanced mobility in these systems. This effect is counterbalanced at higher couplings by the increased caging of the particles, which is more effective for higher κ at higher Γ. The interplay of these effects are expected to give rise to the observed behaviour. An additional caveat is, however, that the comparison of Yukawa systems across different values κ is a challenging task and the scaling of Γ/Γ_c must not be universal for different systems due to the changes (mediated by κ) in the interaction between particles.

As a final remark, we note that the numerical value of α depends on the window of time chosen to extract it from $u_r(t)$. The time dependence of α is studied in more detail in Ref. [26].

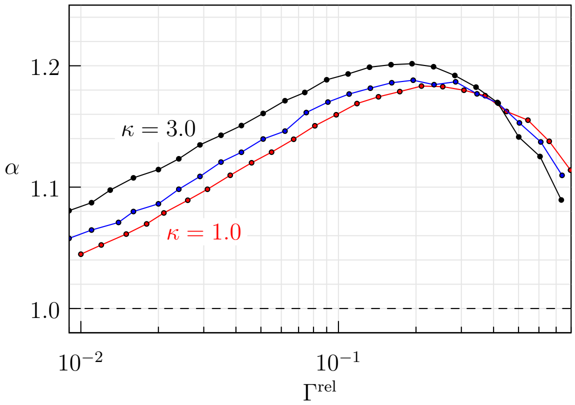

Fig. 4 The diffusion exponent α as a function of the relative coupling parameter for $\kappa = 1$, 2 and 3. (Online colour: www.cppjournal.org)

5 Conclusion

In conclusion, we have presented detailed results for the time-dependence of the MSD for two-dimensional Yukawa systems in the liquids phase. By inspection of the diffusion exponent at long times, we have shown the consistent existence of anomalous (super-)diffusion over a wide range of coupling strengths and screening lengths. The dependence of the diffusion exponent on the coupling was shown to be non-monotonous and confirmed and extended earlier simulations [14–16]. Debye screening was found to be a small but systematic effect which can reduce (at large Γ) or enhance (at small Γ) superdiffusion.

Acknowledgements This work is supported by the Deutsche Forschungsgemeinschaft via SFB-TR24, project A5.

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