Test of the Einstein Relation in Dusty Plasmas

Bin Liu and John Goree

***Abstract*— We test the Einstein relation $D_p = \mu_p k_B T_t$ that connects the diffusion coefficient D_p and mobility coefficient μ_p, where T_t is the temperature of particles that cause the scattering. The test is performed for a 3-D dusty plasma, using results from a Langevin–Yukawa molecular dynamics simulation. The coefficients D_p and μ_p describe the motion of projectile dust particles drifting through a cloud of target particles of a different size due to a constant force. The drift is opposed by collisions with target particles and neutral atoms. The Einstein relation is found to be violated at high driving forces of order $m_p \omega_t^2 a$ or stronger, where m_p is the projectile mass, while ω_t and a are the plasma frequency and Wigner–Seitz radius of the target particles. Because the Einstein relation fails at high forces, another relation is needed to describe diffusion in terms of mobility. We present a generalized Einstein relation, which we find to be satisfied over a wide range of forces.**

***Index Terms*— Complex plasma, diffusion, dusty plasma, Einstein relation, fluctuation-dissipation theorem (FDT), microgravity, mobility, strongly coupled plasma, transport, Yukawa.**

I. Introduction

COLLISIONAL transport processes, such as diffusion and mobility, are fundamentally connected due to the same underlying collisions that are responsible for the transport. An Einstein relation is often used to relate the diffusion to mobility, for example, for the motion of a Brownian particle in thermal equilibrium with an aqueous solution or a gas [1]. It is also used for ions in solution, where the Einstein relation is termed the Nernst–Einstein relation, and it is used for the diffusion of ions in weakly ionized gases [2], where it is sometimes called the Nernst–Townsend relation [3]. From the viewpoint of experimenters, the usefulness of this relation is that one can obtain diffusive properties of a system by measuring a mobility; this can be done by tracking a micron-size particle that is forced to drift through a collection of atoms, molecules, or other target particles in the gas or liquid. Here, we extend the idea of the Einstein relation to a dusty plasma, and we test its validity.

The Einstein relation, for general physical systems, is

$$D/\mu = k_B T \tag{1}$$

where D is a diffusion coefficient and μ is a mobility coefficient, which is the ratio of a drift velocity to a driving force. Equation (1) has the general form of a fluctuation-dissipation theorem (FDT). FDTs describe many physical systems near equilibrium [4], such as electrons in resistors [5] and molecules in fluids [6]. An FDT relates a dissipative process and a scattering process, where both processes are due to the same collisional mechanism. An FDT always involves a temperature T. The Einstein relation is like an FDT because it relates a frictional process (mobility) and a scattering process (diffusion).

In this paper, we investigate the validity of the Einstein relation in a dusty plasma, and we find a regime where it is obeyed and another regime where it is violated. Dusty plasma consists of electrons, ions, neutral gas atoms, as well as micron-size particles of solid matter [7], [8]. The dust particles can develop a large negative electric charge, typically thousands of elementary charges. Different from weakly coupled plasma, strongly coupled dusty plasmas have Coulomb collisions that are so strong that they dominate particle motion [9]. Thus, transport processes may be different from those in weakly coupled plasmas [10], [11].

For a system consisting of molecules in a liquid or gas, a test of the Einstein relation is difficult because of the impossibility of tracking the motion of individual molecules. A dusty plasma has the advantage of allowing the tracking of particle motion microscopically. In [12], this tracking is done using video microscopy, so that transport due to collisions can be observed microscopically. Dust particles can be made to drift by injecting particles of one size into a cloud of particles that have a different size due to unbalanced forces such as confining and ion drag forces [13], [14].

We will test the Einstein relation in the form

$$D_{p\perp}/\mu_p = k_B T_t \tag{2}$$

which describes the diffusion of a projectile particle p that is driven by a constant force $\mathbf{F}$ through a collection of target particles of temperature T_t. The subscripts p and t in the equation identify the projectile and the target (which are the same as test and field particles for collisional transport in plasmas in [15]). The projectile undergoes a combination of three kinds of motion: 1) drift; 2) perpendicular diffusion; and 3) parallel diffusion [15]. The drift velocity u_p is in the direction of $\mathbf{F}$, and it is characterized by a mobility coefficient $\mu_p = u_p/F$. The diffusion is a random walk due to the same type of collisions that are responsible for the mobility. In plasmas, Coulomb collisions generally lead to slightly different rates of diffusion in the directions parallel and perpendicular to the drift [15]; here, we will characterize only the diffusion of projectiles in the direction perpendicular to the drift, as denoted by the subscripts in $D_{p\perp}$.

The Einstein relation (1) in general is intended for small perturbation [4], i.e., near-equilibrium conditions where the microscopic motion of a projectile is dominated by the thermal

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motion of the target particles. Large perturbations can be achieved in dusty plasma by applying large force F; in this case, we expect the Einstein relation will be violated. This violation is already known for ions in gases [16]–[18] at high electric field, where the diffusion of an ion (projectile) is faster than described by (1). To describe transport even when the Einstein relation fails, gaseous electronics researchers have developed a generalized Einstein relation [18] that is useful over a wide range of electric forces; the simplest version is

$$D_{p\perp}/\mu_p = W \tag{3}$$

where W is no longer a temperature of the target (gas) molecules as in the case of near equilibrium, but is instead a combination of a directed energy and a random energy for the projectile (ion). This generalized Einstein relation is an important result of the theory for the diffusion and mobility of ions in gases [18]. Here, we test whether this relation is also satisfied in a dusty plasma. It is not obvious that it should be satisfied because the collisions in a dusty plasma are a combination of Coulomb interactions, which are different from the ion-neutral collisions in the system for which (3) was developed, and collisions of the dust particles with gas molecules.

In this paper, for a projectile dust particle that collides with target dust particles, we will demonstrate the following.

1) The projectile's motion will violate the Einstein relation (2) for a sufficiently large force F at a level that we will quantify.
2) The projectile's motion will obey the generalized Einstein relation (3), with W replaced by the random kinetic energy

$$W_p = m_p \overline{\left(v_y^2 + v_z^2\right)}/2. \tag{4}$$

Here, m_p is the projectile mass and $\overline{v_y^2 + v_z^2}$ is the mean squared velocity for random motion of projectiles in the direction $\perp\mathbf{F}$. For these demonstrations, we carry out further analysis of the 3-D Langevin molecular dynamics simulation data in [19] and [20].

Our work is motivated by experiments with dusty plasmas under microgravity conditions. It has been observed [13], [14] that a collection of target particles can be confined with steady nondrifting conditions due to a balance of forces, and that projectile particles can be introduced so that they drift through the target particles. In those microgravity experiments, the drift of the projectiles was due to unbalanced constant forces.

This situation, with steady forces that are balanced for one size of particles but unbalanced for another, can occur because there are two forces, electric and ion drag, which differently scale with particle size [21]. Electric forces, due to macroscopic electric fields as well as microscopic interparticle repulsion, are proportional to the first power of the dust particle diameter, while the ion drag force is proportional to the second power. A collection of target particles can be confined without drifting motion when these forces are balanced for a given profile of the macroscopic electric field. However, the same electric field will result in unbalanced forces for a differently sized particle. Thus, an isolated projectile particle that is introduced at the edge of a cloud of target particles of a different size will spontaneously drift through the target particles. Such a drift has been observed in the microgravity experiments [13], [14] although the projectiles were so numerous that they interacted among themselves as well as with the target particles, in a phenomenon called lane formation.

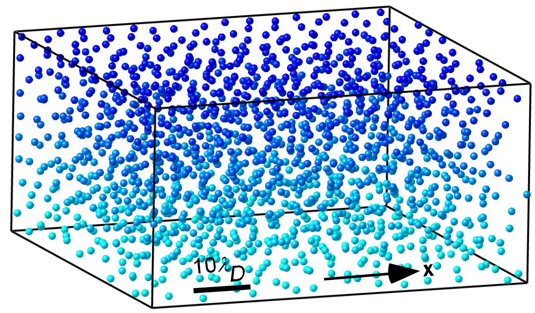

Fig. 1. Snapshot of target particle positions, showing only 1/8 of the $N = 12\,800$ target particles. Note the liquid-like disorder conditions, for $T_t = 2T_m$, i.e., twice the melting point for the collective interactions of the target particles. Not shown here is the projectile, which drifts in the $+x$-direction due to the force $\mathbf{F}$, which is not applied to the target particles due to their different size. The diameter of a particle is exaggerated here for clarity, and its darkness indicates its position in the vertical direction.

In upcoming microgravity experiments using the Plasma Kristall-4 (PK-4) instrument [22] on the International Space Station, we hope to observe this drifting motion of an isolated projectile and test the results predicted in this paper. In anticipation that experiments can be performed with an injection of a smaller number of projectiles than in lane formation experiments, here we consider the case that the projectiles are dilute and do not interact with one another.

II. Simulation Method

The results in this paper are a further analysis of data from the 3-D Langevin dynamics simulation reported in [19] and [20]. We review the simulation briefly here.

In a simplified description of the four-component mixture (dust particles, ions, electrons, and gas), we track only the motion of the dust particles of charge Q. The role of the electrons and ions is described by a screening length λ_D. The dust particles interact among themselves in a binary electric repulsion, modeled by a Yukawa potential $\propto (1/r)\exp(-r/\lambda_D)$ for two particles separated by a distance r. We numerically integrate the equation of motion for each dust particle, including the following forces: a sum of all electric forces due to nearby dust particles, a prescribed confining force which is steady and zero everywhere except a narrow confining edge, and finally two forces due to gas atoms: 1) friction and 2) random kicks. The kicks are Markovian, isotropic, and random in both direction and magnitude, with a Gaussian distribution. The resulting temperature T_t for the target particles is high enough so that the cloud of target particles acts as a liquid, not a solid, as shown in Fig. 1. After the simulation reaches equilibrium for the target particles, an isolated projectile particle is introduced at the simulation boundary. This projectile is accelerated by a prescribed steady force F, which would physically be the

TABLE I
PROJECTILE AND TARGET PARTICLE PARAMETERS

PARAMETERS	Projectile	Target
Particle radius, μm	0.64	3.43
Charge	Q_p = -1590 e	Q_t = -8520 e
Friction constant, s^{-1}	ν_p = 273	ν_t = 51
Mass, kg	$m_p = 1.66 \times 10^{-15}$	$m_t = 2.55 \times 10^{-13}$
Target temperature, T_t		$2T_m$ and $10T_m$
Coupling parameter, Γ		310 and 62

Here, T_m refers to the melting point for a 3D Coulomb crystal of the target particles [23]. The Coulomb coupling parameter is $\Gamma = Q_t^2 / 4\pi\varepsilon_0 a k_B T_t$.

difference between unbalanced electric and ion drag forces. This force F is applied only to the projectile, not to the target particles, due to its different size.

The simulation parameters are based on PK-4 experiment conditions [22]. These include a screening length of 0.083 mm for the Yukawa interaction and a number density of 3×10^4 cm^{-3} for target particles. At this density, the Wigner–Seitz radius for the target particles is $a = 0.02$ cm, the screening parameter is $a/\lambda_D = 2.4$, and the dusty plasma frequency, $\omega_t = (Q_t^2 n_t/\varepsilon_0 m_t)^{1/2}$, is 157 s^{-1}. Other parameters are listed in Table I.

Liu and Goree [19] found the mobility coefficient μ_p by tracking the motion of a number of projectiles, as they drifted through the liquid-like target. For the same conditions, Liu and Goree [20] found the perpendicular diffusion coefficient $D_{p\perp}$ and the perpendicular energy W_p for the projectiles using (4). In this paper, we further analyze these results to test the Einstein relation (2), to find the force at which the Einstein relation fails, and to test the generalized Einstein relation (3).

III. RESULT

A. Test of Einstein Relation

We test the Einstein relation as a theory by comparing it with the simulation results. Results for this test are presented in Fig. 2. The theoretical curve is shown as a horizontal line with a value of unity, $D_{p\perp}/\mu_p k_B T_t = 1$, while the simulation results are presented as data points. In this test, if the Einstein relation is satisfied, we will see data points fall on the horizontal line for the theory, but if it fails, the data points will depart from the horizontal line.

We find that while the Einstein relation is satisfied for small forces F, on the left side of Fig. 2, it is violated for larger forces, as expected. The violation is quite severe, as much as an order of magnitude disagreement for $D_{p\perp}$ as compared with the prediction of (2).

B. Determination of the Transition Force

We quantify the transition force F_c for the Einstein relation to be obeyed. We measure F_c as the intersection of an asymptote in Fig. 2 for the high-force regime, with the horizontal line for the Einstein relation. From Fig. 2, we find that F_c is of order $m_p\omega_t^2 a$.

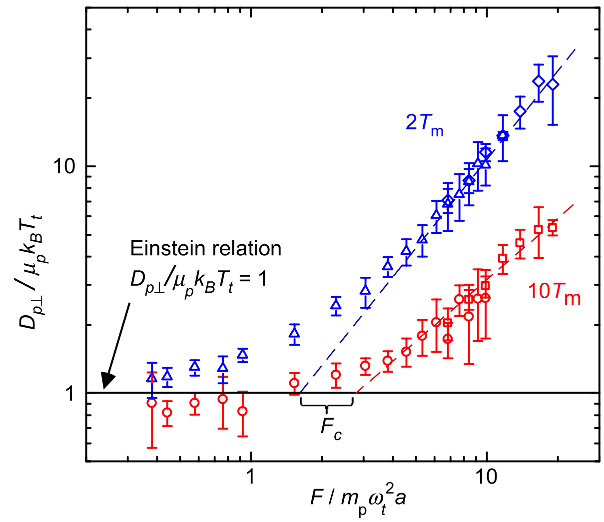

Fig. 2. Test of the Einstein relation (2). The horizontal line represents the theory, i.e., (2), while the data points are from the simulations, for two temperatures for the target particles. We find a large discrepancy at high forces. The Einstein relation is valid only for a force smaller than a transition force F_c of order $m_p\omega_t^2 a$.

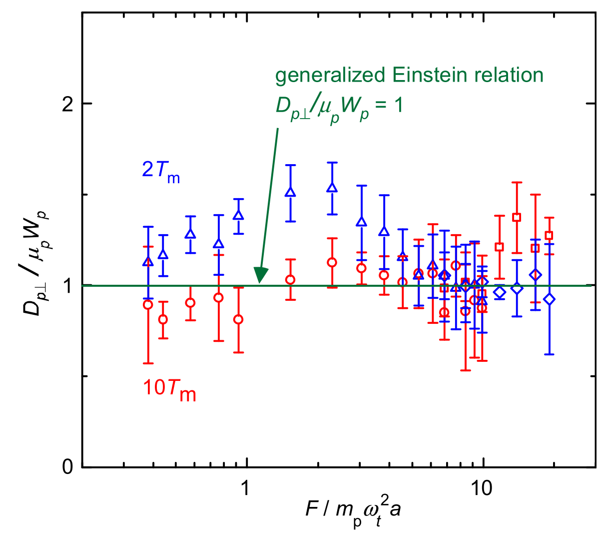

Fig. 3. Test of the generalized relation (5). The theory is represented by a horizontal line. Half of the data points for the simulation fall on this line within ±10%, much better than for the Einstein relation in Fig. 2.

This transition force is also found to weakly depend on the target temperature. In dimensionless units, the transition $F_c/m_p\omega_t^2 a$ is 1.6 for a cold liquid at $T_t = 2T_m$ but 2.9 for a much hotter liquid at $10T_m$. This trend, for F_c to weakly increase with T_t, can be explained in terms of the forces: the random forces for Coulomb collisions with target particles are larger when the target particles have a higher temperature T_t, so that a larger driving force F is needed to overwhelm those random forces.

C. Test of Generalized Einstein Relation

Finally, we test our generalized Einstein relation in Fig. 3, which is motivated by the simplest version of the generalized Einstein relation for ions in gases (3), but with a random energy that is replaced by (4) for the case of a projectile in a target of particles in a dusty plasma. In other words, we hypothesize that diffusion and mobility are connected by a combination of (3) and (4)

$$D_{p\perp}/\mu_p W_p = 1 \tag{5}$$

where the projectile's random energy W_p, instead of the target temperature T_t, is used in calculating the ratio in (3).

Results for this test are shown in Fig. 3, where the horizontal line represents our hypothesis (5). The data points in Fig. 3 are the ratio $D_{p\perp}/\mu_p W_p$ calculated from our previously reported results [19], [20], for $D_{p\perp}$, μ_p, and W_p.

We find that our generalized Einstein relation is satisfied much better than the Einstein relation, over a wide range of driving forces. This is seen by the general agreement of the data points compared with the horizontal line for the theory in Fig. 3. The discrepancy is less than 10% for half the data points. Only for two outlier data points is the discrepancy larger than 40%. Overall, this agreement is much better than the Einstein relation in Fig. 2, where the discrepancy was not just a few percent, but an order of magnitude, at the highest forces that we considered.

IV. Conclusion

We analyzed the simulation results for the drifting motion of a projectile dust particle in a dusty plasma containing mostly nondrifting target particles of a different size. This kind of motion is expected in future dusty plasma experiments performed under microgravity conditions.

We verified that the drifting motion is related to the diffusive motion of the projectile by the Einstein relation, but only for sufficiently small driving forces for the projectile. We found that this violation of the Einstein relation occurs for driving forces larger than a transition force that is a small multiple of $m_p \omega_t^2 a$. This multiple weakly increases with the temperature of the target particles, T_t.

We also hypothesized that a generalized Einstein relation would accurately describe the diffusion of the projectile particles over a wide range of forces. We test the simplest modification to the Einstein relation, replacing the temperature of the target particles with a mean square variation of the kinetic energy of the projectiles. We found that this generalized Einstein relation was satisfied much better than the Einstein relation over a wide range of force, with discrepancies of $\approx$10%, compared with an order of magnitude for the Einstein relation. We expect that this generalized Einstein relation will be useful to experimenters who wish to estimate diffusion coefficients based on drift velocity observations, since the diffusion coefficient can be difficult to measure directly in a 3-D dusty plasma.

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