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Contrib. Plasma Phys. 1 – 7 (2016) / **DOI** 10.1002/ctpp.201500090

Contribution of the 15th International Conference on the Physics of Non-Ideal Plasmas, Almaty, Kazakhstan, from August 30th - September 4th, 2015

Effect of Buffer Gas Induced Friction on the Caging of Particles in a Dusty Plasma

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Received 23 October 2015, revised 28 November 2015, accepted 01 December 2015
Published online 24 February 2016

Key words Dusty plasma, langevin dynamics simulation, cage correlation.

In strongly coupled plasmas the diffusion of the particles takes place on a timescale that is long compared to the timescale of oscillations of the particles in the local minima of the potential landscape. The ensuing quasi-stability of the local particle configurations can be quantified by monitoring the changes of the immediate surroundings, i.e. the "cages", of the particles. Studies of cage correlations are presented here for 2-dimensional Yukawa systems that model dusty plasmas by including the friction exerted on the dust particles by the embedding gaseous environment. We find that the increasing friction enhances the caging time by randomizing the directed motion of the particles.

1 Introduction

Strongly coupled plasmas (SCP-s) – in which the average potential energy per particle dominates over the average kinetic energy – appear in a wide variety of physical systems: colloidal suspensions, dusty plasmas, charged particles in cryogenic traps, liquid metals, electrons trapped on the surface of liquid helium, astrophysical systems, such as the ion liquids in white dwarf interiors, neutron star crusts, supernova cores, and giant planetary interiors, as well as in degenerate electron or hole liquids in two-dimensional or layered semiconductor nanostructures, see e.g. [1–3]. Many of these systems share some properties, which allows one to describe them by the "one-component plasma" (OCP) model [4], 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 form of the potential depends on the nature of the background, which can be either non-polarizable or polarizable. The particle interaction potentials that correspond to these two cases are of Coulomb and Yukawa type, respectively, and the systems are usually refereed to as a (Coulomb) OCP and a Yukawa-OCP (YOCP).

Dusty plasmas represent a notable type of strongly coupled systems and they are often modeled as a YOCP. They appear both in astrophysical environments and can be realized in laboratory experiments. In the latter, dust particles can be grown in a reactive plasma environment, or can be introduced externally. As the length and time scales in dusty plasma experiments are relatively easy to capture, such experiments made it possible during the past two decades to investigate a wide range of physical phenomena (structural properties, transport phenomena, formation of waves, etc.) at the level of the particles, i.e. with "atomic" resolution, e.g. [5–9].

It is a prominent feature of strongly coupled plasmas that the surroundings of the individual particles change on a timescale that is long compared to the timescale of plasma oscillations (oscillations of individual particles in the local minima formed on the slowly varying potential surface). This "quasi-stability" of the surroundings of the particles, or their "quasi-localization" has a primary importance in establishing the properties of SCP-s, including their properties in the liquid state [10], transport characteristics, and collective excitations. The quasi-localization of the particles serves as the physical basis of the Quasi-Localized Charge Approximation that

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makes it possible to derive the dispersion relations of collective excitations from the pair correlation function of the particles [11, 12].

The quasi-localization of the particles can be quantified by computing the *cage correlation functions*, introduced in [13], which account for the changes of particles' neighbor shells. Caging of the particles in 2- and 3-dimensional strongly coupled OCP and YOCP was already investigated [14]. This work has confirmed that in the strongly coupled liquid phase the particles undergo several plasma oscillations before a significant rearrangement of their surroundings takes place (on the timescale of particle diffusion). As a further step, the effect of a homogenous external magnetic field on the cage correlation functions of 2-dimensional (2D) ideal Yukawa liquids was investigated in [15]: the magnetic field was found to increase the caging time in accordance with the expected reduction of particle diffusion across the magnetic field lines.

The purpose of the present work is to study the effect of friction, induced by the buffer gas, on the cage correlation functions in a non-magnetized 2-dimensional system of dust particles, which interact via Yukawa potential. Our computer simulations are carried out based on the Langevin dynamics approach (e.g. [16]). Section 2 of the paper outlines the model and the computational methods, while section 3 presents our results. A brief summary is given in section 4.

2 Model and computational method

To model the effect of friction on the caging in the 2-dimensional YOCP considered here we adopt the following form for the potential energy resulting from the mutual interaction of the particles:

$$\phi(r) = \frac{Q^2}{4\pi\varepsilon_0} \frac{\exp(-r/\lambda_\mathrm{D})}{r}, \tag{1}$$

where Q is the charge of the particles and λ_D is the screening (Debye) length. The equation of motion of the particles (given here for particle i) is

$$m\ddot{\mathbf{r}}_i(t) = \sum_{i \neq j} \mathbf{F}_{ij}(t) - \nu\, m\mathbf{v}_i(t) + \mathbf{F}_\mathrm{Br}, \tag{2}$$

where the first term on the right hand side gives the sum of inter-particle forces, the second, friction term (proportional to the particle velocity) accounts for the presence of the background gaseous environment, while the third term represents an additional randomly fluctuating "Brownian" force that expresses the random kicks of the gas atoms on the dust particles. The first term is computed for (i, j) particle pairs that are separated by a distance that is less than a pre-defined cutoff radius, r_cut, set in a way that contributions from outside r_cut are negligible compared to the total force acting on particle i. (Definition of a cutoff radius is made possible by the exponential decay of the Yukawa potential, in our case we have chosen $r_\mathrm{cut} = L/3$, where L is the length of the simulation box.)

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

$$\Gamma = \frac{Q^2}{4\pi\varepsilon_0 a k_\mathrm{B} T}, \tag{3}$$

where T is temperature. We introduce the screening parameter $\kappa = a/\lambda_\mathrm{D}$, where $a = (1/\pi n)^{-1/2}$ is the two-dimensional Wigner-Seitz radius and n is the areal number density of the particles. The strength of friction is defined by the dimensionless parameter

$$\theta = \nu/\omega_\mathrm{p}, \tag{4}$$

where ω_p is the plasma frequency $\omega_\mathrm{p} = \sqrt{nQ^2/2\varepsilon_0 m a}$. The system is fully characterized by the three parameters Γ, κ, and θ.

We follow $N = 1000$ particles in the simulations. The positions of these particles are chosen randomly at the initialization of the simulations, their velocities are sampled from a Maxwellian distribution with a temperature that corresponds to the value of Γ specified. The equation of motion is integrated using the velocity-Verlet scheme. During the initial phase of the simulations the system is thermalized, but thermostation is stopped before the data collection phase starts.

To quantify the time-dependence of the correlation of the particles' surroundings we adopt the method proposed in [13] and used in [14] for the investigation of strongly coupled Coulomb and Yukawa liquids. We use a generalized neighbor list ℓ_i for particle i, $\ell_i = \{f_{i,1}, f_{i,2}, ..., f_{i,N}\}$. Due to the underlying sixfold symmetry of the system considered here we always search for the six closest neighbors 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*:

$$C_\ell(t) = \frac{\langle \ell_i(t)\ell_i(0)\rangle}{\langle \ell_i(0)^2\rangle}, \tag{5}$$

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

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

$$N_i^{\rm out}(t) = |\ell_i(0)^2| - \ell_i(0)\ell_i(t), \tag{6}$$

where the first term gives the number of particles around particle i at t = 0 (that, actually, equals to six, in our case), while the second term gives the number of "original" particles that remained in the surrounding after time t elapsed. As the next step an integer value c is defined, which is the number of the original neighbors that have to leave the cage before we say that the cage has undergone a "substantial change". The *cage correlation function* $C^c_{\rm cage}(t)$ can be calculated by averaging over particles and initial times, the function $\Theta(c - N_i^{\rm out})$, i.e.

$$C^c_{\rm cage}(t) = \langle\Theta(c - N_i^{\rm out}(0,t))\rangle, \tag{7}$$

where Θ is the Heaviside function. We calculate the cage correlation functions for $c = 3$, i.e. define the "substantial change" quoted above as a situation when half of the original neighbors leave the cage. We adopt the definition of the *caging time* introduced in [14], according to which $t_{\rm cage}$ is defined as the time when $C^3_{\rm cage}$ decays to a value 0.1.

3 Results

Our computations have been carried out for $\Gamma = 20$ and 120, at $\kappa = 1$, 2, and 3, and for a wide range of the friction parameter, $0.0001 \leq \theta \leq 0.5$. The lowest value of θ represents a practically frictionless case, while the highest value corresponds to a strongly damped system, where the frequency associated with collisions with the background particles is comparable to the plasma frequency.

As mentioned earlier, in the calculation of the cage correlation functions we search for the six closest neighbors around each particle. These neighbors are the ones situated within the first coordination shell around the particles, which has a radius of $r_{\rm coord}/a \approx 2.5$, as inferred from the position of the minimum that follow the first peak of the pair correlation function, $g(r)$, shown in Figure 1 for different values of system parameters. The peaks of the pair correlation function increase with the increase of the coupling parameter and with the decreases of the screening parameter, $r_{\rm coord}$, however, remains nearly unaffected. We note that the pair correlation function does not depend on the friction induced by the buffer gas. To visualize the caging effect, we present (x, v_x) phase space trajectory segments of a single particle, for different values of the coupling and friction parameters. Caged motion shows up in these plots as loops on the trajectories. Figure 2(a) and (b) show trajectory samples for low-friction cases ($\theta = 0.0001$). At the lower coupling values (Figure 2(a)) we observe alternating free and localized motion, while at $\Gamma = 120$ the trajectory reveals complete localization during the time of recording ($\omega_{\rm p}\Delta t = 500$). A high value of friction remarkably changes the appearance of the trajectories, which become wiggled due to the randomly fluctuating Brownian force that acts on the particles. Nonetheless, the localization seems to be enhanced, which will be quantified by the computations of the cage correlation functions, displayed in Figure 3. The influence of the friction on the cage correlation function is remarkable, increasing friction prolongs the caging time and leads to a slower decay of the correlation function. This observation can be explained by the fact that a strong friction and the consequent randomized motion (as revealed in trajectories in Figure 2 at high θ) prevents the particles from escaping the cages. At $\Gamma = 20$ we find that the caging time increases by about a factor of three (see Figures 3(a),(b)) when θ is increased to 0.5, from the practically friction-free case of $\theta = 0.001$. An even stronger effect is found at higher coupling, at $\Gamma = 120$ an approximately six-times increase of the caging time is found within the friction values covered.

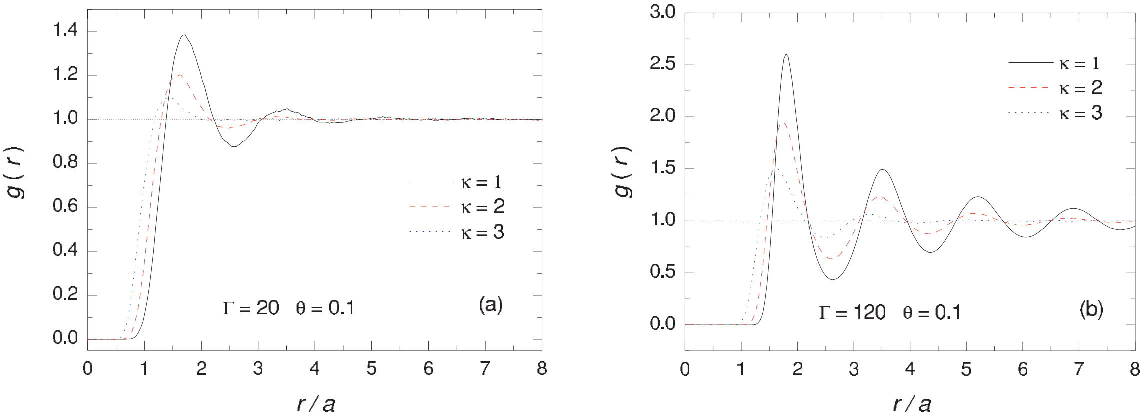

Fig. 1 Pair correlation functions of the 2D Yukawa liquid for different values of κ at $\theta = 0.1$, for $\Gamma = 20$ (a) and $\Gamma = 120$ (b). The position of the first minimum that marks the boundary of the first coordination shell shows little sensitivity on the system parameters.

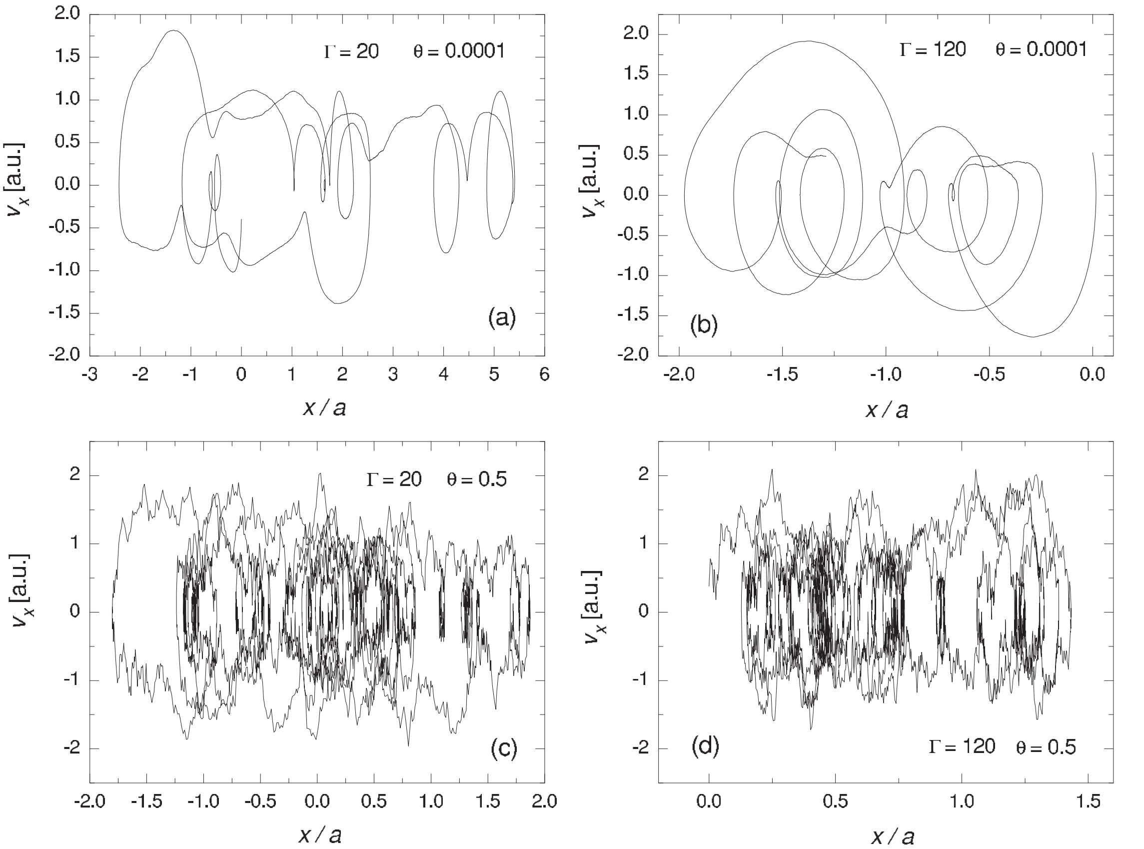

Fig. 2 Samples of (x, v_x) phase space trajectory segments of single particles at low friction (a,b) and at high friction (c,d). $\Gamma = 120$ in (a) and (c), and $\Gamma = 120$ in (b) and (d). $\kappa = 2$ for all plots. The length of trajectory segments in $\omega_{\mathrm{p}}\Delta t = 500$.

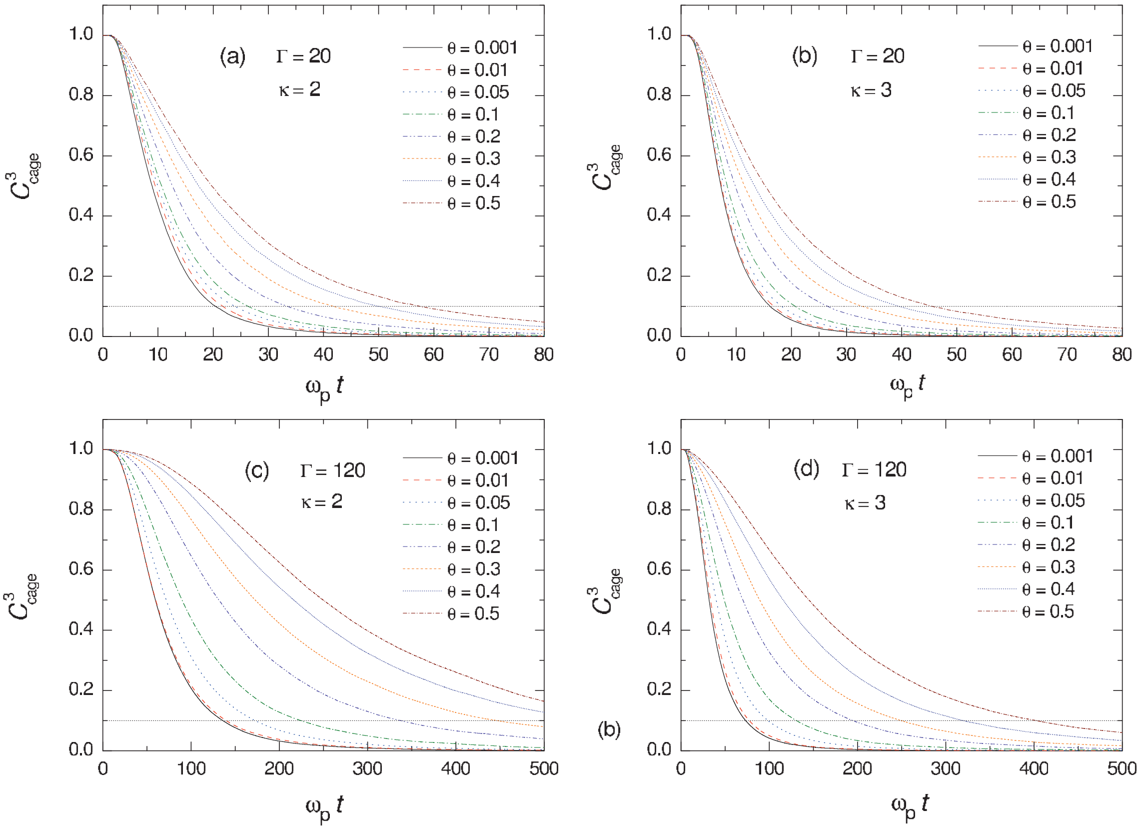

Fig. 3 Cage correlation functions for different values of θ at $\Gamma = 20$, $\kappa = 2$ (a) and $\kappa = 3$ (b), as well as at $\Gamma = 120$, $\kappa = 2$ (c) and $\kappa = 3$ (d).

The caging time (identified as $C^3_{\rm cage} = 0.1$) is displayed in Figure 4 as a function of the friction coefficient for different values of κ at $\Gamma = 20$ and 120. The effect of friction starts to play a role at $\theta \sim 0.03$, above this value the caging time remarkably increases with θ. Bearing in mind the connection between the caging effect and the self-diffusion in the system [14] our observation of the increasing caging time at higher friction parallels the finding of the decrease of the self-diffusion coefficient with increasing friction in a 3D dusty plasma [17, 18], as well as in a 2D system, where a transition from superdiffusion to normal diffusion and to subdiffusion with the increase of the friction coefficient was found [19].

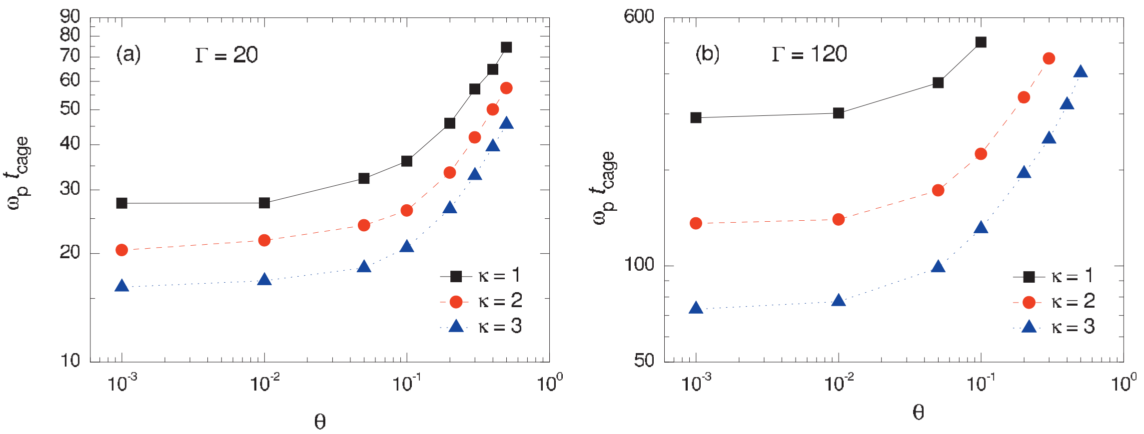

Fig. 4 Dependence of caging time on the friction coefficient for different values of κ at $\Gamma = 20$ (a) and $\Gamma = 120$ (b).

Figure 5 shows values of the caging time $\omega_{\rm p} t_{\rm cage}(\Gamma, \kappa, \theta)$ normalized by $\omega_{\rm p} t_{\rm cage}(\Gamma, \kappa, \theta = 0.001)$. The data points obtained this way for the same Γ but different κ values fall closely on universal curves, implying that the friction enhances the caging time in relative terms to an extent that is (nearly) independent of the screening coefficient. At higher coupling a stronger increase of the caging time is revealed from the data in Figure 5: at $\Gamma = 120$ the increase of $\omega_{\rm p} t_{\rm cage}$ is about twice as high as in the case of $\Gamma = 20$ when θ is increased from 0.001 to 0.5.

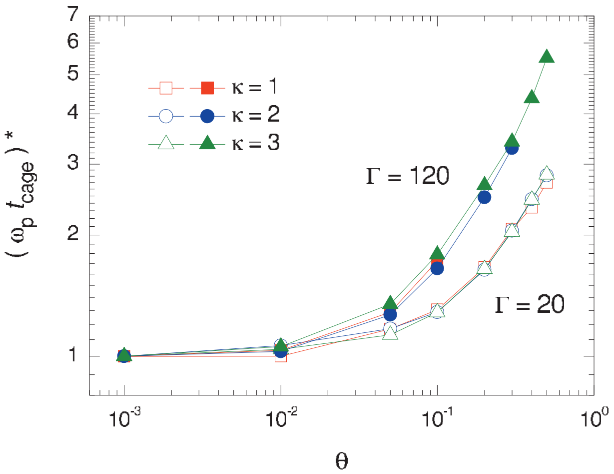

Fig. 5 Dependence of the normalized caging time, $(\omega_{\rm p} t_{\rm cage})^* = \omega_{\rm p} t_{\rm cage}(\Gamma, \kappa, \theta)/\omega_{\rm p} t_{\rm cage}(\Gamma, \kappa, \theta = 0.001)$, on the friction coefficient for different values of κ at $\Gamma = 20$ and $\Gamma = 120$.

4 Summary

In this paper we have investigated the effect of friction – induced by the gas / plasma environment – on the quasi-localization / caging of dust particles in a 2D layer. The system has been described by Langevin Dynamics simulation. We have found that the increasing friction coefficient enhances the caging of the particles, as quantified by the cage correlation functions. These observations match the findings on the self-diffusion coefficient in similar 3D and 2D systems. The enhancement of caging time was found (i) to be remarkable at friction coefficients exceeding $\theta \approx 0.03$, (ii) to exhibit a universal scaling with little sensitivity on the screening coefficient κ, and (iii) to be stronger at higher Γ. Although only 2-dimensional systems have been considered in the present work, a qualitatively similar behavior is expected to take place in 3-dimensional systems, as the effect of friction is foreseen to act similarly, regardless of the dimensionality. A study of the effect of friction induced by the gas on the cage correlation functions in 3-dimensional systems is subject of future work.

Acknowledgements This work was supported by the Ministry of Education and Science of the Republic of Kazakhstan via grant 3087/GF4 and the Hungarian Fund for Scientific Research (OTKA) via grant K105476.

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