Supercomputer Modeling of Stochastic Dynamics of the Mercury Ion Array in an Optical Lattice

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Abstract. Simulations of the resonant ions stochastic dynamics in the polychromatic optical field are presented. We prove the possibility of long-term four- and nine-particle ionic Coulomb planar clusters (crystals) by all-optical method. An estimate of lifetime of a single particle in an optical lattice is also carried out. Our analysis is based on the numerical solution of the stochastic differential equations with multiplicative noise using MVS-100K and MVS-10P supercomputers.

Keywords: Stochastic differential equations, Dissipative optical lattice, Coulomb clusters, Parallel Monte Carlo method, Distributed computing.

1 Introduction

Electromagnetic ion traps have many important applications in quantum informatics, high resolution spectroscopy of ions, metrology, physics of cold collisions and many-body physics [1–4]. A new and interesting trend in this field of research is the so-called all-optical confinement of ions, i.e. optical ion trapping without applying additional radiofrequency or electrostatic and magnetic fields [5–9]. In particular, it is assumed that development of all-optical methods of ion trapping can be useful for creation of ionic clock with better characteristics [10].

In our previous papers [7–9] the solution of all-optical ion trapping problem was proposed, based on using the rectified gradient forces that act on ions in the polychromatic field [11–15]. We demonstrated, by the numerical simulations of stochastic ion motion in the 3D polychromatic optical super-lattice (OSL), the long-term all-optical trapping of two- and three-ion ytterbium clusters in OSL. In the present work, we carried out numerical simulations of dynamics of four- and nine mercury ions in OSL and demonstrated the long-term all-optical trapping of ordered ion array (planar Coulomb cluster) in OSL. Note that a large array of trapped cold ions has attracted special interest from researchers because of its very useful applications [1, 3]. Now there is a broader interest in the form of arrays of ion traps in the context of quantum computings [4]. Stochastic dynamics of a single particle in an optical lattice is also considered.

The mathematical model is a system of stochastic differential equations (SDEs) for positions and velocities of each ionic particle. We take into account four acting forces in the model: the trapping, friction, Coulomb, and stochastic forces. The last force arises due to quantum fluctuations of the optical forces [11]. The Monte Carlo method with parallelization among computing cores is used to evaluate different average characteristics of this physical problem.

2 Equations of Stochastic Motion

Our study is based on the system of stochastic differential equations with multiplicative noise which can be written in the following dimensionless form

$$d\mathbf{r}_\alpha(t,\omega) = \zeta \mathbf{v}_\alpha(t,\omega)dt, \qquad t \in \mathbb{T} = [0, t_f]\,, \tag{1}$$

$$d\mathbf{v}_\alpha(t,\omega) = \mathbf{F}_\alpha(\mathbf{r}_1,\ldots,\mathbf{r}_N,\mathbf{v}_\alpha)dt + \sqrt{2D(\mathbf{v}_\alpha)} \circ d\mathbf{W}_\alpha(t,\omega)\,, \tag{2}$$

$$\mathbf{F}_\alpha(\mathbf{r}_1,\ldots,\mathbf{r}_N,\mathbf{v}_\alpha) \equiv \mathbf{F}^{tr}_\alpha(\mathbf{r}_\alpha,\mathbf{v}_\alpha) + \mathbf{F}^{fr}_\alpha(\mathbf{r}_\alpha,\mathbf{v}_\alpha) + \mathbf{F}^{C}_\alpha(\mathbf{r}_1,\ldots,\mathbf{r}_N)\,, \tag{3}$$

$$\mathbf{r}_\alpha(0,\omega) = \mathbf{r}^0_\alpha(\omega), \quad \mathbf{v}_\alpha(0,\omega) = \mathbf{v}^0_\alpha(\omega), \qquad \alpha = 1,\ldots,N\,, \tag{4}$$

where $\mathbf{r}_\alpha$, $\mathbf{v}_\alpha \in \mathbb{R}^3$ are the position $\mathbf{r}_\alpha$ and velocity $\mathbf{v}_\alpha$ of the center-of-mass of the α-th ion; $\mathbf{r}_\alpha = (r_{\alpha x}, r_{\alpha y}, r_{\alpha z})^{\mathrm{T}}$, $\mathbf{v}_\alpha = (v_{\alpha x}, v_{\alpha y}, v_{\alpha z})^{\mathrm{T}}$; t is time; N is the number of ions; $\mathbf{F}^{tr}_\alpha$, $\mathbf{F}^{fr}_\alpha$, $\mathbf{F}^{C}_\alpha$ are the trapping, friction and Coulomb forces acting on the α-th ion, respectively. The symbol $\circ$ means that this SDEs are interpreted in the Stratonovich sense [16].

$\mathbf{W}_\alpha(t,\omega)$ is a standard three-dimensional vector Wiener process [17]. Recall some of its properties: 1) $\mathbf{W}_\alpha(0,\omega) \equiv \mathbf{0}$; 2) for fixed $\omega \in \Omega$ the vector-function $\mathbf{W}_\alpha(t,\omega)$ is continuous on $\mathbb{T}$; 3) for $\forall m > 1$ and $\forall\{t_k\} \in \mathbb{T}$ $(k = 1,\ldots,m)$ such that $0 < t_1 < t_2 < \cdots < t_m$, the random vectors $\mathbf{W}_\alpha(t_1,\omega)$, $\mathbf{W}_\alpha(t_2,\omega) - \mathbf{W}_\alpha(t_1,\omega), \ldots, \mathbf{W}_\alpha(t_m,\omega) - \mathbf{W}_\alpha(t_{m-1},\omega)$ are independent; 4) for $\forall t_1, t_2 \in \mathbb{T}, (t_1 < t_2)$, the random vector $\mathbf{W}_\alpha(t_2,\omega) - \mathbf{W}_\alpha(t_1,\omega)$ has a Gaussian distribution with mean 0 and dispersion matrix $(t_2 - t_1)I_3$, where I_3 is an unit matrix of the 3-th order. Notice also that for $\forall \alpha_1, \alpha_2$, $(1 \leqslant \alpha_1 < \alpha_2 \leqslant N)$, the random vectors $\mathbf{W}_{\alpha_1}(t,\omega)$ and $\mathbf{W}_{\alpha_2}(t,\omega)$ are independent.

The argument $\omega \in \Omega$ emphasizes that $\mathbf{r}_\alpha$, $\mathbf{v}_\alpha$, and $\mathbf{W}_\alpha$ are the random vector functions in corresponding probability space $(\Omega, \mathfrak{F}, \mathbb{P})$. Below the letter ω will be omitted.

We use the dimensionless variables measuring the positions in units of $L = L_x$, time t in units of ω_R^{-1} (where $\omega_R = \hbar k^2/m$ is the photon recoil frequency, m is the ionic mass), L_i is a period of the OSL cell along i-axis $(i = x, y, z)$, k is the wave number, and velocities in units of $s_0 = \sqrt{T_D/m}$ where $T_D = \hbar\gamma'/2$ is the characteristic temperature determining the so-called Doppler cooling temperature limit [11]. The dimensional time $\breve{t} = t/\omega_R$ is also calculated for describing the simulation results; $\zeta = s_0/\omega_R L \ll 1$ is an analog of the Knudsen number (a small parameter) for the problem under consideration.

Components of the trapping force vector $\mathbf{F}_\alpha^{tr} = (F_{\alpha x}^{tr}, F_{\alpha y}^{tr}, F_{\alpha z}^{tr})^{\mathrm{T}}$ are [7]

$$F_{\alpha i}^{tr} = -\zeta \frac{\partial U_i(r_{\alpha i}, v_{\alpha i})}{\partial r_{\alpha i}}, \qquad i = x, y, z \ , \tag{5}$$

$$U_i(r, v) = -\frac{\cos(2\pi p_i r)}{p_i} \left(\widehat{W}_0 \mathcal{L}\Big(\frac{v}{v_{c0}}\Big) + \widehat{W}_1 \mathcal{L}\Big(\frac{v}{v_{c1}}\Big) \right), \tag{6}$$

where $\widehat{W}_0 = 4a_1 GL \ / \ 9\lambda(b+1)(4\chi+3)$; $\widehat{W}_1 = 2\chi \widehat{W}_0 \ / \ (4\chi+3)$; $p_i = L/L_i$; $\mathcal{L}(u) = 1/(1+u^2)$ is the Lorentzian function; $v_{c0}^2 = (\gamma/6\omega_R)\chi^2$ and $v_{c1}^2 = (\gamma/6\omega_R)(4\chi+3)^2$ are the squares of the so-called capture velocities. The physical constants a_1, G, b, χ, p_i, a_1, γ, λ determine various ion and force characteristics of the three-dimensional OSL; it is supposed that $L \gg \lambda$, where λ is the light wavelength.

Components of the friction force vector $\mathbf{F}_\alpha^{tr}$ are defined as

$$F_{\alpha i}^{fr} = \left(-\kappa_i(r_{\alpha i}, v_{\alpha i}) + \frac{\partial D(v_{\alpha i})}{2 v_{\alpha i} \partial v_{\alpha i}} \right) v_{\alpha i}, \qquad i = x, y, z \ , \tag{7}$$

where

$$\kappa_i(r, v) = \kappa(v)[b + \cos(2\pi p_i r)]/(1+b) \tag{8}$$

are the friction coefficients, $\kappa(v) = \kappa_0 \mathcal{L}(v/v_{c0}) + \kappa_1 \mathcal{L}(v/v_{c1})$, $\kappa_0 = 2a_1 G \ / \ 3\chi(4\chi+3)$, $\kappa_1 = [2\chi^2/(4\chi+3)^2]\kappa_0$.

The velocity diffusion coefficient can be written in the form [15]

$$D(v) = D_s + D_R(v) \ , \tag{9}$$

where $D_s = 2\chi(\chi+1)/3(4\chi+3)$, $D_R(v) = D_0 \mathcal{L}(v/v_{c0}) + D_1 \mathcal{L}(v/v_{c1})$, $D_0 = (2G^2/9\chi)(16\chi^3 + 40\chi^2 + 33\chi + 9)/(4\chi+3)^3$, $D_1 = (16G^2/9)(\chi+1)\chi/(4\chi+3)^3$. An amplitude of the noise $\sqrt{2D(\mathbf{v}_\alpha)}$ in Eq. (2) is calculated on the basis of diffusion coefficients (9).

The long-range Coulombic interaction $\mathbf{F}_\alpha^C$ can be expressed via the dimensionless Coulomb energy $U^C(r) = e^2/(4\pi\varepsilon_0 r L T_D)$ of the ions separated by the distance r in the following way

$$\mathbf{F}_\alpha^C(\mathbf{r}_1, \ldots, \mathbf{r}_N) = -\zeta \sum_{\substack{\alpha'=1 \\ \alpha' \neq \alpha}}^{N} \frac{\partial U^C(|\mathbf{r}_\alpha - \mathbf{r}_{\alpha'}|)}{\partial \mathbf{r}_\alpha} \ . \tag{10}$$

Pay attention, the phases of optical fields forming OSL are set so that friction coefficients (8) reach maximum at the center of OSL cell (unlike the case of our previous articles [7, 8]).

3 Numerical Algorithm

For solution of Eqs. (1)–(4), we developed the numerical algorithm which is a combination of two other computational approaches: 1) the velocity Verlet

method [18] for integrating Newton's ordinary differential equations of particle motion, and 2) the numerical scheme (so called an "integrator") published by R. Mannella et al. [19–21] for solution of the Langevin stochastic equation. The integrator of Mannella has the following advantages: a) ability to reproduce the equilibrium behaviour and properties of dynamical system with a high accuracy; b) ability to well reproduce long-time dynamics of phenomena, such as large rare fluctuations [20], and hence correctly to describe decay of metastable states.

Recall the velocity form of the Verlet algorithm:

$$\begin{aligned}
&\mathbf{r}_\alpha^{n+1} = \mathbf{r}_\alpha^n + \mathbf{v}_\alpha^n h + \mathbf{F}_\alpha^n \frac{h^2}{2} + \mathbf{O}(h^3),\\
&\mathbf{F}_\alpha^{n+1} = \mathbf{F}_\alpha(\{\mathbf{r}^{n+1}\}), \qquad \alpha = 1, \ldots, N,\\
&\mathbf{v}_\alpha^{n+1} = \mathbf{v}_\alpha^n + (\mathbf{F}_\alpha^{n+1} + \mathbf{F}_\alpha^n)\frac{h}{2} + \mathbf{O}(h^2)\ .
\end{aligned}$$

However our numerical algorithm for solving stochastic system of differential equations (1)–(4) turns out considerably more complicated:

$$\begin{aligned}
\mathbf{r}_\alpha^{n+1} = \mathbf{r}_\alpha^n + \zeta \mathbf{v}_\alpha^n h + \zeta \mathbf{F}_\alpha(\mathbf{r}^n, \mathbf{v}^n)\frac{h^2}{2} + \zeta \mathbf{g}_\alpha^n \mathbf{Z}_{2,\alpha}^n + \\
\zeta \mathbf{S}_1 \mathbf{Z}_{3,\alpha}^n + \mathbf{O}(h^{5/2}), \qquad \alpha = 1, \ldots, N\ , \qquad (11)\\
\mathbf{v}_\alpha^{n+1} = \mathbf{v}_\alpha^n + \left[\mathbf{F}_\alpha(\mathbf{r}^n, \mathbf{v}^n) + \mathbf{F}_\alpha(\mathbf{r}^{n+1}, \mathbf{v}^n)\right]\frac{h}{2} + \mathbf{g}_\alpha^n \mathbf{Z}_{1,\alpha}^n + \mathbf{S}_2 \mathbf{Z}_{2,\alpha}^n + \\
\mathbf{S}_1 (\mathbf{Z}_{1,\alpha}^n)^2 + \mathbf{S}_3 \mathbf{Z}_{1,\alpha}^n h + \mathbf{S}_4 (\mathbf{Z}_{1,\alpha}^n)^3 + \mathbf{O}(h^2)\ , \qquad (12)
\end{aligned}$$

where

$$\begin{aligned}
&\mathbf{r}^n = \{\mathbf{r}_\alpha^n\}; \quad \mathbf{v}^n = \{\mathbf{v}_\alpha^n\}; \quad \mathbf{g}_\alpha^n = \sqrt{2D(\mathbf{v}_\alpha^n)}; \quad \mathbf{S}_1 = \mathbf{g}_\alpha^n (\mathbf{g}_\alpha')^n / 2;\\
&\mathbf{S}_2 = -\kappa(\mathbf{r}^n, \mathbf{v}^n)\mathbf{g}_\alpha^n + \hat{\mathbf{f}}_\alpha \mathbf{g}_\alpha^n - (\mathbf{g}_\alpha')^n \mathbf{F}_\alpha(\mathbf{r}^n, \mathbf{v}^n);\\
&\mathbf{S}_3 = (\mathbf{g}_\alpha')^n \mathbf{F}_\alpha(\mathbf{r}^n, \mathbf{v}^n); \quad \mathbf{S}_4 = \{(\mathbf{g}_\alpha'')^n (\mathbf{g}_\alpha^2)^n + [(\mathbf{g}_\alpha')^2]^n \mathbf{g}_\alpha^n\}/6;
\end{aligned}$$

with [20]

$$\begin{aligned}
&\mathbf{Z}_{1,\alpha}(h) = \int_0^h d\mathbf{W}(t) = \mathbf{Y}_{1,\alpha} h^{1/2};\\
&\mathbf{Z}_{2,\alpha}(h) = \int_0^h \mathbf{Z}_{1,\alpha}(t)\, dt = \left[\mathbf{Y}_{1,\alpha} + \mathbf{Y}_{2,\alpha}\frac{1}{\sqrt{3}}\right]\frac{h^{3/2}}{2};\\
&\mathbf{Z}_{3,\alpha}(h) = \int_0^h \mathbf{Z}_{1,\alpha}^2(t)\, dt \approx \left[\left(\mathbf{Y}_{1,\alpha}\right)^2 + \mathbf{Y}_{3,\alpha} + \frac{1}{2}\right]\frac{h^2}{3}\ .
\end{aligned}$$

$\mathbf{Y}_{1,\alpha}, \mathbf{Y}_{2,\alpha}, \mathbf{Y}_{3,\alpha} \in \mathbb{R}^3$ are three uncorrelated random vectors with normal distribution $N(0,1)$ (mean zero and standard deviation one) [19]; $\hat{\mathbf{f}}_\alpha$ is a given function of physical parameters; h is a time step. By definition, we assume here that for any vectors $\mathbf{A}$, $\mathbf{B}$ the record $\mathbf{AB}$ gives the vector $(A_x B_x, A_y B_y, A_z B_z)^{\mathrm{T}}$, and $\sqrt{2D(\mathbf{v}_\alpha^n)} \equiv \left(\sqrt{2D(v_{\alpha x}^n)}, \sqrt{2D(v_{\alpha y}^n)}, \sqrt{2D(v_{\alpha z}^n)}\right)^{\mathrm{T}}$.

The Monte Carlo method is used to evaluate both the average of the solution and the average for different functions from the solution (the size of the cluster, the cluster lifetime, kinetic energy, temperature, etc.). Due to the slow convergence of the Monte Carlo method, the volume of independent samples can be very large. We set different values (from 2^{14} to 2^{16}) in different variants. The number of time steps reached $\sim 6 \cdot 10^7$. Use was made of 128–256 processing cores and the run time reached 12 hours. We used the uniform random number generator with period length $\approx 10^{38}$ from [22, 23].

To implement parallel computing the DVM-system developed in Keldysh Institute of Applied Mathematics of RAS was used. The calculations were carried out using the MVS-100K and MVS-10P supercomputers at the Joint Supercomputer Center of RAS.

Besides, we tested the algorithm by comparing our simulation result (for two-ion cluster [7]) with the analytical predictions of so-called renormalized model of the metastable (cluster) state of ions in the dissipative optical superlattice [9]. As a result, the very good agreement between the results of a numerical simulations and analytical results of renormalized model was obtained.

4 Results of Computation

In all computations we set $\gamma = 1.46 \cdot 10^8\,\mathrm{s}^{-1}$, $m = 199\,\mathrm{amu}$, $\lambda = 194$ nm, $\chi = 0.3$, $G = 2.2$, $b = 1.2$, $v_{c0}^2 = 6.542$, $v_{c1}^2 = 358.1$, $a_1^2 = 0.2$, $\zeta = 2.63 \cdot 10^{-3}$, $\omega_R = 3.35 \cdot 10^5\,\mathrm{s}^{-1}$, $p_x = p_y = 1, p_z = 0.5$ (i.e. the OSL cell is a cuboid). The number of ions N takes values 1, 4, and 9.

In Fig. 1 a general view of the computational domain and initial positions of particles at N=9 is shown. Fig. 2 also shows initial position of ions in more

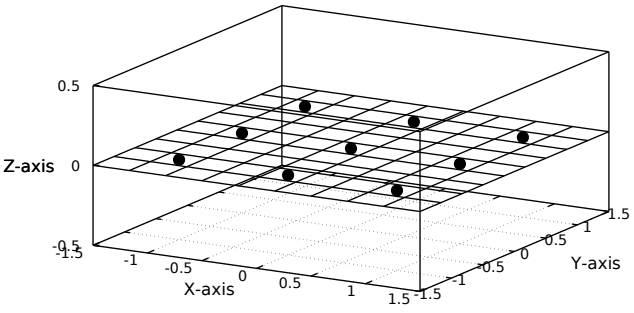

Fig. 1. General view of the computational domain in dimensionless coordinates for the case of nine particles (N=9). Bold points are the initial positions of ions in the XOY-plane at Z=0. Here there are nine OSL cells in all domain.

details.

The example of nine-ion Coulomb cluster formation is shown in Fig. 3. Here the positions of ions (averaged over 2^{14} independent samples) in 0.8 seconds for two values of the parameter L is presented. Average coordinates of the central ion coincide with its initial values.

Fig. 4 shows a behavior of a particle at one partial solution of the basic equations (without averagings).

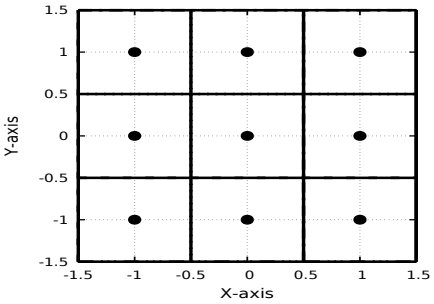

Fig. 2. The initial positions of the ions correspond to the local minimum values of the potential functions, Eq. (6), for trapping forces.

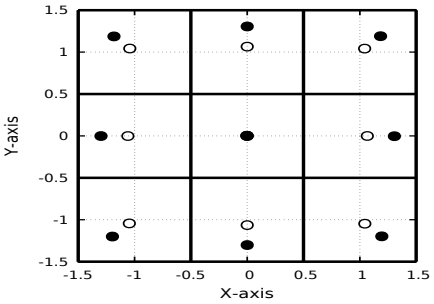

Fig. 3. Formation of the nine-ions metastable Coulomb clusters: projections of the mean ions positions on the plane XOY (the bold points for $L = 0.5$ mm and the circles for $L = 0.6$ mm).

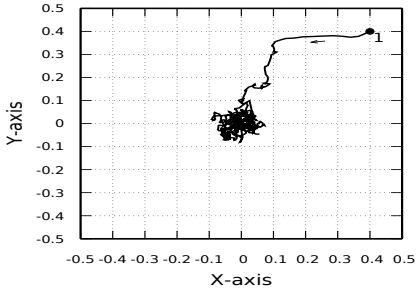

Fig. 4. An example of sample stochastic motion of a single particle in any OSL cell. The point **1** is the initial position, the initial velocity is zero. The particle tends to a point $(0, 0, 0)$ where there is a minimum of potential, and then it makes chaotic fluctuations there.

In Fig. 5 dependence of the clusters lifetime and a single particle on parameter L is shown. The present result, i.e. almost linear dependence of $\ln \tau$ on L, are in a very good agreement with theories of the metastabe states of stochastic dynamical system [26]. For the case of small noises they predict the exponential

dependence of the metastable state lifetime on the relative height of the energetic barrier $\Delta W/T$ (Arrhenius law). Indeed, the $\Delta W \sim L$ (at fixed parameters G and χ), therefore $\ln \tau \sim A + BL$, where A and B are almost independent on L at fixed G and χ. The small deviation from the linear relation probably is caused by influence of a Coulomb interaction of ions on height of an energy barrier.

The relative root-mean-square interionic separation δ is defined as [24, 25]

$$\delta = \frac{2}{N(N-1)} \sum_{i<j} \frac{\sqrt{\langle r_{ij}^2 \rangle - \langle r_{ij} \rangle^2}}{\langle r_{ij} \rangle} , \tag{13}$$

where r_{ij} is a distance between ions i and j. And Coulomb coupling parameter Γ is defined as [3]

$$\Gamma = \frac{e^2}{4\pi\varepsilon_0 k_B L T} , \tag{14}$$

where T is kinetic temperature, L is an OSL period.

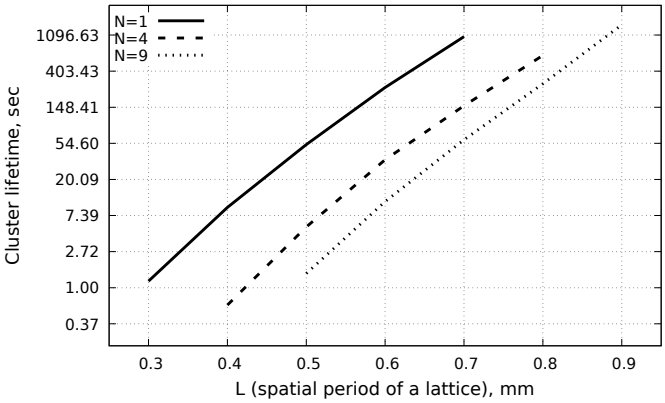

Fig. 5. The lifetime of nine-ions, four-ions clusters, and a single ion (solid line) versus parameter L. The left axis is scaled logarithmically but digits on the axis indicate the actual lifetime (in seconds).

The ordered crystal-like states (Coulomb cluster states) of ion array correspond to small values of δ, $\delta \ll 1$, and large magnitude of large $\Gamma \gg 1$ [7]. It is means that relative fluctuations of ion positions around their mean are small compared to the cluster size and interionic distance but ions are strongly coupled by the Coulomb interactions.

We see from Fig. 6 that for the long-time ion array the both necessary conditions (of Coulomb ion cluster formation) can be satisfied simultaneously. Note, that the case $\delta \simeq 1$ corresponds to breakup of the cluster.

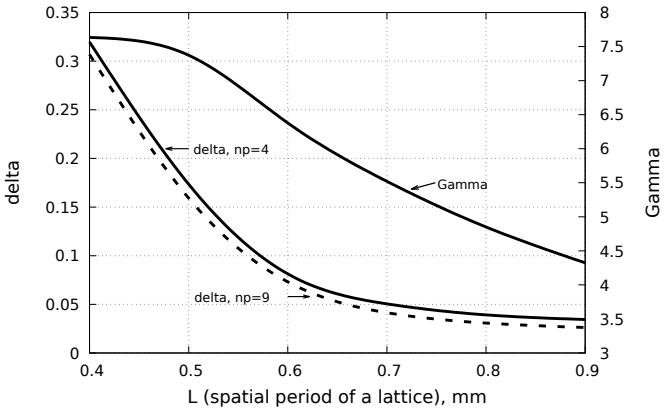

Fig. 6. Correlation parameter δ and parameter of nonideality Γ versus parameter L.

Note also that at $\delta \geq 0.1$ the lifetime of cluster is small (Figs. 5, 6). Cluster states quickly break up in view of a Coulomb interaction and quantum fluctuations of the optical forces. Pay attention that in the theory of clusters [24, 25] the value $\delta = 0.1$ usually defines a point of the cluster melting according to Lindemann's criterion.

5 Conclusion

So, our numerical experiments prove that dissipative optical superlattices are able to form a long-term (up to ~ 1000 seconds) many-particle Coulomb cluster, which is the highly ordered array of mercury ions. Such cluster is characterized by the small values of the relative root-mean-square interionic distance, $\delta \ll 1$, and by the large magnitude of the Coulomb coupling parameter $\Gamma \gg 1$. Dependences of basic parameters of a Coulomb cluster on the period of a dissipative optical superlattice are investigated. They sufficiently well correspond to the known theories of metastable states of stochastic dynamical systems and clusters [25, 26]. Comparison of the obtained numerical results with results of theoretical paper [9] shows very good agreement. For numerical solution of stochastic equations, we give generalization of the well-known velocity Verlet scheme for accounting of a random force.

Our algorithm, Eqs. (11)–(12), allows to consider correctly key features of our stochastic model: a metastability of Coulomb clusters in OSL, non-conservatism of optical trapping forces, nonlinearity of friction coefficients (8), and a multiplicativity of stochastic noise. Parallel realization of this algorithm on supercomputers was performed. In future works, it is planned to increase the number of ions up to several dozens.

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