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Structural transitions in one-dimensionally confined one-component plasmas

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Layered structures occurring in strongly coupled one-dimensionally confined one-component plasmas are studied by means of Monte Carlo simulations. A series of structural transitions with alternating square and hexagonal symmetry is observed with increasing the width of the system. For closer interlayer separation, the square type of lattice (bcc in {100} or {110} plane) is dominating, whereas for wider separations the hexagonal (fcc in {111} plane or hcp) patterns are observed.

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Two-dimensional (2D) and quasi-two-dimensional (quasi-2D) Coulomb systems, i.e., charged many-particle systems confined in one and infinite in the two other directions, attracted considerable interest of researchers in recent decades. Relevant physical examples are charged colloids geometrically confined in a thin layer between two plates [1], dusty plasmas trapped in one-dimensional (1D) potential profiles [2], planar ion structures in Penning traps [3], electronical inversion layers and bilayers in semiconductors [4–6], etc. The distinguishing feature of these systems is their capability to form strongly correlated condensed state at strong coupling.

The basic reference model for strongly coupled Coulomb systems is the model of one-component plasma (OCP). In this model, only one sort of charges is dynamically or statistically taken into account, whereas the total compensating charge is related to the immobile neutralizing background.

While the structure of infinite unbounded strongly coupled OCP is understood currently rather well [7,8], the behavior of 2D and quasi-2D OCP remains much less examined and is the focus of intensive investigations, in particular, by means of Monte Carlo (MC) and molecular dynamics (MD) computer simulations [9–14]. The numerical studies of 2D hexagonal Coulomb lattices [9,10] have demonstrated good agreement with the experiments of C. Grimes and G. Adams on the melting of 2D Wigner lattice formed by electrons on the surface of liquid helium [11]. Computer simulations performed for 1D-confined systems, i.e., with the deviation from the strictly 2D geometry, evidence the formation of layered structures in strongly coupled OCP in this case [12]. Though many of the properties of these systems have been elucidated, the detailed intrinsic structure of the layers remains an open question. According to the theoretical predictions [13] based on minimizing the energy of the system (i.e., for zero temperature) evaluated within the fluid theory, with increasing the width of 1D confined OCP, one should expect a series of structural transitions with alternating square and hexagonal symmetry. Similar transitions were observed in experiments with ions in Penning traps [3], charged colloids [1], and in numerical simulations of closely packed hard spheres [15] confined in quasi-2D geometry. However, direct numerical evidence for these transitions remains up to now absent. The MD simulations of Ref. [12] report only regular hexagonal intralayer structure of multilayered systems.

In this paper, the results of microscopic MC simulations of strongly coupled OCP in quasi-2D geometry are presented. The aim of simulations is structure, in particular, the above question about the structural transitions in few-layered systems.

Thus, the system under examination consists of one kind of pointlike charges in the immobile neutralizing background. The simplest case related to the quasi-2D geometry is that the background is uniform and occupies a volume of a finite width in Z direction ($-H<Z<H$) and infinite in XY directions. Following the treatment conventional for MC simulations, we consider a basic rectangular configurational cell ($0<X,Y<L,-H<Z<H$) with a finite number N_p of particles, which periodically repeats itself in XY directions. The state of the system can be unambiguously specified by the two quantities, the dimensionless width $h=2H/d$ and the coupling $\Gamma=e^2/k_BTd$. The quantity $d=L/\sqrt{\pi N_p}$ has the meaning of the average interparticle distance and is used below as the length unit. Note, that in the case of one layer in

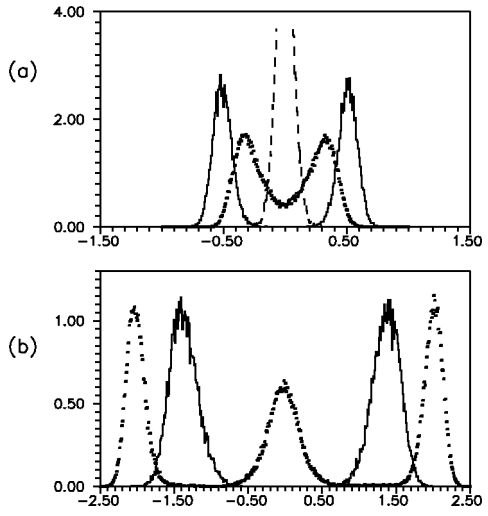

FIG. 1. Transversal probabilty distributions for 1D-confined OCP, $\Gamma=500$; (a) $h=0.92$ (dashed line), $h=1.11$ (dots), $h=1.28$ (solid line); (b) $h=2.73$ (solid line), $h=3.13$ (dots). The transitions from one- to two-layered system, and from two- to three-layered system occur at the points $h\simeq 1.1$ and $h\simeq 2.9$, respectively.

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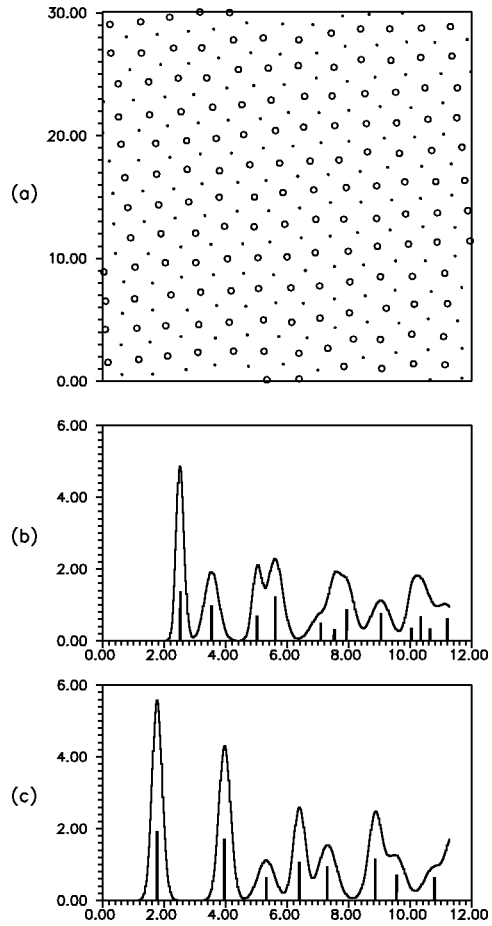

FIG. 2. An equilibrium MC configuration for two-layered square structure (a), ($\Gamma=500$, $h=1.28$, $N_p=288$) and the associated 2D intralayer (b) and interlayer (c) radial distributions. The points and the larger circles (a) relate to the different layers. The vertical impulses in (b) and (c) represent the scaled radial distributions for an ideal bcc {100} lattice with the same spacing.

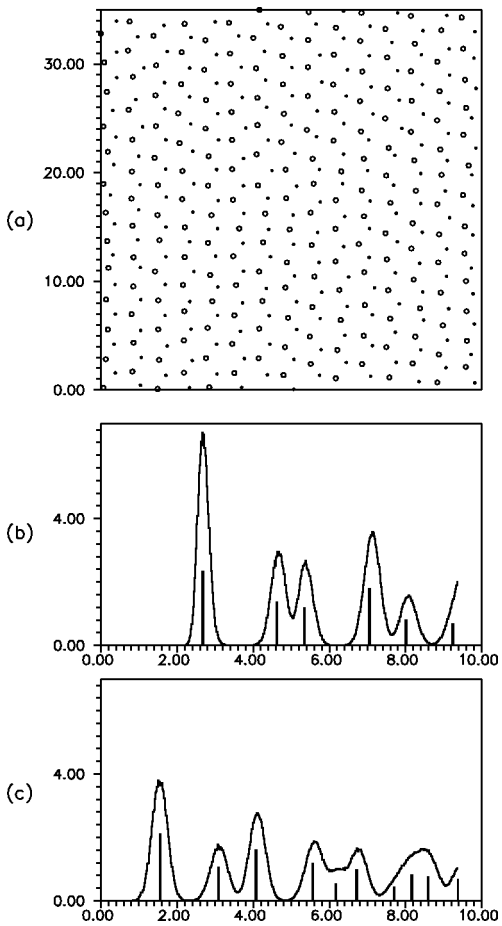

FIG. 3. An equilibrium MC configuration for two-layered hexagonal structure (a), ($\Gamma=500$, $h=2.42$, $N_p=390$) and the associated 2D intralayer (b) and interlayer (c) radial distributions. The points and the larger circles (a) relate to the different layers. The vertical impulses in (b) and (c) represent the scaled radial distributions for an ideal fcc {111} lattice with the same spacing.

the system, the quantities d and Γ coincide with those defined for strictly 2D systems, whereas in the case of K layers they differ from the relevant intralayer parameters by the factor $\simeq\sqrt{K}$. In order to allow for the long-range Coulomb interactions with the image particles, the method developed in Ref. [16] for the computations of Ewald's sums in quasi-2D two-component plasmas is employed. As compared to the expressions obtained in Ref. [16], the allowance for the interaction with the uniform background of the finite width $2H$ in quasi-2D OCP results in only one essential additional term in the potential energy,

$$\frac{U'}{k_BT}=\frac{\Gamma}{h}\sum_{i=1}^{N_p} z_i^2, \tag{1}$$

which can be viewed as a confining oscillator field in Z direction. Here $z_i=Z_i/d$ is the dimensionless Z-coordinate of the ith particle.

Simulations were performed for the range of parameters $\Gamma=300-600$ and $h=0.02-4.8$, which correspond to the crystal structures with 1–3 layers. The structural properties were studied in terms of 2D radial intralayer and interlayer pair distribution functions and the 2D orientational order parameter for the m-fold symmetry [17] defined as

$$O_m=\left\langle\left|\frac{1}{N_L}\sum_l\frac{1}{m}\sum_k e^{im\theta_{lk}}\right|\right\rangle. \tag{2}$$

The inner sum in the above expression is taken over the bonds connecting the lth particle with all the nearest neighbors (θ_{lk} is the angle between such a bond and some fixed axis), i.e., the particles at the distance less than the first minimum r_{min} in the radial intralayer distribution function; the brackets $\langle\cdots\rangle$ denote the canonical averaging; N_L is the number of particles within the layer. The type of 2D symmetry within layers can be simply estimated by the average number of 2D nearest neighbors N_n, which must be close to 4 or 6 for the square or hexagonal types of symmetry, respectively.

MC simulations were carried out for the canonical (NVT) ensemble by using the conventional Metropolis algorithm [18] with the number of particles being within the range

TABLE I. Structural properties of two- and three-layered systems obtained in MC simulations ($\Gamma = 500$). Notation: h = width parameter, K = number of layers, S = structure, N_c = 2D coordination number, N_n = average number of 2D nearest neighbors, O_4/O_6 = orientational order parameter for fourfold/sixfold symmetry, N_p = number of particles in MC cell, D = ratio of the interlayer to the lattice spacing (defined by the first maximum in the relevant radial distributions). The absolute error in the computations of the order parameters does not exceed 0.015.

h	K	S	N_c	N_n	O_4	O_6	D	N_p
	2	bcc{100}	4		1.00[a]		0.50[a]	
1.28				3.98	0.94		0.41	288
1.62				4.00	0.90		0.61	288
	2	fcc{111}	6			1.00[a]	0.82[a]	
2.42				6.00		0.90	0.90	390
2.73				6.00		0.90	1.05	112
	3	bcc{100}	4		1.00[a]		0.50[a]	
3.13				4.18	0.82		0.67	192
	3	bcc{110} (rhombic)	4		0.78[a]		0.82[a]	
3.65				4.41	0.65		0.77	192
	3	fcc{111}	6			1.00[a]	0.82[a]	
4.26				6.00		0.88	0.87	168
	3	hcp	6			1.00[a]	0.82[a]	
4.26				6.00		0.87	0.87	168

[a]"Ideal" lattices.

$N_p = 112–390$. The relative error in the calculation of the Coulomb energy was controlled to be less than 10^{-6}, which was achieved by using appropriate number of the wave vectors in the inverse space and the values of the splitting parameter in computations of 2D Ewald sums. In most of the simulations, the canonical averaging was performed over $\simeq 2000–5000$ statistically independent configurations.

The results of simulations are presented in the figures. The most remarkable result is the observation of transitions in the internal structure of the layers occurring with increasing the width of the system. In Fig. 1, the transversal probability (normalized density) distributions are displayed as a function of the width h. The transitions from one- to two-layered and from two- to three-layered system occur near the points $h \simeq 1.1$ and $h \simeq 2.9$, respectively. The structure obtained for one-layered systems is well known, it is a simple hexagonal lattice quite similar to that observed in strictly 2D case [9,10]. Just above the point $h = 1.1$, the system crystallizes in a two-layered square structure, which is a feature of a bcc lattice in {100} plane. An equilibrium configuration obtained in MC simulations (a perfect lattice) and the associated intralayer and interlayer radial distribution functions

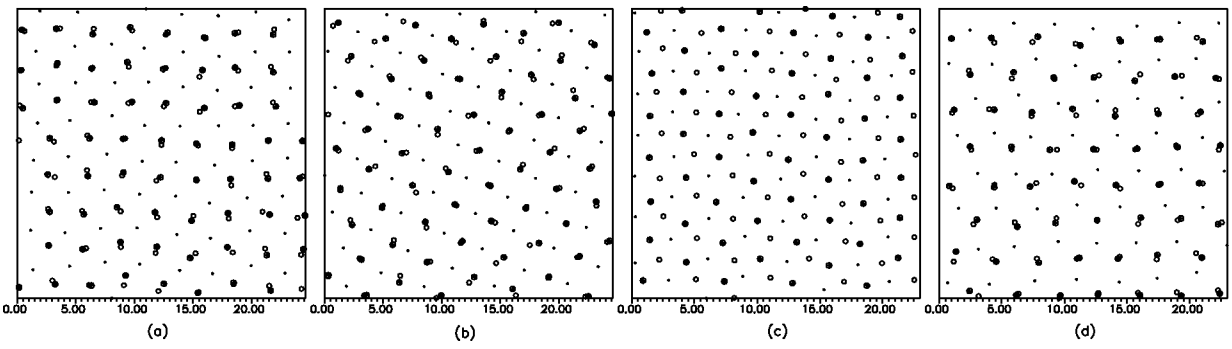

FIG. 4. Equilibrium MC configurations for three-layered structures, $\Gamma = 500$. Structural changes are observed with increasing the width, (a) bcc{100}, $h = 3.13$, (b) bcc{110} (rhombic), $h = 3.38$, (c) and (d) the competing fcc{111} and hcp structures for the same width $h = 4.26$. The positions of particles are marked with points (the inner layer), and with larger circles (the outer layers).

are given in Fig. 2. Comparison with distributions of an ideal bcc lattice clearly indicates this type of structure. The number of the nearest 2D neighbors computed for this region, is close to 4, in agreement with the fourfold symmetry. Let us mention, that with increasing the width parameter, i.e., with growing the interlayer separation, the structure acquires a deviation from square geometry (large-scale deformation), which is reflected by the changes in distribution functions and in some decrease of the order parameter O_4 (see Table I).

Above the point $h \simeq 1.8$, the system undergoes a transition to a hexagonal ''honeycomb'' structure with the same number of layers $K=2$, which can be observed visually, Fig. 3, and is evidenced by the change in the position of the first minimum in the intralayer distribution function from 3.0 to 3.6. The associated number of the nearest 2D neighbors increases therewith to $N_n=6$. In contrast to the square lattice with dominating interlayer correlations, in the case of two-layered hexagonal structure the intralayer correlations are more pronounced. The behavior of 2D distributions indicates that the latter hexagonal structure represents a piece of fcc lattice in {111} plane. A similar transition from the square to hexagonal structure is observed in three-layered systems within the range $h=2.9$–4.8, Fig. 4. Note that at larger interlayer separations, two competing hexagonal structures with equal average energies are observed, fcc{111} and hcp, as dependent on initial random configurations. This indicates that the type structure is determined by the interactions between the nearest layers only (i.e., the interaction between the outer layers is negligible). The intermediate deformed square lattice consisting of elongated squares is better defined in this case and can be regarded as the same bcc structure in {110} orientation, or, more generally, as a rhombic lattice. The MC simulations performed for the range $\Gamma = 300$–600 resulted in similar structural properties, except that the radial distributions are broader for higher temperatures. Some information related to a number of selected runs is summarized in the table. The results of MC simulations correlate with the theoretical predictions of Ref. [13] and are in very good agreement with the experiments with the planar ion structures in Penning traps [3], Fig. 5, representing the most accurate implementation of OCP in 1D oscillator confinement. The evident similarity of the results obtained with the properties of other systems (charged colloids [1], hard spheres [15]) in quasi-2D geometry indicates that the structural transitions under consideration are the general feature of 1D-confined systems weakly dependent on the nature of repulsive interparticle interaction.

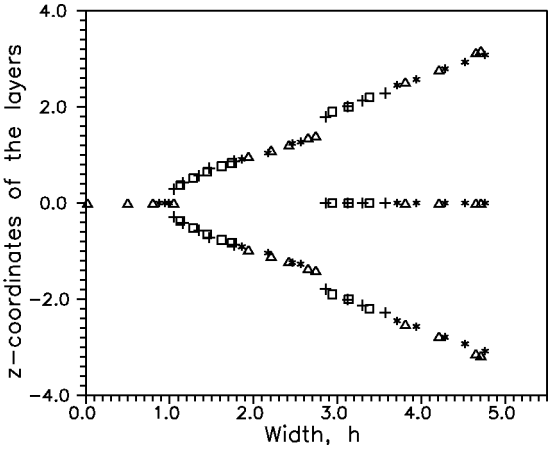

FIG. 5. Structure of 1D-confined OCP. Comparison of the results of these MC simulations ($\Gamma=300$) and experimental data of Ref. [3] ($160<\Gamma<3150$) recalculated for $(z-h)$-plane. The positions of layers are marked with symbols of triangles/squares (MC simulations), and $*/+$ (experiment) for the hexagonal/square type of symmetry, respectively.

To conclude, layered structures occurring in strongly coupled one-dimensionally confined one-component plasmas are studied by means of Monte Carlo simulations. A series of structural transitions with alternating square and hexagonal symmetry is observed with increasing the width of the system. For closer interlayer separation, the square type of lattice (bcc in {100} or {110} plane) is dominating, whereas for wider separations the hexagonal (fcc in {111} plane or hcp) patterns are observed.

[1] C.A. Murray and D.H. Van Winkle, Phys. Rev. A **64**, 562 (1986).
[2] H. Thomas, G.E. Morfill, V. Demmel, J. Goree, B. Feuerbacher, and D. Möhlmann, Phys. Rev. Lett. **73**, 652 (1994).
[3] T.B. Mitchell, J.J. Bollinger, D.H.E. Dubin, X.-P. Huang, W.M. Itano, and R.H. Baughman, Science **282**, 1290 (1998).
[4] A.B. Fowler and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[5] G.J. Kalman, Z. Donko, and K.I. Golden, Contrib. Plasma Phys. **41**, 191 (2001).
[6] C.B. Hanna, D. Haas, and J.C. Diaz-Velez, Phys. Rev. B **61**, 13 882 (2000).
[7] E.L. Pollock and J.P. Hansen, Phys. Rev. A **8**, 3110 (1973).
[8] S.G. Brush, H.L. Sahlin, and E. Teller, J. Chem. Phys. **45**, 2102 (1966).
[9] R.C. Gann, S. Chakravarty, and G.V. Chester, Phys. Rev. B **20**, 326 (1979).
[10] R.H. Morf, Phys. Rev. Lett. **43**, 931 (1979).
[11] C.C. Grimes and G. Adams, Phys. Rev. Lett. **42**, 795 (1979).
[12] J.P. Schiffer, Phys. Rev. Lett. **61**, 1843 (1988).
[13] D.H.E. Dubin, Phys. Rev. Lett. **71**, 2753 (1993).
[14] H. Totsuji and J.-L. Barrat, Phys. Rev. Lett. **60**, 2484 (1988).
[15] B. Pansu, Pi. Pieransky, and Pa. Pieransky, J. Phys. (France) **45**, 331 (1984).
[16] O.V. Bystrenko, Phys. Rev. E **65**, 037702 (2002).
[17] A. Zippelius, B.I. Halperin, and D.R. Nelson, Phys. Rev. B **22**, 2514 (1990).
[18] K. Binder, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer-Verlag, Berlin, 1979).