Layered Structure in Condensed, Cold, One-Component Plasmas Confined in External Fields

John P. Schiffer
Argonne National Laboratory, Argonne, Illinois 60439-4843, and
University of Chicago, Chicago, Illinois 60637
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Novel features of solids that may be formed from cold, condensed plasmas confined in external fields (storage rings or ion traps) have been investigated with molecular-dynamics calculations. Such plasmas have well defined outer surfaces and interior layers that are parallel to the outer surface. In each layer the particles are arranged in an approximate hexagonal pattern of a two-dimensional Coulomb lattice. The interactions between layers have also been investigated: They are relatively stronger in the straight (commensurate) and virtually absent in the curved (incommensurate) directions.

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The prospects for achievement of cold one-component plasmas in ion traps[1] and storage rings[2] look promising for the near future. Molecular-dynamics (MD) studies of such plasmas, with an external confining force that approximates the average focusing fields on a particle beam in a storage ring,[3] have been reported. It was found that above a critical linear density, the particles arrange themselves in one or more, well defined, cylindrical shells. The particles within each shell form a hexagonal pattern, very similar to the one characteristic of a two-dimensional Coulomb lattice,[4] while (for a multishell beam) the overall correlation function in three dimensions shows structures with a coordination of 14 and 58, characteristic of body-centered-cubic (bcc) symmetry.[5] Since the two symmetries are incompatible, their presence in the same array must be approximate. In Ref. 3 it was also reported that a system with three-dimensional confinement that approximates the geometry of ion traps shows spherical shells with similar features.

In the present work, the properties of such systems have been investigated further with one- as well as two- and three-dimensional confinement, and very similar results are obtained in each case. A harmonic restoring force was assumed: for three-dimensional confinement, $F=-K[(x^2+y^2+z^2)]^{1/2}$; for two-dimensional confinement, $F=-K[(y^2+z^2)]^{1/2}$; and for one-dimensional confinement, $F=-Kx$, where K is the force constant. A $1/r^2$ interparticle force was used throughout.

These systems were studied with the methods of molecular dynamics[3] with repeating boundary conditions to allow for extension in the unconfined directions. Various systems of 200, 700, or 2000 particles were allowed to settle gradually into a state sufficiently cold for thermal oscillations to be small. The systems started with random coordinates which were allowed to settle for at least a hundred steps (0.5 time unit, as defined below) at each temperature, starting with $\Gamma=1$ and finishing at $\Gamma\simeq 2000$, changing through at least three intermediate levels of temperature. [$\Gamma\equiv(q^2/a)/kT$, q being the charge, $a\equiv(3/4\pi\rho)^{1/3}$ the average spacing, ρ the density, and kT the temperature.[1]] Calculations with different initial conditions or cooling procedures resulted in qualitatively similar, though not precisely identical, results. The density profile of particles along the direction of

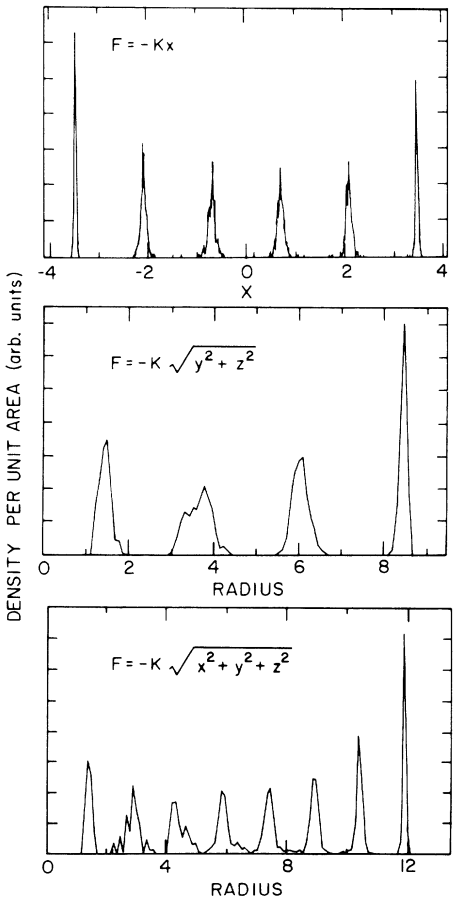

FIG. 1. Particle density (per unit area) as a function of distance for one-, two-, and three-dimensional confinement. The distance for the top figure is that from the central $x=0$ plane; in the middle figure it is the radial distance from the $(y=0,z=0)$ line; and on the bottom it is the radial distance from the origin, all in units of the appropriate a.

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confinement is shown in Fig. 1, from which it is clear that the feature of a layered structure is common to all these systems: A one-dimensional force produces flat sheets; two- and three-dimensional forces produce cylindrical and spherical shells, respectively. The two-dimensional order within each layer is particularly striking: Correlation functions are shown in Fig. 2. The distances in these systems may be compared in terms of the average particle spacing a, defined above, which is equivalent to $a^3=(3q^2/K)$, $(3q^2/2K)$, and (q^2/K) for the one-, two-, and three-dimensional systems, respectively. In units of the appropriate a, the following spacings are compared in Table I: the average spacing between shells (or sheets) D_{sh}, the average nearest-neighbor spacing between particles within a shell S, and the widths (FWHM) of the outermost shell and the second from outer shell, W_{sh}(outer) and W_{sh}(2). The

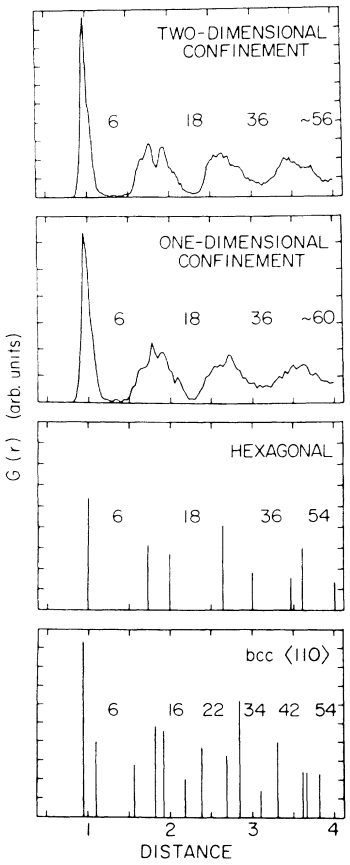

FIG. 2. The correlation function (probability of finding a particle a given distance from any other particle) within one sheet or shell is shown in the top and second frames for one- and two-dimensional confinement. That for three-dimensional confinement is similar. The numbers on the figures indicate the coordination for the peaks: the total number of particles up to that distance. The distance scale is normalized to 1 for the nearest-neighbor peak. The third frame shows the correlation function expected for an ideal "hexagonal" pattern; while the bottom one is that for the ⟨110⟩ plane of a bcc lattice.

TABLE I. Spacings for ordered Coulomb solids with external confining forces.

	D_{sh}	S	S/D_{sh}	W_{sh}(outer)	W_{sh}(2)
1D	1.38	1.74	1.26	0.040	0.094
2D	1.48	1.80	1.22	0.038	0.10
3D	1.49	1.80	1.21	0.046	0.15
bcc ⟨110⟩	1.44	1.85	1.29		
fcc ⟨111⟩	1.48	1.81	1.22		

widths are approximate ($\pm 20\%$); they seem quite sensitive to the details of the MD calculation. Repeated calculations with different numbers of particles and different initial conditions gave very similar results as far as the correlation functions and the quantities in Table I are concerned, though the detailed arrangement of particles within each shell (where the hexagonal patterns generally have some defects, since a perfect hexagonal pattern is not possible on a closed curved surface of arbitrary size), as well as the relative arrangement of particles between different shells, was not the same when conditions were varied. Smaller values of Γ (down to about 200) showed the same general pattern, with the correlation functions and the widths of the layers becoming broader for higher temperatures.

All the systems studied show very similar characteristics. For each, the outermost shell is extremely sharp, on the order of a few percent of the intershell spacing; the following shell is a factor of 2–3 thicker, but after that there is no strong increase in the widths of subsequent layers. The limit to the number of shells has not been explored; up to eight layers, the maximum obtainable in

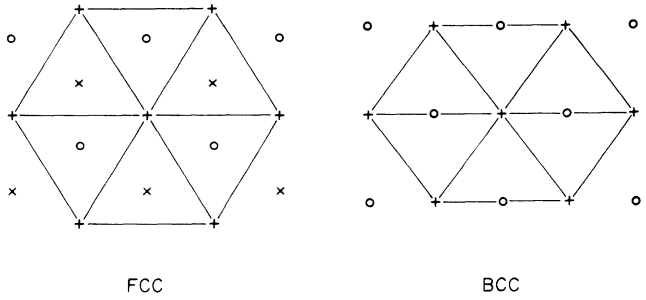

FIG. 3. The pattern of +'s connected by lines on the left-hand figure is that for regular hexagons, similar to that seen in the MD calculations, and corresponding to the ⟨111⟩ planes of an fcc lattice. The O's and ×'s show the lattice positions in subsequent fcc planes. The right-hand figure shows the position of lattice sites in the ⟨110⟩ plane of a bcc lattice, with the O's showing the next plane. The correlation between particles *within* layers in the MD calculations are similar to that corresponding to the pattern on the left, while the correlation *between* layers is more like that in the bcc lattice shown on the right.

the present calculations, have been seen. Values calculated for ⟨110⟩ planes in a bcc lattice are similar, yet not directly comparable. These planes contain elongated hexagons as shown in Fig. 3, and the two-dimensional correlation function in such a plane is not consistent with that found for the individual layers in the confined systems in the MD calculations, as was demonstrated in Fig. 2. The values for fcc ⟨111⟩ planes are also shown in Table I.

Since, for one-dimensional confinement, the particles are in plane sheets, and the complications of curvature are absent, the correlations between particles in adjacent sheets are of interest. Here, however, the exact number of particles and the exact cell size becomes significant, since the symmetry may be sensitive to the exact size of the repeating cell. Within the limitations of the available computer time, it has not been practical to study systems much larger than about 2000 particles. The cell size was chosen to yield six layers with about 340 particles each, two layers on the outside, two second from the outside, and two on the inside.

The "hexagonal" pattern discussed in the context of Fig. 2 is a feature of the ⟨111⟩ planes of a face-centered-cubic lattice; however, there the planes alternate in an $(a,b,c,a,b,c,\ldots)$ pattern. The lattice in the present one-dimensionally confined systems does not show such a pattern; instead, adjacent planes show regular hexagons within each layer, as is evident from the correlation function of Fig. 1, but alternate in an $(a,b,a,b,\ldots)$ sequence, which is characteristic of the ⟨110⟩ bcc planes, shown in Fig. 3. Of course, for many layers, this pattern must lead to a transition to an overall bcc symmetry in the interior, since this is the result of calculations for an infinite plasma[5]; the hexagonal pattern seems to be associated with the surface and near-surface planes, perpendicular to the confining force; all six planes exhibit it in the present calculation. For the two- and three-dimensional confinement there is no repeating pattern evident between adjacent shells: There cannot be any clear correlation since the surfaces are not commensurate because of the curvature. For these systems, the hexagonal pattern is clear in all except the innermost shells, which contain very few particles.

For the three-dimensionally confined plasmas, the number of layers n_s must be independent of the magnitude of the confining force—it depends only on the number of particles as long as the system is sufficiently cold ($\Gamma \gtrsim 200$). The equilibrium configuration is independent of this force; only the overall size scales with it. The number of shells determined from a series of calculations is $n_s \approx (N/4)^{1/3}$. If λ is the number of particles per unit length (in units of a) then for the cylindrical case $n_s \simeq 0.8\lambda^{1/2}$; and $n_s \approx 0.43\sigma$ for one-dimensional confinement, with σ the areal density in the same units.

The interaction between shells has been studied with the MD method. The particles in one shell (the second

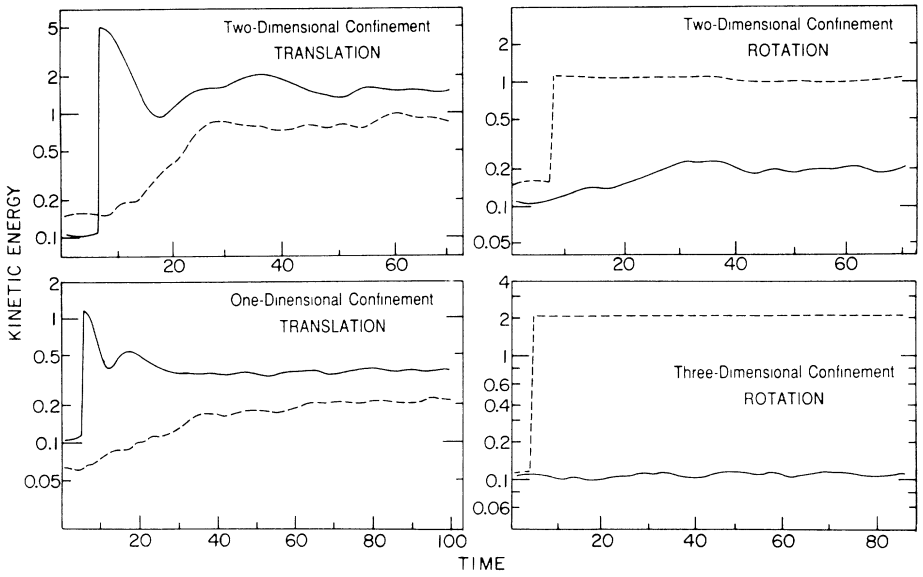

FIG. 4. Components of kinetic energy in various systems plotted as functions of time, in units of $1/\omega_{\text{plasma}}$ [where $\omega_{\text{plasma}} \equiv (4\pi\rho q^2/m)^{1/2}$], the reciprocal of the plasma frequency characteristic for each system. At a given time the particles in one layer (the second from the outside) are given a linear or rotational velocity in a direction perpendicular to the confining force. For the upper two figures the solid line represents translational kinetic energy along the symmetry axis ($\sum \frac{1}{2} m v_x^2$, in units of the dimensionless temperature for $\Gamma = 200$), and the dashed line is the kinetic energy associated with rotation about that axis. On the lower left, the solid line is for translational kinetic energy along the imposed motion and the dashed one is for motion perpendicular to the first, both along the planes; for the lower right the dashed line is for rotational and the solid one for radial kinetic energy.

from the outside) were given a small velocity with respect to the others; the calculations were used to explore whether there are any restoring forces, and the extent to which kinetic energy of a particular mode of motion of one shell is damped into kinetic energy associated with other degrees of freedom. The results of these calculations are shown in Fig. 4. It is evident that, for three-dimensional confinement, the rotation of one spherical shell of particles and, for the two-dimensional case, the rotation of a cylindrical shell both proceed relatively unhindered (within the limits of these calculations) and with no observable elastic restoring force or frictional dissipation into other microscopic modes. On the other hand, the longitudinal motion of a cylindrical shell and, for one-dimensional confinement, the lateral motion of one plane with respect to the others both are subject to a relatively much larger restoring force, and are damped by frictional heating, transferring kinetic energy into other degrees of freedom.

It appears that motion along the degrees of freedom that are represented by curved coordinates (rotation), where the particles cannot interlock, since the surfaces are incommensurate, can proceed relatively unhindered. In the straight directions, where the surfaces are commensurate, the interparticle forces between the shells or layers become appreciable, and the motion is damped.

In conclusion, it seems that all systems of Coulomb solids that are reported here have a number of common characteristics induced by the external confining forces. These are a well defined surface layer, perpendicular to the direction of the confining (harmonic) force, hexagonal ordering within that surface, subsequent regularly spaced inner layers with similar ordering, and forces between the surfaces that are much weaker for relative displacements in the direction of curvature than in straight directions.

Some work has been done on the extension of these calculations to anisotropic confinement ($F_y \neq F_z$ for two-dimensional confinement or $F_x \neq F_y = F_z$ for the three-dimensional case) with similar results. The layered properties of these plasmas under external confinement appear to be a rather general phenomenon. Results showing similar layered structures from molecular-dynamics calculations for three-dimensional confinement, using a Hamiltonian with the "guiding center" approximation representing a magnetic Penning trap, have been published since this work was submitted.[6]

This is the continuation of work started with the late Aneesur Rahman, and his adaptation of the MD method to this class of problems opened the way to this line of inquiry. Discussion with other colleagues is gratefully acknowledged, in particular with M. Marder, S. Pieper, and P. Vashista. This work was supported by the U.S. Department of Energy, Nuclear Physics Division, under Contract No. W-31-109-ENG-38. Calculations reported were done on ERCRAY, and the Cray-2 at the University of Minnesota.

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