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STRUCTURE OF A ONE-COMPONENT PLASMA IN AN EXTERNAL FIELD: A MOLECULAR DYNAMICS STUDY OF PARTICLE ARRANGEMENT IN A HEAVY-ION STORAGE RING

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ABSTRACT

A one-component plasma has been studied by molecular dynamics calculations to simulate the behavior of charged particles in heavy-ion storage rings. The Hamiltonian used confines the plasma in the directions lateral to the direction of travel in the ring in the frame of reference which is moving with the beam. The results show an unexpected stratification of density in the lateral direction, and a tendency towards a first-neighbor coordination of 14(8+6) seems incipient. On each shell we observe a triangular pattern of particle arrangement.

INTRODUCTION

In heavy-ion storage rings a plasma of bare or heavily ionized nuclei, all with the same mass and positive charge, is kept circulating, with magnetic (or electric) focussing arranged so as to confine the plasma to a narrow region around the equilibrium orbit in the ring. The plasma may be cooled by several methods: among them electron cooling and the newly suggested method of laser cooling, such that the relative thermal motion of the particles with respect to each other is lowered, although the whole plasma is moving around the ring with velocities of 10^{10} cm/sec or more. The number densities in such a plasma can be between 10^5 and 10^8 ions/cm^3 and temperatures of relative motion of 1 deg.K have been reported, temperatures down to the mK range are anticipated with laser cooling. The possibility of observing condensation phenomena in such systems has been noted [1].

We have made an attempt to simulate these conditions by computer molecular dynamics [2] which, within the limitations of the Hamiltonian assumed, give fully detailed information on the structure and dynamics of the system. The basic assumption is that we have a Cartesian reference frame moving with the plasma beam and that the classical, Newtonian, equations of motion may be used to determine the dynamics of the ions. In addition, as will be seen in the next section, there are simplifying assumptions about the confining potential, which imply idealizations of the magnetic fields that contain the plasma in a real storage ring. The results obtained are rather unexpected and hence are being reported even though the more realistic aspects of the conditions prevailing in storage rings have not yet been incorporated.

THE HAMILTONIAN AND BOUNDARY CONDITIONS

We use here a periodically repeating cubic box of length L (expressed in terms of some unit of length = ξ cm) in which there are N ions with potential energy V (the summation over all periodic boxes being implicit),

$$V = \Sigma_i \Sigma_{j>i}\ 1/r_{ij} + \Sigma_i\ 1/2K(y_i{}^2+z_i{}^2),$$

where x_i, y_i, z_i (i=1,N) are the coordintates of the N particles in the box, r_{ij} is the distance between the particles i and j (all in units of ξ) and V is the energy in units of Z^2e^2/ξ. (In a typical storage ring for ions with charge Z the values of KZ^2e^2/ξ^3 range between 10^{-6} and 10^{-12} erg/cm^2.) If the value of K is large, the coordinates y_i and z_i will be confined to a narrow region around the x axis and the plasma will be spread in a cylinder along this axis, continuing to the edges of the box and joining onto the cylinder of plasma in the adjoining boxes.

In the usual manner of treating a one-component plasma with periodic boundary conditions the double summation in V is evaluated using the standard Ewald summation method first used in this context by Brush, Sahlin and Teller [3], then by Hansen and collaborators [4] in an extensive study of the one-component plasma, and then by Slattery et al. [5] in a particularly detailed study of such systems.

We note here that if the external field potential energy is modified to include the x coordinate, i.e. if it is $1/2K(x_i{}^2+y_i{}^2+z_i{}^2)$, one can dispense with the periodic boundary condition altogether. We shall mention this point again below.

The only parameters in our Hamiltonian are the dimensions of the box L, the number of particles N, the confining potential K and the temperature T at which the system is maintained using standard methods of molecular dynamics [2].

For such a calculation to be meaningful as an approximate simulation of conditions in a storage ring, the paramaters used must be appropriate, in other words the value of K should be sufficiently large to confine the particles in a pencil-like narrow region around the x axis with a diameter much less than the cell size L. We may then expect that the dynamics of the structure in the pencil will be only slightly perturbed by the periodic boundary conditions.

It should be noted that the present calculations only roughly approximate conditions in the storage rings that are under construction at several laboratories. The time average of the focusing forces that contain particles in a ring is proportional to the displacement from a mean equilibrium orbit. Although most storage rings have periodic strong-focusing elements, it is possible, at least in principle, to have a weak focusing ring where the restoring forces are constant in time. In weak focusing, the magnetic field that causes the particles to follow a closed orbit, is proportional to $r^{-1/2}$, where r is the bending radius, and the focusing force is equal in the horizontal (bending plane) and the vertical (perpendicular to the bending plane) directions. This idealized restoring force corresponds to the assumptions in the present calculations, with the circular motion neglected.[1]

N=2000, L=4, K=10,000, T=1/9

Under these condition the diameter of the pencil of plasma is found to be less than 0.6. Before presenting the detailed results let us consider what physical conditions such a calculation would represent.

Suppose that the unit length ξ is 0.1 cm. The beam diameter will then be <0.06 cm; the temperature would be 2°mK for Z=1 and 20°K for Z=90; while $K=2.3\times10^{-12}$ dyn/cm and 2.0×10^{-8} dym/cm for the two temperatures. The number density $\sim\xi^{-2}$ for this pencil with N=2000, 0.06 cm in diameter and 0.4 cm in length, will be 2×10^{6} cm^{-3}. These values include the parameter range of storage rings envisioned at present.

Figure 1 shows the projection of the 2000 particles onto the y-z plane. The stratification in the direction perpendicular to the beam is

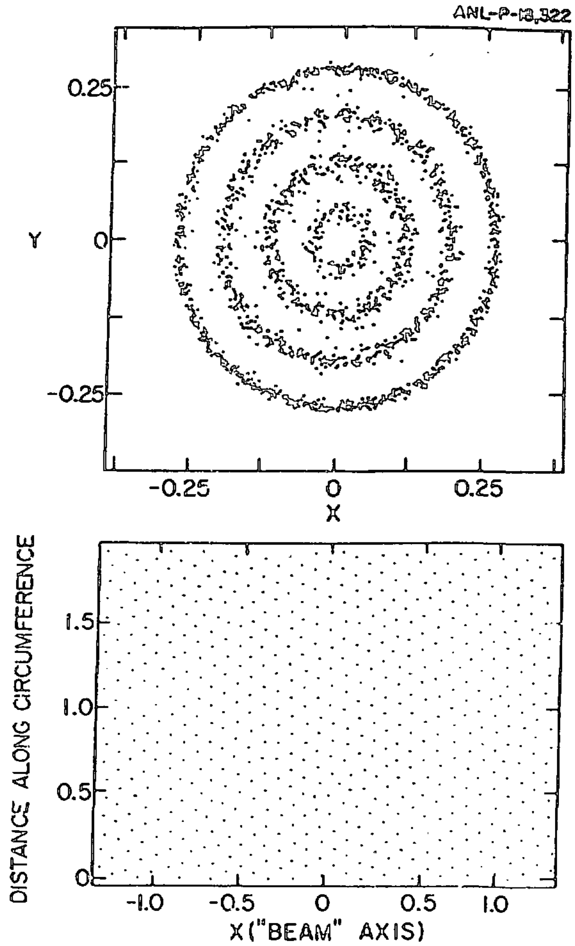

Figure 1 Upper part: Projection of 2000 particles in a molecular dynamics calculation onto the plane perpendicular to the beam (x-axis) for Γ=180. Lower part: distribution of particles in the outer shell with the shell unfolded into a plane. All but the innermost shell show a similar pattern.

quite dramatic, and immediately leads to the conclusion that there must be many more intriguing properties to be analyzed. Here we shall present a few structural properties of this system; dynamical properties will be presented elsewhere. The 3-dimensional pair correlation g(r) in the system as a whole shows a sharp peak at r=0.092 and clear but broader peaks at r=0.17 and 0.245. Since, as seen in Figure 1, a large number of the particles are in the outer shell, the overall pair correlation is distorted by the fact that particles in this shell have no neighbors on the outer side. We have therefore analyzed the 3-dimensional g(r) separately for each shell. Moreover, instead of the standard procedure of presenting g(r) as a function of r, we plot it instead in Figure 2, as a function of the coordination number n(r). It is clear that, except for the outermost shell, the first peak in g(r) has a coordination of 14.

In the lower part of Figure 2 we also show the two-dimensional pair correlation between particles in the same shell. It is clear that for all but the innermost shell, there are six neighbors under a sharp first peak at r=0.092 and 12 more neighbors under the broader second peak. In a projection of particle coordinates, which corresponds to unrolling the cylindrical shells onto a plane, the triangular pattern of particle

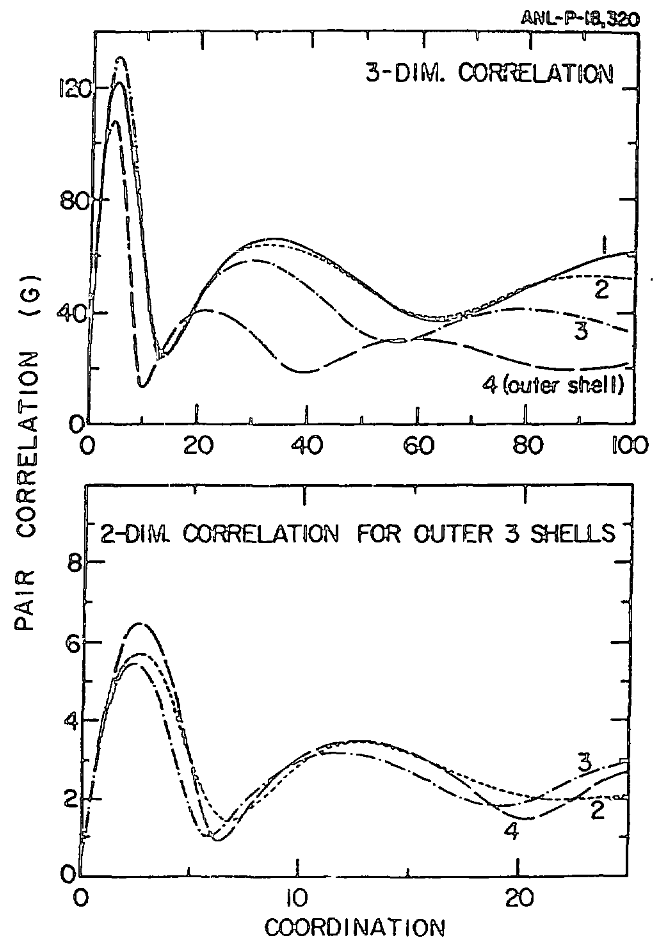

Figure 2 Upper part: Three-dimensional pair correlation function g(r) computed separately with respect to particles within the four shells shown in figure 1. It is plotted against the coordination: the number of particles included up to a given radius. Lower part: The 'two-dimensional' pair correlation function restricted to particles within one shell, for the three outer shells.

positions is clearly seen. The radii of the shells are 0.052, 0.13, 0.20, and 0.28 in the reduced units, and their population 128, 370, 616, and 886. Assuming each of these surfaces to form perfect cylinders (an assumption that becomes less valid as the radius gets smaller) and using constant surface densities for the particles with nearest neighbor distances $a=0.092$ and six first neighbors in a perfect triangular arrangement, one would estimate 177, 443, 682, and 955 particles.

The innermost shell has a simpler structure. There the particles form a helical pattern around the x axis, rotating about 120 degrees about that axis between successive particles. There is a tendency for the sense of rotation to maintain itself for a number of particles; it does not appear to be randomly distributed.

A calculation with only 100 particles (somewhat less than the number in the inner shell) shows a clearly defined single shell of radius 0.04 (somewhat smaller than the .058 for the inner shell seen with 128 particles) and similar ordering. When the number of particles is reduced to 40, the ions get distributed along the axis with only thermal deviations.

For the 2000 particle system the parameter Γ, which plays a central role in determining the properties of a uniform one-component plasma, can be worked out for our system. Using the volume per particle to define a radius r_s for this volume, $\Gamma=1/(r_s T)$. Substituting the data deduced from this case we get $\Gamma=180$.

$N=2000$, $L=4$, $K=5000$, $T=0.411$

In this calculation with higher temperature and less severe confining force, the shell structure in the lateral direction is less well defined; there are two reasonably well defined outer shells with the outer one being at a distance 0.4 from the x axis. The value of Γ for this calculation is ~40 and the presence of a two dimensional triangular arrangement on the surface of the last outer shell is still quite clearly seen. Thus "ordering": the presence of shells and a triangular two-dimensional arrangement of ions within the shells, can occur at rather low values of Γ.

ISOTROPIC CONFINEMENT WITH $N=2000$, $L=4$, $K=10,000$, $T=1/9$

This case was studied in order to ascertain whether the shell structure observed might have been induced by the presence of the periodic boundary conditions that had to be assumed for the cylindrical cases in order to allow the Ewald sums to be evaluated. With the confining potential spherically symmetric ($1/2\ K\ (x^2+y^2+z^2)$) one may remove the boundary conditions and compare the results with and without them. We find very clear spherical shell structure in both cases, with radii at 0.58, 0.48, 0.41, 0.34, 0.27, 0.21. On the outer shell the two-dimensional pair correlations show peaks at $r=0.080$ and 0.151 in both cases, with coordination 6 and 18. Figure 3 shows the shell structure in the case where periodic boundary conditions were not used. The figure caption explains the manner in which the results are presented. Figure 4 is the usual Mercator projection of particle positions on the outermost shell.

The close similarity of the results with and without the periodic boundary conditions leads us to the conclusion that in the isotropic case the boundary conditions are not responsible for the ordering, and thus it seems reasonable to assume that the order seen in the cylindrical case is likewise insensitive to the periodic boundary condition.

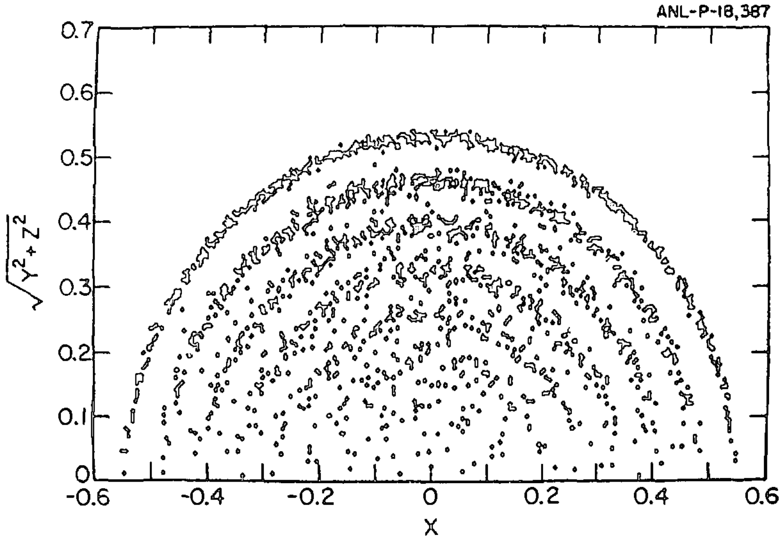

Figure 3 The abscissa is the distance along a line joining two poles of the spherical distribution obtained with 3 dimensional confinement and no periodic boundary conditions. The ordinate is the distance of the particle from this line.

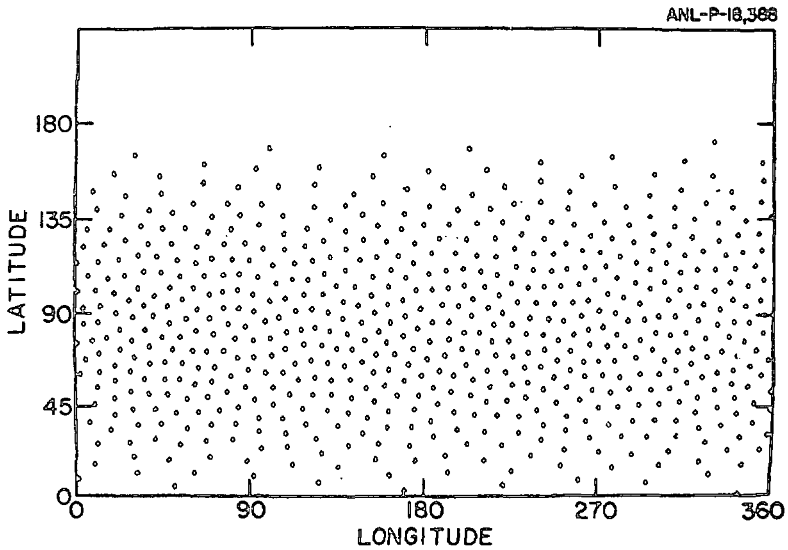

Figure 4 For the calculation mentioned in Figure 3, the Mercator projection is displayed for the positions of particles in the outermost shell.

CONCLUDING REMARKS

The calculations reported here indicate clearly that under the conditions that seem to be within reach of currently planned storage rings ordered structures can occur which are more complex and richer than the liquid-like and Wigner-solid structures that are calculated in uniform one-component plasmas. To what extent the ordering into shells and the consequent triangular ordering within the well defined surfaces will persist when the Hamiltonian is made more realistic than the one used here is now being investigated.

The assumptions made here cannot be satisfied precisely in a real storage ring. First of all, the horizontal focusing must be exerted on particles traveling in circular orbits. It is obvious, that if a beam is cooled such that all particles are travelling at accurately the same linear velocity, the order cannot be sustained if they are to each maintain their velocity and travel in circular orbits of differing radii. In other words, the horizontal focusing force has a shearing component in the direction of travel. The elastic limits againt shear of a condensed array of charged particles may be sufficient to resist slippage of rows of particles within the beam, but these limits will depend on the magnitude of the focusing forces. If slippage does occur, the beam may become heated from the frictional forces.

Another complication is the effect of a restoring force that is periodic in time, and that more nearly approximates the design of the actual focusing elements in storage rings under construction, the so called beta function. The detailed nature of the cooling process will also have to be considered. These aspects of real storage rings will need investigation before one can predict with any reasonable confidence whether this form of order might actually be achievable in currently envisioned facilities.

Finally, a theoretical basis to account for the calculational consequences of the Hamiltonian used here would be a very valuable addition to our understanding of ordering in one-component plasmas.

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