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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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.

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Recently the possibility was considered that within storage rings for highly stripped heavy ions, where cooling techniques are employed, sufficiently low temperatures may be reached that the large Coulomb repulsion between ions may produce an ordered, condensed state within the beam.[1] Storage rings for heavy ions with cooling are under construction at several laboratories (Gesellschaft für Schwerionenforschung in Darmstadt, Max Planck Institut in Heidelberg, and the University of Aarhus). The circulating beam in a storage ring forms a plasma of bare or heavily ionized nuclei, all with the same mass and positive charge, with magnetic (or electric) focusing arranged so as to confine the plasma to a narrow region around the equilibrium orbit in the ring. The cooling of the plasma is to be accomplished either by electron cooling or by the recently 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 high velocity, 10^{10} cm/sec or more. The number of particles stored in the ring may be up to 10^9, and particle densities may be between 10^5 and 10^8 ions/cm^3. Temperatures of relative motion of 1 K have been reported in electron-cooled proton beams.[2]

We have made an attempt to simulate these conditions by computer molecular dynamics[3] which, within the limitations of the Hamiltonian assumed, gives 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 representing the 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 length ξ) in which there are N ions experiencing a restoring force that is proportional to their displacement from the x axis ("beam" direction): $F=K(y^2+z^2)^{1/2}$, with potential energy V (the summation over all periodic boxes being implicit),

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

where x_i, y_i, z_i $(i=1,\ldots,N)$ are the coordinates of the N particles in the box, r_{ij} is the distance between the particles i and j (all in units of ξ), V is the energy in units of Z^2e^2/ξ, and K is in units of Z^2e^2/ξ^3. (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} dyn/cm.) 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 cylinders 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 by the standard Ewald summation method first used in this context by Brush, Sahlin, and Teller,[4] then by Hansen and collaborators[5] in an extensive study of the one-component plasma, and then by Slattery, Dooley, and DeWitt[6] in a particularly detailed study of such systems. In these earlier calculations there was no external restoring force and a bcc solid was observed at low temperatures.

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, in the same energy units as V, at which the system is maintained by standard methods of molecular dynamics.[3]

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. This idealized restoring force corresponds to the assumptions in the present calculations, with the circular motion neglected.[1]

$N=2000$, $L=4$, $K=10\,000$, $T=\frac{1}{9}$.—Under these conditions the diameter of the pencil of plasma is found to be less than 0.6ξ. 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} dyn/cm for the two temperatures. The number density $\sim\xi^{-3}$ 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 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 three-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 Fig. 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 three-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 Fig. 2 as a function of the coordination number $n(r)$, the average number of ions within a distance r from any ion in the shell. 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 Fig. 2 we also show the two-dimensional pair correlation between particles in the same shell. It is clear that in the three outer shells, 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 positions is clearly seen in the lower part of the Fig. 1. 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.

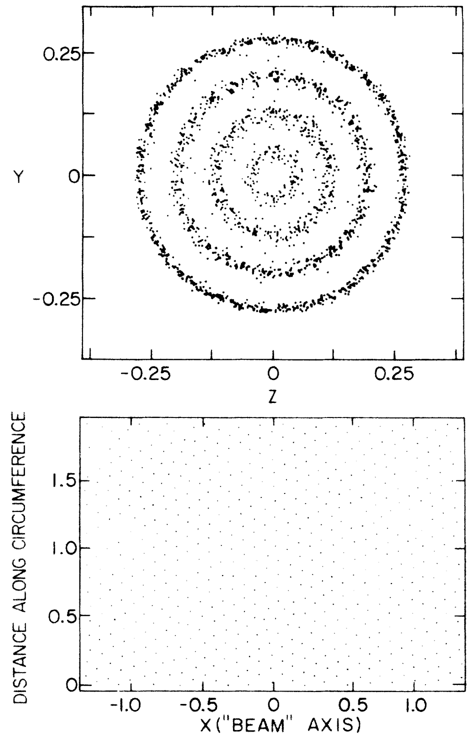

FIG. 1. Upper part: Projection of 2000 particles in a molecular-dynamics calculation onto the plane perpendicular to the beam (x axis) for $\Gamma=180$. Lower part: distribution of particles in the outer shell with the shell unfolded into a plane. All shells but the innermost show a similar pattern.

The innermost shell has a simpler structure. There the particles form a helical pattern around the x axis, rotating about 120° 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 0.048 and similar ordering. When the number of particles is reduced to 40, the ions get distributed along the axis in a straight line with only thermal deviations.

For the 2000-particle system the parameter Γ, which plays a central role in determining the properties of a

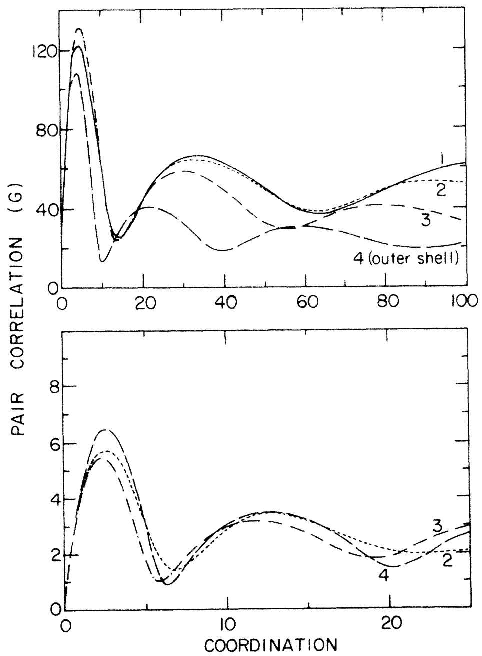

FIG. 2. Upper part: Three-dimensional pair correlation function $g(r)$ computed separately with respect to particles within the four shells shown in Fig. 1. It is plotted against the coordination, the number of particles included up to a given radius. Lower part: The "two-dimensional" pair correlation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

uniform one-component plasma, can be worked out for our system. With use of 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, T=0.411, K=5000.—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, $T=\frac{1}{9}$.—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 $[\frac{1}{2}K(x^2+y^2+z^2)]$ 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.

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.

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 liquidlike 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. The particles are cooled and travel at accurately the same linear velocity. The order cannot be sustained if the particles are to maintain their velocity and travel in circular orbits of differing radii. In other words, in the plane of the ring there is a shearing force in the direction of travel. The elastic limits against 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 most storage rings. 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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