A CONDENSED STATE IN A SYSTEM OF STORED AND COOLED IONS

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1. INTRODUCTION

In heavy-ion storage rings a beam of particles with uniform mass and (positive) charge, is confined to a narrow region around an equilibrium orbit. The internal temperature in the co-moving reference frame for such beams (travelling with a velocity that is at least a few percent of the velocity of light) may be lowered by stochastic or electron cooling to very low values: 1°K has been reported for proton beams. If such conditions are indeed realized in heavy-ion beams, new types of condensation phenomena should appear [1,2]. For laser cooling techniques [3] even lower temperatures are anticipated. We here present a progress report on studies of computer simulations of such systems using the method of Molecular Dynamics.

If beams of highly charged particles can reach internal temperatures similar to the ones already reported they have to be ordered; when the electrostatic potential energy corresponding to random order is greater

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than the temperature contained in the average kinetic energy, disorder and temperature become synonymous. In accelerator physics it is often said that the limiting factor in getting high beam quality (low internal temperature) is 'intra-beam scattering', which arises from the Coulomb interaction between beam particles. However, it is these very same Coulomb interactions that force particles into an ordered state at low temperatures.

In the Molecular Dynamics calculations [4] the classical Newtonian dynamics of the interacting particles is studied with the external constraints represented by a model Hamiltonian that approximates some of the principal features of the storage ring. First results of such calculations showing pronounced shell structures were reported before [2]; we review this earlier work and go on to present more recent results incorporating some of the principal complicating features of storage rings in the model Hamiltonian. The calculations with a confining focusing field in that contain a beam, indicate significant differences from the pioneering calculations of infinite one component plasmas [5].

The principal issue to investigate is the extent to which the design of a storage ring can prevent the large kinetic energies in a stored beam from coupling into heating the particles, in other words how successfully the beam may be cooled.

2. 'STATIC' CALCULATIONS

2.1 Cylindrical Geometry for Storage Rings

The first calculations were carried out with boundary conditions designed to approximate the time-average of the constraints in a storage ring. With the coordinate frame chosen to be travelling along with the

beam velocity one may assume a constant (time-averaged) cylindrically symmetric focusing force, $F = -Kr$, where $r = (y^2 + z^2)^{1/2}$ is the radial displacement from the 'beam' (x) axis, and K is a constant. The potential energy is then given by $V = \sum_i \sum_{j>i} \left[\frac{q^2}{r_{ij}} + \frac{1}{2} K(y_i^2 + z_i^2) \right]$, where q is the charge, x_i, y_i, z_i are the coordinates of the individual particles and r_{ij} is the distance between particles i and j . More details were given in reference 2. The temperature was simply controlled in the calculation separately in x, y and z , by renormalizing the appropriate components of the velocities when the average kinetic energy in a direction differed from the specified value by more than 20%. The calculations were carried out in dimensionless units, with the value of Γ , (proportional to the reciprocal of the temperature) specified: $\Gamma \equiv \frac{q^2/a}{kT}$, where a is the interparticle spacing related to the density by $\frac{4}{3} \pi a^3 \equiv 1/\rho$ and kT is the temperature. Length and time units are dimensionless; their actual value would depend on the values assumed for the charge of the particles and the strength of the focusing force. Calculations were carried out mostly for $\Gamma \approx 180$ and 1800 - the infinite plasma calculations indicate condensation into a bcc solid for $\Gamma \gtrsim 170$. To keep the dimensions of the problem manageable, a finite length of beam was considered. Periodic boundary conditions were imposed, that is the particles at one end were assumed to continue with the particles from the other end. The length of the cell was longer than its cross section by a factor of 2; the largest transverse extent of the particles in equilibrium was about 8 times longer than the length of the cell.

The results of the first calculations were intriguing and have been reported in brief form [2], they are shown in figure 1. Macroscopically, the particles arrange themselves in a cylinder, which is what one would

expect from the cylindrically symmetric restoring force. More surprisingly, however, the internal arrangement is that of concentric cylindrical shells, with the particles within a shell arranged in a hexagonal pattern characteristic of two-dimensional order as is illustrated in the lower part of figure 1. The number of particles in each shell is proportional to its radius and thus the average density is uniform.

2.2 Symmetries and Correlation Functions

The correlation function for particles in a shell, shown in figure 2 on the left, exhibits peak structure with six particles in the first peak and 18 in the second, as expected in two-dimensional order. The correlation including all particles shown in figure 2 on the right however, shows nearest neighbors clustering in a peak with 14 particles, which is the signature of bcc order. Thus the cylindrical shells seem to accommodate the hexagonal pattern characteristic of two dimensional order and yet the combination of shells shows approximate bcc symmetry. These two symmetries are not, strictly speaking, compatible with each other; it seems to be the curvature of the cylinders that permits their approximate coexistence.

2.3 Helicity in the Inner Cylinder

When the calculation starts with a sufficiently small number of particles, the focusing force tends to keep them all on the axis in a straight line, with only thermal excursions taking place. As more particles are added, their repulsion becomes sufficient to bulge away from the axis in a pattern that tends to be helical over short sections, with successive particles positioning themselves about 120° apart around the axis, as is shown in figure 3. A very similar helical pattern is present

in a bcc lattice along the $[111]$ direction. In the Molecular Dynamics calculation the system seems to settle with long regions of the inner tube having the same helicity; the number of changes in helicity seems a sensitive function of the temperature and the prior treatment of a system of particles. The pattern of particles in the central tube is also shown in figure 4; minute disorder causes this triangular arrangement to gradually smear out into the circle that was shown in figure 1.

2.4 Shells as a Function of Particle Number

The influence of the number of particles on the shell structure is shown in figure 5. As particles are added to a system consisting of a single tube, the helical order persists and the radius of the tube expands. Eventually a new row of particles appears on the axis; with yet more particles the outer tube grows further and the inner row again expands into a tube. The helical pattern is more difficult to define in the outer cylinders, though there are some qualitative indications that it does persist. The radii of the shells seem to depend on the number of particles in an approximately linear way as is illustrated in Figure 6, with no apparent large discontinuities. The ordering seems sufficiently flexible to accommodate a continuously increasing number of particles with no major 'quantized' jumps, the possible exception is at the smallest radii where there may be a small deviation from the linear relationship between particle number and radius.

2.5 Spacings between particles and between shells

To first approximation, the spacings between particles are uniform. However, the spacings of particles within the shells is significantly different from the intra-shell particle spacings, which again is different from the spacing of average shell radii. These numbers are shown in Table I.

The outermost shell is appreciably thinner than the inner ones, though the innermost shell again is appreciably sharper than the others. The width of the shells also changes significantly with temperature.

It appears that the outermost shell forms a well defined surface, much as the surface of the ocean is well defined by an equipotential. Given this surface, where particles are packed as tightly as possible, the next shell forms at as close a spacing as is permitted by the interparticle repulsion. It therefore seems reasonable that the inner shells could have larger widths, though the quantitative relationship is not well understood.

2.6 Spherical Geometry

A very few calculations were also carried out with a constraining force that had spherical symmetry: $F = -K(x^2+y^2+z^2)^{1/2}$. These calculations were done to check the generality of the results, and also to eliminate the remote possibility that the periodic boundary conditions could somehow be responsible for the observed patterns; the repeating periodic boundary condition is not required in the spherical case. The results for such a calculation are shown in Figure 7. The particles are now arranged in spherical shells, with the same type of two-dimensional order within each shell as was seen in the cylindrical case, and the overall correlation still showing structure characteristic of bcc order. For 2000 particles there are a larger number of shells and the shells in the inner region are not so well defined. The spherical calculations were carried out for $\Gamma = 180$ only, it is possible that the inner shells would be better defined for a colder system. No spherical calculations have been carried out so far with fewer particles or colder systems.

The spherical geometry may perhaps be regarded as a very rough first approximation to Penning or other forms of ion traps, where values of Γ of about 10 [6] have been reported and the ion cloud appears to be spheroidal in shape. The understanding of the dynamical coupling between the degrees of freedom that arise from the magnetic confinement in two dimensions and electrostatic in two others may benefit from computer simulations by the techniques of Molecular Dynamics.

3. DYNAMICAL EFFECTS IN STORAGE RINGS

There are several effects not included in the static calculations described so far, that may cause problems in coupling the large laboratory kinetic energies of the particles into thermal modes. These are

- (a) the time-dependent nature of the focusing field, and
- (b) the shear associated with circular motion.

To include these in the model Hamiltonian of the Molecular Dynamics calculations one has to relate the dimensionless parameters in the calculation to the parameters of storage rings under construction. The focusing force is related to the ring through the appropriate average beta function (~ 2.5), and from this distance and time scales may be set and the temperature corresponding to a given Γ may be calculated. These are listed in Table II for some typical values. Since the assumption of a given particle charge and ring parameter fixes the distance and time scales, the time-dependent effects from the periodicity in focusing and the effects of the shear associated with the rotation may be assigned numerical values in the calculations.

3.1 Periodic Focusing

The ideal condition of a constant and cylindrically symmetric focusing force may actually be attained in a ring with so-called weak focussing, where the magnetic field strength varies as $1/\sqrt{R}$, R being the radius of the circular orbit. Here the horizontal focusing that is inherent in the bending of a beam in a uniform field, decreases to half the uniform-field value and a restoring force of equal magnitude is present in the vertical (perpendicular to the bend plane) direction. The actual focusing in most storage rings is not of this type but is based primarily on alternating-gradient quadrupole (hexapole) elements yielding an average focusing force about 5-6 times as strong as weak focusing for the same ring radius. The restoring force then becomes periodic in time and alternating in sign, with the vertical and horizontal components out of phase.

We used the Molecular Dynamics method to calculate what oscillations would occur in the beam envelope with periodic focusing, and then to investigate whether this process could couple into heating, the disordered thermal degrees of freedom. The calculations done so far were simplified, in that the force was always assumed to be focusing and turned on and off at time intervals roughly corresponding to the spacing between quadrupole elements in a ring. As a consequence of this, an oscillation was induced in the radius of the beam envelope as is seen in figure 8. However, the period of this oscillation is not that of the imposed frequency, but seems to be related to the plasma frequency of the medium. The temperature of the system was not adjusted during this calculation and the average kinetic energies corresponding to the directions orthogonal to this motion (along the axis and azimuthally) were monitored and are also shown in

figure 8. While these energies do oscillate in time as the radial envelope of the beam oscillates (particles are accelerated as they move closer), the minima and maxima of the kinetic energies do not increase very rapidly and the rate of increase appears to be within the limits that may be controllable.

Since the period of the beam oscillations does not seem to be related to the periodicity of the focusing field, it appears unlikely that the further complications that happen on a shorter time scale (alternating gradients, with the vertical and horizontal forces out of phase) would appreciably alter the results. Such calculations would have to be done in considerably finer time steps and be quite expensive of computer time. The order in the system, as measured by the sharpness of maxima and minima in the correlation functions, was not appreciably altered by the application of periodic focusing.

We conclude, that periodic focusing does not appear to be a serious problem in heating the system of charged particles in a storage ring.

3.2 Shear Associated with Motion in a Circular Path

It is evident that for a beam of particles travelling in a storage ring there is a problem in keeping particles side by side. By a cold beam one means that the particles in the beam are travelling with the same linear velocity, while two particles travelling side by side would require the same angular velocity in order to remain in a fixed relative position. If the particles are separated by a distance Δ in the transverse direction, then after one orbit, the outer one will have fallen behind by an amount $2\pi\Delta$. If, in the moving frame we choose the origin ($z = 0$) to be at the central ray, then particles displaced from this central ray in the bend plane acquire an incremental velocity along the

beam axis (x) that is proportional to their displacement in z (a shearing motion): $\Delta \vec{v} = \vec{\omega} \times \vec{z}$, where $\vec{\omega}$ is the angular velocity.

The question then is whether the repulsive forces between the particles condensed in the fashion observed in the static calculations have a sufficiently stiff elastic constant to resist the imposed shearing motion, or whether they will slip, disrupt the order, and cause the system to heat. Calculations were carried out with two systems of particles in order to investigate the effect of such shear. In one, there were sufficient particles (2000) to form four cylinders (as in figure 1), in the other the number of particles was reduced (to 150) until there was only one tube remaining. The shear velocity increment was added and subtracted to the motion of each particle depending on its z -coordinate (corresponding to alternating bending and straight sections) with the focusing force kept constant in time. The shear displacement of the system was monitored both during the 'bending regions' and the 'straight sections'.

The behavior of the larger system is shown in figure 9, where the bending regions correspond to ~ 22 degree turns (assuming that the focusing strength of the ring, which determines the time scale, is similar to that of the rings under construction) followed by long straight sections. The mean kinetic energies of the particles in the orthogonal directions, radial (z) and perpendicular to the bend plane (y). While the system does slip under the imposed shear, it then seems to recover the displacement in the straight sections. However, the time constant associated with this recovery is rather slow and adequate recovery would require much more time than is available in straight sections around an actual ring. The heating of the system is appreciable, reaching temperatures almost three times the

initial ($\Gamma = 1800$, in this case) value, for a 90° turn; the temperature is brought down by a short period of cooling before the next bend.

In contrast, the smaller system resists slippage and has a much faster recovery time. The corresponding results are shown in figure 10 and indicate that even after a 90 degree turn the system recovers rapidly. The heating is much smaller and much more likely to be controllable.

3.3 Conclusion on Dynamical Effects

The results of calculations so far are encouraging, in that it may be reasonable for a cold beam to continue in an ordered state once it has reached it. How such a state may be reached from a disordered hot beam has not yet been addressed by calculations, and is beyond the presently envisioned study.

One may conclude that the effects of rotation for the focusing strength used here may be tolerable for modest beams but cause difficulty as the number of particles increases. Of course, one will have to combine the effects of periodic focusing with the rotation and follow the detailed parameters of particular rings. Were it is possible to produce a waist while the particles are in a bending region the shear would, of course, be reduced; the smaller the extent of the beam in the bend direction the better.

Although the problems are by no means trivial, no obvious insurmountable difficulties have been encountered in these model calculations. The dynamics of the cooling process for electron cooling and laser cooling need to be investigated. The equilibration time in temperature between the three dimensions seems to be sufficiently fast (comparable to the period of the ring) that the directional nature of cooling may not be a serious problem.

4. ONE DIMENSIONAL SYSTEM

The systems in which the above dynamical problems are almost certainly minimized are ones with sufficiently few particles that their Coulomb interactions will not cause them to be displaced from the central axis. If the particles are cold, they will not have sufficient transverse temperature to get past each other and will be effectively confined to one dimension. In a one-dimensional system there are no phase transitions, the regularity of spacings increases gradually. The thermodynamic properties of a classical one-dimensional Coulomb gas were investigated by Dyson [7] in the context of the repulsion in level spacings between compound nucleus resonances. His parameter β is the same as Γ defined above, and he investigated the properties of systems with $\beta = 1, 2$ and 4 (orthogonal, symplectic, and unitary ensembles) in some detail, but also in the more general case.

5. EXPERIMENTAL EVIDENCE

The only piece of experimental information that may be relevant to the present consideration is that obtained in Novosibirsk [8] with a cooled proton beam. Here it was deduced that the particles reached an internal temperature at least as low as 1°K . In looking at noise as a function of proton current with a normal and a cooled beam, an interesting difference was observed: the normal beam shows a smooth increase in noise with increasing beam current, while the cooled beam shows no detectable noise until a threshold value of about 10-20 microamperes, as is shown in figure 11. A rough estimate suggests that this is approximately the beam current at which the particles would no longer fit into a single shell and

it is conceivable that this noise threshold is associated with conditions where the internal structure with finite width can no longer withstand the shear produced in the rotating system.

6. POSSIBLE METHODS OF DETECTION

The most obvious detection techniques are ones that are almost inherent in the diagnostic systems of storage rings. Pickup signals, such as the ones studied in the Novosibirsk work [8] and the absence of noise would be the first sign of condensation. More subtle effects may also appear, such as a change in the velocity of signal propagation along the beam. New modes (e.g. torsional waves) may become possible in a condensed beam, and compressional waves would travel with different characteristics. To explore the detailed nature of the order, however, diffraction studies are likely to be needed -- Bragg scattering with infrared lasers seems the most promising technique -- though this technique is likely to be useful only for partially ionized particle beams.

7. CONCLUSION

The calculations carried out so far are encouraging in continuing to suggest that an ordered beam may be achievable in planned heavy-ion storage rings, where the highly charged ions will produce larger values of Γ for a given temperature and thus conditions would be more favorable for ordering. More powerful cooling techniques, such as that of laser cooling applicable to partially ionized beams, may produce lower temperatures more rapidly. It may well be that the parameters of storage rings will have to be adjusted to favor an ordered state, it may even turn out that new designs (stronger focusing) for storage rings may be necessary to attain

order in larger beams. If such order is achieved, this will have profound effects on the beam optics in a ring, since new collective oscillations (e.g. torsional modes) will appear. Thus present understanding of beam properties and wave propagation along beams is likely to need reexamination. An ordered and condensed beam would also have important implications for many studies to be carried out at these storage rings in nuclear or atomic physics.

More generally though, attainment of an ordered system of the type discussed here would represent a new condensed state, many orders of magnitude less dense than the ones with which we are familiar. The simultaneous approximate accommodation of two-dimensional and bcc order, that appears under the cylindrical and spherical boundary conditions, needs to be understood more fully.

Quantum mechanical effects have not been investigated; the system considered here would be classical, with the wavelength of particles small compared to their spacings. Only if cooling techniques into the mK regime become eventually feasible, are quantum effects likely to be significant. The study of the properties of a new form of condensed matter could be of considerable interest in its own right.

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Table I
 Spacings with Four Cylindrical Shells ($\Gamma = \sim 1800$)
 (dimensionless units)

Radius and rms widths of shells	.276	.0022
	.198	.0056
	.121	.0103
	.048	.0052
mean spacing between shells	.076	

Spacings between nearest neighbors		
and rms fluctuations for all particles	.100 $\pm$.010	
for particles within		
one shell	.097 $\pm$.007	
for particles in		
different shells	.103 $\pm$.012	

TABLE II

Parameters for Various Particles Typical of Planned
Storage Rings for $\Gamma = 180$

Particle	Energy (MeV/u)	Temperature (°K)	Inter-particle Spacing (μ)	Institute
$^{238}\text{U}^{92+}$	500	45	32	GSI
$^{58}\text{Ni}^{26+}$	8	2.5	44	Heidelberg
$^7\text{Li}^+$	.03	.003	66	Aarhus
$^9\text{Be}^{3+}$	1	.1	20	"
p	50	1 ($\Gamma = \sim 4$)	8	Novosibirsk

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Figure Captions

- Figure 1) The upper part of the figure shows the results of a Molecular Dynamics calculation with 2000 particles in the cell, $\Gamma = 180$. The particle coordinates are projected onto the plane perpendicular to the beam (x) axis. The lower part of the figure shows the distribution of particles in the outermost shell on the surface of the shell.
- Figure 2) The upper parts of the figure show the correlation function $g(r)$ for particles in one shell (on the left) and for all particles in the cell on the right. The lower part of the figure shows the number of neighbors (coordination) as a function of distance, with the numbers corresponding to two dimensional ordering (left) and bcc order (right) indicated by dashed horizontal lines.
- Figure 3) The behavior of particles in the innermost tube. The top part of the figure shows the azimuthal angle between successive particles along the beam axis; the points are the angles in three dimensions. The middle curve shows the average azimuthal angle for cases with different numbers of particles in the inner tube. It appears to take more than 60 particles to form a clearly discernible cylinder. The bottom curve shows the ratio of the average distance between successive particles ordered in x, $\langle r_{12} \rangle$, to that between every fourth particle $\langle r_{14} \rangle$; the ratio would be 1.0 for a bcc section along the [111] direction.

Figure 4) A projection of particles from a segment (1/4) of a 2000 particle calculation (with $\Gamma = 1800$) onto the plane perpendicular to the axis. The triangular pattern in the inner tube is clearly discernible and there seems to be a corresponding slight distortion in the next shell. In the full set of particles these distortions are severed and into a circular pattern.

Figure 5) Projection of calculations with 40, 150, 300, and 600 particles in the unit cell onto the plane perpendicular to the axis. Γ was 180 for all but the 150 particle calculation where it was 1800.

Figure 6) Mean radius of cylindrical shells as a function of number of particles in the shell. Data from calculations with various total number of particles are combined. The line is a best fit passing through the origin. The bottom curve shows the percent deviation from the linear fit.

Figure 7) Results of a Molecular Dynamics calculation with an isotropic restoring force; $\Gamma = 180$. The top curve shows all the particles projected on a half circle; the bottom is a Merkator projection of the outermost shell.

Figure 8) Molecular Dynamics calculation with the constraining force turned on and off for equal periods of time. The top curve shows the mean radius of the particles as a function of time. The dashed curve indicates the time when the focusing force is on. The bottom curve shows the mean temperature components in the directions perpendicular to the constraining force: along the axis, and in the azimuthal direction. The initial value of Γ was 1800; the kinetic energies are in units of the initial temperature. No 'cooling' adjustment to the temperature was applied during this series of calculations.

Figure 9) Shear velocity from a Molecular Dynamics calculation for 2000 particles in the cell, with a shear imposed periodically, corresponding to bending the beam through 90° in four ($\sim 22^\circ$) segments. Each segment is followed by a relaxation period and then cooling is applied. The temperature control is set for $\Gamma = 1800$. The lower part of the figure shows the components of temperature in the directions perpendicular to the shear; the units of temperature are in units corresponding to the initial temperature.

Figure 10) Shear velocity from a Molecular Dynamics calculation for 150 particles in the cell, with a shear imposed corresponding to bending the beam through 90° in one step. No 'cooling' adjustment to the temperature was applied; the initial temperature corresponds to $\Gamma = 1800$. The lower part of the figure shows the components of temperature in the direction of shear and perpendicular to it in units of the initial temperature.

Figure 11) Measured noise power as a function of proton current (or number of particles in the ring) from the Novosibirsk measurement [8]. The top part of the figure is for an uncooled beam; the bottom for one that was subjected to electron cooling and whose temperature was estimated at 1°K ($\Gamma = \sim 4$). Based on Molecular Dynamics calculations one would estimate that the beam would probably be one dimensional below $\sim 5 \mu\text{A}$ and that it may condense into a single shell (if sufficiently cold) between roughly 10 and 20 μA .

FIG. 1

FIG. 2

FIG. 3

FIG. 4

FIG. 5

FIG. 6

FIG. 7

FIG. 8

90 DEGREE TURN IN 4 SEGMENTS WITH COOLING

FIG. 9

90 DEGREE ROTATION, NO COOLING

FIG. 10

FIG. 11

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