# NUMERICAL SIMULATIONS OF A CRYSTALLIZED NON-NEUTRAL PLASMA

Jinhyung Lee* and John R. Cary†
CIPS‡ and Department of Physics, University of Colorado, Boulder, CO

*Abstract*

Crystalline non-neutral plasmas and beams have both been observed, though the crystalline beams show regularity in only one dimension. Our research is oriented towards understanding the phase transitions that occur with non free-particle dynamics, as is the case in particle beams. To this end we have studied phase transitions in strongly magnetized, non-neutral plasma through molecular dynamics. Our preliminary results show that in the Coulomb system the transition occurs at a certain value of the plasma parameter, and that in the limit of small gyroradius the transition may also occur at the same value of the parameter provided the plasma parameter is calculated using the parallel temperature.

## 1 INTRODUCTION

The concept of crystalline non-neutral plasma, regarded as a new state of matter, has been studied for a variety of fundamental and applied physics areas, including the study of space-charge-dominated beams, the study of Coulomb crystal, the realization of high luminosity ion colliders, the application to ultrahigh resolution nuclear experiments and to the atomic physics research, etc. In recent years, many theoretical and experimental works on the Coulomb crystal where the particle density and the strength and range of effective pair potential can be varied continuously over large ranges has elicited interest in the new classical state. A lot of static and dynamic phenomena, such as melting transition from the crystalline phase to fluid under certain applied conditions have been observed.[1][2].

In high energy physics, Penning traps and antiparticle storage rings have been used for experimental tests of the $CPT$ theorem, which predicts equivalence of various physical parameters such as masses, charge-to-mass ratio, magnetic moments, and gyromagnetic ratio for particle and antiparticle. Charged particles can be confined perfectly in an ideal cylindrically symmetric trap with a uniform axial magnetic field, which is the basic setup of the Penning trap. This approach, the use of Penning trap, has been favored and widely used because the particle can be cooled down to a temperature of order 1 K[3]. The other approach, the use of antiparticle storage rings, has more problems than the first approach. In this trap the idea of producing beams of antiparticle atoms is closely related to the technique of electron cooling. However, owing to the difficulties in performing experiments involving atoms of relativistic velocities, there has been little achievement of the cooling[4].

* Email: jinhyung@colorado.edu
† Email: cary@colorado.edu
‡ Center for Integrated Plasma studies

Despite the considerable success in Coulomb crystallization and the large amount of work in beam crystallization, there has not been a successful experiment that reaches the beam crystalline state. It was demonstrated theoretically that the crystallization can be achievable in a properly designed storage ring with a sufficiently strong 3D cooling force[5]. In experiments, laser cooling, which is supposed to be one of the most promising method to obtain the crystalline beam has been employed to achieve a longitudinal beam temperature in the mK range. However, since intrabeam heat exchanging rate between the longitudinal and transverse directions is too slow, still the transverse temperature is too high, while theoretically the transverse temperature can be in the range of 0.01 K or less which is far below what has been achieved in the current experiments. In theoretical studies, one of the first approaches to understand the nature of beam crystal was molecular dynamics simulations(MD simulations). The simulations has been used to find the phase transition of non-neutral plasma. Hamaguchi and coworkers have found this kind of transition in Yukawa system with the simulations[6]. As seen in many Penning trap experiments, the non-neutral plasma has three different phases-bcc, fcc, and fluid. However, the theoretical studies of the phase transition for a magnetized non-neutral plasma are quite open so far, although many experimental results have shown those kinds of transitions. Especially when the gyroradius is very small compared to interparticle distance, the system gives a possible intuition of beam crystallization because longitudinal and transverse temperatures are different before the plasma equilibriates.

From these various reasons, we already concluded that analysis of non-neutral plasma in Penning trap would allow study of beam crystallization and found the ideal equilibria of non-neutral plasma in a modified Penning trap with a center conductor that is electrically biased. By changing the radial potential difference slowly, all physical parameters including temperature can be controlled and the plasma profile is wider and colder as the potential difference is smaller[7]. Therefore, in the range of 1 eV or less the system can be considered as an idealized model comprising of sufficiently large number of identical piece where the particles interact through Coulomb potential with a uniform magnetic field, so that the thermodynamics of a piece with a periodic boundary condition may be the same as that of the entire plasma.

In addition, in order to understand the nature of the crystalline phase, we have developed a code of molecular dynamics. In the following section, we briefly explain how to get the physical properties from the simulations. In the next section, results of unmagnetized and magnetized systems are shown and the phase transition from fluid phase to bcc is observed in the unmagnetized Coulomb system.

## 2 MD SIMULATIONS

The thermodynamics of the non-neutral plasma can be described in terms of some dimensionless physical parameters. One of the parameters, namely the Coulomb coupling parameter, is

$$\Gamma = \frac{Q^2}{ak_BT} \tag{1}$$

where $Q$ is the total charge of a particle, and $k_BT$ is thermal energy, and $a$ is the Wigner-Seitz radius ($a \equiv (3/4\pi n)^{1/3}$). When $\Gamma$, roughly the ratio of the Coulomb potential energy to the thermal energy per particle, exceeds a certain threshold ($\Gamma_c \approx 170$), the highly ordered state can be formed in the non-neutral plasma.

With the Wigner-Seitz radius and the inverse of the plasma frequency ($\omega_p \equiv \sqrt{4\pi nQ^2/m}$) as units of length and time, the dimensionless equations of motion in MD simulations are

$$\frac{d^2\vec{\xi_k}(\tau)}{d\tau^2} = -\sum_{j\neq k}^{N} \vec{F}_k(\vec{\xi_k} - \vec{\xi_j}) \tag{2}$$

where $\tau = \omega_p t$ is the dimensionless time, $\vec{\xi_k} = \vec{r}_k/a$ is the dimensionless location of $k$-$th$ particle, and $\vec{F}$ is the dimensionless force which is determined from the dimensionless potential $\hat{\Phi} = a\Phi/Q^2$ and the dimensionless magnetic field. For the one component plasma (OCP), the dimensionless OCP potential

$$\begin{aligned}\hat{\Phi}(\vec{\xi}) &= \sum_{\vec{n}} \frac{erfc(\sqrt{\pi}|\vec{\xi}+\vec{n}\Lambda|/\Lambda)}{|\vec{\xi}+\vec{n}\Lambda|} \\ &+ \sum_{\vec{n}\neq 0} \frac{exp(-\pi|\vec{n}|^2)cos(2\pi\vec{n}\cdot\vec{\xi}/\Lambda)}{\pi|\vec{n}|^2\Lambda} \end{aligned} \tag{3}$$

which is the well-known Ewald potential for the OCP[8], is the effective pair potential describing the interaction of any two particles ($\vec{\xi} = \vec{\xi_k} - \vec{\xi_j}$) with all periodic images of the latter ($\Lambda \equiv (4\pi N/3)^{1/3}$). This cubically-symmetric potential can be approximated by a tensor-product cubic spline function interpolating an array of 3D discrete values[9]. The function interpolating an array of $40 \times 40 \times 40$ values has a fractional deviation from the exact value of no more than $10^{-6}$.

In MD simulations with appropriate equations of motion of the system and a given initial state ($bcc\ or\ fluid$), all the thermodynamic quantities are determined as time averages of the physical quantities including internal energy for a canonical ensemble after a typical relaxation time. Taking possible initial states, such as bcc or fluid with their initial velocities of particles, the energies can be calculated, and then the phase transition can be found from a sudden change in the internal energy.

### 2.1 Coulomb System Immersed in a Heat Bath

A Coulomb system immersed in a heat bath finally equilibriates with the bath, so that the temperature of the system is identical to the bath. Therefore, the system can be described by a dissipative system with a fluctuation. The dissipative force continues to take the energy out of the system before the system equilibriates to a stable state due to the equalization between the dissipation and the fluctuation.

The recursive forms of equations for $k$-$th$ particle are

$$\vec{\xi}_k^{(n+1)} - \vec{\xi}_k^{(n)} = d\tau\, \vec{V}_k^{(n)} \tag{4}$$

$$\begin{aligned}\vec{V}_k^{(n+1)} - \vec{V}_k^{(n)} &= -d\tau \sum_{j\neq k} \nabla\hat{\Phi}(\vec{\xi}_k^{(n)} - \vec{\xi}_j^{(n)}) \\ &\quad -d\tau\,\nu\,\vec{V}_k^{(n)} + \vec{\delta}_k^{(n)}\sqrt{dt}\end{aligned} \tag{5}$$

where $\nu$ is the dissipative coefficient and $\vec{\delta}_k$ is the fluctuation. From the equations we get the coupling parameter of the equilibrium state,

$$\Gamma \approx \frac{6\nu}{\langle \sum\limits_k |\vec{\delta}_k|^2\rangle} \tag{6}$$

with a small $\nu$ and a constraint, $\langle \sum\limits_k |\vec{\delta}_k|^2\rangle = const.$

### 2.2 Strongly Magnetized System

For an isolated system with a strong magnetic field ($\vec{B} = B\hat{z}$), the gyromotion is clearly so fast compared to bounce and drift motion that the adiabatic invariance of the magnetic moment effectively reduces the system from the actual motion to a very good approximation, guiding center approximation. In this case the guiding center position, $X$ and $Y$ are conjugate to each other, so that the system can be described by two pairs of conjugate variables. The equations of motion are

$$\frac{d^2\xi_z}{d\tau^2} = -\frac{\partial\hat{\Phi}}{\partial\xi_z} \tag{7}$$

$$\frac{d\xi_X}{d\tau} = -\frac{\omega_p}{\sqrt{3}\Omega}\frac{\partial\hat{\Phi}}{\partial\xi_Y} \tag{8}$$

$$\frac{d\xi_Y}{d\tau} = \frac{\omega_p}{\sqrt{3}\Omega}\frac{\partial\hat{\Phi}}{\partial\xi_X} \tag{9}$$

where the longitudinal motion is much faster in the strongly magnetized system than the transverse motion because of the small coefficient, $\omega_p/\Omega$.

## 3 RESULTS

### 3.1 Coulomb System Immersed in a Heat Bath

With a random initial state and an appropriate $\langle\sum|\vec{\delta}_k|^2\rangle$ for desired $\Gamma$ which is larger than $\Gamma_c$, we got the phase transition from fluid to solid from fluid to solid ($bcc\ state$).

For a sufficiently large coupling ($\Gamma > \Gamma_c$), the system equilibriates to a meta-stable random state and then the state is changed to a bcc after a typical time.

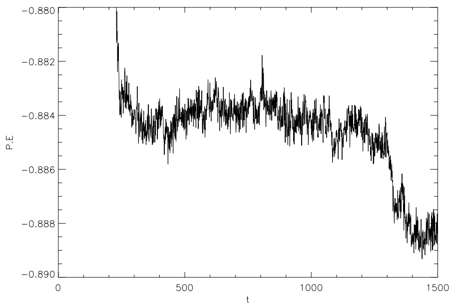


Figure 1: The potential is suddenly changed at $\tau \approx 1350$.

In Fig. 1, a sudden change in the potential of a particle is seen at $\tau \approx 1350$. At this time, the transition from fluid to bcc can be found. Fig. 2 shows that the random state is changed to a bcc state after $\tau \approx 1350$.

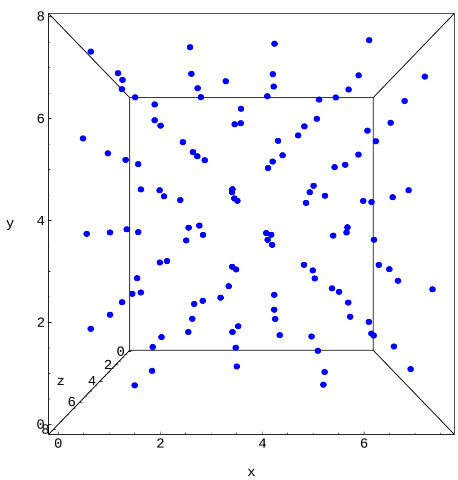


Figure 2: The state is changed to a $bcc$ after 1500 time unit.

For a small coupling ($\Gamma < \Gamma_c$), the system equilibriates to the same kind of random state with the initial state and the transition is not observed after the equilibration.

### *3.2 Strongly Magnetized System*

By taking various temperature with bcc states as their initial states, we calculated a lot of internal energies for the various temperature. In most of the cases, the systems keep their initial state during the entire simulation, even though the particles have their own oscillations due to the exchanges between kinetic and potential energies. With the internal energies for the various temperature[6], we got a reasonable result that the two systems ($magnetized\ and\ unmagnetized\ systems$) are nearly the same thermodynamically in the range of low temperatures ($high\ \Gamma$) as seen in Fig. 3.

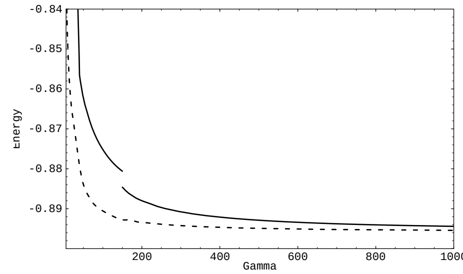


Figure 3: The internal energy of a particle, $u/\Gamma\ vs\ \Gamma$. Solid line-Unmagnetized plasma ($Hamaguchi's\ data$), Dashed line-Magnetized plasma ($Our\ data$).

In the range of low temperatures, the motion of particles in both systems are very limited in range and slow. As a result, the potential energies are dominant in both system. Therefore, the thermodynamics are nearly the same to each other.

## 4 DISCUSSION

MD simulations can be applied both to an unmagnetized and a magnetized one component plasma. In the case of the unmagnetized one component plasma, the phase transition from fluid to bcc is found when the random initial state is immersed in a sufficiently cool background. In the limit where the gyroradius is small compared with the mean interparticle distance in a strongly magnetized system, the transfer rate between $E_{||}$ and $E_{\perp}$ is very small, so that the two temperatures are nearly independent to each other ($\Gamma_{||} \neq \Gamma_{\perp}$) before a typical relaxation time. For this reason, guiding center approximation is valid and plasma crystal could be found irrespective of $T_{\perp}$ with $T_{||}$ decreased as much as desired before the time. In this case, the result is nearly the same to the unmagnetized one at low temperature where the initial state is taken as a bcc state. In addition, the phase transition for a strongly magnetized plasma is expected with a random initial state immersed in a sufficiently cool background.

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