

Crystalline Beam Ground State*

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Abstract

In order to employ Molecular Dynamics method, commonly used in condensed matter physics, we have derived the equations of motion for a beam of charged particles in the rotating rest frame of the reference particle. We include in the formalism that the particles are confined by the guiding and focusing magnetic fields, and that they are confined in a conducting vacuum pipe while interacting with each other via a Coulomb force. Numerical simulations have been performed to obtain the equilibrium structure. The effects of the shearing force, centrifugal force, and azimuthal variation of the focusing strength are investigated. It is found that a constant gradient storage ring can not give a crystalline beam, but that an alternating-gradient (AG) structure can. In such a machine the ground state is, except for one-dimensional (1-D) crystals, time-dependent. The ground state is a zero entropy state, despite the time-dependent, periodic variation of the focusing force. The nature of the ground state, similar to that found by Rahman and Schiffer[1], depends upon the density and the relative focusing strengths in the transverse directions. At low density, the crystal is 1-D. As the density increases, it transforms into various kinds of 2-D and 3-D crystals. If the energy of the beam is higher than the transition energy of the machine, the crystalline structure can not be formed for lack of radial focusing.

I. INTRODUCTION

The ground states of crystalline beams were first studied, in seminal work, by J. Schiffer[1] and his colleagues. Their work assumed a storage ring model in which particles are subject to time-independent harmonic forces in both transverse directions. Subsequently, they studied the crystallization in a time-dependent, AG focusing potential.[2]

In order to employ Molecular Dynamics method for quantitative studies, we first derive in section 2 the equations of motion for the particles in the rotating rest frame of the reference particle. Qualitative studies pertaining to the crystallization in the weak and AG focusing rings are presented in section 3. Section 4 describes the molecular dynamics calculation and the numerical results.

II. ROTATING BEAM FRAME HAMILTONIAN

The motion of the particles under Coulomb interaction

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and external electromagnetic (EM) forces can be most conveniently described in the rotating rest frame (x, y, z, τ) of the reference particle of which the orientation of the axes are constantly aligned to the radial (x), tangential (z) and vertical (y) direction of the motion, and τ is the proper time. The equations of motion are derived using the general relativity formalism. First, we express the equations of motion in a general tensor formalism applicable to any arbitrary coordinate system. The Lorentz force experienced by the particle is constructed as a product of the EM field tensor and the four-velocity. Starting from the laboratory frame, the EM field tensor is written by means of the components of the EM fields. Then, tensor algebra is used to transform this field tensor into the rest frame. With a similar transformation, the metric tensor of the rest frame is also obtained. The equations of motion and the Hamiltonian can thus be constructed in the rest frame.

Consider the case that the beam is guided by a bending field B_0 , and focused by a quadrupole field of gradient B_1

$$B_x = B_1 y, \quad B_y = B_0 + B_1 x, \quad B_z = 0, \quad (1)$$

where the magnet end effect is neglected. Assume that there exists no electric field so that the beam is not focused azimuthally. The magnitude of B_0 is determined by the velocity βc and the bending radius R of the reference particle $eB_0 R = m_0 c^2 \beta \gamma$. Let $n = -B_1 R/B_0$ represent the strength of the focusing field. The Hamiltonian $H(x, P_x, y, P_y, z, P_z; t)$ of the particle system is derived as

$$H = \frac{1}{2} (P_x^2 + P_y^2 + P_z^2) - \gamma x P_z + \frac{1}{2} [(1-n)x^2 + ny^2] + V_C, \quad (2)$$

where V_C is the Coulomb potential, the time t is in unit of $R/\beta \gamma c$, the space coordinates x, y, z are in unit of ξ ($\xi \equiv (r_0 R^2/\beta^2 \gamma^2)^{1/3}$ with $r_0 = e^2/m_0 c^2$), and the energy is in unit of $\beta^2 \gamma^2 e^2/\xi$. Here, ξ is a characterization of the inter-particle distance in the presence of Coulomb interaction. The equations of motion are given by the Hamilton's equations.

III. CONDITIONS FOR CRYSTALLIZATION

In a weak-focusing machine, the constant n provides pure focusing (and defocusing) in the vertical (and radial) direction. Typically, radial (or horizontal) focusing emerges from the difference in the centrifugal forces experienced by the particles of different radial displacements. Among particles of the same energy, the difference in the centrifugal force always focuses the particles towards the reference orbit. The effective radial focusing is $1 - n$, and [†]us if $0 < n < 1$, there is focusing in both planes.

The situation becomes different when the beam is crystallized. In the ground state, particles circulate around with the same angular velocity. Contrary to the conventional case, the centrifugal force provides a defocusing force. Using the equations in the rest frame, it has been proven in general that crystalline beam can not exist in any dimension in a weak-focusing machine.

In the case of AG focusing, however, the amount of magnetic net focusing can easily prevail over the centrifugal defocusing caused by crystallization. Qualitatively, the conditions of crystallization can be estimated using the smooth approximations. Consider a ring consisting of N_c identical lattice cells. In the rest frame, the potential produced by the external magnetic field varies periodically with period $T_c = 2\pi/N_c$ in the reduced unit. The equilibrium state is defined as the one when the motions of all the particles are periodic in T_c . After linearizing the Coulomb force by expanding around the equilibrium orbit (x_j, y_j, z_j) of each particle i , the transverse equations become

$$\begin{aligned} \ddot{x} + \left\{ \nu_x^2 - \gamma^2 - \sum_j \left[\frac{1}{r_{ij}^3} - \frac{3(x_i - x_j)^2}{r_{ij}^5} \right] \right\} x &= \sum_j \frac{x_i - x_j}{r_{ij}^3}, \\ \ddot{y} + \left\{ \nu_y^2 - \sum_j \left[\frac{1}{r_{ij}^3} - \frac{3(y_i - y_j)^2}{r_{ij}^5} \right] \right\} y &= \sum_j \frac{y_i - y_j}{r_{ij}^3}, \end{aligned} \quad (3)$$

where r_{ij} is the distance between i and j , and ν_x and ν_y are the horizontal and vertical tunes in the absence of the Coulomb interaction. Similar to the weak focusing case, the crystal can only exist when the effective transverse focusing is sufficiently strong i.e. $\nu_x^2 > \gamma^2$ and $\nu_y^2 > 0$. Since typically $\nu_x \approx \gamma_T$, it is implied that the AG machine has to operate below the transition energy.

When the particle density is low, the equilibrium state is a 1-D chain where all the particles are aligned along the $x = y = 0$ axis and uniformly distributed in z . As the density increases, it transforms into 2-D. If the net radial focusing is weaker (or stronger) than the vertical one i.e. $\nu_x^2 - \gamma^2 < \nu_y^2$ (or $\nu_x^2 - \gamma^2 > \nu_y^2$), the 2-D structure lies in the horizontal (or vertical) plane. As the density is increased further, the equilibrium state eventually becomes 3-D.

To estimate the threshold density at which the 1-D crystal becomes 2-D, consider a 1-D crystal chain with the nearest-neighbor azimuthal distance Δ_z . The vibrational frequencies $\omega_x(k)$ in x direction can be expressed as

$$\omega_x^2(k) = (\nu_x^2 - \gamma^2) - \frac{2}{\Delta_z^3} \sum_m \frac{1}{m^3} + \frac{2}{\Delta_z^3} \sum_m \frac{\cos(mk)}{m^3}, \quad (4)$$

where k is the crystal momentum. Apparently $\omega_x(k)$ takes its minimum at $k = \pi$, which corresponds to two neighboring particles moving in the opposite direction. The transition from 1-D to 2-D occurs in x direction at the Δ_z value where the smallest $\omega_x(k)$ becomes imaginary. Therefore, in the case that $\nu_x^2 - \gamma^2 < \nu_y^2$, the condition for a stable 1-D crystal is given by the equation

$$\nu_x^2 - \gamma^2 > 4.2/\Delta_z^3. \quad (5)$$

IV. MOLECULAR DYNAMICS RESULTS

When Coulomb interaction and AG focusing are present, it is impossible to solve the Hamiltonian in Eq. 2 analytically. We therefore seek numerical solutions using molecular dynamics. Since the Coulomb interaction is long ranged, an Ewald-type summation has to be performed to calculate the energy and the forces. Rahman and Schiffer[1] used periodic boundary conditions in all three directions in order to utilize the standard Ewald summation method. However, in a realistic accelerator, the system may be considered infinite only in z direction. Also, the infinitely long collection of positively charged particles give a logarithmically diverging energy. In general, a negatively charged background has been added to the system to cancel this infinity. To simulate a real accelerator, we consider instead a bunch of charged particles confined in a perfectly conducting, infinitely long pipe. The periodic boundary condition is used only in the z direction, where the "supercell" of length L (in unit of ξ) repeats itself to infinity. The energy $\phi(\mathbf{x}_i, \mathbf{x}_j)$ due to two particles at $\mathbf{x}_i$ and $\mathbf{x}_j$, after all the image charges and equivalents in other supercells are included, is

$$\begin{aligned} \phi = \frac{1}{r_{ij}} + \frac{4}{L} \int_0^\infty \frac{\cosh(2z_{ij}k/L) J_0(2\rho_{ij}k/L) - 1}{\exp(2k) - 1} dk + \\ + \frac{2}{L} [\log(\pi b/L) + C], \end{aligned} \quad (6)$$

where $z_{ij} = z_i - z_j$, $\rho_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$, $r_{ij} = \sqrt{z_{ij}^2 + \rho_{ij}^2}$, b is the radius of the pipe. The condition $\rho_{ij} \ll b$ is used and z_{ij} is understood to be between $-L/2$ and $L/2$. Apart from the last term which is an unimportant constant, Eq. (6) is the same as the formula given by Avilov[4], but the physical environments are different.

The integration in Eq. (6) is performed by a 15th order Gauss-Laguerre method. The equations of motion is integrated by the 4th order Runge-Kutta algorithm. The storage ring is assumed to consist of 10 identical FODO cells. Within each cell, the lengths of the F, O, D, and O elements are assume to be 15%, 35%, 15%, and 35% of the cell length, respectively. The focusing and defocusing gradients n are set to be 50 and -50 , respectively. This arrangement results in $\nu_x = 2.7$, $\nu_y = 2.3$, and γ_T is about 2.5. γ is set to 1.4. The time step for the integration is $1/20$ of the period T_c of the focusing field.

Notice that the Hamiltonian we are solving is time dependent, therefore the total energy is not a constant of motion, and the "temperature" as conventionally defined is no longer meaningful. Initially, the positions and momenta of the particles are randomly chosen. At the end of each FODO period, a periodic condition is imposed on all positions and momenta. The "drifting velocity" $v_z = [z(T_c) - z(0)]/T_c$ is then subtracted from P_z for each particle to correct "shearing" in the beam. Our experience shows that this is a very effective method to "cool" the system down to reach the ground state.

Here, we report the preliminary results with $L = 10$ and number of particles N in the supercell ranging from 5 to 100. When $N = 5$, the crystal is 1-D, and does not change

with time in spite of the change of the focusing force. When $N = 10$, the crystal is 2-D — a zig-zag chain in the $x - z$ plane. The reason that the crystal is in the $x - z$ plane instead of the $y - z$ plane is because of the relatively stronger vertical focusing. Now the particles move with time — a symmetrical breathing in x direction. The crystal transforms from 1-D to 2-D when N goes from 8 to 9.

With the current lattice and beam energy, the critical density at which the crystal transforms from 2-D to 3-D is approximately twice that from 1-D to 2-D. It is trivial to change the parameters in the simulation as well as in a real accelerator so that these effective focusing strengths are different, and therefore the crystal remains 2-D at a much higher density.

Fig. 1 show the plots for $N = 40$. The crystal is 3-D. Basically the particles form elliptical cylinders. They fall on ellipses when projected onto the $x - y$ plane, and form spirals on the cylinders. At lower densities (e.g. $N = 40$), one cylinder is formed, but at higher densities (e.g. $N = 60$), a second one is formed in the center.

Many of the features discussed above are similar to those found by Schiffer *et al.*[1,5] with static focusing and without the shearing force. However, the ground state we found is time dependent. The shape of the crystals and the position of the particles are both periodic in time. The foci of the ellipses move as functions of time, and the principal axes can be either the x or the y axis. To show the dramatic change of the crystal shape in one period of time, we take $N = 60$ as an example and plot four snap shots of the particle positions (projected onto the $x - y$ plane) in Fig. 2. The particles move as much as one hundred percent of their coordinates in the $x - y$ plane and then all move back to their previous locations after one period. The crystal “breathes” transversely with no drifting and almost no oscillation in z .

V. CONCLUSION

We have studied the ground state of a crystalline particle beam under time-dependent, realistic storage ring environment. The equations of motion for the particles are derived in the rest frame of the reference particle that circulates around the ring with constant velocity. It has been shown that in a weak-focusing storage ring, the crystalline beams can not be formed for lack of transverse focusing. In an AG focusing ring, on the other hand, the crystalline beams can exist in spite of the variation in the focusing strengths, as long as the energy of the beam is less than the transition energy of the machine. If γ is higher than γ_T , the crystalline structure can not be formed for lack of radial focusing.

The quantitative investigation is performed using the molecular dynamics method. The ground state is obtained by, at the end of each focusing period, imposing the periodic condition on all the positions and momenta of the particles and then subtracting the “drifting velocity” from the z component P_z of the canonical momentum for each particle.

The nature of the crystalline beam is determined by the density of the particles and the effective strengths of the transverse focusing. When the density is low so that Eq. 5 is approximately satisfied, the beam is a 1-D crystal. When the density is increased, the crystal becomes a 2-D zig-zag chain in the plane of relatively weaker transverse focusing. The critical density at which the crystal transforms from 2-D to 3-D depends on the ratio of the effective focusing strengths between radial and vertical directions. In both 2-D and 3-D cases, the time-dependent crystalline structure has the same periodicity as that of the focusing forces. The crystal “breathes” transversely with no shearing and almost no oscillation in the azimuthal direction.

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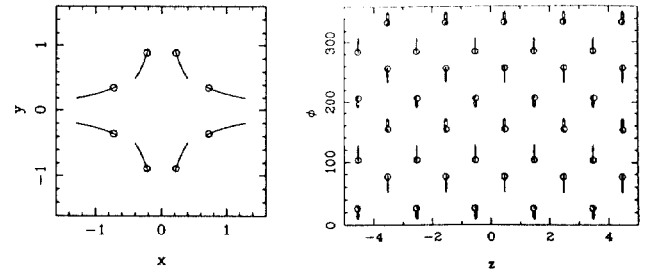


Fig. 1 Particle positions for $N = 40$. (a) Projected onto the $x - y$ plane. (b) The $\phi - z$ plot (ϕ is the polar angle). Circles are the positions at beginning and end of the focusing period. Solid lines are the trajectories within one period.

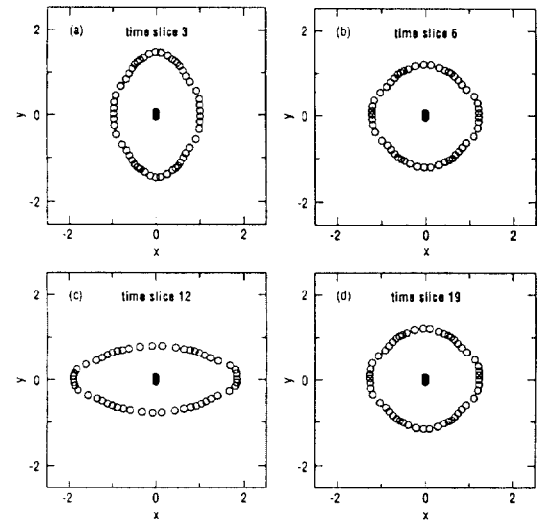


Fig. 2 Snap shots of the particle positions (projected onto the $x - y$ plane) in one time period for $N = 60$ (20 time slices per focusing period).