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CRYSTALLINE BEAM GROUND STATE

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Crystalline Beam Ground State^{*}

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Abstract

In order to employ molecular dynamics (MD) methods, 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 using MD methods has been performed to obtain the equilibrium crystalline beam structure. The effect 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

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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 Schiffer *et al.*[1 - 10] 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 studied, first in seminal work by Schiffer and his colleagues,[1 - 3] and then by others[4 - 10]. Their work assumed a storage ring model in which charged particles are subject to time-independent harmonic forces in both transverse directions. Subsequently, Schiffer and Rahman studied the crystallization in a time-dependent, alternating-gradient (AG) focusing potential.[11, 12]

In a realistic storage ring, however, the beam of particles are subject to more complicated forces. As the beam circulates around the ring under the guiding and focusing magnetic fields, the angular revolution frequency is in general different for particles of different momenta. If the energy of the particle beam is higher (or lower) than the transition energy of the ring, a particle of momentum larger than the synchronous value circulates with a lower (or higher) revolution frequency. The difference effectively produces a shearing force in the beam. Besides, the centrifugal force experienced by the particle is determined by the momentum and orbit radius. When particles are crystallized so that they move with the same angular velocity, the difference in the centrifugal force effectively defocuses the beam in radial direction. Furthermore, a storage ring as would be typically constructed may consist of AG focusing elements and straight sections for cooling, injection, acceleration, and observations. Consequently, the external forces experienced by the particles are in general time dependent.

In order to employ molecular dynamics (MD) method, commonly used in condensed matter physics for quantitative studies, we first derive in section II the equations of motion for the particles in the rotating rest frame of the reference particle. We include in the formalism that the particles are confined by the external guiding and focusing magnetic fields, and that they are confined in a conducting vacuum pipe while interacting with each other via a Coulomb force. Qualitative studies pertaining to the crystallization in the weak

and AG focusing rings are summarized in sections III and IV, respectively. Section V briefly describes the method and models used in MD calculation. Numerical results on the equilibrium crystalline-beam structure is discussed in section VI. The conclusions are given in section VII.

II. EQUATIONS OF MOTION IN THE ROTATING BEAM FRAME

The motion of the particles under Coulomb interaction and external electromagnetic (EM) forces can be most conveniently described in the rotating rest frame of the reference particle of which the orientation of the axes are constantly aligned to the radial, tangential, and vertical direction of the motion. In this frame, particle motion becomes non-relativistic, and a periodic, zero-entropy state simply corresponds to the desired crystalline state.

In this section, the equations of motion of a charged particle 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 can thus be constructed in the rest frame which include centrifugal force, Coriolis force (which contributes to shearing), time-dependent external EM forces, and electrostatic Coulomb forces. Finally, these equations are re-scaled in terms of dimensionless quantities for the convenience of computer simulation and analysis.

A. Tensor formalism

Adopting the formalism used by Møller,[13] we consider the motion of a particle in an

arbitrary system of coordinates (x^i) , where $i = 1, 2, 3, 4$ indicate the space-time components.

The metric tensor $\{g_{ij}\}$ is defined in terms of the differential line element ds as

$$ds^2 = g_{ij}dx^i dx^j, \quad (1)$$

where the summation is performed over the four indices. Let

$$x^i = x^i(\tau)$$

be the equation of the time track of the motion, τ being the proper time of the particle.

The contravariant components of the four-velocity are

$$U^i \equiv \frac{dx^i}{d\tau} = (\Gamma u^\iota, \Gamma c),$$

where $u^\iota = dx^\iota/dt$ are the contravariant components of the spatial velocity, the Greek letter ι indicates the three spacial components, c is the speed of light, and

$$\Gamma = \left\{ \left[(-g_{44})^{\frac{1}{2}} - \frac{g_{\kappa 4} u^\kappa}{c \sqrt{-g_{44}}} \right]^2 - \frac{u^2}{c^2} \right\}^{-\frac{1}{2}} \quad (2)$$

is the generalized Lorentz factor. The contravariant components of the four-momentum are

$$P^i = m_0 U^i,$$

where m_0 is the proper mass of the particle.

If the particles are acted upon by non-gravitational forces, the equations of motion can be written in this general system of coordinates as

$$\frac{DP^i}{d\tau} = g^{ik} F_k, \quad F_i U^i \equiv 0, \quad (3)$$

where $\{F_i\}$ is the non-gravitational four-force, the 4×4 matrix $\{g^{ij}\}$ is the inverse of $\{g_{ij}\}$, and the covariant differentiation is defined as

$$\frac{DP^i}{d\tau} \equiv \frac{dP^i}{d\tau} + \Gamma_{ik}^l U^k P^l, \quad \Gamma_{ik}^l = \frac{g^{lm}}{2} \left(\frac{\partial g_{mi}}{\partial x^k} + \frac{\partial g_{mk}}{\partial x^i} - \frac{\partial g_{ik}}{\partial x^m} \right). \quad (4)$$

Among the non-gravitational forces, for instance, the external EM force acting upon the particles is expressed by means of the EM field tensor $\{F_{ij}\}$ as

$$F_i = \frac{e}{c} F_{ik} U^k, \quad (5)$$

where e is the electric charge, and $\{F_{ij}\}$ is anti-symmetric. The Maxwell's equations is given by

$$\begin{cases} \frac{\partial F_{ik}}{\partial x^l} + \frac{\partial F_{kl}}{\partial x^i} + \frac{\partial F_{li}}{\partial x^k} = 0, \\ \frac{1}{\sqrt{|g|}} \frac{\partial}{\partial x^i} (\sqrt{|g|} F^{ik}) = \frac{\rho_0 U^i}{c}, \end{cases} \quad (6)$$

where

$$F^{ij} = g^{il} g^{jm} F_{lm},$$

$|g|$ is the absolute value of the determinant of the metric $\{g_{ij}\}$, and ρ_0 is the charge density measured in a local rest system of inertia.

B. Laboratory frame

In the Cartesian coordinate system of inertia (X^i), the so-called laboratory frame, Eq. 3 can be written in the conventional vector form. In this frame, the only non-zero components of the metric tensor are

$$g_{11} = g_{22} = g_{33} = 1, \quad \text{and} \quad g_{44} = -1. \quad (7)$$

In terms of the conventionally defined electric and magnetic fields

$$\mathbf{E} = (E_1, E_2, E_3), \quad \mathbf{B} = (B_1, B_2, B_3). \quad (8)$$

the EM field tensor becomes

$$\{F_{ij}\} = \begin{pmatrix} 0 & B_3 & -B_2 & E_1 \\ -B_3 & 0 & B_1 & E_2 \\ B_2 & -B_1 & 0 & E_3 \\ -E_1 & -E_2 & -E_3 & 0 \end{pmatrix}. \quad (9)$$

It is straightforward with these expressions to verify that Eq. 3 is equivalent to the equations

$$m_0 \frac{d(\Gamma \mathbf{u})}{dt} = e \mathbf{E} + \frac{e}{c} \mathbf{u} \times \mathbf{B}, \quad m_0 c^2 \frac{d\Gamma}{dt} = e \mathbf{u} \cdot \mathbf{E}. \quad (10)$$

where $dt = \Gamma d\tau$, and $\Gamma = (1 - u^2/c^2)^{-1/2}$ is in this case the Lorentz factor.

C. Beam rest frame of fixed orientation

Consider a reference particle circulating around the vertical axis X^2 with a uniform angular velocity ω at the radius R . Its time track $\{f^i\}$ may be described in the laboratory frame in terms of the proper time τ

$$f^i(\tau) = (R \cos \theta, 0, R \sin \theta, \gamma \tau), \quad (11)$$

where $\theta = \omega \gamma \tau$ is the revolution angle, $\gamma = (1 - \beta^2)^{-1/2}$, and $\beta c = R\omega$ is the velocity. Introduce a rigid system of coordinates (x^i) which follows the reference particle in its motion, so that the particle is constantly situated at the origin of this frame of reference, and that the spacial axes have constant orientations. The transformation connecting the variables (X^i) and (x^i) are

$$X^i = f^i(\tau) + \check{\alpha}_{i\kappa} x^\kappa, \quad \text{and} \quad x^4 = \tau, \quad (12)$$

where the check $(\check{})$ denotes the inverse operation, the summation over κ is on spacial components 1, 2, 3, and the coefficients α_{ij} are obtained by means of successive infinitesimal Lorentz transformations without rotation of the spatial axes,[13]

$$\{\alpha_{ij}\} = \begin{pmatrix} \cos \theta \cos \bar{\theta} + \gamma \sin \theta \sin \bar{\theta} & 0 & \sin \theta \cos \bar{\theta} - \gamma \cos \theta \sin \bar{\theta} & \gamma \beta \sin \bar{\theta} \\ 0 & 1 & 0 & 0 \\ \cos \theta \sin \bar{\theta} - \gamma \sin \theta \cos \bar{\theta} & 0 & \sin \theta \sin \bar{\theta} + \gamma \cos \theta \cos \bar{\theta} & -\gamma \beta \cos \bar{\theta} \\ \gamma \beta \sin \theta & 0 & -\gamma \beta \cos \theta & \gamma \end{pmatrix}, \quad (13)$$

where

$$\bar{\theta} = \omega \gamma^2 \tau = \gamma \theta.$$

The fact that $\tilde{\theta}$ differs from the revolution angle θ by the Lorentz factor γ is the consequence of the Thomas precession. This kinematic effect may be observed explicitly by considering at the time of one revolution period $\gamma\tau_1 = 2\pi/\omega$. $\{\alpha_{ij}\}$ can be written as the product of a pure rotation and a Lorentz transformation without rotation

$$\{\alpha_{ij}(\tau_1)\} = \begin{pmatrix} \cos \tilde{\theta}_1 & 0 & -\sin \tilde{\theta}_1 & 0 \\ 0 & 1 & 0 & 0 \\ \sin \tilde{\theta}_1 & 0 & \cos \tilde{\theta}_1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \gamma & -\beta\gamma \\ 0 & 0 & -\beta\gamma & \gamma \end{pmatrix}. \quad (14)$$

Therefore, the total angle of precession in one revolution is just $2\pi(\gamma - 1)$.

To obtain the metric tensor of the rest frame, we need to derive the relation between the line elements of the two coordinate systems. Differentiation of Eq. 12 gives

$$dX^i = \tilde{\alpha}_{i\kappa} dx^\kappa + \left[\frac{f^i(\tau)}{d\tau} + \frac{\tilde{\alpha}_{i\kappa}(\tau)}{d\tau} x^\kappa \right] d\tau \equiv \tilde{\alpha}_j^i dx^j, \quad (15)$$

where

$$\{\alpha_j^i\} = \{\tilde{\alpha}_j^i\}^{-1} \quad (16)$$

is the transformation matrix between the line elements of the laboratory and the rest frame. The metric tensor $\{g'_{ij}\}$ of the rest frame is related to $\{g_{ij}\}$ of the laboratory frame by the relation

$$g'_{ij} = \tilde{\alpha}_i^l \tilde{\alpha}_j^m g_{lm}. \quad (17)$$

Using the transformation matrix, the contravariant components of a vector $\{a^i\}$ in the laboratory frame are transformed into the rest frame (denoted by a prime) as

$$a'^i = \alpha^i_\kappa a^\kappa. \quad (18)$$

On the other hand, the covariant components of a tensor of rank 2, e.g. the EM field tensor, are transformed as

$$F'_{ij} = \tilde{\alpha}_i^l \tilde{\alpha}_j^m F_{lm}. \quad (19)$$

With Eqs. 17 and 19, the equation of motion in the beam rest frame of fixed orientation can be obtained from Eq. 3 by explicitly evaluating Eq. 4. These equations, however, can be greatly simplified if they are expressed in terms of the variables tangential and normal to the direction of the motion of the reference particle. We thus seek for another transformation into the rotating beam rest frame of which the orientation of the spacial axes are constantly aligned to the radial (x), tangential (z), and vertical (y) direction of the motion of the reference particle.

D. Rotating beam rest frame

Define the rotating beam frame as the rest frame of which the orientation of the spacial axes x and z rotate an angle $\tilde{\theta}$ per revolution relative to those of the fixed orientation x^1 and x^3

$$\begin{pmatrix} x \\ y \\ z \\ \tau \end{pmatrix} = \begin{pmatrix} \cos \tilde{\theta} & 0 & \sin \tilde{\theta} & 0 \\ 0 & 1 & 0 & 0 \\ -\sin \tilde{\theta} & 0 & \cos \tilde{\theta} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x^1 \\ x^2 \\ x^3 \\ x^4 \end{pmatrix}. \quad (20)$$

Express the electric and magnetic fields in the laboratory frame in terms of the tangential component in z and the normal component in x

$$\begin{cases} E_x = E_1 \cos \theta + E_3 \sin \theta, & B_x = B_1 \cos \theta + B_3 \sin \theta, \\ E_y = E_2, & B_y = B_2, \\ E_z = -E_1 \sin \theta + E_3 \cos \theta, & B_z = -B_1 \sin \theta + B_3 \cos \theta. \end{cases} \quad (21)$$

The equations of motion can be obtained from Eqs. 3 and 4 by using Eqs. 19, 9, and 17

$$\begin{cases} \frac{m_0}{\Gamma} (\ddot{x} - 2\gamma^2 \omega \dot{z} - \gamma^4 \omega^2 x) - m_0 \Gamma \gamma^2 \omega^2 R(1 - \chi) = e(1 - \chi) E'_x + \\ \quad + \frac{e}{\Gamma c} [B'_z \dot{y} - B'_y (\dot{z} + \gamma^2 \omega x)] - \frac{\partial V_C}{\partial x}, \\ \frac{m_0}{\Gamma} \ddot{y} = e(1 - \chi) E'_y + \frac{e}{\Gamma c} [B'_x (\dot{z} + \gamma^2 \omega x - B'_z (\dot{x} - \gamma^2 \omega z))] - \frac{\partial V_C}{\partial y}, \\ \frac{m_0}{\Gamma} (\ddot{z} + 2\gamma^2 \omega \dot{x} - \gamma^4 \omega^2 z) = e(1 - \chi) E'_z + \frac{e}{\Gamma c} [B'_y (\dot{x} - \gamma^2 \omega z) - B'_x \dot{y}] - \frac{\partial V_C}{\partial z}, \end{cases} \quad (22)$$

where

$$\begin{cases} E'_x = \gamma(E_x - \beta B_y), & B'_x = \gamma(B_x + \beta E_y), \\ E'_y = \gamma(E_y + \beta B_x), & B'_y = \gamma(B_y - \beta E_x), \\ E'_z = E_z, & B'_z = B_z, \end{cases} \quad (23)$$

are the electric and magnetic fields after a Lorentz transformation without rotation.

$$V_C(x, y, z) = \sum_j \frac{Z^2 e^2}{\sqrt{(x_j - x)^2 + (y_j - y)^2 + (z_j - z)^2}} \quad (24)$$

is the Coulomb potential energy, e is the unit electric charge, Z is the charge state of the particle, and the summation is performed over all the other particles j and their image charges. Since the particle motion in the rest frame is typically non-relativistic, the Lorentz factor Γ has been simplified as

$$\Gamma \approx (1 - \chi)^{-1}, \quad \text{with } \chi \equiv \beta^2 \gamma^2 \frac{x}{R}. \quad (25)$$

Typically, the dimensionless quantity χ is much smaller than 1. The terms on the left hand side of Eq. 22 include the centrifugal and Coriolis forces. Those on the right hand side are external EM forces and electrostatic Coulomb forces. Again, since the particle motion is non-relativistic, the magnetic force produced by the motion of the particles is negligible compared with the electrostatic force.

In the following, we consider the case that the beam is guided by a bending field B_0 and focused by a quadrupole field of gradient B_1

$$B_x = B_1 y, \quad B_y = B_0 + B_1 x, \quad B_z = 0, \quad (26)$$

where B_1 may vary for different piece of magnets, and the field variation at the magnet end is neglected. Assume that there exists no electric field so that the particle beam is not focused azimuthally. The magnitude of the B_0 is determined by the velocity βc and the bending radius R of the reference particle

$$e B_0 R = m_0 c^2 \beta \gamma. \quad (27)$$

With this model, the equations of motion can be simplified by linearizing Eq. 22

$$\begin{cases} m_0 (\ddot{x} - \gamma^2 \omega \dot{z}) - m_0 \gamma^2 \omega^2 R \chi = -e\beta\gamma B_1 x - \frac{\partial V_C}{\partial x}, \\ m_0 \ddot{y} = e\beta\gamma B_1 y - \frac{\partial V_C}{\partial y}, \\ m_0 (\ddot{z} + \gamma^2 \omega \dot{x}) = -\frac{\partial V_C}{\partial z}. \end{cases} \quad (28)$$

Here, χ has been assumed small compared with 1.

E. Equations of motion in dimensionless variables

For the convenience of later analysis, the equations of motion Eq. 28 will be written in terms of dimensionless variables. Let

$$n \equiv -B_1 R / B_0 \quad (29)$$

represent the strength of the focusing magnetic field, and

$$\xi \equiv \left(\frac{r_0 R^2}{\beta^2 \gamma^2} \right)^{\frac{1}{3}} \quad (30)$$

be a characterization of the inter-particle distance in the presence of Coulomb interaction in the storage ring, where $r_0 = Z^2 e^2 / m_0 c^2$ is the classical radius of the particle. Express the time t in unit of $R / \beta \gamma c$, the spacial coordinates x , y , and z in unit of ξ , and the energy in unit of $\beta^2 \gamma^2 Z^2 e^2 / \xi$. Eq. 28 becomes in these reduced units

$$\begin{cases} \ddot{x} - \gamma \dot{z} + (-\gamma^2 + 1 - n)x = -\frac{\partial V_C}{\partial x}, \\ \ddot{y} + ny = -\frac{\partial V_C}{\partial y}, \\ \ddot{z} + \gamma \dot{x} = -\frac{\partial V_C}{\partial z}. \end{cases} \quad (31)$$

Here, the dots denote differentiations with respect to the reduced time t . In the reduced units, the revolution period of the reference particle in the storage ring is 2π .

F. Hamiltonian formalism

Using the canonical momentum (P_x, P_y, P_z) , the particle system of Eq. 31 can be described by the Hamiltonian

$$H(x, P_x, y, P_y, z, P_z; t) = \frac{1}{2} (P_x^2 + P_y^2 + P_z^2) - \gamma x P_z + \frac{1}{2} [(1-n)x^2 + ny^2] + V_C, \quad (32)$$

where the cross term $-\gamma x P_z$ describes the coupling between the tangential and normal motion that leads to shearing. The Hamilton's equations are

$$\begin{cases} \dot{x} = P_x, & \dot{P}_x = \gamma P_z - (1-n)x - \frac{\partial V_C}{\partial x}, \\ \dot{y} = P_y, & \dot{P}_y = -ny - \frac{\partial V_C}{\partial y}, \\ \dot{z} = P_z - \gamma x, & \dot{P}_z = -\frac{\partial V_C}{\partial z}. \end{cases} \quad (33)$$

It can be easily verified that Eqs. 31 and 33 are equivalent.

In the absence of the Coulomb interaction, $V_C \equiv 0$, the component P_z of the canonical momentum is a constant of motion. Eqs. 33 show that the particle is focused horizontally with the strength $1-n$, and vertically with the strength n .

G. Motion in a storage ring with straight sections

The formalism presented in the previous sections can be easily generalized to a storage ring that consists of both bending and straight sections. Denote the guiding field and bending radius in the bending section as B_0 and R , respectively. The equations of motion in the bending sections are given by Eq. 31 or Eq. 33, while the system Hamiltonian is given by Eq. 32.

In the straight sections where the guiding field is zero, the strength n of the focusing field can be defined using Eq. 29 by normalizing the gradient B_1 in the straight section to B_0 in the bending section. Since both centrifugal and Coriolis forces vanish for lack of

bending, the equations of motion that corresponds to Eq. 31 become

$$\begin{cases} \ddot{x} - nx = -\frac{\partial V_C}{\partial x}, \\ \ddot{y} + ny = -\frac{\partial V_C}{\partial y}, \\ \ddot{z} = -\frac{\partial V_C}{\partial z}. \end{cases} \quad (34)$$

With the Hamiltonian formalism, the cross term in Eq. 32 that couples x and z motion disappears. The Hamiltonian becomes

$$H(x, P_x, y, P_y, z, P_z; t) = \frac{1}{2} (P_x^2 + P_y^2 + P_z^2) + \frac{1}{2} [-nx^2 - ny^2] + V_C. \quad (35)$$

The Hamilton's equation that corresponds to Eq. 33 becomes

$$\begin{cases} \dot{x} = P_x, & \dot{P}_x = nx - \frac{\partial V_C}{\partial x}, \\ \dot{y} = P_y, & \dot{P}_y = -ny - \frac{\partial V_C}{\partial y}, \\ \dot{z} = P_z, & \dot{P}_z = -\frac{\partial V_C}{\partial z}. \end{cases} \quad (36)$$

If the circumference of the ring is C , the revolution period of the reference particle is C/R in the reduced unit.

For simplicity but without losing generality, we assumed in the following discussion a circular storage ring with no straight sections. With Eqs. 31 and 34, it is straightforward to study the more general case.

III. CRYSTALLIZATION IN A WEAK-FOCUSING MACHINE

In a weak-focusing machine, the constant n provides pure focusing (and defocusing) in the vertical (and radial) direction. Typically, radial 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 particle

towards the reference orbit. The effective radial focusing is $1 - n$. Thus, if

$$0 < n < 1, \quad (37)$$

there is focusing in both planes. Particles perform harmonic oscillation in the transverse directions with horizontal tune $\sqrt{1 - n}$ and vertical tune $\sqrt{n}$, respectively.

The situation becomes different when the beam is crystallized. In the ground state, particles circulate around the machine with the same angular velocity. Contrary to the conventional case, the centrifugal force is now linearly proportional to the orbit radius of the particle. Effectively, it defocuses the particles away from the reference orbit. Therefore, particle motion in the radial direction is always unstable if the particles are focused vertically.

The same conclusion can be obtained in the rotating beam rest frame. In the rest frame, the crystalline state corresponds to the condition

$$\dot{x} = \dot{y} = \dot{z} = 0. \quad (38)$$

When the Coulomb interaction is neglected, Eq. 31 implies that the conditions for stable radial and vertical motion are, respectively,

$$n < 1 - \gamma, \text{ and } n > 0. \quad (39)$$

Since the Coulomb force is repulsive, and that $1 - \gamma$ is always negative, the stability conditions can never be satisfied.

Although the previous analysis indicates that a crystalline beam does not exist in a weak-focusing machine, it is still tempting to believe that a 1-D or 2-D crystalline structure may exist having all the particles in the plane $x = 0$. This is in fact not true. It is however instructive to go through the detailed analysis.

Consider a test particle in a 2-D crystalline structure with its equilibrium azimuthal coordinate z_0 chosen as 0. In equilibrium, the azimuthal component of the Coulomb force

is also zero

$$\sum_j \frac{z_j}{r_j^3} = 0. \quad (40)$$

Assume that the test particle has perturbative displacements $x \ll r_j$ and $z \ll r_j$ from the equilibrium position. Since the motion in y direction is not coupled to that in x and z , the relevant equations of motion can be expressed by using Eq. 33 while expanding the Coulomb forces around the equilibrium position

$$\begin{cases} \dot{x} = P_x, \\ \dot{P}_x = \gamma P_z - (1 - n - C_x)x, \\ \dot{z} = P_z - \gamma x, \\ \dot{P}_z = -C_z z, \end{cases} \quad (41)$$

where

$$C_x = \sum_j \frac{1}{r_j^3} > 0, \quad \text{and} \quad C_z = \sum_j \frac{1}{r_j^3} \left(\frac{3z_j^2}{r_j^2} - 1 \right). \quad (42)$$

The stability condition in x and z is obtained by requiring all the eigenmodes of the linear system Eq. 41 being stable, i.e.

$$\gamma^2 - 1 \leq -n - C_x. \quad (43)$$

Since $C_x > 0$, the conditions for stable radial (Eq. 43) and vertical ($n > 0$) motion can not be simultaneously satisfied. Obviously, this conclusion also applies to the 1-D case when particles are distributed azimuthally with $x = y = 0$. Thus, it is proven in general that crystalline beam can not exist in any dimension in a weak-focusing machine.

IV. CONDITIONS OF CRYSTALLIZATION IN AG FOCUSING MACHINE

In the previous section, we concluded that crystalline beam can not exist in a weak-focusing machine for lack of simultaneous focusing in both transverse planes. In the case of AG focusing, however, magnetic net focusing can be achieved in both transverse planes.

The amount of 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 storage ring of circumference C consisting of N_c identical FODO cells. Within each cell, the polarity of the quadrupole magnet field alternates from the radially focusing ($n > 0$) F magnet to the radially defocusing ($n < 0$) D magnet. In the rest frame, the potential produced by the external magnetic field varies periodically with period

$$T_c = \frac{C}{N_c R}$$

in the reduced time unit. The equilibrium state is defined as the one when the motions of all the particles are periodic in T_c . Linearize the Coulomb force by expanding around the equilibrium orbit (x_i, y_i, z_i) of each particle i , the transverse equations of motion become under the smooth approximations

$$\begin{cases} \ddot{x} + \left[\nu_x^2 - \gamma^2 - \sum_j \left(\frac{1}{r_j^3} - \frac{3(x_i - x_j)^2}{r_j^5} \right) \right] x = \sum_j \frac{x_i - x_j}{r_{ij}^3}, \\ \ddot{y} + \left[\nu_y^2 - \sum_j \left(\frac{1}{r_j^3} - \frac{3(y_i - y_j)^2}{r_j^5} \right) \right] y = \sum_j \frac{y_i - y_j}{r_{ij}^3}, \end{cases} \quad (44)$$

where ν_x and ν_y are the horizontal and vertical tunes in the absence of the Coulomb interaction. The equilibrium condition is thus for every particle i of the beam to satisfy

$$\begin{cases} \left[\nu_x^2 - \gamma^2 - \sum_j \left(\frac{1}{r_j^3} - \frac{3(x_i - x_j)^2}{r_j^5} \right) \right] x_i = \sum_j \frac{x_i - x_j}{r_{ij}^3}, \\ \left[\nu_y^2 - \sum_j \left(\frac{1}{r_j^3} - \frac{3(y_i - y_j)^2}{r_j^5} \right) \right] y_i = \sum_j \frac{y_i - y_j}{r_{ij}^3}. \end{cases} \quad (45)$$

The stability condition for this equilibrium state is approximately

$$\nu_x^2 - \gamma^2 > \sum_j \left(\frac{1}{r_j^3} - \frac{3(x_i - x_j)^2}{r_j^5} \right), \quad \text{and} \quad \nu_y^2 > \sum_j \left(\frac{1}{r_j^3} - \frac{3(y_i - y_j)^2}{r_j^5} \right). \quad (46)$$

Similar to the weak-focusing case, the crystal can only exist when the effective transverse focusing is sufficiently strong, i.e.

$$\nu_x^2 > \gamma^2, \text{ and } \nu_y^2 > 0. \quad (47)$$

Since in typical storage rings ν_x is approximately equal to the transition energy γ_T of the machine, Eq. 47 implies 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 direction. As the density increases, it transforms into 2-D. If the net radial focusing is weaker (or stronger) than the vertical one, i.e.

$$\nu_x^2 - \gamma^2 < \nu_y^2 \text{ (or } \nu_x^2 - \gamma^2 > \nu_y^2), \quad (48)$$

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 where the nearest-neighbour azimuthal distance is Δ_z . Since Δ_z is usually much smaller than the radius of the conducting vacuum pipe that confines the beam, the effect of the image charges can be neglected. The vibrational frequencies $\omega_x(k)$ in x direction can be expressed as

$$\omega_x(k)^2 = (\nu_x^2 - \gamma^2) - \frac{2}{\Delta_z^3} \sum_m \frac{1}{m^3} + \frac{2}{\Delta_z^3} \sum_m \frac{\cos(mk)}{m^3}, \quad (49)$$

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

$$\nu_x^2 - \gamma^2 > \frac{4.2}{\Delta_z^3}. \quad (50)$$

V. MOLECULAR DYNAMICS

When Coulomb interaction and AG focusing are present, it is impossible to solve the Hamiltonian in Eq. (32) analytically. We therefore seek numerical solutions using molecular dynamics.

Since Coulomb interaction is long ranged, an Ewald-type summation[14] has to be performed to calculate the energy and the forces. Schiffer *et al.*[1-10] used periodic boundary conditions in *all* three directions in order to utilize the standard Ewald summation method. However, in a realistic storage ring, the system may be considered infinite only in the 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. In a realistic machine, however, such a negative background does not exist. To simulate a real storage ring, we consider 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 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

$$\phi(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{r_{ij}} + \frac{4}{L} \int_0^\infty \frac{\cosh(2z_{ij}k/L) J_0(2\rho_{ij}k/L) - 1}{\exp(2k) - 1} dk + \frac{2}{L} [\log(\pi b/L) + C], \quad (51)$$

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 $L/2$ (if z_{ij} falls outside this range, an integral multiple of L is added to bring it to the correct range). Apart from the last term which is an unimportant constant, Eq. (51) is the same as the formula given by Avilov[15], but the physical environments of the two cases are different.

The integration in Eq. (51) is performed by a 15th order Gauss-Laguerre method. The equations of motion in Eq. (33) is integrated by the 4th order Runge-Kutta algorithm. The storage ring is assumed to consist of 10 identical focusing-drift-defocusing-drift (FODO)

lattice cells. Within each cell, the lengths of the F, O, D, and O elements are assumed 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 transverse tunes $\nu_x = 2.7$ and $\nu_y = 2.3$ in the absence of the Coulomb interaction. The transition energy γ_T is about 2.5. The energy γ of the reference particle 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. Thus care must be taken when we try to lower the “temperature” and to find the “ground state” of the system. 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. After 10,000 time steps (or 500 FODO cells) of the simulated cooling, the ground-state crystalline structure (if it exists) is recorded. Then, the motion of the particles is tracked for a testing period of another 10,000 time steps without the simulated cooling to assure the stability of the crystal. All of the crystalline structures to be presented in the next section are stable at their ground state during the testing period.

VI. NUMERICAL RESULTS

Since to evaluate Eq. (51) is an order of N^2 process, the simulations are quite time consuming, especially when the number of particles, N , in the supercell is large. Here, we report the preliminary results with $L = 10$ and N ranging from 5 to 100.

Fig. 1(a) shows the positions of the particles projected to the $x - y$ plane when $N = 5$.

Only one particle at (0,0) is seen because all the others are exactly in behind. Fig. 1(b) shows them in the ϕ - z plane, where ϕ is the polar angle. This is an example of 1-D crystal, where all the particles are in the middle of the $x - y$ plane and uniformly distributed in z direction. The particles do not move at all although the focusing field is time-dependent.

The $N = 10$ case is shown in Fig. 2. The circles are the positions of the particles at the beginning and the end of a period, and the solid lines attached to the circles represent the trajectories of the particles within a period. Apparently, 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 the effective focusing in y direction is stronger than that in x direction. Now the particles move with time — a symmetrical breathing in x direction.

The crystal transforms from 1-D to 2-D when the number of particles N goes from 8 to 9. The transition density is slightly smaller than the one given by Eq. (50). This is partly because the effective focusing strength ν_x is only approximate.

The critical density at which the crystal transforms from 2-D to 3-D is approximately twice that from 1-D to 2-D. This is because the parameters of the ring is such that the effective focusing strengths in the x and y directions are about the same. It is trivial to change the parameters in the simulation as well as in a real storage ring so that these effective focusing strengths are different, and therefore the crystal remains as 2-D at a much higher density.

Figs. 3 to 6 show the same plots for $N = 20, 40, 60$ and 80 , respectively. All of them are 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 ($N = 20$ and 40), one cylinder is formed, but at higher densities ($N = 60$ and 80), a second one is formed in the center. In the latter cases, only the outer cylinders are shown in the ϕ - z plots. In Fig. 5(a), particles are seen all over the ellipse because they are not lined up exactly parallel to the x axis, as also shown in Fig. 5(b). For the $N = 80$ case, the system is not cooled to

the “zero temperature” during the 10,000 time steps, as shown by Fig. 6(a).

Many of the features discussed above are similar to those found by Schiffer *et al.*[1 - 10] with static focusing and without the shearing force. In contrast to the static focusing case, as previously observed by Schiffer *et al.*[11, 12] 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. 7. 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 .

VII. CONCLUSION

We have studied the ground state of a crystalline particle beam under time-dependent, realistic storage ring environment. As would be typically constructed, such a ring consists of arc sections for bending and focusing, and straight sections for cooling, injection, acceleration, and observations. 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. The Hamiltonian is obtained in terms of the reduced variables for the particle system.

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 MD 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. 50 is approximately satisfied, the beam is a 1-D crystal, where all the particles are in the origin of the transverse plane and uniformly distributed in azimuthal direction. The particles are static in the rest frame, although the focusing forces are time-dependent. 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 azimuthal direction.

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Figure Captions

Fig. 1 Particle positions. (a) Projected onto the $x - y$ plane. (b) The ϕ - z plot where ϕ is the polar angle. The total number of particles is $N = 5$. This is an example of 1-D crystal. The particles do not move at all although the focusing field is time-dependent.

Fig. 2 The same as Fig. 1 except that $N = 10$. This is an example of 2-D crystal. The particles moves periodically with time, and the solid lines show the trajectories of the particle motion within one focusing period. Circles are the positions at beginning and end of the period.

Fig. 3 The same as Fig. 2 except that $N = 20$. This is an example of 3-D crystal.

Fig. 4 The same as Fig. 3 except that $N = 40$.

Fig. 5 The same as Fig. 3 except that $N = 60$. A new ring starts in the center. (b) only shows the outer ring.

Fig. 6 The same as Fig. 5 except that $N = 80$. The system is not cooled to “zero temperature”, thus (a) show some scattering.

Fig. 7 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).

Fig. 1

Fig. 2

Fig. 3

Fig. 4

$N=60$

$N=60$

Fig. 5

Fig. 6

Fig. 7

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