

# PHONON MODES AND THE MAINTENANCE CONDITION OF A CRYSTALLINE BEAM\*

X.-P. Li, Skyworks Solutions, Newbury Park, USA

H. Enokizono, H. Okamoto, and Y. Yuri, Hiroshima University, Higashi-Hiroshima, Japan

A.M. Sessler, Lawrence Berkeley National Laboratory, Berkeley, USA

J. Wei†, Brookhaven National Laboratory, Upton, USA

## Abstract

Previously it has been shown that the maintenance condition for a crystalline beam requires that there not be a resonance between the crystal phonon frequencies and the frequency associated with a beam moving through a lattice of  $N_l$  periods. This resonance can be avoided provided the phonon frequencies are all below half of the lattice frequency. Here we make a detailed study of the phonon modes of a crystalline beam. Analytic results obtained in the smooth approximation using the ground-state crystalline beam structure is compared with numerical evaluation employing Fourier transform of the molecular dynamics (MD) modes. The MD also determines when a crystalline beam is stable. The maintenance condition, when combined with either the simple analytic theory or the numerical evaluation of phonon modes, is shown to be in excellent agreement with the MD calculations of crystal stability. A confirmed maintenance condition based on the linear resonance criteria is that the lattice frequency must not be equal to the sum of any two phonon frequencies.

## INTRODUCTION

In the work that first considered the formation of crystals in “real” machines; i.e., machines that allow the formation and maintenance of crystal, two criteria were presented. The first is that the machine can not be weak focusing (i.e., a constant gradient at all azimuths), but must be a strong focusing machine operating below transition [1]. The second is a maintenance condition for a crystalline beam. It requires that there not be a linear resonance between the crystal phonon frequencies and the frequency associated with a beam moving through a lattice of  $N_l$  periods [2, 3].

Previously, the maintenance condition is stated as that the lattice frequency must be larger than two times the maximum phonon frequency, because if this condition is not satisfied, a linear resonance occurs and any crystalline beams will be destroyed. For a typical beam of high density with near-equal transverse (betatron) tunes, the maximum phonon frequency is near  $\sqrt{2}$  times the higher single-particle (bare) tune. Practically, the resonance can be avoided if the lattice periodicity  $N_l$  is larger than  $2\sqrt{2}$  times the higher bare tune of  $(\nu_x, \nu_y)$ . Here, we closely examine cases from low to high beam density, and study in detail phonon modes and the maintenance condition.

The phonon modes are evaluated first under the so-called

smooth approximation analytically for a one-dimensional (1D) structure and numerically in general using the ground-state crystalline-beam structure, and then augmented with computational evaluation employing Fourier transform of particle trajectory simulated with the molecular dynamics (MD) method. The maintenance condition based on the evaluated phonon modes is shown to be in excellent agreement with the MD simulation on the stability.

In Section 2, we present the Hamiltonian employed and evaluate analytically the phonon spectrum. In Section 3, we introduce the MD method and employ it to determine, by Fourier transform, the phonon spectrum. In Section 4, we confront these spectra with crystals that are stable, or unstable, in MD. Section 5 is a discussion.

## ANALYTICAL PHONON SPECTRUM

The phonon modes may be calculated under the assumption that the external focusing is uniform in time (the smooth approximation). In this case the Hamiltonian is:

$$H = \frac{1}{2} \sum_i (P_{x,i}^2 + P_{y,i}^2 + P_{z,i}^2) - \gamma x_i P_{z,i} + \frac{1}{2} (\nu_x^2 x_i^2 + \nu_y^2 y_i^2) + V_C \quad (1)$$

where the Coulomb potential is  $V_C = \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$ ,

$|\mathbf{r}_i - \mathbf{r}_j| \equiv r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$   
The only non-linear terms are derivatives of  $V_C$ , which should be Taylor-expanded around the equilibrium positions retaining only the linear terms. Assume that

$$\begin{aligned} x_i &= X_i + \delta x_i, & \delta x_i &= \tilde{x}_i \exp[i(\omega t - kZ_i)], \\ y_i &= Y_i + \delta y_i, & \delta y_i &= \tilde{y}_i \exp[i(\omega t - kZ_i)], \\ z_i &= Z_i + \delta z_i, & \delta z_i &= \tilde{z}_i \exp[i(\omega t - kZ_i)]. \end{aligned} \quad (2)$$

Assume that the unit cell length is  $L$ , and that there are  $N$  particles per unit cell. We obtain the linearized equations of motion in a circular accelerator,

$$\begin{aligned} \omega^2 \tilde{x}_i &= -i\gamma\omega \tilde{z}_i + (\nu_x^2 - \gamma^2) \tilde{x}_i + \sum_{n=-\infty}^{\infty} \sum_{j=1}^N \\ &\left\{ \left[ \frac{1}{R_{nij}^3} - \frac{3(X_i - X_j)^2}{R_{nij}^5} \right] \left[ e^{ik(Z_i - Z_j - nL)} \tilde{x}_j - \tilde{x}_i \right] \right. \\ &- \frac{3(X_i - X_j)(Y_i - Y_j)}{R_{nij}^5} \left[ e^{ik(Z_i - Z_j - nL)} \tilde{y}_j - \tilde{y}_i \right] \\ &\left. - \frac{3(X_i - X_j)(Z_i - Z_j - nL)}{R_{nij}^5} \left[ e^{ik(Z_i - Z_j - nL)} \tilde{z}_j - \tilde{z}_i \right] \right\} \quad (3) \end{aligned}$$

\* Work performed under the auspices of the US Department of Energy.

† jwei@bnl.gov

$$\omega^2 \tilde{y}_i = \nu_y^2 \tilde{y}_i + \sum_{n=-\infty}^{\infty} \sum_{j=1}^N \left\{ -\frac{3(X_i - X_j)(Y_i - Y_j)}{R_{nij}^5} \left[ e^{ik(Z_i - Z_j - nL)} \tilde{x}_j - \tilde{x}_i \right] + \left[ \frac{1}{R_{nij}^3} - \frac{3(Y_i - Y_j)^2}{R_{nij}^5} \right] \left[ e^{ik(Z_i - Z_j - nL)} \tilde{y}_j - \tilde{y}_i \right] - \frac{3(Y_i - Y_j)(Z_i - Z_j - nL)}{R_{nij}^5} \left[ e^{ik(Z_i - Z_j - nL)} \tilde{z}_j - \tilde{z}_i \right] \right\} \quad (4)$$

$$\omega^2 \tilde{z}_i = i\gamma\omega \tilde{x}_i + \sum_{n=-\infty}^{\infty} \sum_{j=1}^N \left\{ -\frac{3(X_i - X_j)(Z_i - Z_j - nL)}{R_{nij}^5} \left[ e^{ik(Z_i - Z_j - nL)} \tilde{x}_j - \tilde{x}_i \right] - \frac{3(Y_i - Y_j)(Z_i - Z_j - nL)}{R_{nij}^5} \left[ e^{ik(Z_i - Z_j - nL)} \tilde{y}_j - \tilde{y}_i \right] + \left[ \frac{1}{R_{nij}^3} - \frac{3(Z_i - Z_j - nL)^2}{R_{nij}^5} \right] \left[ e^{ik(Z_i - Z_j - nL)} \tilde{z}_j - \tilde{z}_i \right] \right\} \quad (5)$$

where  $R_{nij} = \sqrt{(X_i - X_j)^2 + (Y_i - Y_j)^2 + (Z_i - Z_j - nL)^2}$  and  $i = 1, \dots, N$ . Also,  $R_{nij} = 0$  term is excluded from the double sum.

### 1D crystalline beam

For a 1D chain of intra-particle distance  $L$ ,  $N = 1$  and  $(X, Y, Z) = (0, 0, 0)$ , the phonon bands are given by

$$\begin{aligned} \omega_1^2 &= \frac{1}{2} \left\{ \nu_x^2 + \Omega^2 + \sqrt{(\nu_x^2 + \Omega^2)^2 - 8\Omega^2(\nu_x^2 - \gamma^2 - \Omega^2)} \right\} \\ \omega_2^2 &= \nu_y^2 - \Omega^2 \\ \omega_3^2 &= \frac{1}{2} \left\{ \nu_x^2 + \Omega^2 - \sqrt{(\nu_x^2 + \Omega^2)^2 - 8\Omega^2(\nu_x^2 - \gamma^2 - \Omega^2)} \right\} \end{aligned} \quad (6)$$

where

$$\Omega^2 = 2 \sum_{n=1}^{\infty} \frac{1 - \cos(knL)}{n^3 L^3} \geq 0 \quad (7)$$

and  $k$  varies from  $-\frac{\pi}{L}$  to  $\frac{\pi}{L}$ . The phonon bands satisfy

$$\sum_{i=1}^3 \omega_i^2 = \nu_x^2 + \nu_y^2, \quad \omega_1^2 + \omega_3^2 = \nu_x^2 + \Omega^2, \quad \text{and} \quad \omega_3^2 \leq \omega_1^2.$$

The frequency  $\omega_2$  corresponds to the motion polarized in  $y$ , while the frequencies  $\omega_1$  and  $\omega_3$  correspond to the motion coupled in  $x$  and  $z$  directions.

A test particle deviating from its equilibrium position experiences through Coulomb interaction defocusing forces in both the horizontal ( $x$ ) and vertical ( $y$ ) directions, and focusing force in the longitudinal ( $z$ ) direction. At a low beam density, the phonon frequencies in both mode 1 and 2 shift downwards from the base tune, while the frequency in mode 3 shifts upwards from 0, as shown in Fig. 1. The typical density of states is shown in Fig. 2.

When the beam density increases, the amount of frequency shift downwards in mode 2 and upwards in mode 3 also increases, as shown in Figs. 1 and 2. Because of

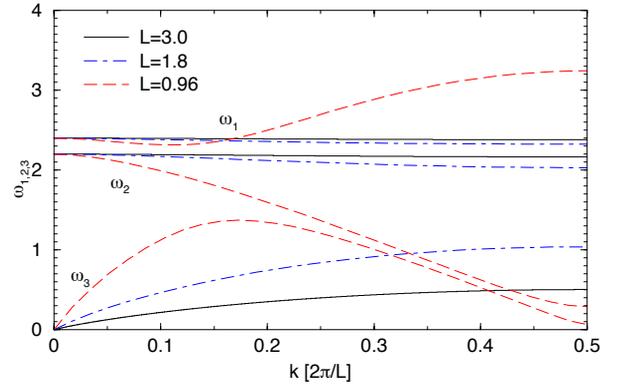


Figure 1: Dispersion function evaluated under the smooth approximation of three 1D crystalline beams with  $L = 3.0$ , 1.8, and 0.96, respectively. The tunes are  $\nu_x = 2.4$  and  $\nu_y = 2.2$ , respectively, and  $\gamma = 1.000016$ .

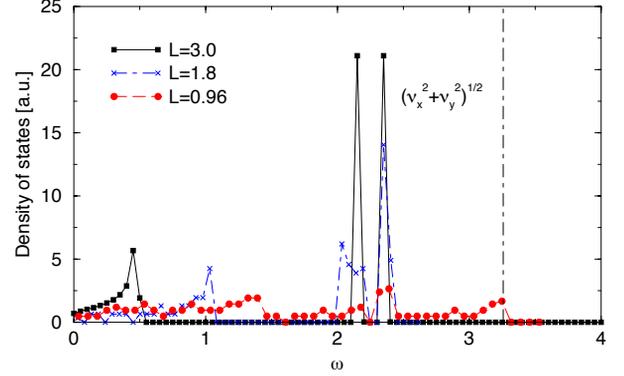


Figure 2: Density of states corresponding to Fig. 1 evaluated under the smooth approximation at three beam densities with  $L = 3.0$ , 1.8, and 0.96, respectively.

the coupling in horizontal and longitudinal motion, the frequency in mode 1 can also shift upwards from the base tune  $\nu_x$ . The amount of upward frequency shift reaches a maximum when the density approaches the threshold of 1D to 2D transition (Fig. 2). The maximum phonon frequency for a stable 1D crystalline beam satisfies

$$\omega_{1,3,\max} \leq \sqrt{\nu_x^2 + \nu_y^2}, \quad \omega_{2,\max} \leq \nu_y. \quad (8)$$

The maximum frequency is achieved when  $k = \pi/L$ , i.e., when nearest-neighbor particles  $i$  and  $i + 1$  move in the opposite phase in each direction. The motion in the horizontal and longitudinal directions are 90 degrees out of phase. In the case when the equivalent focusing in the horizontal and vertical directions are equal,  $\nu_x^2 - \gamma^2 = \nu_y^2$ , the threshold density corresponds to

$$L = \left( \frac{4.2}{\nu_x^2 - \gamma^2} \right)^{1/3} = \left( \frac{4.2}{\nu_y^2} \right)^{1/3}. \quad (9)$$

At this density value, the mode 2 frequency is down-shifted to zero when  $k$  reaches the maximum ( $k = \pi/L$ ).

### 2D and 3D crystalline beams

For a crystalline beam beyond 1D, the dispersion relation in general can not be solved analytically. We first obtain the equilibrium crystalline structure under the smooth

approximation. Then, we obtain the dispersion relation and the density of states by numerically solving Eqs. 3-5. Fig. 3 shows the density of states of a series of 2D and 3D crystalline beams. The maximum frequency of the  $3N$  phonon bands satisfies the relation

$$\omega_{\max} \leq \sqrt{\nu_x^2 + \nu_y^2}. \quad (10)$$

Eq. 10 is expected to be a general relation independent of the choice of machine lattice parameters.

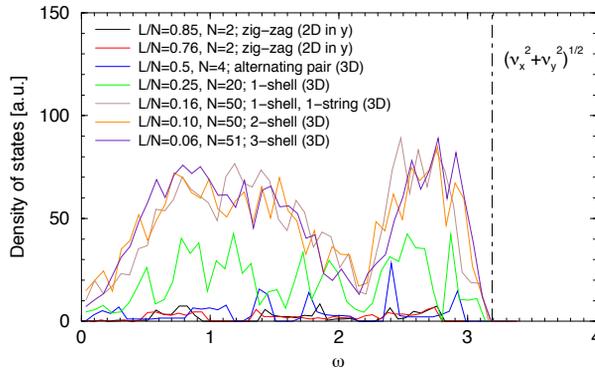


Figure 3: Density of states evaluated under the smooth approximation for various 2D and 3D crystalline beams with  $\nu_x = 2.4$ ,  $\nu_y = 2.1$ , and  $\gamma = 1.000016$ .

### PHONON SPECTRUM FROM MD

The phonon spectrum can be directly evaluated for a “real” lattice without using the smooth approximation by the MD method, first determining the ground state and then evaluating the density of states in the frequency domain by Fourier-analyzing the particle trajectory under small-amplitude vibrations. The agreement with those obtained using the analytical method under the smooth approximation is good ( $L = 3.0$  case in Figs. 2 and 4) [2, 3].

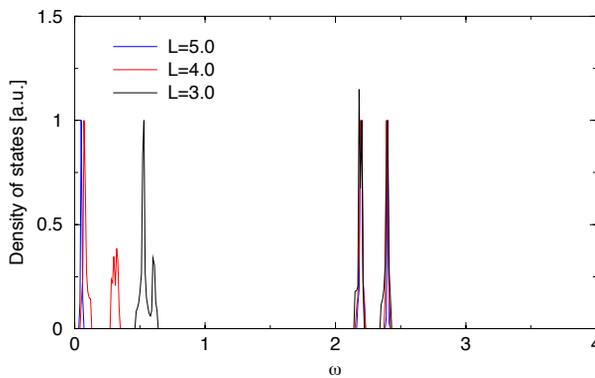


Figure 4: Density of states evaluated with MD using a “real” lattice with  $N_l = 3$  as discussed in Section 4.

### MAINTENANCE CONDITION

The maintenance condition based on the linear resonance criteria is that the lattice frequency must not be equal to the sum of any two phonon frequencies. In order to verify this condition, we study six slightly different “real” storage ring lattices of 12 FODO cells with  $\nu_x = 2.4$ ,  $\nu_y = 2.2$ ,

and  $\gamma = 1.000016$ . The strength of the 12 FODO cells are adjusted such that the lattice super-periodicity  $N_l$  is 12, 6, 4, 3, 2, and 1, respectively. (1) With  $N_l = 12$ , the 1D crystal is stable for  $L \geq 0.96$ . At higher densities the crystal becomes 2D and 3D. Resonances at  $\omega = 6$  are of no concern. (2) With  $N_l = 6$ , the 1D crystal is stable also for  $L \geq 0.96$ , below this value the crystal becomes 2D and 3D. The resonance condition forbids phonon frequency at  $\omega_1 = 3$ . (3) With  $N_l = 4$ , the 1D crystal is stable only for  $L \geq 2.2$ . At higher densities the down-shift of  $\omega_2$  to 2 causes resonance. (4) With  $N_l = 2$ , the 1D crystal is stable again only for  $L \geq 2.2$ . At higher densities the down-shift of  $\omega_2$  to 2 causes resonance. (5) With  $N_l = 1$ , the 1D crystal is stable only for  $L \geq 3.2$ . At higher densities the up-shift of  $\omega_3$  to 0.5 causes resonance.

The  $N_l = 3$  case is worth special discussion. According to MD result, the 1D crystal is stable only for  $L \geq 3.0$  (Fig. 5). At the density of  $L \geq 3.0$ , however, there is no power density at half of the lattice frequency, i.e. 1.5. The resonance originates from the sum of the modes near  $\omega_1 = 2.5$  and  $\omega_3 = 0.5$  hitting 3 (Fig. 4).

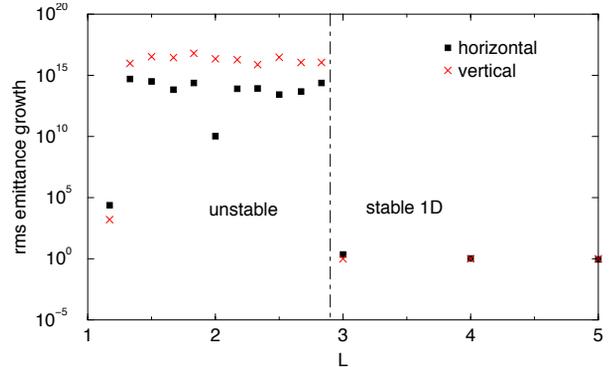


Figure 5: 1D crystalline beam stability for the  $N_l = 3$  lattice obtained by MD.

### DISCUSSIONS

In this paper we have focused on the maintenance condition for a crystalline beam. We have derived the phonon spectrum in the smooth approximation and then compared with that obtained by Fourier transform from MD calculation. The maintenance condition based on linear resonance criteria is that the lattice frequency must not be equal to the sum of any two phonon frequencies. The maximum phonon frequency is  $\sqrt{\nu_x^2 + \nu_y^2}$ . For crystalline beams of high density, this condition states that the lattice super-periodicity  $N_l$  must be larger than  $2\sqrt{\nu_x^2 + \nu_y^2}$ , or  $2\sqrt{2}$  times the bare transverse tune when the two tunes are near equal.

The formalism can be applied to crystal formation in traps where  $\gamma = 0$ . Similar maintenance condition holds.

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