Singularities of particle trajectory caustics and beam shaping in bunch compressors

T. K. Charles^{*}

European Organization for Nuclear Research (CERN), Geneva, Switzerland

School of Physics, University of Melbourne, 3010, Victoria, Australia *E-mail: tessa.charles@cern.ch

D. M. Paganin

School of Physics and Astronomy, Monash University, Clayton, VIC 3800, Australia

R. T. Dowd

Australian Synchrotron, Clayton, VIC 3168, Australia

M. J. Boland

Canadian Light Source, Saskatoon SK S7N 3V4, Canada

Caustics are a common occurrence in optics, describing the bright lines seen in a well-lit coffee cup or the dancing networks of light seen at the bottom of a swimming pool on a sunny day. Recently, caustic formation in electron trajectories was identified as the mechanism driving strong current modulations in accelerated charged-particle beams. Under certain conditions, neighboring electron trajectories coalesce to form caustics, resulting in current spikes. Caustic lines and surfaces are regions of maximum electron density, and are often witnessed in accelerator physics as folds in the transverse or longitudinal phase space distribution. Knowledge of caustics can allows us to shape the longitudinal beam shape to our advantage.

Keywords: Beam dynamics; Caustics; Current spikes; CSR; Bunch Compression

1. Caustics in Accelerator Physics

On occasion, phenomenon encountered in other fields of physics find themselves an equivalence in accelerator physics. Caustics are one such example. Within the fields of optics and electron microscopy, caustics are commonly recognized and are well-understood. The same effect can be seen in various accelerator physics scenarios, although it might not be referred to by the name caustics. Instead of rays of light reflecting or refracting, relativistic particle trajectories can be focused and defocused to form an envelope of trajectories associated with current peaks.

1.1. What are caustics?

Caustics are a form of 'natural focusing', whereby particle trajectories coalesce to form regions of greatly enhanced charge density.

In optics, caustics appear as the bright lines that can be seen in a well–lit coffee cup as shown in Fig. 1, or the dancing networks of light appearing at the bottom of swimming pools on a sunny day^{1,2}. Figure 1b shows how the reflected rays of light in the coffee cup coalesce to form the bright line tracing out a cardioidal shape.

Recently published work considered applications of caustics to accelerator physics³. One such example, which is explored further in Sec. 2, is current horns that can appear in strong bunch compression⁴.

1.2. Tell-tail signs of caustics

In his book "Natural Focusing and the Fine Structure of Light" ², Nye described the intensity profile along a line crossing a caustic. At the position of the caustic, in ray theory of light, a singularity is encountered. Moving away from the caustic, the intensity of the light drops away rapidly, following the relationship, $I \propto d^{-1/2}$, where d is the position away from the caustic (Fig. 1c).



Fig. 1. Optical caustics, which are analogous to electron-trajectory caustics found in accelerator physics. (a) image of caustic lines appearing in a coffee cup. (b) illustration of light rays forming the caustic (red line), and (c) intensity of the rays in the vicinity of the caustic

Numerous examples in accelerator physics exhibit the same steeply rising linear charge density, with a sharp drop off (similar to Fig. 1c). Some examples can be seen in References⁵⁻¹⁰. These sharply rising current profiles appear from folds in phase space being projected onto the x, y, or z axes (where x, y, and z are transverse and longitudinal position coordinates). An example is shown in Fig. 2. Similarly if the longitudinal phase space where projected onto energy axis, spikes can be witness in the energy spectrum which are also caustic in nature (For example, see¹¹).

1.3. Caustics in Partilce Trajectories

A caustic expression has been previously derived⁴. This parametric expression describes the longitudinal position of the caustics for a given set of control parameters,

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Fig. 2. Folds in the longitudinal phase space distribution correspond to spikes in the associated current profile.

 R_{56}, T_{566} , and U_{5666} (i.e. the first-, second-, and third-order longitudinal dispersion);

$$\tilde{z}(z_i) = z_i - \frac{\delta(z_i)}{\delta'(z_i)} - T_{566}\delta^2(z_i) - 2U_{5666}\delta^3(z_i)$$
(1a)

$$\tilde{R_{56}}(z_i) = \frac{-1}{\delta'(z_i)} - 2T_{566}\delta(z_i) - 3U_{5666}\delta^2(z_i),$$
(1b)

where $\delta(z_i)$ is the shape of the initial longitudinal phase space (or chirp), often described by a high-order polynomial and $\delta'(z_i)$ is the derivative with respect to z_i .

When a bunch is subjected to strong bunch compression, often the compressed bunch will exhibit a double-horned current profile (e.g. Fig. 2). These current spikes are detrimental to FEL performance, leading to greater CSR which can increase the horizontal projected emittance^{12,13}.

The caustic expression [Eq. (1)] describes where (i.e. at what longitudinal positions, z) and under what conditions (i.e. at what values of R_{56} , T_{566} , etc.) caustics will form. Figure 3 shows the caustic expression [Eq. (1)] as a function of R_{56} for various values of T_{566} and U_{5666} evaluated with an initial bunch that can be described by the first-, second-, and third-order chirp values: $h_1 = 81.06 \text{ m}^{-1}$,

 $h_2 = 5929.08 \text{ m}^{-2}$, and $h_3 = 1.30 \times 10^8 \text{ m}^{-3}$. Each plot in Fig. 3 is a catastrophe of codimension 2, named a cusp. Just as was shown in the coffee cup example, the cusp involves two fold caustic lines meeting, and at the point of meeting, the two caustic lines share the same tangent.

The current profiles associated with the three plots in Fig. 3a, at an R_{56} value of -11 mm, is shown in Fig. 3b-d. It is evident that the current profile shapes vary greatly depending upon the value of T_{566} . This information can be gleaned from Fig. 3a where the caustic lines are shown to skew with changing T_{566} value.

Typically, varying T_{566} has the property of varying the charge distribution from either the head of the bunch to the tail or vice versa. For example, if two current horns are present, tweaking T_{566} can change the relative heights of the two peaks. Taken one step further, if T_{566} is increased or decreased to a larger degree, the size of the two peaks becomes so disparate that the second smaller peak disappears.



Fig. 3. Top: Caustic expression evaluated for three possible bunch compressors characterized by T_{566} and U_{5666} . In each case the bunch entering the compressor has the following properties, $h_1 = 81.06 \text{ m}^{-1}$, $h_2 = 5929.08 \text{ m}^{-2}$, and $h_3 = 1.30 \times 10^8 \text{ m}^{-3}$. b) Histogram of charge density evaluated at $R_{56} = -11 \text{ mm}$, and for $T_{566} = 20 \text{ mm}$ and $U_{5666} = -0.15 \text{ m}$. c) Histogram of charge density evaluated at $R_{56} = -11 \text{ mm}$, and for $T_{566} = 80 \text{ mm}$ and $U_{5666} = -0.15 \text{ m}$. d) Histogram of charge density evaluated at $R_{56} = -11 \text{ mm}$, and for $T_{566} = 80 \text{ mm}$ and $U_{5666} = -0.15 \text{ m}$. d) Histogram of charge density evaluated at $R_{56} = -11 \text{ mm}$, and for $T_{566} = -30 \text{ mm}$ and $U_{5666} = 0.71 \text{ m}$.

Figure 4 also shows the caustic expression [Eq. (1)], evaluated for the same bunch properties as that shown in Fig. 3, that is: $h_1 = 81.06 \text{ m}^{-1}$, $h_2 = 5929.08$

m⁻², and $h_3 = 1.30 \times 10^8$ m⁻³. However the difference between Fig. 3 and Fig. 4 is largely due to the larger value of U_{5666} used in Fig. 4. In Fig. 4, $T_{566} = 0.015$ m and $U_{5666} = 4.6$ m. This results in what is known as a butterfly catastrophe¹⁴. Despite being significantly more complex than the cusp catastrophe shown in Fig. 3, both catastrophes shown in Figs. 3 and 4 are calculated using the same expression, Eq. (1), evaluated with different values of T_{566} and U_{5666} .

The caustic expression can predict the position of the current spikes in both Fig. 3 and Fig. 4 without needing to track many individual particles and inspect the result.

2. Current Profile Shaping

As mentioned previously, current horns experienced in FEL linacs can cause CSRinduced emittance growth and degrade FEL performance¹². The influence of CSR is particularly detrimental when these sharp current peaks are present as the rate of change of energy induced by CSR is proportional not only to the peak current value but also to the derivative of the current profile¹⁵.

Through considering of the underlying dynamics as caustic, this reveals options for current profile shaping to avoid the current horns forming. Being catastrophric in nature, this indicates that only slight deviations in the chirp away from linear can result in these strong peaks forming. Equation (1) also indicates that it is not solely the second- and third-order chirp that are responsible for the current horns, but also the influence of T_{566} and U_{5666} .

The boundaries between the regions of parameter space where caustics will and will not form can be calculated using the following expression that was derived in Reference³, as the following:

$$f(R_{56}, T_{566}, U_{5666}, h_1, h_2, h_3; z_{\min/\max}) =$$

$$1 + h_1 R_{56} + 2h_2 R_{56} z_{\min/\max} + 3h_3 R_{56} z_{\min/\max}^2 + 2T_{566} h_1^2 z_{\min/\max} + 6T_{566} h_1 h_2 z_{\min/\max}^2 + 3h_1^3 U_{5666} z_{\min/\max}^2.$$
(2)

where $z_{\min/\max}$ are the maximum and minimum values of the initial bunch, R_{ij} , T_{ijk} , U_{ijkl} are the elements of the first-, second- and third-order transfer matrices, respectively. Where $f(R_{56}, T_{566}, U_{5666}, h_1, h_2, h_3; z_{\min/\max}) = 0$, defines the boundaries between the regions of one and zero caustics expected, as well as boundaries between regions of catastrophes of codimension one or two forming.

Therefore, for a particular scenario where the first-order chirp of the bunch and R_{56} of the compressor are known, we have two methods for creating conditions under which caustics (and the associated current horns) cannot form, in accordance with Eq. (2). The first is through manipulating T_{566} and U_{5666} of the compressor. The second is altering h_2 , h_3 of the incoming bunch. The following section details an example utilising the second approach.



Fig. 4. The caustic expression calculated for a bunch compressor with $T_{566} = 0.015$ m and $U_{5666} = 4.6$ m, and with a bunch entering the compressor with the properties of $h_1 = 81.06$ m⁻¹, $h_2 = 5929.08$ m⁻², and $h_3 = 1.30 \times 10^8$ m⁻³. (a) Caustic expression (green, bold) overlayed on many individual trajectories (blue) and (b) without the individual trajectories for clarity. Also included in (b) are vertical lines marking R_{56} values equaling -11 mm, -11.5 mm, -12 mm, and -12.75 mm. (c)-(f) Histograms of the charge density along the bunch for the various values of R_{56} indicated by the vertical grey lines shown visible in (b). Note that each peak in the charge density histogram is predicted by the caustics expression shown in (b).

2.1. Example Application

In this section we consider an S-band linac for an FEL, where the bunch compression is shared between two chicane compressors. Figure 5 shows a schematic of the linac layout, including the bunch compressors' longitudinal dispersion values, both for the standard 4-dipole chicane (BC1) and also for when an octupole magnet is included in the first bunch compressor. An X-band (12 GHz) harmonic cavity is placed for BC1 in order to cancel the second-order effects of bunch compression. With the addition of the harmonic cavity but with no other measures (e.g. without measures such as collimation) double-horn current profile often emerges after the second bunch compressor (BC2).



Fig. 5. FEL linac layout schematic, including the longitudinal dispersion values for the two options for the first bunch compressor (BC1) and the dispersion values for the second bunch compressor (BC2).

Using Eq. (2), with the properties of BC2: $R_{56} = -19.38$ mm, $T_{566} = 29.10$ mm, and $U_{5666} = -38.76$ mm, where the bunch approaching the bunch compressor has a first-order chirp of $h_1 = 44.87$ m⁻¹, the boundaries between the caustics and non-caustics regions can be calculated. Figure 6 shows the resulting expressions plotted over a range and domain of second-order and third-order chirp values.

Also shown in Fig. 6 is the initial working point, which was calculated through simulations to be $(h_3, h_2) = (1.30 \times 10^8 \text{ m}^{-2}, 3893.8 \text{ m}^{-3})$. This places the working point in the region where we expect to see the double current-horn profile forming, and indeed current horns are seen in simulations results (as shown later in Fig. 7c). Through adding an octupole with a normalized field strength of K_3 =-1007 m⁻³ to BC1, the longitudinal phase space distribution is altered, with the third-order component of the chirp being most strongly influenced. Passing through Linac 2, also alters the second- and third-order of the bunch through the influence of the longitudinal wakefields. Nevertheless with the addition of the octupole in BC1, the third-order chirp is reduced to a large enough degree, that the bunch arriving at BC2 has the property of $(h_2, h_3) = (0.83 \times 10^8 \text{ m}^{-2}, 4425.2 \text{ m}^{-3})$. This places the working point in the non-caustic region of Fig. 6.



Fig. 6. Regions of h_2 , h_3 space where single, multiple, or zero caustics are expected to be found. Position (1) indicates the working point of the standard 4-dipole chicane where $R_{56} = -19.38$ mm. Through addition of an octupole to BC1, the working point can be moved from position (1) to position (2) which lies in a non-caustic region, and therefore is a working point for which current horns will not form.

Particle tracking simulations were written in "Electron Generation and Tracking" (elegant) software toolkit¹⁶, to test this theoretical analysis. Figure 7 shows the the longitudinal phase space and associated current profile at the end of linac 2 without and with the inclusion of the octupole in BC1. With the absence of any higher-order magnets in the chicanes, the current spikes are clearly visible in Fig. 7c. After the inclusion of an octupole in the low-energy compressor, the current spikes have been suppressed, resulting in a more uniform current profile (see Fig. 7d).

Figure 8 shows the slice properties (slice emittances, mean x' position, and mean x centroid position) for this S-band example. Again the data shows the two cases of without and with the inclusion of an octupole in BC1. The slice emittance in x and y is maintained between the two cases. However Fig. 8c shows that the x-centroid position remains closer to zero for the case of the second layout where the octupole in used. This results in the overall lower projected horizontal emittance.

Table 1 lists the beam properties at the end of linac 2 for the two configurations. Included in the table are the emittance values (both projected and slice), showing that it is possible to reduce the projected emittance by 48.45% with an octupole included in BC1.

It should be noted that inclusion of an octupole in a dispersive region is just one method of suppressing current horns through this caustic approach. Alternative solutions are discussed in Sec. 2.2. It can also be noted that placing a single octupole in a chicane causes the T_{166} and T_{266} to no longer go to zero at the end of the bunch compressor. Due to the large correlated energy spread, this residual horizontal dispersion terms can create a slice variation of the twiss parameters along the bunch which can lead to emittance growth (although the overall effect of removing the current horns is still a reduction in the emittance, see Table 1), and could make matching of the beam to the undulator section more difficult. Promising alternative methods for manipulating U_{5666} , which avoid slice variation in the Twiss parameters, are currently being investigated.



Fig. 7. Longitudinal phase space distribution and current profiles at the end of the S-band linac without CSR or laser heating included in the simulation for (a) without any multipole magnets and (b) with an octupole included in BC2. Note the head of the bunch corresponds to negative values of longitudinal position.

Table 1. Beam properties at the end of the final linac section, for the Baseline layout and Layout 2 which includes the octupole in BC1.

Parameter	Symbol	Units	Baseline	Layout 2
Bunch length	σ_z	$\mu \mathrm{m}$	7.80	7.78
Energy spread	$\sigma_{\Delta E/E}$	%	0.0183	0.0157
Total compression ratio	$C\dot{R}$	-	103.75	103.38
Bunch charge	Q	pC	250	250
Electron energy	\mathbf{E}	${\rm GeV}$	6.46	6.46
Projected horizontal emittance	$\epsilon_{n,x}$	mm mrad	1.241	0.836
Mean horizontal slice emittance	$\epsilon_{s,n,x}$	mm mrad	0.422	0.357
Projected vertical emittance	$\epsilon_{n,y}$	mm mrad	0.281	0.281
Mean vertical slice emittance	$\epsilon_{s,n,y}$	mm mrad	0.242	0.248

2.2. Alternative Solutions

In the previous section, we outlined one method to find a non-caustic solution as defined by Eq. (1). From Eq. (1), we can see that the control parameters are R_{56} , T_{566} , U_{5666} , h_1 , h_2 and h_3 . Therefore in order to control how or if caustic current spikes form, we can modify either the optics of the dispersive region (R_{56} , R_{56} , M_{566} , M_{5666} , M_{56} , M_{566} , M_{566} , M_{566} , M_{566} , M_{566} , M_{566} , M_{56} , M_{566} , M_{566} , M_{56} , M_{566} , M_{56} , M_{566} , M_{56}



Fig. 8. Slice properties of the bunch at the end of the S-band linac for without an octupole (\bullet) , and with an octupole (*) in BC1. The *x* centroid offset and the variation in x' along the length of the bunch cause increased projected emittance growth of the baseline design.

 T_{566} , and U_{5666}), or the properties of the bunch entering the dispersive region $(h_1, h_2 \text{ and } h_3)$. In the previous section, we altered h_3 (and to a lesser extent h_2) through changing the optics of the compressor upstream. Collective effects, such as wakefields and space charge forces, also influence these higher-order components of the chirp and should be taken into account when manipulating the chirp at one position along the accelerator to achieve a particular chirp at a later stage of the accelerator. Aside from adding sextupole or octupole magnets to a dispersive region upstream of the compressor of interest, there are other mechanisms that could alter the bunch properties to achieve a similar effect. For example the choice of RF phase in a harmonic cavity can significantly influence h_2 , but will also influence h_3 .

As mentioned earlier, T_{566} , and U_{5666} could be directly manipulated through placing sextupole and/or octupole magnets placed in a dispersive region. A recent publication detailed this option for both an X-band and an S-band linac³. Finally there is an option for dividing this longitudinal phase manipulation over two or more dispersive sections. These are just a few of many possible techniques that could be employed to enhance or avoid caustics as necessary.

3. Conclusion

These proceedings summarize what caustics are and how they present in accelerator physics. An example of beam shaping using caustic theory was presented, showing how a double-horned current profile could be shaped into a more uniform current profile. This was achieved through consideration of the underlying caustic formation and altering the high-order components of the chirp of a bunch entering the bunch compressor.

Acknowledgments

T. K. Charles would like to thank Sven Reiche and Sara Thorin for independently pointing out the importance of the second-order horizontal dispersion, and the useful discussions that followed.

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