Improving inverse Compton sources by removing non-linearities

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We present a new, more nuanced understanding of non-linear effects in inverse Compton sources. Contrary to what has been heretofore understood, deleterious non-linear effects can arise even at low laser intensities, a regime previously viewed as linear. After laying out a comprehensive survey of all non-linear phenomena which degrade the effectiveness of inverse Compton sources, we discuss two powerful techniques designed to remove these non-linearities. Starting with the known technique of longitudinal chirping of the laser pulse, which we developed earlier to mitigate adverse non-linear effects in the high laser field regime, we have discovered that the simple stretching of the laser pulse, while keeping the energy constant, can significantly increase the spectral density of the scattered radiation in many operating regimes. Our numerical simulations show that combining these two techniques removes detrimental non-linearities and improves the performance of inverse Compton sources over an order of magnitude.

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X-rays enable scientists to see the internal structure of materials on all length scales from the macroscopic down to the positions of individual atoms. This capability has had profound impact on science, technology, and on the world economy. It is impossible to overstate this impact, from Nobel Prize winning science to the everyday dental x-ray. The science and technology community agrees that future advances in many areas depend on understanding structure/function relationships at the nano-scale where new properties emerge, and controlling the fabrication of complex materials at that scale to achieve transformative physical, chemical, and biological functionality.

The sources of x-ray radiation relying upon Compton scattering [1, 2] possess a notable advantage over the traditional bremsstrahlung sources—the narrow-band nature of the radiation emerging from them. This motivated creation of designated facilities featuring inverse Compton sources (ICS) [3], which have been applied to x-ray structure determination [4], dark-field imaging [5, 6], phase contrast imaging [7], and computed tomography [8].

As a significantly more affordable alternative to large facility sources, inverse Compton sources (ICS) of x-rays may allow a multitude of studies not easily accomplished at the large facilities. These potentially groundbreaking studies in medicine, pharmaceutical industry, chemistry, material science, homeland security and many other fields of human endeavor, hold a promise of fundamentally improving our lives. However, in order to bring about this new era, we first need to develop a deeper understanding of physical processes in ICS.

In this letter, we map out the regimes of operations for ICS and describe the non-linear effects which plague each of these regimes. We then present two precise techniques which combine to largely remove these non-linearities, thereby substantially improving the peak spectral density of the scattered radiation emerging from these sources.

In ICS, a relativistic electron beam interacts with a high-field laser beam, producing intense and highly collimated electromagnetic radiation via Compton scattering [2]. Through relativistic upshifting and the relativistic Doppler effect, highly energetic polarized photons are radiated along the electron beam motion when the electrons interact with the laser light.

The strength of the laser field is quantified by the amplitude \( a_0 \) of the normalized vector potential \( \hat{A}(\xi) = eA(\xi)/m_ec = a(\xi)\cos(2\pi\xi/\lambda) \), where \( a(\xi) \) is the amplitude envelope, \( \xi = z + ct \) is the coordinate along the laser pulse, \( \lambda \) the wavelength of the laser. At high laser field intensities, the spectrum of backscattered radiation

\[ \text{FIG. 1: Regimes of operation of ICS, as listed in Table 1. Blue line pointing downward represents stretching the laser pulse (increasing its length } \sigma_{l,z} \text{), while keeping the energy of the laser constant } (a_0^2\sigma_{l,z} \text{ = const.}). \text{ Red lines pointing to the left represent chirping the laser pulse, which removes subsidiary peaks. Stars denote parameters for simulations carried out in Fig. 2 and 3, each color corresponding to the spectrum of the same color.} \]
is considerably broadened because of the changes in the longitudinal velocity of the electrons during the pulse. Such ponderomotive line broadening in the scattered radiation makes the bandwidth too large for some applications and reduces the spectral brilliance.

The onset of non-linear ponderomotive line broadening has been associated with the increase of the laser field strength \[8,10\]. However, we present a more nuanced analysis of the origins of non-linearities which fall under the umbrella of ponderomotive broadening. This analysis, illustrated in Fig. 1 and detailed in the text, helps us devise ways of removing non-linearities from ICS.

The two main mechanisms which bring about non-linear ponderomotive broadening of the spectra are: (1) non-linear subsidiary peaks and (2) non-linear redshift. The interplay between the two effects is shown in Fig. 1 with each axis quantifying the importance of each.

Linear spectrum features solitary, narrow peaks. One of the signatures of spectral non-linearities is the appearance of multiple peaks around each harmonic. These non-linear subsidiary peaks in the scattered spectra at high laser intensities been observed and their number empirically approximated for a gaussian laser envelope and \(\lambda = 800\) nm in Refs. \[11,12\]. The exact number of subsidiary peaks for an arbitrary laser envelope and wavelength was derived in Ref. \[9\]. For a gaussian envelope we consider here, it is

\[
N_\tau = \sqrt{\pi} \, \frac{a_0}{\lambda} \, \sigma_{l,z}, \tag{1}
\]

where \(\sigma_{l,z}\) is the length of the laser pulse. For \(N_\tau > 1\), additional peaks appear in the spectrum, thereby reducing the spectral density in the primary peak.

From the Eq. (1), it follows that the number of subsidiary peaks does not depend on the strength of the laser field \(a_0\) alone, but on the combination of the strength of the laser field and the length of the laser, \(a_0^2 \sigma_{l,z}\). Therefore, it is possible for a spectrum to feature non-linear subsidiary peaks even at low \(a_0\), a regime previously viewed as linear, if the laser is long enough. The spectrum shown in blue in Fig. 2, which represents \(a_0 = 0.1\), is an illustration of such a case.

Removing subsidiary peaks and restoring the narrow-band nature of the spectrum is accomplished by exact laser chirping, which changes the normalized vector potential to \(A(\xi) = a(\xi) \cos(2\pi \xi f(\xi)/\lambda)\), where \(f(\xi)\) is the chirping prescription \[9\].

\[
f(\xi; a_0) = \frac{1}{1 + a_0^2/2} \left( 1 + \frac{1}{2 \xi} \int_0^{\xi} a^2(\xi') d\xi' \right). \tag{2}
\]

Exact laser chirping was shown to be perfectly effective for restoring narrow-band property of the scattered radiation produces in scattering a 1D plane wave laser with an on-axis, single-electron \[9\] and an electron beam with an energy spread \[13\]. Improving the laser model to a 3D laser pulse, brought about a generalized chirping prescription when colliding with a single on-axis electron \[13\], which, while not perfect, is still quite effective. Finally, in a realistic scenario of a collision between a 3D laser pulse and a general electron beam distribution, we have shown that the optimal form of laser chirping can be found using an optimization over the parameters of the chirping prescription \[10\]. The effectiveness of such chirping depends on the relative transverse sizes of the two colliding beams and can still be quite effective when the transverse size of the laser pulse is roughly the size of the electron beam or larger \[10\].

Therefore, the laser chirping removes subsidiary peaks, leaving only one dominant peak per harmonic. The effect on laser chirping on the landscape of regimes of operation for ICS shown in Fig. 1 is to move horizontally from the region where \(N_\tau \gg 1\) to the region where \(N_\tau \approx 1\).

Linear spectrum contains a narrow peak centered around the frequency \(\omega_0 = (1 + \beta)^2 \gamma^2 2\pi c/\lambda\). As the magnitude of the normalized vector potential \(a_0\) grows, the peak experiences non-linear red-shift:

\[
\omega = \frac{\omega_0}{1 + a_0^2 / 2}. \tag{3}
\]

The non-linear shift is accompanied by widening of the peaks. This is evident from the comparison of the location of the primary harmonic in spectra in Figs 2a,2b.

From the Eq. (3), it is clear that the non-linear shift will be reduced if \(a_0\) is reduced. If the total energy in the laser pulse is kept constant, the reduction in \(a_0\) can only come at an appropriate increase in the laser volume \(V\), because the laser intensity \(I\) is given by

\[
I = \frac{c E}{V} = \frac{2\pi^2 m_e^2 c^3}{\lambda^2 e^2 \mu_0} a_0^2, \tag{4}
\]

where \(E\) is the laser energy

\[
E = \frac{2\pi^2 m_e^2 c^3}{\lambda^2 e^2 \mu_0} a_0^2 V. \tag{5}
\]

For a gaussian laser pulse, both transversally and longitudinally, \(V = (2\pi)^{3/2} \sigma_{l,x} \sigma_{l,y} \sigma_{l,z}\), where \(\sigma_{l,x}\) is the horizontal and \(\sigma_{l,y}\) vertical size of the laser pulse. \(m_e\) is the mass of the electron, \(c\) is the speed of light, \(e\) is the elementary charge and \(\mu_0\) is the permeability of vacuum. Therefore, to keep energy constant, reducing \(a_0\) by some factor is accomplished by making the volume (the transverse or longitudinal size, or combination thereof) larger by a square of that factor. In the case of the 1D laser pulse model, the only way to increase the volume of the laser is by stretching it (increasing its longitudinal size). In the case of a 3D laser pulse model, the increase in volume can be done by either stretching the beam or increasing its cross-section (transverse size). However, increasing
the cross-section of the laser while keeping the energy constant will result in the net reduction of peak spectral density. While increasing the transverse size of the laser pulse leads to a more favorable distribution of effective laser field strength parameter \(a_0\) that electrons experience [10], the peak spectral density will be dominated by its dependence on \(a_0^2\sigma_{l,z}^2\) [13].

This realization suggests a simple method of reducing the deleterious effects of non-linear red-shift: stretching the laser beam while keeping its energy constant. The effects of this approach on peak spectral density are presented next, first for the 1D plane wave and then for the 3D pulse laser model.

We verify these ideas through numerical simulations. The theory and the code for an on-axis, single-electron collision with a 1D laser pulse was developed in Ref. [8]. In Ref. [9], we modified it to model an arbitrary laser chirp. The code has been further improved to carry out simulations for electron beams with energy spread [14].

Finally, we recently developed another code, still based on the original theory developed for a single-electron scattering off a 1D laser pulse [8, 9], to model scattering of a 3D laser pulse (chirped or unchirped) off a realistic electron beam (with emittances and energy spread). This is the most general code, named SENSE (Simulation of Emitted Non-linear Scattering Events), subsuming all previous versions. It is described in detail in Ref. [10]. It is valid in a regime where electron recoil can be neglected, or, in terms of the subsidiary peaks, \(N_r \lesssim 3/(4a_0) \approx 103\), where \(a_0\) is the fine structure constant. This is not a very restrictive range, because most, if not all, existing and future ICS are situated comfortably within this regime. SENSE can be used to compute a spectrum from a single, on-axis electron scattering off a 1D plane wave (using a 3D model in the 1D limit \(\sigma_{l,x}, \sigma_{l,y} \gg \sigma_{l,z}\)). We can also use it for fully realistic simulations—including electron beams with energy spread and emittance and a 3D laser pulse with finite transverse extent—of an existing ICS.

The individual effects of stretching of the laser and chirping are best visualized separately. We do that by following the path marked by the colored stars in Fig. 1. We start with an unchirped case with high \(a_0\) (the black star in Fig. 1 and the black line in Fig. 2a) and stretch the laser pulse to the unchirped case with a low \(a_0\) (the blue star in Fig. 1 and the blue line in Fig. 2a), shown in Fig. 2a. We then chirp the laser for both the low-\(a_0\) (the red star Fig. 1 and the red line in of Fig. 2a), and the high-\(a_0\) case (the green star Fig. 1 and the green line in Fig. 2a), shown in Fig. 2b.

While at constant energy \((a_0^2\sigma_{l,z} = \text{const.})\), the spectra look similar in shape when scaled by the non-linear offset \(1/(1 + a_0^2/2)\). In the low-\(a_0\) regime, the height of the peak is directly proportional to \(a_0^2\sigma_{l,z}^2\) [13]:

\[
\frac{d^2E}{dE'd\Omega} = \frac{\pi\alpha}{2}\gamma^2(1 + \beta)^2a_0^2\sigma_{l,z}^2/\gamma^2,
\]

where it is assumed that the collecting aperture is small enough that the spread it generates is less than the spread from the pulse and the spectral height is less than the pedestal level [14]. Therefore, at constant \(a_0^2\sigma_{l,z}\), the peak spectral density scales as \(a_0^2\). This dependence is verified in simulations for \(a_0 \lesssim 0.5\), carried out for the fixed laser energy \((a_0^2\sigma_{l,z} = \text{const.})\) and is shown in Fig. 2a, for both unchirped and chirped lasers. For \(a_0 \gtrsim 0.5\), the drop in peak spectral density with increasing \(a_0\) is even more precipitous because of (1) the relative importance of the higher-order harmonics increases with \(a_0\), from being negligible at \(a_0 \lesssim 0.5\) to rivaling the primary harmonic at \(a_0 \gtrsim 1\) [13]; and (2) the complete merger of all harmonics at \(a_0 \gtrsim 2\).

Taking a couple of steps forward in terms fidelity of computational modeling to the physical problem, we carry out numerical simulations with SENSE for a collision of an electron beam—specified by its bulk properties of emittance, size and energy spread—and a 3D laser pulse. We use parameters from an actual experiment, and simulate what would happen if the laser in the experiment was changed—stretched and/or chirped. Chirping is implemented by varying \(a_0\) in Eq. (2).

We model an experiment at the ICS in Dresden, reported in Ref. [16], which we recently simulated in detail [10]. In our simulation, the electron beam is kept constant, possessing the same properties as the electron beam in the Dresden experiment [16]. Here we focus on the largest laser field strength reported, \(a_0 = 1.6\), because in this case the non-linearities are most pronounced.

Again, we visualize the individual effects of stretching of the laser and chirping separately by following the path marked by the colored stars in Fig. 1. We do that by following the path marked by the colored stars in Fig. 1. We start with an unchirped case with high \(a_0\) (the black star in Fig. 1 and the black line in Fig. 3a) and stretch the laser pulse to the unchirped case with a low \(a_0\) (the blue star in Fig. 1 and the blue line in Fig. 3a), shown in Fig. 3a. We then chirp the laser for both the low-\(a_0\) (the red star Fig. 1 and the red line in Fig. 3a), and the high-\(a_0\) case (the green star Fig. 1 and the green line in Fig. 3a), shown in Fig. 3b.

The improvements in peak spectral density due to chirping are considerably more modest for scattering off an electron beam than in the case of a single, on-axis electron. As the electrons from a beam distributions

| Regime             | \(\sigma_{l,z}^2\) | \(a_0\) | Non-linearities |
|--------------------|--------------------|--------|----------------|
| Linear (white)     | \(N_r \leq 1\)     | \(a_0 \leq 0.5\) | none            |
| Non-linear (green) | \(N_r \geq 1\)     | \(a_0 \leq 0.5\) | subs. peaks     |
| Non-linear (blue)  | \(N_r \leq 1\)     | \(a_0 \geq 0.5\) | red-shift       |
| Non-linear (aqua)  | \(N_r \geq 1\)     | \(a_0 \geq 0.5\) | red-shift, subs. peaks |

TABLE I: Regimes of operations for ICS, as shown in Fig. 1, color-coded.
collide with a laser pulse, they will experience a wide range of laser field strength parameters $a_0$ \[^\text{[10]}\]. Exact chirping prescription in Eq. (2) depends on $a_0$, and can perfectly compensate the non-linearities in the spectrum only for electrons experiencing one value of the laser field strength. Therefore, the majority of the electron distribution does not see the perfect chirping prescription.

As the laser field strength $a_0$ reduces while keeping the energy constant, the longitudinal size of the laser $\sigma_{l,z}$ increases, and the energy spread of the pulse decreases. Stretching the laser pulse reduces its energy spread—in both chirped and unchirped case—and its contribution to the scattered linewidth becomes negligible when compared to the other sources, such as electron beam emittance. This is indeed observed from Fig. [3]: a spectrum dominated by electron beam emittance where chirping is a non-factor. A comprehensive discussion of the scaling laws in ICS is presented in Refs. [15–19], along with clear illustrations of what spectra dominated by various sources of linewidth look like. The asymmetry and the hard high-energy edge in the spectrum in Fig. [3] are clear signs of dominace of electron beam emittance.

In Ref. [10], we demonstrate that the effectiveness of chirping in improving the peak spectral density becomes more pronounced as the electron beam emittance is reduced. This is to be expected, since reducing the beam emittance, reduces its size relative to that of the laser pulse, thereby approaching the 1D plane wave limit [10].

The impact of laser stretching on peak spectral density is still substantial. In the case simulated here, beam stretching from the nominal experimental setup for $a_0 = 1.6$ to $a_0 = 0.1$ increases the peak spectral density by about a factor of 10.

As the laser pulse is stretched, it experiences an hourglass effect which reduces the rate of interaction [20]. The reduction with respect to the nominal parameters at $a_0 = 1.6$ and $\sigma_{l,z} = 4.46 \, \mu m$ is shown in Fig. [1]. For the case considered here, it is not significant—on the order of 30% at $a_0 = 0.1$.

We put forward a new, more subtle, understanding of non-linearities in ICS. One novel realization is that non-linear subsidiary peaks in the scattered spectra can arise even at low values of the laser field strength parameter $a_0$, a region previously thought of as linear. Another new idea presented here, more profound and consequential in magnitude, is that the deleterious non-linear redshift can be removed by stretching the laser pulse while keeping its energy constant. This stretching alone improves the peak spectral density by over an order of magnitude. In cases when the linewidth of scattered radiation is not dominated by the electron beam emittance, laser chirping can be useful removing subsidiary peaks from individual spectra, thereby further improving the peak spectral density. Overall, combining these two approaches—stretching and chirping of the laser beam—removes both non-linear manifestations which are detrimental to spectral linewidth: non-linear red-shift and subsidiary peaks, thereby substantially improving the performance of ICS.

The most important implication of our findings is that the ICS do not need high-field lasers to produce high-yield radiation. In fact, given the same laser energy, operating at lower field strengths increases the peak yield by a substantial factor, often exceeding an order of magnitude. Our findings substantially reduce the challenge of designing and operating high-field lasers, thereby lowering their cost and increasing the prospect of their widespread availability.

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FIG. 3: Spectra for a scattering event as for $a_0 = 1.6$ in Ref. [10]: 45 MeV electron beam with normalized transverse emittances $\epsilon_{x,n} = 20.3$ mm mrad, $\epsilon_{y,n} = 18$ mm mrad, transverse size $\sigma_x = 41 \mu m$, $\sigma_y = 81 \mu m$, and the energy spread of 0.00175, colliding with a 3D plane wave laser with wavelength of $\lambda = 800$ nm and transverse size $\sigma_{1,x} = \sigma_{1,y} = 13.59 \mu m$. Panels (a) and (b) use the same arbitrary units. (a): Unchirped (black line) and chirped (green line) laser with $a_0 = 1.6$; experimental data from Ref. [10] (grey points). Chirping increases the peak spectral density by 16%. (b): The laser pulse is stretched longitudinally so as to keep $a_0^2 \sigma_{1,x} = \text{const.}$: unchirped (blue line) and chirped (red line) laser with $a_0 = 0.1$ (blue line) and $\sigma_{1,x} = 1.14$ mm. Chirping is a non-factor. Stretching increases the peak spectral density by about 12 times for both unchirped and chirped lasers. (c): The relative increase in peak spectral density, normalized to the spectral density of the unchirped case at $a_0 = 1.6$, as a function of the laser field strength parameter $a_0$.

FIG. 4: Hourglass reduction factor as a function of the size of the laser pulse, normalized to the value at nominal parameters $a_0 = 1.6$ and $s = 5.57$.

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