Tutorial of Fourier Transform for ultrafast optics

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This tutorial is designed for individuals who are new to the field of ultrafast optics. It was written in response to the apparent lack of comprehensive introductions to the basic Fourier Transform, extending beyond the flat-phase description. Additionally, there is a need for complete derivations of several relations involving the Fourier Transform, maintaining its most general formulation. This approach avoids the arbitrary selection of Fourier-Transform coefficients and ensures a complete understanding. It shows the importance of having Fourier-Transform coefficients as parameters, which I would like to advocate people to do. Most important of all, I've seen misuse of Fourier Transform over my years of discussion in the lab and from others' questions since I shared my code publicly on Github. Surprisingly, since people check the correctness of numerical implementation only by seeing if the simulation result is smooth and if it duplicates the "overall physics," this seems to be a widespread problem from my perspective, which can be solved by a simple tutorial (see Sec. 2B). This is why I hope that this tutorial can help people understand more about the Fourier Transform, especially in the context of ultrafast optics.

Feel me to send me an email if there is any confusion, or you think that there is more to add to this tutorial.

1. ANALYTIC SIGNAL

When we learn ultrafast optics with textbooks, such as Boyd's Nonlinear Optics [1], they usually start with the field equation for the real-valued field:

$$\mathbb{E}(t) = \frac{1}{2}\left(\mathcal{E}(t) + \mathcal{E}^*(t)\right) = \frac{1}{2}\left(E(t)\mathrm{e}^{-i\omega_0 t} + E^*(t)\mathrm{e}^{i\omega_0 t}\right) \tag{S1}$$

or simply assume, for the complex-valued field:

$$\mathcal{E}(t) = E(t)\mathrm{e}^{-i\omega_0 t}. \tag{S2}$$

These two equations make intuitive sense if the field is a simple sinusoidal wave that follows $\mathbb{E}(t) = \sin(\omega t) = \frac{\mathrm{e}^{i\omega t} - \mathrm{e}^{-i\omega t}}{2i}$ so that the coefficient $E(t)$ in Eq. (S1) is just $\frac{-1}{2i}$. During nonlinear studies, there are usually conversions between temporal and spectral components through Fourier Transform. However, a lack of deep understanding about how to correctly decompose the field following the form of Eq. (S1) results in a mixed use of Fourier Transform of the real-valued $\mathbb{E}(t)$ and complex-valued $\mathcal{E}(t)$. This mistake even misleads researchers from obtaining all generated frequencies and leads to the paper discussing negative frequencies [2]. The correct decomposition should follow the analytic-signal decomposition, which decomposes the real-valued signal into its positive- and negative-frequency components. The positive-frequency part is called the "analytic signal," whose complex conjugate is the negative frequency part of the real-valued signal.

Any derivations of nonlinear optics should start with the real-valued $\mathbb{E}(t)$, followed by its decomposition into the "analytic signal." If a derivation starts with a single complex-valued $\mathcal{E}(t)$ (either the positive- or negative-frequency part), then readers need to be cautious about two things: (1) whether there is any missing frequency component due to ignoring the complex-conjugate part, and (2) whether there is a deviation of a factor of two. As an example, [3] starts with the complex-valued field for deriving the Raman-induced index change, which eventually deviates from the result that correctly starts with the real-valued field [Eq. (S1)] by a factor of $\frac{1}{2}$. This is why in their paper, they reported a deviation of a factor of two between their theory and experiments. (Correct derivation with analytic signal, as well as generalization to an arbitrary polarization, is in my work [4].) I have seen several other examples (in research papers) throughout the years. Therefore, in this section, I will introduce analytic signal that underlies correct complex-valued decomposition of any real-valued signal.

An analytic signal is a complex-valued function that has no negative-frequency part. If $s(t)$ is a real-valued function with Fourier Transform $S(f)$, then it exhibits the Hermitian symmetry about $\nu = 0$.

$$S(-\nu) = S^*(\nu). \tag{S3}$$

Thus, there is redundancy if both frequencies are considered; negative-frequency components can be discarded without loss of information.

We define $S_a(\nu)$ to represent the positive-frequency part as the following:

$$\begin{aligned} S_a(\nu) &= \begin{cases} 2S(\nu) & ,\nu > 0 \\ S(\nu) & ,\nu = 0 \\ 0 & ,\nu < 0 \end{cases} \\ &= S(\nu) + \mathrm{sgn}(\nu)S(\nu), \end{aligned} \tag{S4}$$

so that

$$\begin{aligned} S(\nu) &= \begin{cases} \frac{1}{2}S_a(\nu) & ,\nu > 0 \\ S_a(\nu) & ,\nu = 0 \\ \frac{1}{2}S_a^*(-\nu) & ,\nu < 0 \end{cases} \\ &= \frac{1}{2}\left(S_a(\nu) + S_a^*(-\nu)\right) \end{aligned} \tag{S5}$$

and thus

$$s(t) = \frac{1}{2}\left(s_a(t) + s_a^*(t)\right). \tag{S6}$$

$s(t)$ is a combination of its analytic signal $s_a(t)$ and the corresponding complex conjugate, which is the negative-frequency part of the $s(t)$.

Since analytic signal of $s(t)$ is the inverse Fourier Transform of $S_a(\nu)$,

$$\begin{aligned}
s_a(t) &= \mathfrak{F}^{-1}\left[S(\nu) + \mathrm{sgn}(\nu)S(\nu)\right] \\
&= s(t) + C_{\mathfrak{F}}\mathfrak{F}^{-1}\left[\mathrm{sgn}(\nu)\right] * \mathfrak{F}^{-1}\left[S(\nu)\right] \quad \text{with the convolution theorem [Eq. (S10a)]} \\
&= s(t) + C_{\mathfrak{F}}\left[\left(C_{\mathfrak{I}\mathfrak{F}}c_s\frac{2}{it}\right) * s(t)\right] \quad \because \mathfrak{F}^{-1}\left[\mathrm{sgn}(f)\right] = C_{\mathfrak{I}\mathfrak{F}}c_s\frac{2}{it} \\
&= s(t) + \left[\left(-\frac{ic_s}{\pi t}\right) * s(t)\right], \quad \because C_{\mathfrak{F}}C_{\mathfrak{I}\mathfrak{F}} = \frac{1}{2\pi}
\end{aligned} \tag{S7}$$

With the analytic signal, any real-valued signal can be decomposed into its positive-frequency (analytic-signal) and negative-frequency parts. This underlies the decomposition of Eq. (S1). In addition, this tells us that the Fourier Transform of the real-valued field $\mathbb{E}(t)$ is different from that of the analytic signal $\mathcal{E}(t)$. Hence, it is crucial to define clearly what is being used, especially in studies of, for example, four-wave mixing and Raman scattering that involves nonlinear evolutions of different frequencies. For example, $\vec{\mathbb{P}}(t) = \int_{-\infty}^{\infty}\chi^{(3)}(t_1,t_2,t_3)\vdots\vec{\mathbb{E}}(t-t_1)\vec{\mathbb{E}}(t-t_2)\vec{\mathbb{E}}(t-t_3)\,\mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3$ is apparently different from $\vec{\mathcal{P}}(t) = \int_{-\infty}^{\infty}\chi^{(3)}(t_1,t_2,t_3)\vdots\vec{\mathcal{E}}(t-t_1)\vec{\mathcal{E}}(t-t_2)\vec{\mathcal{E}}(t-t_3)\,\mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3$, where $\vec{\mathcal{P}}(t)$ lacks all frequency components that result from combinations including the negative-frequency components of $\vec{\mathbb{E}}(t)$.

2. SPECTRAL FOURIER TRANSFORM

In this section, we explain the Fourier Transform in its continuous and discrete formats. In addition, all coefficients are represented as parameters to be compatible with various conventions people in different fields use. I would also like to advocate people to derive their equations based on parametrized Fourier Transform, as in Eq. (S8). As I will show later, many relations are dependent on the Fourier-Transform convention and its coefficients. Various conventions out there in the world (*e.g.*, $C_{\mathfrak{F}} = 1$ or $C_{\mathfrak{F}} = \frac{1}{\sqrt{2\pi}}$ [Eq. (S8)]) can create misleading equations. For example, if an equation has π, we do not know whether it is dependent on Fourier-Transform convention or not; it can come from anywhere, such as the frequency relation $\omega = 2\pi\nu$ during derivation. Furthermore, losing the information of Fourier-Transform coefficients prevents people from correctly deriving the equations with discrete Fourier Transform used in numerical computations, as I would show later in Sec. 2C.

Here in this tutorial, the overall trend of notation follows the physical convention whose inverse spectral Fourier Transform follows $A(t) \sim \int A(\omega)\mathrm{e}^{i(k_z z - \omega t)}\,\mathrm{d}\omega$, which is the spectral Fourier Transform in mathematics or engineering. Note that in contrast to the spectral Fourier Transform, the physical convention ($k_z z - \omega t$) potentially shows that the spatial Fourier Transform $\mathfrak{F}_{k_z}$ is consistent with mathematical convention; however, we typically do not calculate based on the k_z-space. Here, we will focus only on spectral Fourier Transform.

A. Definition

In general, the Fourier Transform is defined as

$$\begin{aligned} A(\omega) &= \mathfrak{F}[A(t)] \equiv C_{\mathfrak{F}} \int_{-\infty}^{\infty} A(t)\mathrm{e}^{ic_s\omega t}\,\mathrm{d}t \\ A(t) &= \mathfrak{F}^{-1}[A(\omega)] \equiv C_{\mathfrak{I}\mathfrak{F}} \int_{-\infty}^{\infty} A(\omega)\mathrm{e}^{-ic_s\omega t}\,\mathrm{d}\omega. \end{aligned} \tag{S8}$$

If $c_s = 1$, the Fourier Transform follows the physical convention; whereas it follows the mathematical convention if it is -1. Its coefficients satisfy $C_{\mathfrak{F}}C_{\mathfrak{I}\mathfrak{F}} = \frac{1}{2\pi}$, which is found with

$$\begin{aligned} A(t) &= C_{\mathfrak{I}\mathfrak{F}} \int_{-\infty}^{\infty} A(\omega)\mathrm{e}^{-ic_s\omega t}\,\mathrm{d}\omega \\ &= C_{\mathfrak{I}\mathfrak{F}} \int_{-\infty}^{\infty} \left(C_{\mathfrak{F}} \int_{-\infty}^{\infty} A(\tau)\mathrm{e}^{ic_s\omega\tau}\,\mathrm{d}\tau \right) \mathrm{e}^{-ic_s\omega t}\,\mathrm{d}\omega \\ &= C_{\mathfrak{F}}C_{\mathfrak{I}\mathfrak{F}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A(\tau)\mathrm{e}^{ic_s\omega(\tau-t)}\,\mathrm{d}\omega\,\mathrm{d}\tau \\ &= C_{\mathfrak{F}}C_{\mathfrak{I}\mathfrak{F}} \int_{-\infty}^{\infty} A(\tau)\frac{2\pi}{|c_s|}\delta(\tau - t)\,\mathrm{d}\tau \\ &= C_{\mathfrak{F}}C_{\mathfrak{I}\mathfrak{F}} A(t)2\pi \quad \because |c_s| = 1 \\ \Rightarrow C_{\mathfrak{F}}C_{\mathfrak{I}\mathfrak{F}} &= \frac{1}{2\pi}. \end{aligned} \tag{S9}$$

Since the convolution theorem is a commonly-used relation, we show it below:

$$\mathfrak{F}[A * B] = \frac{1}{C_{\mathfrak{F}}}\mathfrak{F}[A]\mathfrak{F}[B] \tag{S10a}$$

$$\mathfrak{F}^{-1}[A * B] = \frac{1}{C_{\mathfrak{I}\mathfrak{F}}}\mathfrak{F}^{-1}[A]\mathfrak{F}^{-1}[B]. \tag{S10b}$$

The discrete counterpart is

$$\begin{aligned} \mathfrak{F}_{D_c}[A * B] &= \frac{1}{C_{\mathfrak{F}}}\mathfrak{F}_{D_c}[A]\mathfrak{F}_{D_c}[B] \\ \mathfrak{F}_{D_c}^{-1}[A * B] &= \frac{1}{C_{\mathfrak{I}\mathfrak{F}}}\mathfrak{F}_{D_c}^{-1}[A]\mathfrak{F}_{D_c}^{-1}[B] \end{aligned} \quad \text{if} \quad \begin{aligned} A(\omega) &= \mathfrak{F}_{D_c}[A(t_n)] \equiv C_{\mathfrak{F}} \sum_{n=1}^{\mathfrak{N}} A(t_n)\mathrm{e}^{ic_s\omega t_n}\triangle t \\ A(t) &= \mathfrak{F}_{D_c}^{-1}[A(\omega_m)] \equiv C_{\mathfrak{I}\mathfrak{F}} \sum_{m=1}^{\mathfrak{N}} A(\omega_m)\mathrm{e}^{-ic_s\omega_m t}\triangle\omega \end{aligned}. \tag{S11}$$

$\mathfrak{F}$ and $\mathfrak{F}_{D_c}$ are the continuous and discrete versions of Fourier Transform, respectively. $\mathfrak{N}$ is the number of discrete points. In the discrete manner, $t_n = n\triangle t$ and $\omega_m = m\triangle\omega$. The time window is $T^w = \mathfrak{N}\triangle t$, and the frequency window $\nu^w = \frac{1}{\triangle t} = \frac{\mathfrak{N}}{T^w} = \mathfrak{N}\triangle\nu$. The angular-frequency spacing $\triangle w = 2\pi\triangle\nu = \frac{2\pi}{T^w}$. If the sampling frequency is high enough, $\mathfrak{F}_{D_c}[\cdot] \approx \mathfrak{F}[\cdot]$ and $\mathfrak{F}_{D_c}^{-1}[\cdot] \approx \mathfrak{F}^{-1}[\cdot]$.

In practice, during numerical computations, we sloppily treat the result from the following discrete Fourier Transform (DFT) simply as Fourier Transform, which differs from Eq. (S11) in constants and units ($\mathfrak{F} = \frac{C_{\mathfrak{F}}}{C_{\mathfrak{F}_D}} \triangle t \mathfrak{F}_D$ and $\mathfrak{F}^{-1} = \frac{C_{\mathfrak{I}\mathfrak{F}}}{C_{\mathfrak{I}\mathfrak{F}_D}} \triangle \omega \mathfrak{F}_D^{-1}$):

$$\begin{aligned} A_D(\omega) = \mathfrak{F}_D[A(t_n)] &\equiv C_{\mathfrak{F}_D} \sum_{n=1}^{\mathfrak{N}} A(t_n) \mathrm{e}^{ic_s \omega t_n} \\ A(t) = \mathfrak{F}_D^{-1}[A_D(\omega_m)] &\equiv C_{\mathfrak{I}\mathfrak{F}_D} \sum_{m=1}^{\mathfrak{N}} A_D(\omega_m) \mathrm{e}^{-ic_s \omega_m t}. \end{aligned} \tag{S12}$$

If we replace variables following $\omega_m = m\triangle\omega = m\frac{2\pi}{T^w} = m\frac{2\pi}{\mathfrak{N}\triangle t}$ and $t_n = n\triangle t$, Eq. (S12) becomes

$$\begin{aligned} A_D(\omega_m) = \mathfrak{F}_D[A(t_n)] &\equiv C_{\mathfrak{F}_D} \sum_{n=1}^{\mathfrak{N}} A(t_n) \mathrm{e}^{ic_s \frac{2\pi}{\mathfrak{N}} mn} \\ A(t_n) = \mathfrak{F}_D^{-1}[A_D(\omega_m)] &\equiv C_{\mathfrak{I}\mathfrak{F}_D} \sum_{m=1}^{\mathfrak{N}} A_D(\omega_m) \mathrm{e}^{-ic_s \frac{2\pi}{\mathfrak{N}} nm}, \end{aligned} \tag{S13}$$

where $C_{\mathfrak{F}_D} C_{\mathfrak{I}\mathfrak{F}_D} = \frac{1}{\mathfrak{N}}$, found with the similar process to Eq. (S9).

The DFT $A_D(\omega)$ [Eq. (S12)] is denoted with an extra "D" subscript to distinguish it from $A(\omega)$ of Eqs. (S8) and (S11). Therefore, it is important to derive a relationship between $A(\omega)$ and $A_D(\omega)$, which follows

$$\frac{1}{C_{\mathfrak{F}_D}} A_D(\omega) \triangle t = \frac{1}{C_{\mathfrak{F}}} A(\omega) \tag{S14}$$

so that they obtain the same $A(t)$. For the commonly-used Fourier-Transform convention in the laser field (and the one we emphasize in this article), $c_s = 1$ so that the inverse Fourier Transform is consistent with the use of $A(t) \sim \int A(\omega) \mathrm{e}^{i(k_z z - \omega t)} \, \mathrm{d}\omega$ in physical representation. With this convention, the inverse Fourier Transform in mathematics becomes the Fourier Transform in physics, so we define $C_{\mathfrak{F}_D} = \frac{1}{\mathfrak{N}}$, the constant of the mathematical inverse DFT, such that Eq. (S14) becomes $A_D(\omega) = A(\omega)\triangle\nu / C_{\mathfrak{F}}$ in this convention.

B. Important correct application of the Fourier-Transform convention

Many physics equations are derived by assuming the phase following $(k_z z - \omega t)$, which implies that the Fourier Transform in physics is that the inverse Fourier Transform in mathematics, *i.e.*, $c_s = 1$. For example in unidirectional pulse propagation equation:

$$\begin{aligned} \partial_z A_p(z,\Omega) = & \, i\left[\beta_p(\omega) - \left(\beta_{(0)} + \beta_{(1)}\Omega\right)\right] A_p(z,\Omega) \\ & + i\frac{\omega n_2}{c} \sum_{\ell mn} \Bigg\{ \left(1 - f_R\right) S^K_{p\ell mn} \mathfrak{F}\left[A_\ell A_m A_n^* + \tilde{\Gamma}^K_{p\ell mn}\right] \\ & + f_R \Bigg\{ f_a S^{R_a}_{p\ell mn} \mathfrak{F}\left[A_\ell \left\{ h_a(t) * \left[A_m A_n^* + \tilde{\Gamma}^{R_a}_{p\ell mn}\right]\right\}\right] + f_b S^{R_b}_{p\ell mn} \mathfrak{F}\left[A_\ell \left\{ h_b(t) * \left[A_m A_n^* + \tilde{\Gamma}^{R_b}_{p\ell mn}\right]\right\}\right] \Bigg\} \Bigg\}, \end{aligned} \tag{S15}$$

where the explanation of notations can be found in [5]. Its derivation can be found in the supplement of [4] and we can see that A_p results from

$$\vec{\mathbb{E}}(\vec{r},t) = \sum_p \int \mathrm{d}\omega \frac{1}{2} \left\{ \frac{\vec{F}_p(\vec{r}_\perp,\omega)}{N_p(\omega)} A_p(z,\omega) \mathrm{e}^{i\left[\beta_p(\omega) z - \omega t\right]} + \text{c.c.} \right\}, \tag{S16}$$

where shows that A_p represents the slowly-varying envelope of the analytic signal of the real-valued electric field $\vec{\mathbb{E}}(\vec{r},t)$. Some might rewrite it in the time domain (with a narrowband assumption with Taylor-series expansion around center

frequency ω_0) as

$$\partial_z A_p(z,T) = \left\{ i\left[\beta_p^{(0)}(\omega_0) - \beta_{(0)}\right] - \left[\beta_p^{(1)}(\omega_0) - \beta_{(1)}\right]\partial_T \right\} A_p(z,T) + i\sum_{m\geq 2} \frac{(i\partial_T)^m}{m!}\beta_p^{(m)}(\omega_0) A_p(z,T)$$
$$+ \frac{i\omega_0 n_2}{c}\left[1 + \tau_{p\ell mn}(i\partial_t)\right] \sum_{\ell mn} \left\{ (1-f_R)\, S^K_{p\ell mn}\left[A_\ell A_m A_n^* + \tilde{\Gamma}^K_{p\ell mn}\right] \right.$$
$$\left. + f_R \left\{ f_a S^{R_a}_{p\ell mn}\left[A_\ell \left\{ h_a(t) * \left[A_m A_n^* + \tilde{\Gamma}^{R_a}_{p\ell mn}\right]\right\}\right] + f_b S^{R_b}_{p\ell mn}\left[A_\ell \left\{ h_b(t) * \left[A_m A_n^* + \tilde{\Gamma}^{R_b}_{p\ell mn}\right]\right\}\right] \right\} \right\}, \quad \text{(S17)}$$

but the term with $i\partial_T A(z,T)$ resulting from $\Omega A(z,\Omega)$ is related to the convention of Fourier Transform with $c_s = 1$:

$$\partial_T A(z,T) \xrightarrow{\mathfrak{F}} -ic_s \Omega A(z,\Omega). \quad \text{(S18)}$$

As a result, it is crucial to apply the correct DFT that satisfies the physical convention; *i.e.*, use mathematical (MATLAB's) ifft for Fourier Transform into the spectral domain and use mathematical (MATLAB's) fft for inverse Fourier Transform into the temporal domain. Some might think that the wrong use of Fourier Transform might simply create a signal that is a complex conjugate of the correct one. Since the analytic signal is in general complex-valued, the spectral signal transformed with mathematical fft is not a complex conjugate of the spectral signal transformed with mathematical ifft. A wrong convention of Fourier Transform simply creates a wrong result.

C. Conversion of quantities with physically-useful units between FT and DFT

In this section, we derive several formulae for conversion of physical quantities between Fourier Transform and discrete Fourier Transform.

$$\begin{aligned}
\int_{-\infty}^{\infty} |A(t)|^2 \,\mathrm{d}t &= \int_{-\infty}^{\infty} C^2_{\mathfrak{IF}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A(\omega)A^*(\omega')\mathrm{e}^{-ic_s(\omega-\omega')t}\,\mathrm{d}\omega\,\mathrm{d}\omega'\,\mathrm{d}t \\
&= C^2_{\mathfrak{IF}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A(\omega)A^*(\omega')\left[\int_{-\infty}^{\infty}\mathrm{e}^{-ic_s(\omega-\omega')t}\,\mathrm{d}t\right]\mathrm{d}\omega\,\mathrm{d}\omega' \\
&= C^2_{\mathfrak{IF}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A(\omega)A^*(\omega')\left[2\pi\delta\left(c_s(\omega-\omega')\right)\right]\mathrm{d}\omega\,\mathrm{d}\omega' \\
&= 2\pi C^2_{\mathfrak{IF}} \int_{-\infty}^{\infty} |A(\omega)|^2\,\mathrm{d}\omega, \quad \delta\left(c_s(\omega-\omega')\right) = \frac{\delta(\omega-\omega')}{|c_s|} = \delta(\omega-\omega') \\
&= \frac{C_{\mathfrak{IF}}}{C_{\mathfrak{F}}} \int_{-\infty}^{\infty} |A(\omega)|^2\,\mathrm{d}\omega. \quad \because C_{\mathfrak{IF}} = \frac{1}{2\pi C_{\mathfrak{F}}}
\end{aligned} \quad \text{(S19)}$$

Eq. (S19) leads to the general formulation of the Parseval's theorem:

$$\frac{1}{C_{\mathfrak{IF}}}\int_{-\infty}^{\infty} |A(t)|^2\,\mathrm{d}t = \frac{1}{C_{\mathfrak{F}}}\int_{-\infty}^{\infty} |A(\omega)|^2\,\mathrm{d}\omega. \quad \text{(S20)}$$

With Eq. (S14) and $\triangle\omega = \frac{2\pi}{\mathfrak{N}\triangle t}$, we can derive the discrete version of the Parseval's theorem:

$$\frac{1}{C_{\mathfrak{IF}_D}}\sum_{n=1}^{\mathfrak{N}} |A(t_n)|^2 = \frac{1}{C_{\mathfrak{F}_D}}\sum_{m=1}^{\mathfrak{N}} |A_D(\omega_m)|^2. \quad \text{(S21)}$$

Rewriting the Parseval's theorem in powers leads to $\int_{-\infty}^{\infty} P(t)\,\mathrm{d}t = \int_{-\infty}^{\infty} P(\omega)\,\mathrm{d}\omega$, where $P(t) = |A(t)|^2$. Since $P(t)$ has the unit of "W=J/s," $P(\omega) = \frac{C_{\mathfrak{IF}}}{C_{\mathfrak{F}}}|A(\omega)|^2 = \frac{1}{2\pi C^2_{\mathfrak{F}}}|A(\omega)|^2$ has the unit of "J/(rad · Hz)" [ω has a unit of "Hz/(2π) = rad · Hz"]. To calculate the spectrum with the unit of "J/Hz" numerically,

$$P(\nu) = 2\pi P(\omega) = \frac{1}{C^2_{\mathfrak{F}}}|A(\omega)|^2 = \left(\frac{\triangle t}{C_{\mathfrak{F}_D}}\right)^2 |A_D(\omega)|^2, \quad \text{(S22)}$$

by applying Eq. (S14) and $C_{\mathfrak{F}}C_{\mathfrak{IF}} = \frac{1}{2\pi}$. $\int P(\omega)\,\mathrm{d}\omega = \int P(\nu)\,\mathrm{d}\nu$ leads to $P(\nu) = 2\pi P(\omega)$. With the DFT convention we use here ($C_{\mathfrak{F}_D} = \frac{1}{\mathfrak{N}}$), it becomes $P(\nu) = (T^w)^2|A_D(\omega)|^2$.

The Parseval's theorem assumes the unit of energy (J) after the integral. However, for continuous waves, a unit in terms of *power* makes more sense in the frequency domain. With a known time window $T^w = \mathfrak{N}\triangle t$, the continuous-wave spectral energy in this time window is $P_{\text{CW}}(\omega)T^w = \frac{1}{2\pi C_{\mathfrak{F}}^2}\left|A_{\text{CW}}(\omega)\right|^2$, where $P_{\text{CW}}(\omega)$ is in "W/(rad $\cdot$ Hz)." Hence,

$$\left|A_{\text{CW}}(\omega)\right| = C_{\mathfrak{F}}\sqrt{2\pi P_{\text{CW}}(\omega)T^w} = C_{\mathfrak{F}}\sqrt{P_{\text{CW}}(\nu)T^w}, \tag{S23}$$

by use of the relation $P_{\text{CW}}(\nu) = 2\pi P_{\text{CW}}(\omega)$. $P_{\text{CW}}(\nu)$ is in W/Hz. This leads to, with Eq. (S14),

$$\left|A_{D,\text{CW}}(\omega)\right| = \frac{C_{\mathfrak{F}_D}}{\triangle t}\sqrt{2\pi P_{\text{CW}}(\omega)T^w} = \frac{C_{\mathfrak{F}_D}}{\triangle t}\sqrt{P_{\text{CW}}(\nu)T^w}, \tag{S24}$$

which results in $\left|A_{D,\text{CW}}(\omega)\right| = \sqrt{\frac{P_{\text{CW}}(\nu)}{T^w}} = \sqrt{P_{\text{CW}}(\nu)\triangle\nu}$ with the DFT convention we use here (note that $T^w = 1/\triangle\nu$).

In the common model of adding noise photon (*e.g.*, shot noise), the noise is added as a CW background with one noise photon per frequency mode/bin, or equivalently, with an one-noise-photon spectral distribution (J = W/Hz) $P_{\text{noise}}(\nu) = h\nu$ [6–9]. Eq. (S23) leads to

$$\left|A_{\text{noise photon}}(\omega)\right| = C_{\mathfrak{F}}\sqrt{T^w h\nu} \tag{S25a}$$

$$\left|A_{D,\text{noise photon}}(\omega)\right| = \frac{C_{\mathfrak{F}_D}}{\triangle t}\sqrt{T^w h\nu}, \tag{S25b}$$

Eq. (S25b) gives $\left|A_{D,\text{noise photon}}(\omega)\right| = \sqrt{h\nu/T^w} = \sqrt{h\nu\triangle\nu}$ with the DFT convention we use here.

The power spectral density $P(\omega)$ or $P(\nu)$ can also be represented in the wavelength domain. First, we derive the relation

$$\begin{aligned} & c = \nu\lambda \\ & \Rightarrow 0 = \lambda\,\mathrm{d}\nu + \nu\,\mathrm{d}\lambda \\ & \Rightarrow \mathrm{d}\nu = -\frac{\nu}{\lambda}\,\mathrm{d}\lambda = -\frac{c}{\lambda^2}\,\mathrm{d}\lambda \end{aligned} \tag{S26}$$

which leads to

$$\begin{aligned} \int P(\lambda)|\mathrm{d}\lambda| &= \int P(\nu)\,\mathrm{d}\nu \\ &= \int P(\nu)\left|-\frac{c}{\lambda^2}\,\mathrm{d}\lambda\right| = \int\left(\frac{c}{\lambda^2}P(\nu)\right)|\mathrm{d}\lambda| \\ &\Rightarrow P(\lambda) = \frac{c}{\lambda^2}P(\nu) \end{aligned} \tag{S27}$$

Because wavelength and frequency have an inverse relation, and the power is always positive, an absolute value is taken in derivation. $P(\lambda)$ has the unit "J/m," whose CW version [Eqs. (S23) and (S24)] is in "W/m."

3. DISCRETE FOURIER TRANSFORM (DFT)

In this section, I show the periodic relation of DFT (Fig. S1), which has confused me a lot before. Hope this figure can help others when thinking about when to use MATLAB's "fftshift" and "ifftshift." It is important to note that the periodicity occurs for both temporal and spectral domains. Despite various conventions of Fourier Transform, fftshift is used to shift the signal to the center of the window (move $t_x = 0$ or $\nu_x = 0$ to window's center), whether it is in temporal or spectral domain. On the other hand, ifftshift is to cancel the fftshift effect and shifts the signal to center at $t_x = 0$ or $\nu_x = 0$ (left edge of the window). t_x and ν_x represent the sampling coordinates in the temporal and spectral domains, respectively. They should not be used simply as a pair of (fft,fftshift) and (ifft,ifftshift) due to different Fourier-Transform conventions. For example, to compute the spectrum, we should follow

```
Nt = size(field,1); % the number of sampling points
dt = mean(diff(t)); % ps; temporal sampling spacing
c = 299792.458; % nm/ps; speed of light
f = f0+(-Nt/2:Nt/2-1)'/(Nt*dt); % THz; frequency coordinate; f0 is the center frequency of the freuqnency
    window, defined elsewhere
wavelength = c./f; % nm
factor_correct_unit = (Nt*dt)^2/1e3; % to make the spectrum of the correct unit "nJ/THz" [Eq. (S22)]
                                     % "/1e3" is to make pJ into nJ
spectrum = abs(fftshift(ifft(field),1)).^2*factor_correct_unit; % nJ/THz; centered at the frequency window
```

In practice, the time coordinate is placed such that the pulse at the center of the numerical time window locates at $t = 0$ in real-time (t) coordinates [Fig. S1(b)]. Do not confuse it with the pulse locating at $t_x = 0$ [Fig. S1(a)]. In principle, the time coordinate can be placed arbitrarily because numerical computations see only the sampling-point coordinate t_x or ν_x.

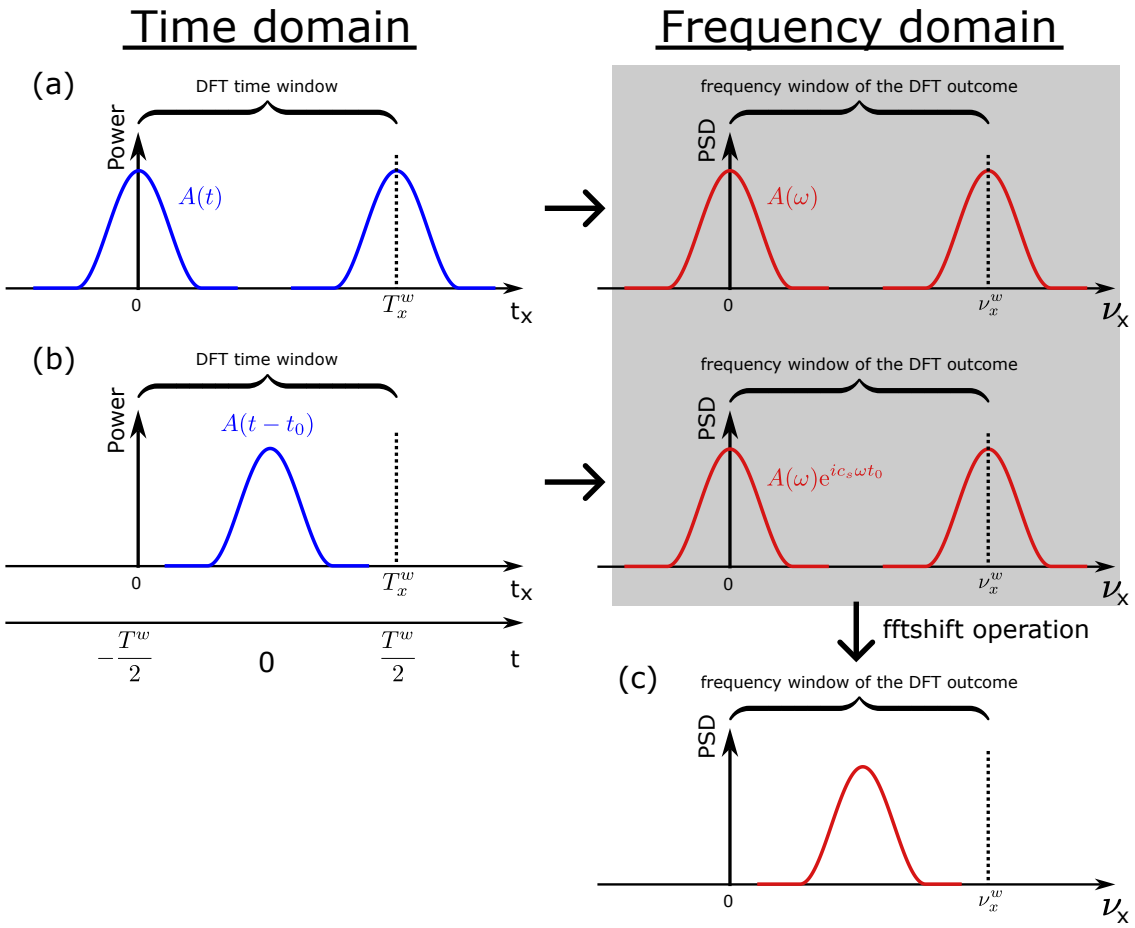

Fig. S1. DFT conversion. (a) is the "formal" use of DFT when the temporal profile $|A(t)|^2$ is centered at $t = 0$. However, in numerical simulations, it is common to place the pulse at the center of the time window for visualization purpose (b), resulting in a spectral phase shift that doesn't affect the spectral shape. (c) is the result after fftshift centers the spectrum with respect to the frequency window. PSD: power spectral density $\sim |A(\omega)|^2$. Here, the subscript "x" represents the coordinate of sampling points, rather than the actual time and frequency coordinates.

Since in nonlinear optics, convolution is commonly used, such as in computations of Raman scattering [4, 10], it is worth bringing it up again. Here, we use single-mode Raman scattering as an example, which has a term $\partial_z A(t) \propto A(t)\left(R(t) * \left|A(t)\right|^2\right)$ in limited conditions (*e.g.*, ignoring the shock-wave effect, *i.e.*, frequency dependence of nonlinearities). It follows

$$
\begin{aligned}
R(t) * \left|A(t)\right|^2 &= \frac{1}{C_{\mathfrak{F}}} \mathfrak{F}^{-1}\left[\mathfrak{F}\left[R(t)\right] \mathfrak{F}\left[\left|A(t)\right|^2\right]\right] \quad \text{with Eq. (S10a)} \\
&= \frac{1}{C_{\mathfrak{F}}}\left(\frac{C_{\mathfrak{I}\mathfrak{F}}}{C_{\mathfrak{I}\mathfrak{F}_D}} \triangle\omega\right) \mathfrak{F}_D^{-1}\left[\left(\frac{C_{\mathfrak{F}}}{C_{\mathfrak{F}_D}} \triangle t \mathfrak{F}_D\left[R(t)\right]\right)\left(\frac{C_{\mathfrak{F}}}{C_{\mathfrak{F}_D}} \triangle t \mathfrak{F}_D\left[\left|A(t)\right|^2\right]\right)\right] \quad \text{with} \begin{cases} \text{Eq. (S14)} \\ \mathfrak{F}^{-1} = \frac{C_{\mathfrak{I}\mathfrak{F}}}{C_{\mathfrak{I}\mathfrak{F}_D}} \triangle\omega \mathfrak{F}_D^{-1} \end{cases} \\
&= \frac{\triangle t}{C_{\mathfrak{F}_D}} \mathfrak{F}_D^{-1}\left[\mathfrak{F}_D\left[R(t)\right] \mathfrak{F}_D\left[\left|A(t)\right|^2\right]\right] \quad \because \triangle t \triangle\omega = \frac{2\pi}{\mathfrak{N}}
\end{aligned} \tag{S28}
$$

In our convention ($C_{\mathfrak{F}_D} = \frac{1}{\mathfrak{N}}$), $R(t) * \left|A(t)\right|^2 = T^w \mathfrak{F}_D^{-1}\left[\mathfrak{F}_D\left[R(t)\right] \mathfrak{F}_D\left[\left|A(t)\right|^2\right]\right]$, where the time window $T^w = \mathfrak{N}\triangle t$. The factor of $\frac{\triangle t}{C_{\mathfrak{F}_D}}$ [Eq. (S28)] is important and can be easily forgotten if people simply treat this as DFT convolution theorem: $R(t) * \left|A(t)\right|^2 \sim \mathfrak{F}_D^{-1}\left[\mathfrak{F}_D\left[R(t)\right] \mathfrak{F}_D\left[\left|A(t)\right|^2\right]\right]$.

4. PHENOMENA WITH COMPLEX-VALUED FOURIER TRANSFORM

Figs. S2 and S4 shows how the phase affects the signal. When the pulse has a flat phase in time domain, it is called "a transform-limited pulse." Its temporal and spectral width satisfy a fixed time-bandwidth product: a more-broadband pulse has a smaller duration. By adding a temporally (or spectrally) varying phase to the pulse, it modulates the signal. For example, adding a parabolic (second-order) phase to the temporal profile of a transform-limited signal creates a chirp, *i.e.*, varying frequency at different temporal slices, broadening the spectrum [Figs. S2(b) and S3]. The temporal frequency change follows $\triangle\omega(t) = \frac{1}{-c_s}\frac{\mathrm{d}\phi}{\mathrm{d}t}(t)$, so the phase effect to the signal is also dependent on the convention of Fourier Transform. Similarly, adding a parabolic phase to the spectral profile increases the pulse duration, which is the "dispersion" effect: different frequencies moves at different speeds, widening the pulse's temporal profile [Fig. S2(c)]. Fig. S4 shows the effect of a cubic phase.

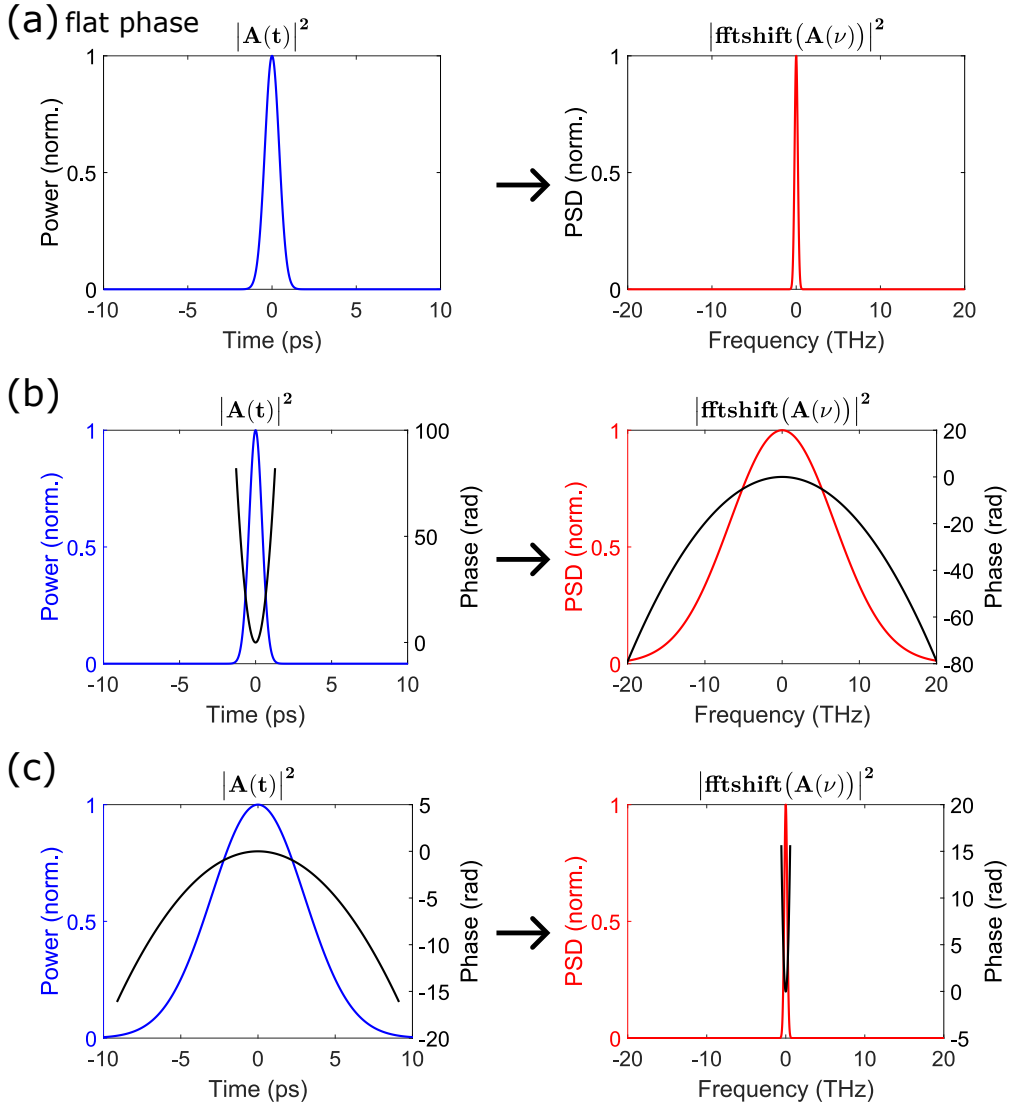

Fig. S2. DFT conversion of a second-order chirped signal. (a) transform-limited pulse that has only flat phase in time domain. (b) and (c) add a parabolic phase to the temporal and spectral profiles, respectively.

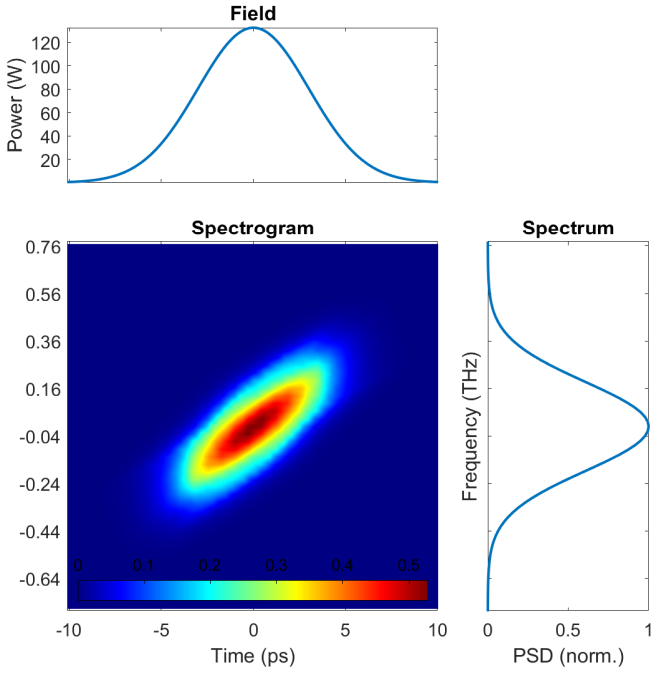

Fig. S3. Spectrogram of a parabolically-chirped signal [Fig. S2(c)]. Here, the signal is positively-chirped such that lower-frequency components are in the temporal leading edge.

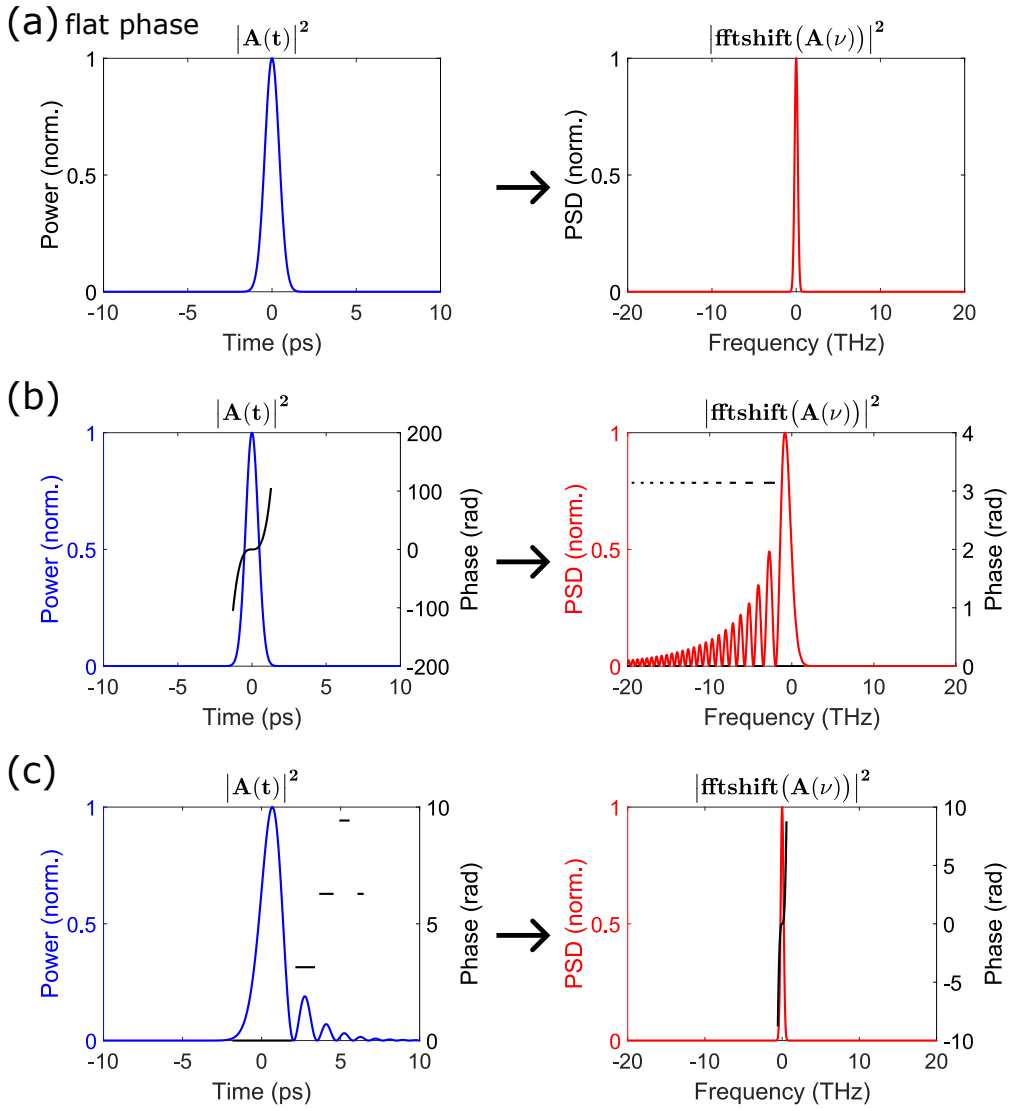

Fig. S4. DFT conversion of a third-order chirped signal. (a) transform-limited pulse that has only flat phase in time domain. (b) and (c) add a cubic phase to the temporal and spectral profiles, respectively.

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