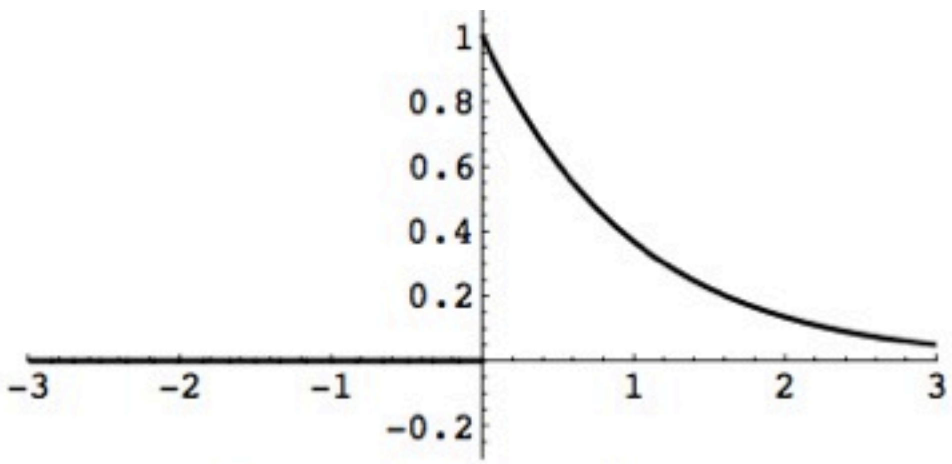
KRAMERS-KRONIG RELATION

and applications

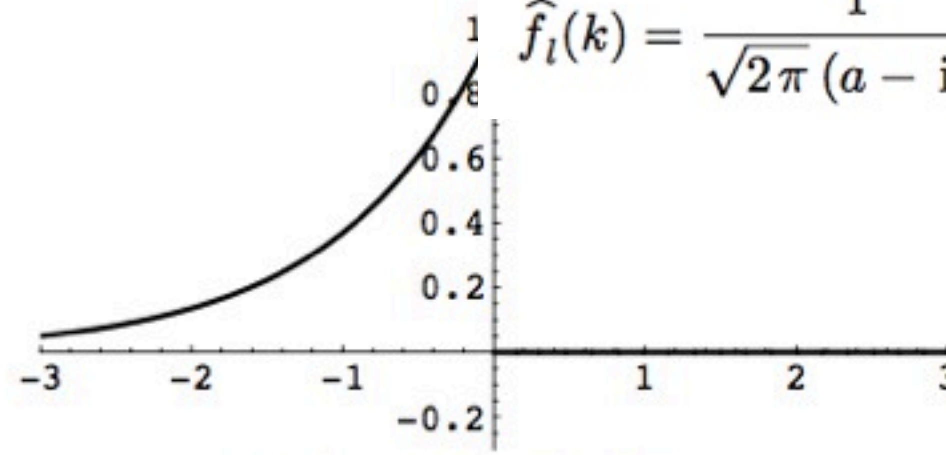
Fourier transform of pulse functions

$$\widehat{f}_r(k) = \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{-a x} e^{-\mathrm{i} k x}\, dx = -\frac{1}{\sqrt{2\pi}} \frac{e^{-(a+\mathrm{i} k)x}}{a+\mathrm{i} k} \Bigg|_{x=0}^{\infty} = \frac{1}{\sqrt{2\pi}\,(a+\mathrm{i} k)}.$$

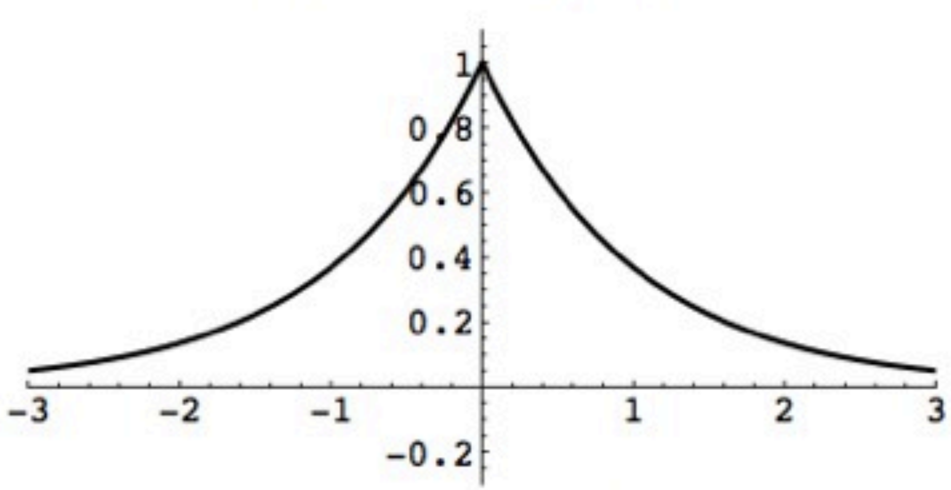
$$\widehat{f}_l(k) = \frac{1}{\sqrt{2\pi}\,(a-\mathrm{i} k)}.$$



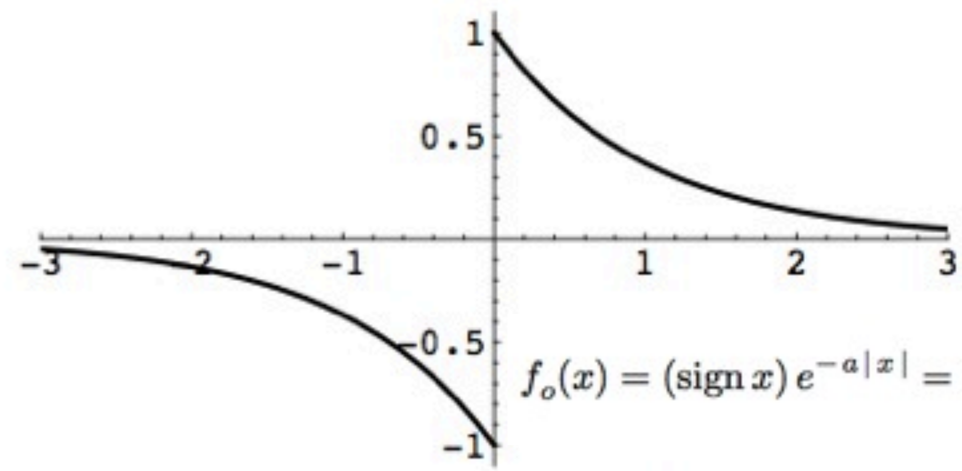
Right Pulse $f_r(x)$



Left Pulse $f_l(x)$



Even Pulse $f_e(x)$



Odd Pulse $f_o(x)$

$$f_o(x) = (\operatorname{sign} x)\, e^{-a|x|} = \begin{cases} e^{-ax}, & x > 0 \\ -e^{ax}, & x < 0 \end{cases}$$

$$f_e(x) = e^{-a|x|}$$

$$\widehat{f}_o(k) = \widehat{f}_r(k) - \widehat{f}_l(k) = \frac{1}{\sqrt{2\pi}\,(a+\mathrm{i} k)} - \frac{1}{\sqrt{2\pi}\,(a-\mathrm{i} k)} = -\mathrm{i}\sqrt{\frac{2}{\pi}}\,\frac{k}{k^2+a^2}$$

$$\widehat{f}_e(k) = \widehat{f}_r(k) + \widehat{f}_l(k) = \frac{1}{\sqrt{2\pi}\,(a+\mathrm{i} k)} + \frac{1}{\sqrt{2\pi}\,(a-\mathrm{i} k)} = \sqrt{\frac{2}{\pi}}\,\frac{a}{k^2+a^2}$$

Fourier Transform, properties

Theorem 1 *If the Fourier transform of the function $f(x)$ is $\widehat{f}(k)$, then the Fourier transform of $\widehat{f}(x)$ is $f(-k)$.*

Theorem 2 *The Fourier transform of the convolution $h(x) = f(x) * g(x)$ of two functions is a multiple of the product of their Fourier transforms:*

$$\widehat{h}(k) = \sqrt{2\pi}\, \widehat{f}(k)\, \widehat{g}(k).$$

Vice versa, the Fourier transform of their product $h(x) = f(x)\, g(x)$ is, up to multiple, the convolution of their Fourier transforms:

$$\widehat{h}(k) = \frac{1}{\sqrt{2\pi}}\, \widehat{f}(k) * \widehat{g}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widehat{f}(k-\kappa)\, \widehat{g}(\kappa)\, d\kappa.$$

Proof: Combining the definition of the Fourier transform with the convolution formula (8.52), we find

$$\widehat{h}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} h(x)\, e^{-\,i\,k\,x}\, dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x-\xi)\, g(\xi)\, e^{-\,i\,k\,x}\, dx\, d\xi.$$

Applying the change of variables $\eta = x - \xi$ in the inner integral produces

$$\widehat{h}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\eta)\, g(\xi)\, e^{-\mathrm{i}\, k(\xi+\eta)}\, d\xi\, d\eta$$

$$= \sqrt{2\pi} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\eta)\, e^{-\mathrm{i}\, k\eta}\, d\eta \right) \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(\xi)\, e^{-\mathrm{i}\, k\xi}\, d\xi \right) = \sqrt{2\pi}\, \widehat{f}(k)\, \widehat{g}(k).$$

Example: *Use the symmetry property of the Fourier transform to obtain FT of the product.*
The FT for a rectangular pulse is given by:

$$f(x) = \sigma(x+a) - \sigma(x-a) = \begin{cases} 1, & -a < x < a, \\ 0, & |x| > a, \end{cases}$$

or *box function*, of width $2a$, is easily computed:

$$\widehat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} e^{-\mathrm{i}\, kx}\, dx = \frac{e^{\mathrm{i}\, ka} - e^{-\mathrm{i}\, ka}}{\sqrt{2\pi}\, \mathrm{i}\, k} = \sqrt{\frac{2}{\pi}}\, \frac{\sin ak}{k}\, .$$

EXAMPLE:

$$f(x) = \frac{\sin x}{x}$$

is the box function

$$\widehat{f}(k) = \sqrt{\frac{\pi}{2}}\,\left[\,\sigma(k+1) - \sigma(k-1)\,\right] = \begin{cases} \sqrt{\frac{\pi}{2}}, & -1 < k < 1, \\ 0, & |\,k\,| > 1. \end{cases}$$

We also know that the Fourier transform of

$$g(x) = \frac{1}{x} \qquad \text{is} \qquad \widehat{g}(k) = -\,\mathrm{i}\,\sqrt{\frac{\pi}{2}}\,\operatorname{sign} k.$$

Therefore, the Fourier transform of their product

$$h(x) = f(x)\,g(x) = \frac{\sin x}{x^2}$$

can be obtained by convolution:

$$\begin{aligned} \widehat{h}(k) &= \frac{1}{\sqrt{2\pi}}\,\widehat{f}(k) * \widehat{g}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widehat{f}(\kappa)\,\widehat{g}(k-\kappa)\,d\kappa \\ &= -\,\mathrm{i}\,\sqrt{\frac{\pi}{8}} \int_{-1}^{1} \operatorname{sign}(k-\kappa)\,d\kappa = \begin{cases} \mathrm{i}\sqrt{\frac{\pi}{2}} & k < -1, \\ -\,\mathrm{i}\sqrt{\frac{\pi}{2}}\,k, & -1 < k < 1, \\ -\,\mathrm{i}\sqrt{\frac{\pi}{2}} & k > 1. \end{cases} \end{aligned}$$

Peter Olver: www.math.umn.edu (lecture notes)

Pairs of Fourier transforms

$f(x)$	$\widehat{f}(k)$
1	$\sqrt{2\pi}\,\delta(k)$
$\delta(x)$	$\dfrac{1}{\sqrt{2\pi}}$
$\sigma(x)$	$\sqrt{\dfrac{\pi}{2}}\,\delta(k) - \dfrac{\mathrm{i}}{\sqrt{2\pi}\,k}$
$\operatorname{sign} x$	$-\mathrm{i}\,\sqrt{\dfrac{2}{\pi}}\,\dfrac{1}{k}$
$\sigma(x+a) - \sigma(x-a)$	$\sqrt{\dfrac{2}{\pi}}\,\dfrac{\sin a\,k}{k}$
$e^{-a\,x}\,\sigma(x)$	$\dfrac{1}{\sqrt{2\pi}\,(a+\mathrm{i}\,k)}$
$e^{a\,x}\,(1-\sigma(x))$	$\dfrac{1}{\sqrt{2\pi}\,(a-\mathrm{i}\,k)}$

Pairs of Fourier transforms

$e^{ax}(1-\sigma(x))$	$\dfrac{1}{\sqrt{2\pi}\,(a - \mathrm{i}\,k)}$
$e^{-a\lvert x\rvert}$	$\sqrt{\dfrac{2}{\pi}}\,\dfrac{a}{k^2+a^2}$
e^{-ax^2}	$\dfrac{e^{-k^2/(4a)}}{\sqrt{2a}}$
$\tan^{-1} x$	$\dfrac{\pi^{3/2}}{\sqrt{2}}\,\delta(k) - \mathrm{i}\sqrt{\dfrac{\pi}{2}}\,\dfrac{e^{-\lvert k\rvert}}{k}$
$f(cx+d)$	$\dfrac{e^{\mathrm{i}\,k\,d/c}}{\lvert c\rvert}\,\widehat{f}\left(\dfrac{k}{c}\right)$
$\overline{f(x)}$	$\overline{\widehat{f}(-k)}$
$\widehat{f}(x)$	$f(-k)$
$f'(x)$	$\mathrm{i}\,k\,\widehat{f}(k)$
$x\,f(x)$	$\mathrm{i}\,\widehat{f}\,'(k)$
$f * g(x)$	$\sqrt{2\pi}\,\widehat{f}(k)\,\widehat{g}(k)$

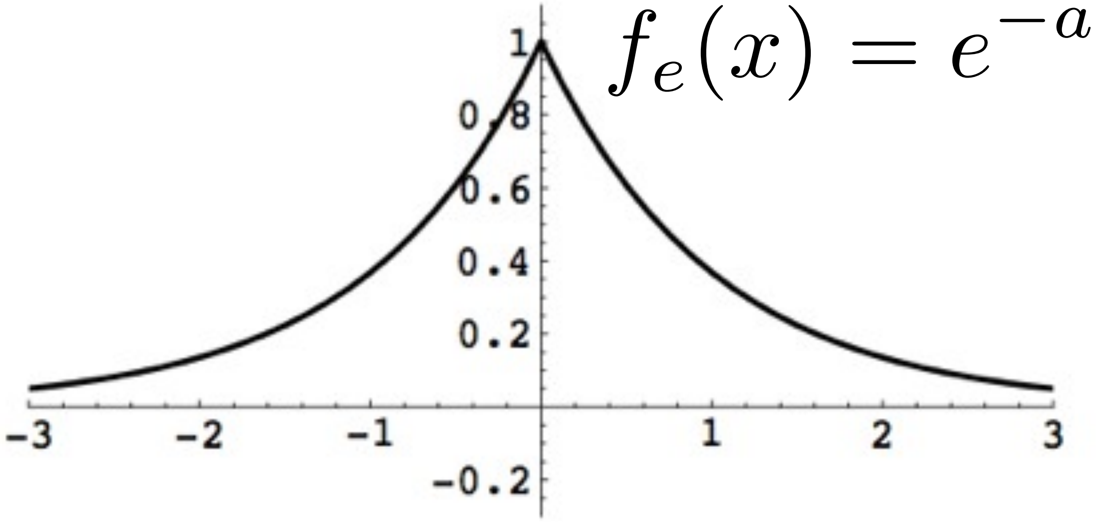
Note: The parameters a, c, d are real, with $a > 0$ and $c \neq 0$.

$$f(x) = \operatorname{sign} x = \sigma(x) - \sigma(-x) = \begin{cases} +1, & x > 0, \\ -1, & x < 0. \end{cases}$$

$$\widehat{f}(k) = -\,\mathrm{i}\,\sqrt{\frac{2}{\pi}}\,\frac{1}{k}\,.$$

$$\hat{f}(k) = \mathcal{F}[\sigma(x)] = ?$$

$$f_e(x) = e^{-a|x|}$$



Even Pulse $f_e(x)$

$$\lim_{a\to 0} f_e(x) \equiv 1$$

$$\lim_{a\to 0} \hat{f}_e(k) = \lim_{a\to 0} \sqrt{\frac{2}{\pi}} \frac{a}{k^2 + a^2}$$

$$= \begin{cases} 0 & \text{for} \quad k \neq 0 \\ \infty & \text{for} \quad k = 0 \end{cases}$$

Remind that $\delta(x) = \lim_{n\to\infty} \dfrac{n}{\pi\,(1 + n^2 x^2)} = \lim_{a\to 0} \dfrac{a}{\pi\,(a^2 + x^2)}$

FOURIER TRANSFORM OF THE HEAVISIDE FUNCTION

$$\mathcal{F}(\sigma(x)) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikx} \sigma(x) dx$$

$$\hat{f}(k) = \mathcal{F}[\sigma(x)] = ?$$

$$= \lim_{\epsilon \to 0} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikx} e^{-\epsilon x} \sigma(x) dx$$

$$= \lim_{\epsilon \to 0} \frac{1}{\sqrt{2\pi}} \frac{1}{ik + \epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{1}{\sqrt{2\pi}} \left[\frac{\epsilon}{\epsilon^2 + k^2} + \frac{-ik}{\epsilon^2 + k^2} \right]$$

$$\sqrt{\frac{\pi}{2}}\, \delta(k) - \frac{\mathrm{i}}{\sqrt{2\pi}\, k}$$

estimated as for an exponentially decaying right-handed pulse...

Causality of the response:

$$\chi(t) \to \sigma(t)\chi(t)$$

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} = \epsilon_0 (1 + \chi)\mathbf{E} = \epsilon \mathbf{E} = \epsilon_0 \epsilon_r \mathbf{E}.$$

EXAMPLE: After-effect and polarization

dielectric constant (→ ϵ)

relative permittivity (→ ϵ_r)

The polarization response is not instantaneous (the charges take time to redistribute themselves in an instantaneous application of an external electric field).

$$\mathbf{P}(t) = \epsilon_0 \int_{-\infty}^{t} \chi(t - t')\mathbf{E}(t')dt'$$

$$= \epsilon_0 \int_0^{\infty} \chi(\tau)\mathbf{E}(t - \tau)d\tau$$

C. F. Bohren, „What did Kramers and Kronig do and how did they do it ?," Eur. J. Phys. ***31*** *(2010) 573*

Evaluation of $\mathcal{F}[\sigma(t)\chi(t)]$

$$\hat{f}(k) = (\sqrt{2\pi})^{-1}\int_{-\infty}^{\infty} f(x)e^{-ikx}dx$$

$$f(x) = (\sqrt{2\pi})^{-1}\int_{-\infty}^{\infty} \hat{f}(k)e^{ikx}dk$$

$$\mathcal{F}[f(x)\equiv 1] = \hat{f}(k) = \sqrt{2\pi}\delta(k)$$

$$\delta(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}dx$$

$$\mathcal{F}[\sigma(t) * \chi(t)] = \sqrt{2\pi}\hat{\sigma}(k)\hat{\chi}(k)$$

$$\mathcal{F}[\sigma(t)\chi(t)] = (\sqrt{2\pi})^{-1}\hat{\sigma}(k) * \hat{\chi}(k)$$

$$\begin{aligned}
&\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\hat{\sigma}(k-s)\hat{\chi}(s)ds \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[\sqrt{\frac{\pi}{2}}\delta(k-s) - \frac{i}{\sqrt{2\pi}(k-s)}\right]\hat{\chi}(s)ds \\
&= \frac{1}{2}\hat{\chi}(k) - \frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{\hat{\chi}(s)}{k-s}ds \\
&= \ldots\hat{\chi}(k)
\end{aligned}$$

$$\hat{\chi}(k) = -\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{\hat{\chi}(s)}{k-s}ds$$

$$\hat{\chi}(k) = -\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{\hat{\chi}(s)}{k-s}ds$$ *AND* $$\hat{\chi}(k) = \hat{\chi}'(k) + i\hat{\chi}''(k)$$

ACCORDINGLY:

$$\hat{\chi}'(k) = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\hat{\chi}''(s)}{k-s}ds$$
$$\hat{\chi}''(k) = -\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\hat{\chi}'(s)}{k-s}ds$$

If $\chi(t)$ *real, even* ⇒ $\hat{\chi}(k)$ *real, even*

If $\chi(t)$ *real, odd* ⇒ $\hat{\chi}(k)$ *imaginary, odd*

$$\chi(t) = \chi_e(t) + \chi_o(t) \qquad \hat{\chi}(k) = \hat{\chi}_e(k) + \hat{\chi}_o(k)$$

$$\hat{\chi}'(k) = \hat{\chi}'(-k) \qquad \hat{\chi}''(k) = -\hat{\chi}''(-k)$$

Kramers-Kronig relations:

$$\hat{\chi}'(k) = \frac{2}{\pi}\int_{0}^{\infty}\frac{s\hat{\chi}''(s)}{k^2-s^2}ds$$
$$\hat{\chi}''(k) = -\frac{2k}{\pi}\int_{0}^{\infty}\frac{\hat{\chi}'(s)}{k^2-s^2}ds$$

POWER ABSORPTION

... we have defined $f(t) = Re f_0 e^{-i\omega t} = f_0 \cos\omega t \quad \hat{f}(\omega) = \pi f_0[\delta(\omega-\omega_0) + \delta(\omega+\omega_)]$

...monochromatic wave

$$ABS = \frac{1}{T}\int_0^T dt f(t)\frac{dA(t)}{dt} = -\frac{1}{T}\int_0^T \dot{f}(t)A(t)$$

$$-f(t)\frac{dA}{dt} = (A \rightarrow < A >) = -f(t)\frac{d}{dt}\int_{-\infty}^{\infty} dt'\chi(t-t')f(t')$$

$$< A(t) > = \int_{-\infty}^{\infty} dt'\chi(t-t')f(t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt'\hat{\chi}(\omega)\hat{f}(\omega)e^{-i\omega t}d\omega$$

$$= \frac{f_0}{2}\left[(\hat{\chi}'(\omega_0) + i\hat{\chi}''(\omega_0))e^{-i\omega_0 t} + (\hat{\chi}'(-\omega_0) + i\hat{\chi}''(-\omega_0))e^{i\omega_0 t}\right]$$

$$= f_0\left[(\hat{\chi}'(\omega_0)\cos\omega_0 t + \hat{\chi}''(\omega_0)\sin\omega_0 t)\right]$$

$$\boxed{\frac{1}{T}\int_0^T dt f(t)\frac{dA(t)}{dt} = \frac{1}{2}f_0^2\omega_0\hat{\chi}''(\omega_0)}$$

power dissipated

Sochocki-Plemelj formula

can be used to derive the above longly calculated integrals...

Let f be a complex-valued function which is defined and continuous on the real line, and let a and b be real constants with $a < 0 < b$. Then

$$\lim_{\varepsilon\to 0^+}\int_a^b \frac{f(x)}{x \pm i\varepsilon}\,dx = \mp i\pi f(0) + \mathcal{P}\int_a^b \frac{f(x)}{x}\,dx,$$

where $\mathcal{P}$ denotes the Cauchy principal value.

A simple proof is as follows.

$$\lim_{\varepsilon\to 0^+}\int_a^b \frac{f(x)}{x \pm i\varepsilon}\,dx = \mp i\pi \lim_{\varepsilon\to 0^+}\int_a^b \frac{\varepsilon}{\pi(x^2+\varepsilon^2)} f(x)\,dx + \lim_{\varepsilon\to 0^+}\int_a^b \frac{x^2}{x^2+\varepsilon^2}\frac{f(x)}{x}\,dx.$$

For the first term, we note that $\varepsilon/\pi(x^2+\varepsilon^2)$ is a nascent delta function, and therefore approaches a Dirac delta function in the limit. Therefore, the first term equals $\mp i\pi f(0)$.

For the second term, we note that the factor $x^2/(x^2+\varepsilon^2)$ approaches 1 for $|x| \gg \varepsilon$, approaches 0 for $|x| \ll \varepsilon$, and is exactly symmetric about 0. Therefore, in the limit, it turns the integral into a Cauchy principal value integral.

Sochocki-Plemelj formula

wide application in physics...

In quantum mechanics and quantum field theory, one often has to evaluate integrals of the form

$$\int_{-\infty}^{\infty} dE \int_0^{\infty} dt\, f(E) \exp(-iEt)$$

where E is some energy and t is time. This expression, as written, is undefined (since the time integral does not converge), so it is typically modified by adding a negative real coefficient to t in the exponential, and then taking that to zero, i.e.:

$$\lim_{\varepsilon\to 0+} \int_{-\infty}^{\infty} dE \int_0^{\infty} dt\, f(E) \exp(-iEt - \varepsilon t)$$

$$= -i \lim_{\varepsilon\to 0+} \int_{-\infty}^{\infty} \frac{f(E)}{E - i\varepsilon}\, dE = \pi f(0) - i\mathcal{P} \int_{-\infty}^{\infty} \frac{f(E)}{E}\, dE,$$

where the latter step uses this theorem.