Ambiguities in bunch shape reconstruction from spectroscopic data

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Longitudinal bunch form factor

Phase computation using theory of complex functions
Kramers-Kronig dispersion relation

Ambiguities in bunch shape reconstruction and their origin

Model calculations

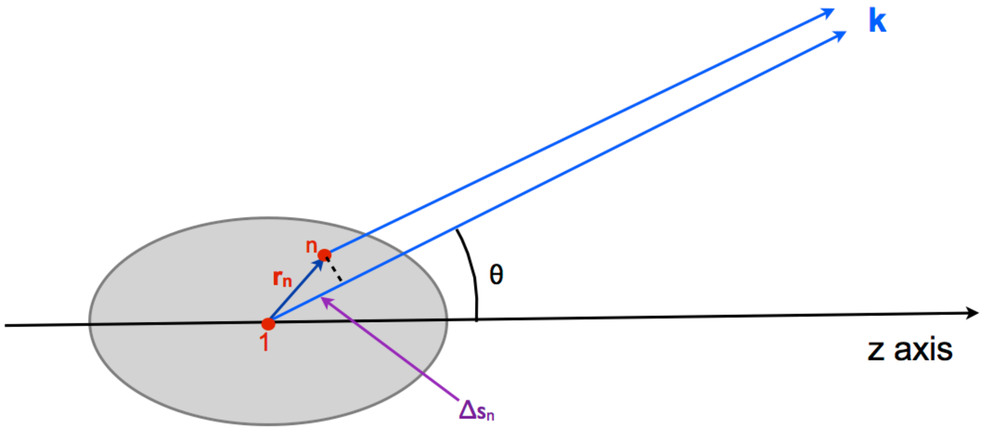
Iterative phase retrieval

Some experimental results and comparison with TDS measurements

Remarks on far-field and near-field transition radiation

Suppression of short wavelengths by transverse form factor

Coherent radiation from an electron bunch



reference electron at $r_1=0$
arbitrary electron at r_n

phase difference $\Delta\varphi_n = \Delta s_n\,(2\pi/\lambda) = \boldsymbol{k}\cdot\boldsymbol{r}_n$

total field at large distance $\tilde{E}_{\rm tot}(\boldsymbol{k}) = \tilde{E}_1(\boldsymbol{k}) \sum_{n=1}^{N} \exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}_n)$

$$\tilde{F}_{\rm 3D}(\boldsymbol{k}) = \int \rho(\boldsymbol{r}) \exp(\,i\,\boldsymbol{k}\cdot\boldsymbol{r})\,d^3r \quad \text{with} \quad \int \rho(\boldsymbol{r})\,d^3r = 1\,.$$

3D form factor

$$\left[\frac{d^2U}{d\omega d\Omega}\right]_{\rm coh} = N^2 \left[\frac{d^2U}{d\omega d\Omega}\right]_1 |\tilde{F}_{\rm 3D}(\boldsymbol{k})|^2$$

coherent radiation intensity

radiation from single electron

simplifying assumption: transverse charge density is independent of longitudinal position

$$\rho(x, y, z) = \rho_{\text{trans}}(x, y)\, \rho_{\text{long}}(z)$$

Then: 3D form factor is product of transverse and longitudinal form factor

$$\tilde{F}_{\text{3D}}(\boldsymbol{k}) = \tilde{F}_{\text{trans}}(k_x, k_y)\, \tilde{F}_{\text{long}}(k_z)\,.$$

Longitudinal bunch profile (beam radius zero)

we use time t as longitudinal coordinate

$$\mathcal{F}(\omega) = \int_{-\infty}^{\infty} \rho(t) \exp(i\,\omega\,t) dt$$

longitudinal form factor

$$\rho(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathcal{F}(\omega) \exp(-i\,\omega\,t) d\omega \quad \text{with} \quad \int_{-\infty}^{\infty} \rho(t) dt = 1$$

$$\mathcal{F}(\omega) = F(\omega)\, e^{i\,\Phi(\omega)}$$

form factor is a complex function

magnitude can be measured, phase is unknown

How can we determine the phase?

Method 1: Kramers-Kronig dispersion relation

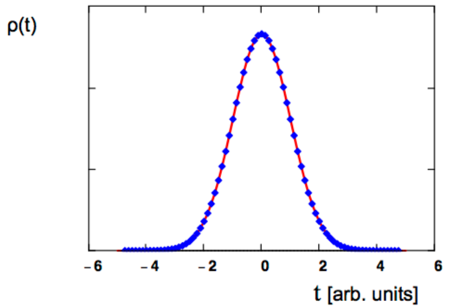
Method 2: Iterative phase retrieval

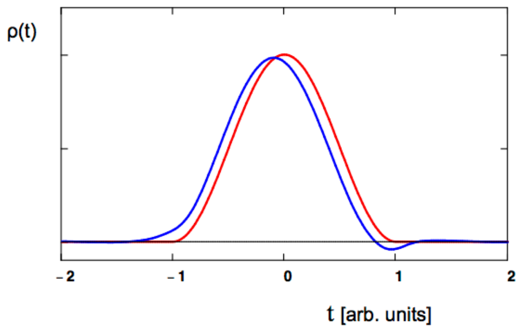
Kramers-Kronig dispersion relation

$$\Phi_{\mathrm{KK}}(\omega) = \frac{2\omega}{\pi}\mathcal{P}\int_0^{\omega_{\mathrm{cut}}} \frac{\ln(|\mathcal{F}(\omega')|) - \ln(|\mathcal{F}(\omega)|)}{\omega^2 - \omega'^2}\, d\omega'$$

rigorous derivation in Appendix A

KK works well for single Gaussian or cosine half wave





red: input distribution
blue: reconstruction

Remarks on dispersion relations

A dispersion relation is an integral formula relating a dispersive process to an absorptive process. An example is the relation between the refractive index $n(\omega)$ of an optical medium and its extinction coefficient $k(\omega)$, or the relation between real part and imaginary part of the dielectric function of a solid. Dispersion relations follow rigorously from causality. In this appendix we follow closely the book *Optical Properties of Solids* by F. Wooten [24] but we go into more detail and present several mathematical proofs that are missing in [24]. A comprehensive treatment can be found in [20].

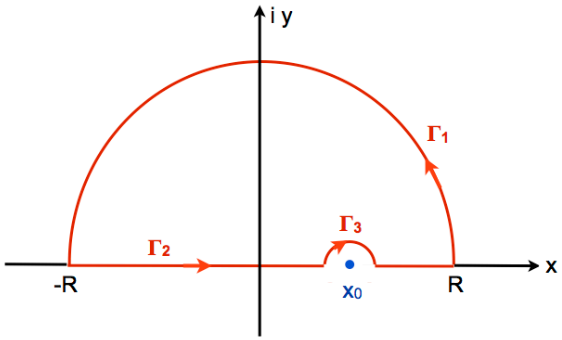
suppose want to evaluate the integral

$$\int_{-\infty}^{\infty} \frac{e^{ix}}{x - x_0} dx$$

go into the complex plane

$$\oint_{\Gamma} \frac{e^{iz}}{z - x_0} dz = \int_{\Gamma_1} \frac{e^{iz}}{z - x_0} dz + \int_{\Gamma_2} \frac{e^{iz}}{z - x_0} dz + \int_{\Gamma_3} \frac{e^{iz}}{z - x_0} dz = 0$$

Cauchy Intregral Theorem



$$\lim_{R\to\infty} \int_{\Gamma_1} \frac{e^{iz}}{z - x_0} dz = 0$$

$$\lim_{\varepsilon\to 0} \int_{\Gamma_3} \frac{e^{iz}}{z - z_0} dz \quad = \quad e^{iz_0} \lim_{\varepsilon\to 0} \int_{2\pi}^{\pi} \frac{1}{\varepsilon\, e^{i\theta}}\, i\,\varepsilon e^{i\theta} d\theta = -\pi\, i e^{iz_0}$$

$$\boxed{\mathcal{P} \int_{-\infty}^{\infty} \frac{e^{iz}}{z - x_0} dz = i\,\pi\, e^{iz_0}\,.}$$

$$\mathcal{P} \int_{-\infty}^{\infty} \frac{e^{iz}}{z - x_0} dz = \lim_{\varepsilon\to 0} \left[\int_{-\infty}^{x_0-\varepsilon} \frac{e^{iz}}{z - x_0} dz + \int_{x_0+\varepsilon}^{\infty} \frac{e^{iz}}{z - x_0} dz \right]$$

The famous Kronig-Kramers dispersion relation in solid state physics

An important application is the relation between real part and imaginary part of the electric susceptibility $\chi_e(\omega) = \varepsilon(\omega) - 1 = \varepsilon_1(\omega) - 1 + i\,\varepsilon_2(\omega)$ of a solid (see [24])

$$\varepsilon_1(\omega) - 1 = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\varepsilon_2(\omega')}{\omega' - \omega} d\omega' , \quad \varepsilon_2(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\varepsilon_1(\omega') - 1}{\omega' - \omega} d\omega' . \tag{54}$$

Real part of dielectric function can be computed by principal- value integral over imaginary part, and vice versa

Reflection of an electromagnetic wave from a solid body:

$$\tilde{E}_r(\omega) = r(\omega)\tilde{E}_i(\omega) \qquad r(\omega) = \rho(\omega)e^{i\Phi(\omega)}$$

$$R(\omega) = |r(\omega)|^2 = (\rho(\omega))^2$$

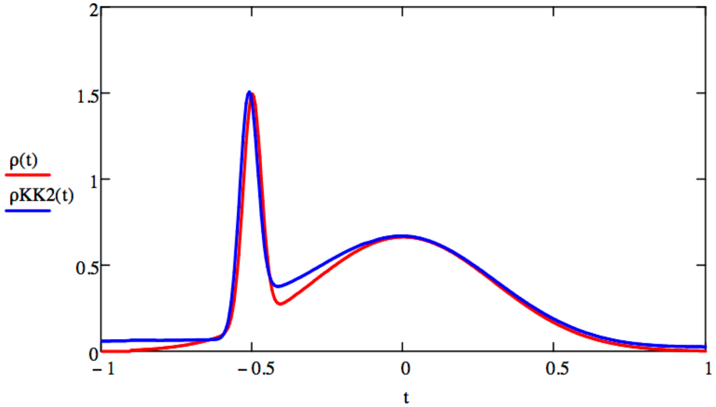
R(ω) is measured, phase Φ(ω) is unknown

$$\Phi(\omega_0) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{(1 + \omega_0\omega)\ln(\rho(\omega))}{(1 + \omega^2)(\omega_0 - \omega)} d\omega$$

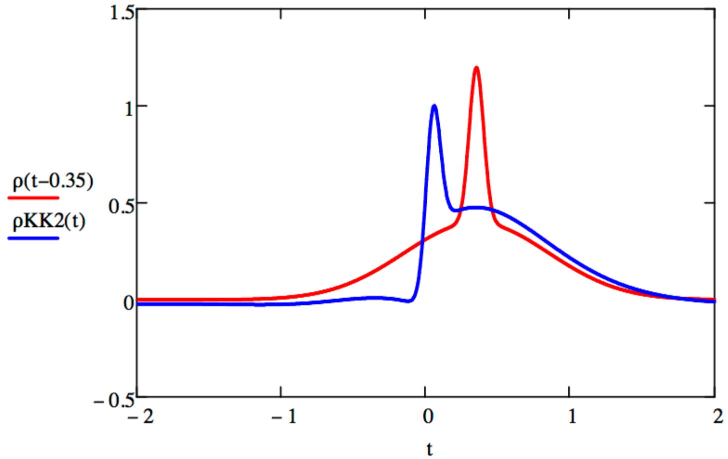
another form of the Kronig-Kramers relation
Derivation: see F. Wooten and App. A

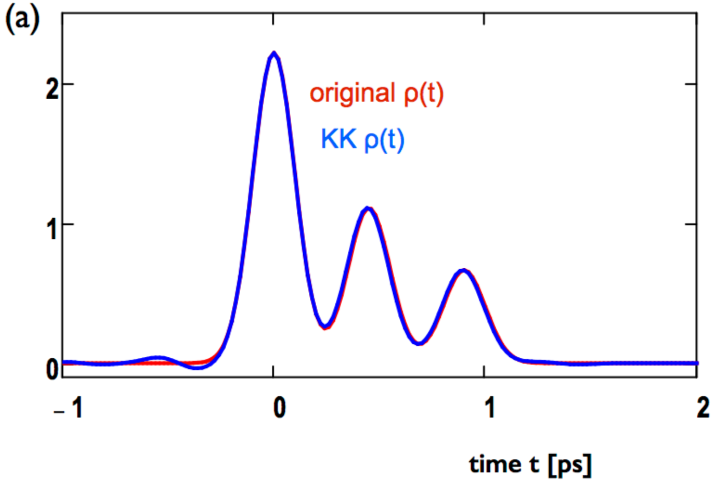
confusing results when two or more peaks are present

narrow peak at front

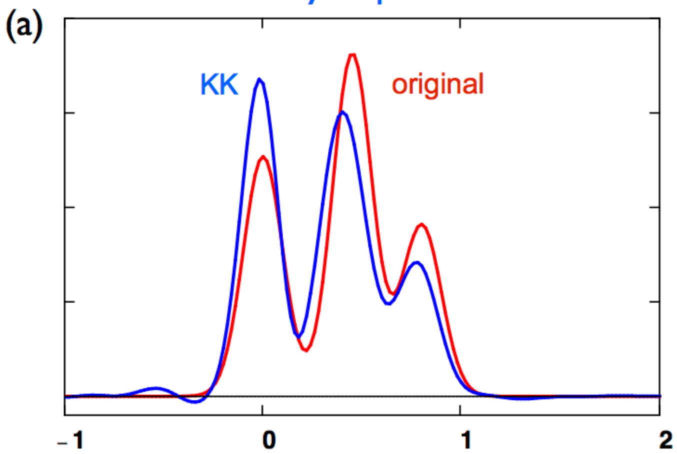


narrow peak at center





only KK phase

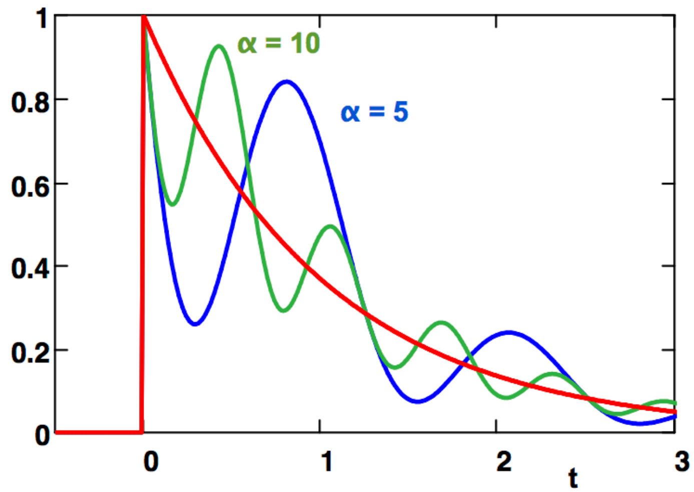


What is the reason for "right" or "wrong" reconstructions?

Akutowicz functions

$$f_1(t) = e^{-\beta t}$$

$$f_2(t) = e^{-\beta t}\left(1 + \frac{4\beta^2(1-\cos(\alpha t))}{\alpha^2} - \frac{4\beta\sin(\alpha t)}{\alpha}\right)$$



The complex Fourier transforms are different

$$\mathcal{F}_1(\omega) = \frac{1}{\beta + i\omega}, \qquad \mathcal{F}_2(\omega) = \frac{\alpha^2 + (\beta + i\omega)^2}{[\alpha^2 + (\beta - i\omega)^2](\beta - i\omega)}$$

But their absolute magnitude is identical for real ω

$$|\mathcal{F}_1(\omega)| = |\mathcal{F}_2(\omega)| = \frac{1}{\sqrt{\beta^2 + \omega^2}}$$

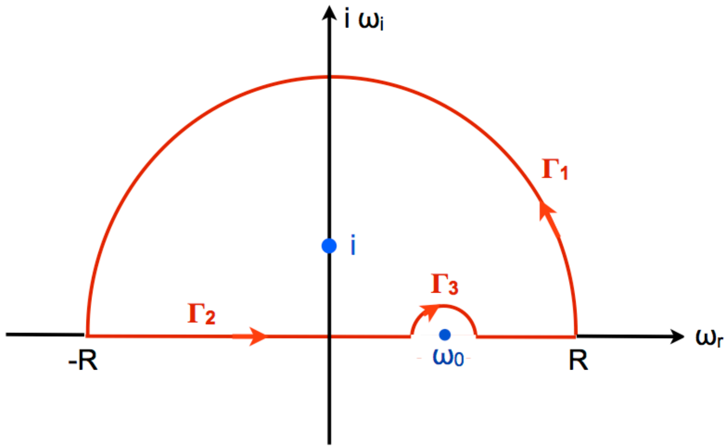
The unique reconstruction of a signal from the magnitude of its Fourier transform is mathematically impossible

E. J. Akutowicz, *On the Determination of the Phase of a Fourier Integral*, Trans. Amer. Math. Soc. **83**, 179 (1956).

Something is missing: Blaschke phase

$$\Phi_{\rm KK}(\omega) = \frac{2\omega}{\pi}\mathcal{P}\int_0^{\omega_{\rm cut}} \frac{\ln(|\mathcal{F}(\omega')|) - \ln(|\mathcal{F}(\omega)|)}{\omega^2 - \omega'^2}\,d\omega'$$

principal value integral



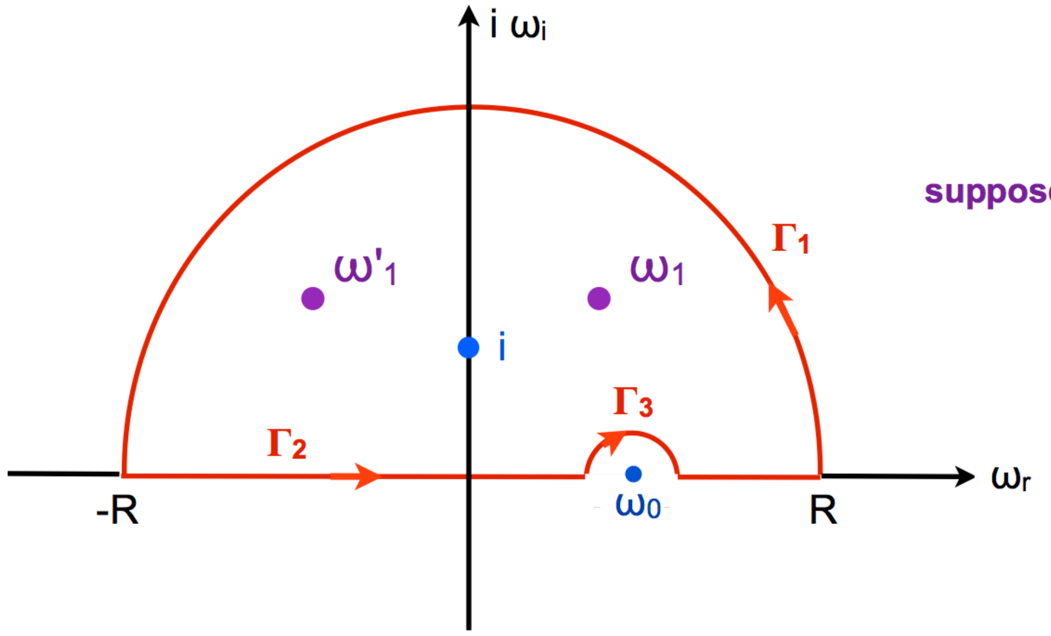
evaluation in complex ω plane

integrand has a pole at ω=i but is not allowed to have another singularity inside the loop

The complex form factor must be different from zero in the entire upper half plane
otherwise its logarithm diverges

Suppose now that the form factor has a zero at some complex frequency $\omega_1 = a + ib$ in the right upper quarter of the ω plane $(a, b > 0)$. An interesting observation is that zeros occur always in pairs, at $\omega_1 = a + ib$ in the right upper quarter and at $\omega_1' = -a + ib$ in the left upper quarter.

define modified form factor $$\mathcal{F}_{\rm mod}(\omega) = \mathcal{F}(\omega)B(\omega)$$



suppose form factor has one pair of zeros

$$\omega_1 = a + ib$$

$$\omega_1' = -a + ib$$

Blaschke factor

$$B(\omega) = \frac{\omega - \omega_1^*}{\omega - \omega_1} \cdot \frac{\omega - \omega_1'^*}{\omega - \omega_1'} = \frac{\omega - (a - ib)}{\omega - (a + ib)} \cdot \frac{\omega - (-a - ib)}{\omega - (-a + ib)}$$

$$\mathcal{F}_{\text{mod}}(\omega) = \mathcal{F}(\omega) B(\omega)$$ modified form factor has no zero

$$|B(\omega)| = 1 \quad \Rightarrow \quad |\mathcal{F}_{\text{mod}}(\omega)| = |\mathcal{F}(\omega)| \quad \text{for real} \quad \omega$$

modified form factor yields same radiation spectrum

$$\mathcal{F}_{\mathrm{mod}}(\omega) = \mathcal{F}(\omega) B(\omega)$$

modified form factor has no zero
so its phase is identical with the KK phase

$$\Phi(\omega) = \Phi_{\mathrm{KK}}(\omega) - \Phi_{\mathrm{B}}(\omega)$$

phase of original form factor

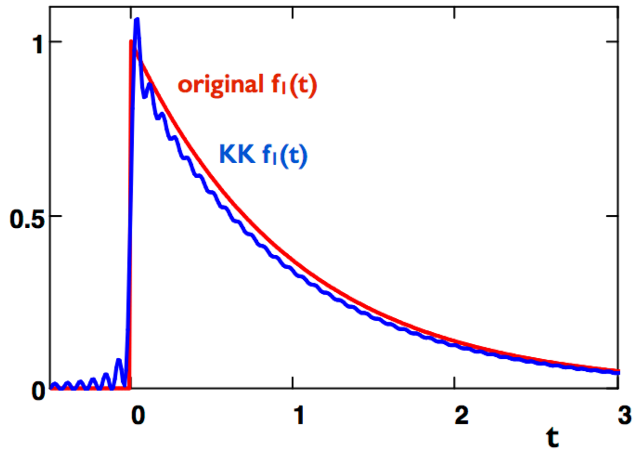
$$\Phi_{\mathrm{B}}(\omega) = \arg(B(\omega))$$

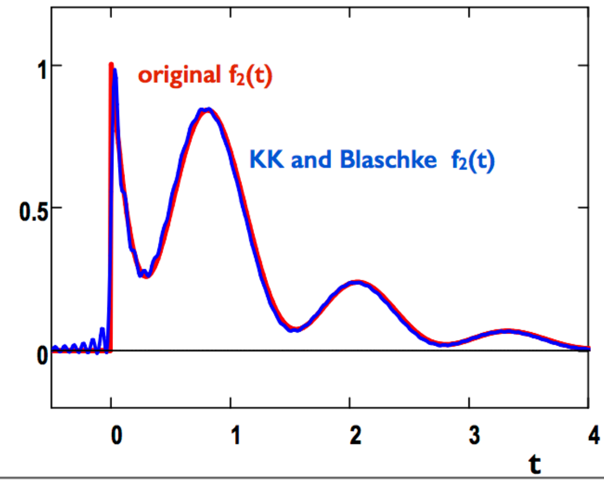
check with Akutowicz function $f_2(t)$

$$f_2(t) \;=\; e^{-\beta t}\left(1 + \frac{4\beta^2(1-\cos(\alpha t))}{\alpha^2} - \frac{4\beta\sin(\alpha t)}{\alpha}\right)$$

$$\mathcal{F}_2(\omega) = \frac{\alpha^2 + (\beta + i\omega)^2}{[\alpha^2 + (\beta - i\omega)^2](\beta - i\omega)}$$

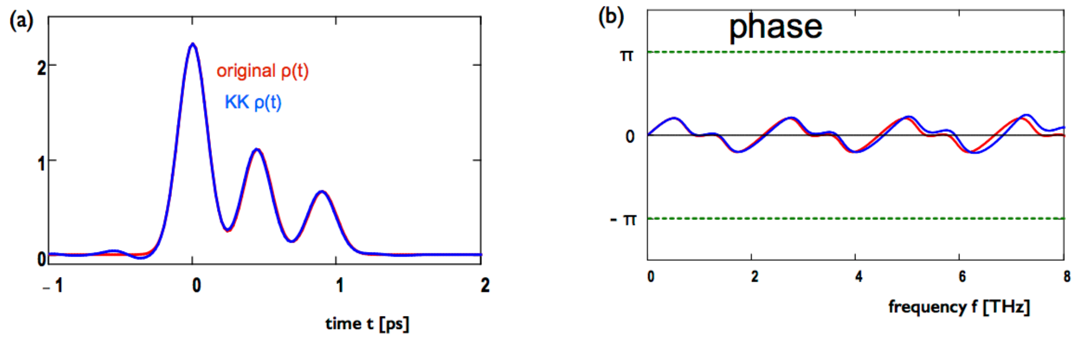
zeros of form factor: $\omega_1 = \alpha + i\beta$ $\quad \omega_1' = -\alpha + i\beta$



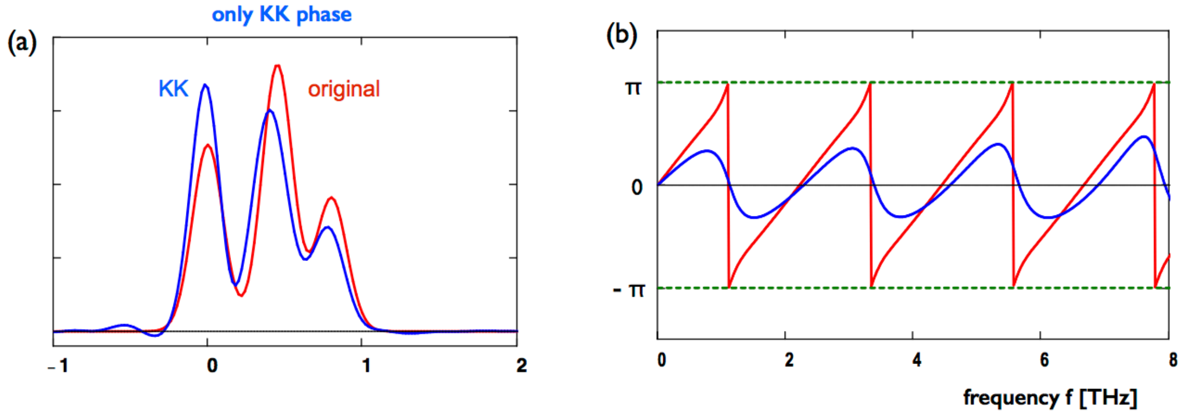


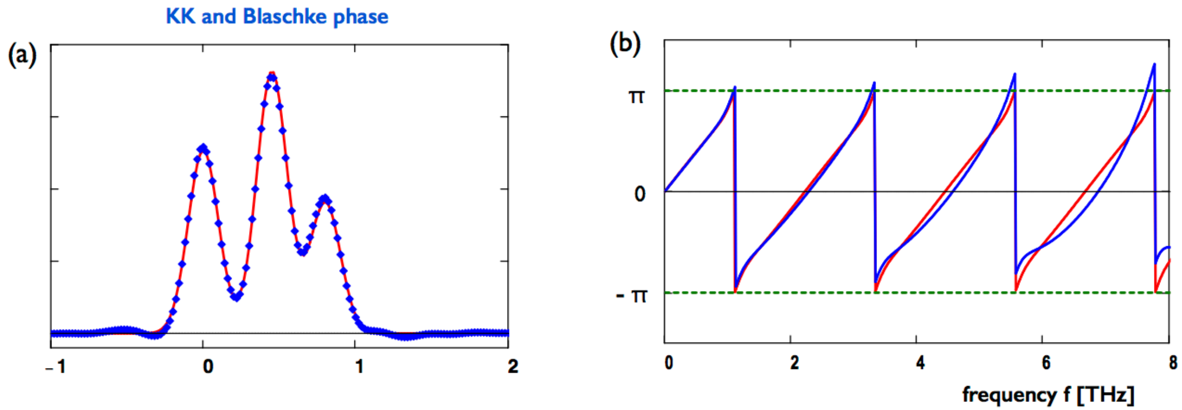
Example 1:
3 Gaussians of equal width, equidistant

case 1
large peak at front

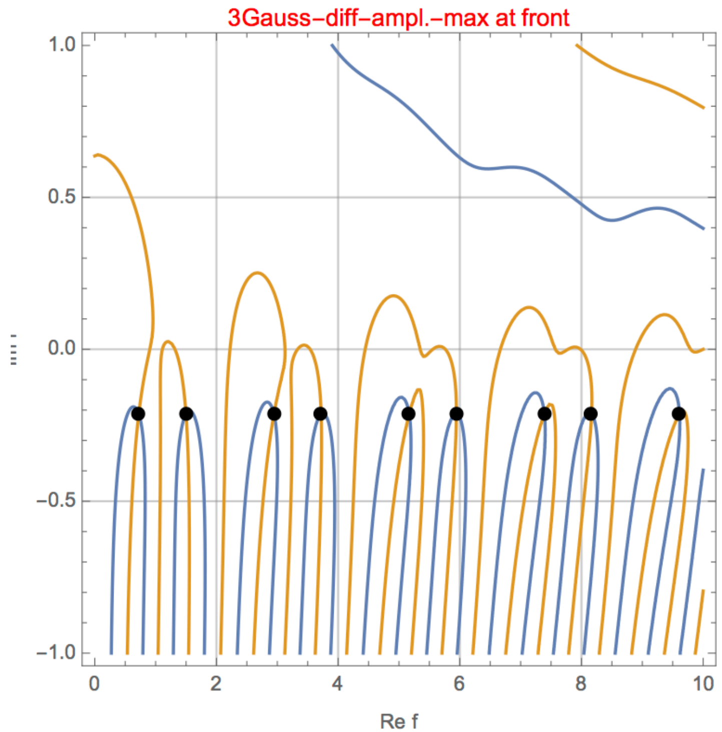


case 2
large peak at center



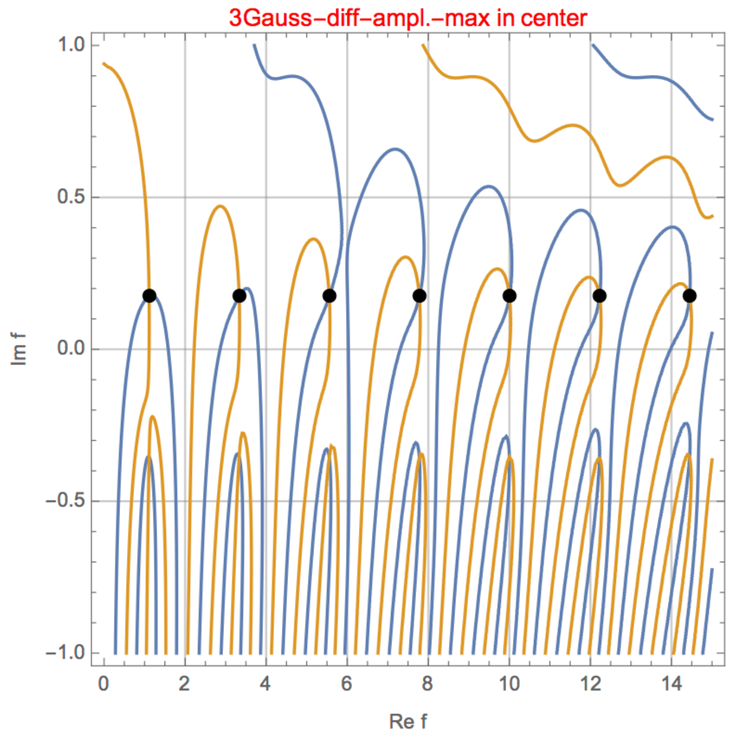


numerical determination of form factor zeros (Bernhard Schmidt)



case 1

no zeros in upper half plane, Φ_B=0

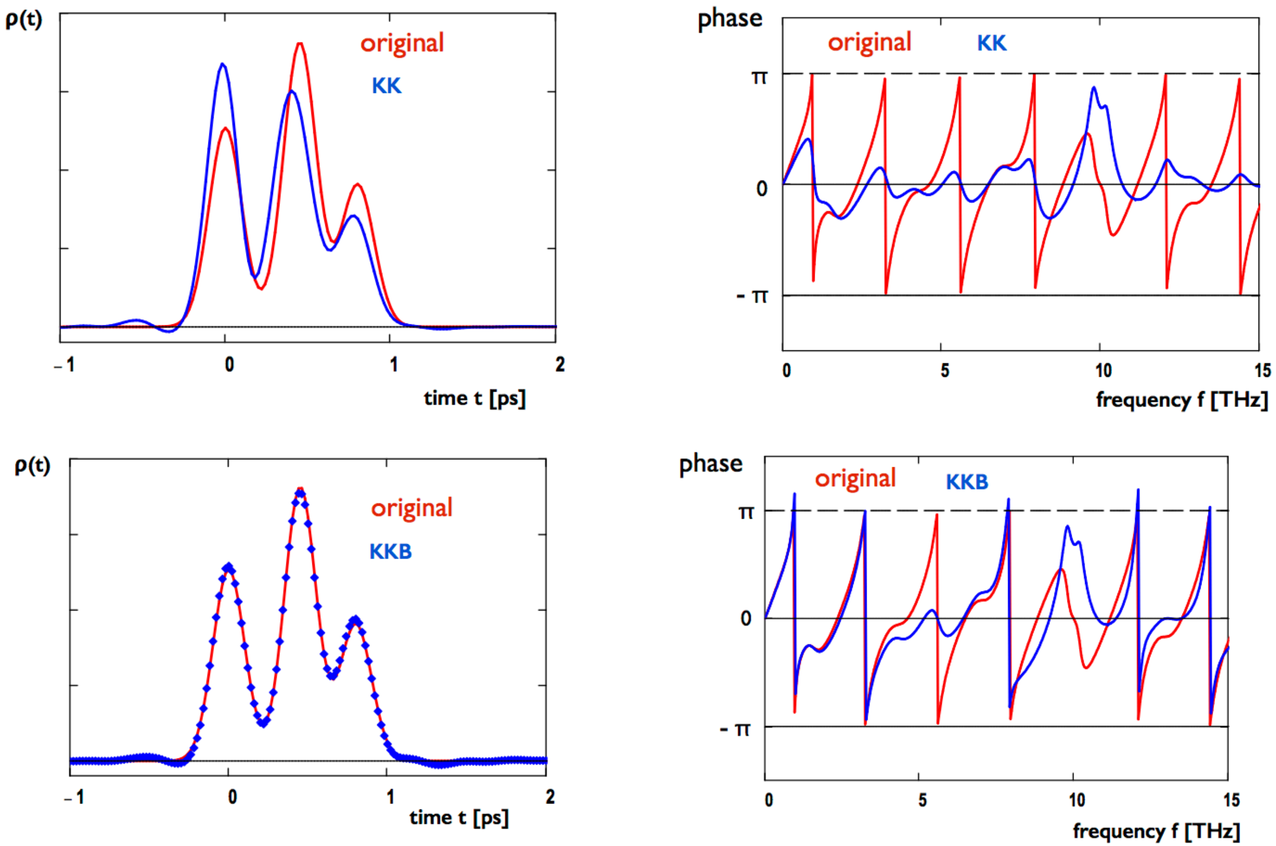


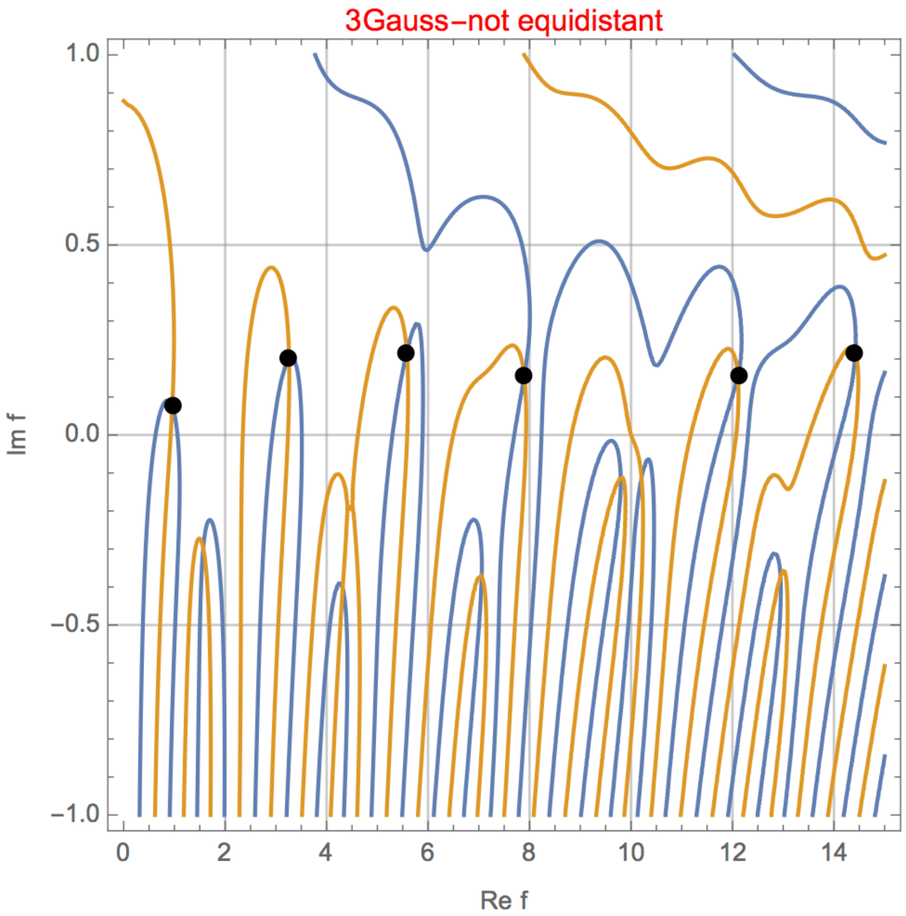
case 2

many zeros in upper half plane, Φ_B nonzero

blue curves: $\Re(\mathcal{F}(\omega)) = 0$ yellow curves: $\Im(\mathcal{F}(\omega)) = 0$

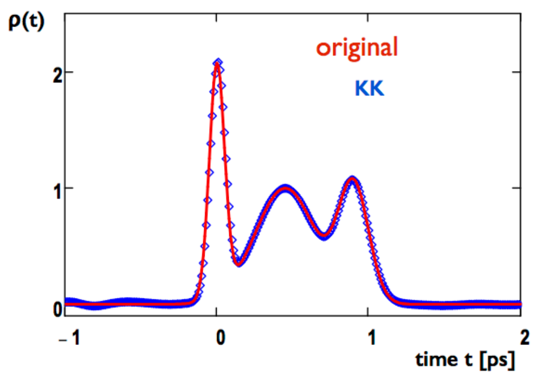
Example 2:
3 Gaussians of equal width, not equidistant

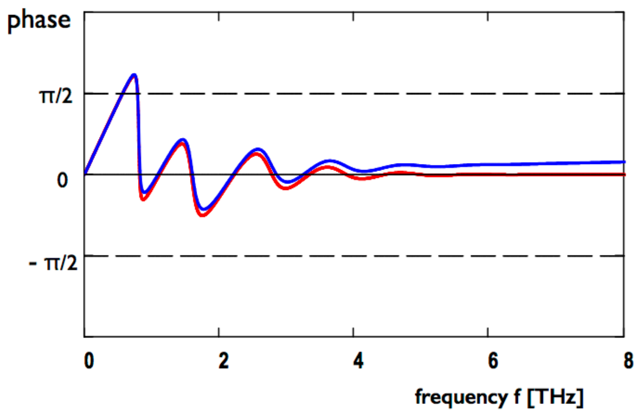



3Gauss−not equidistant
1.0
0.5
0.0
−0.5
−1.0
Im f
0
2
4
6
8
10
12
14
Re f

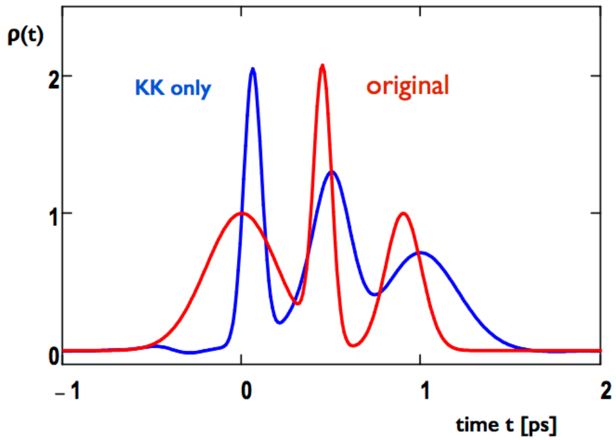
Example 3:
3 Gaussians of different width, equidistant

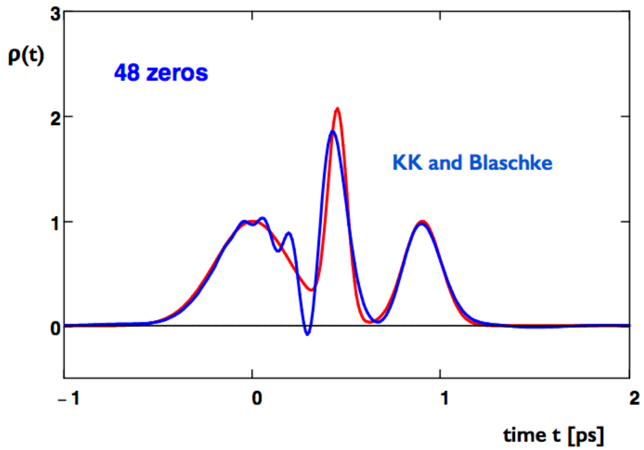
case 1
narrow peak at front

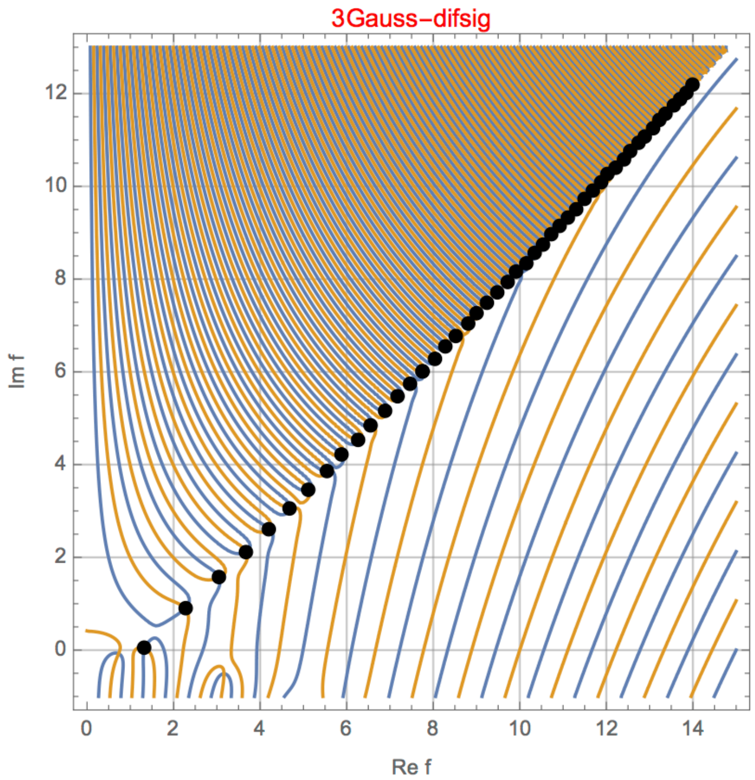




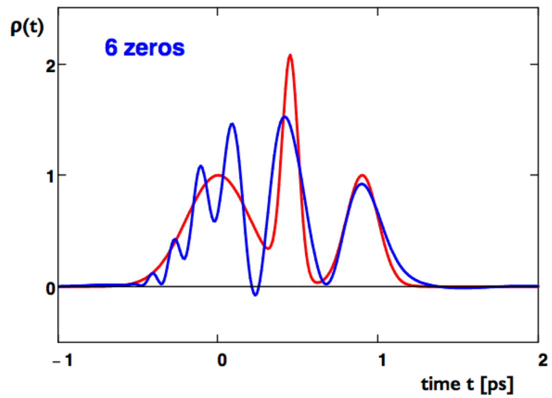
case 2
narrow peak at center

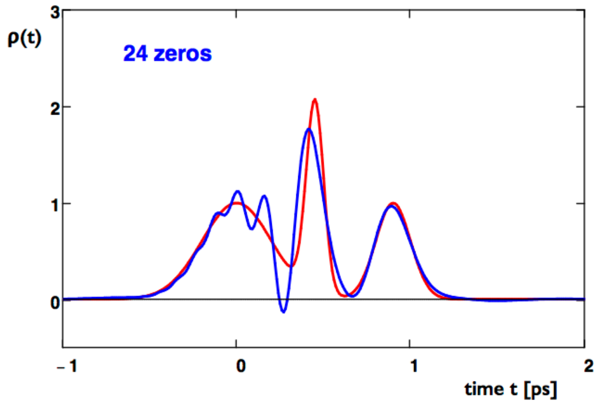






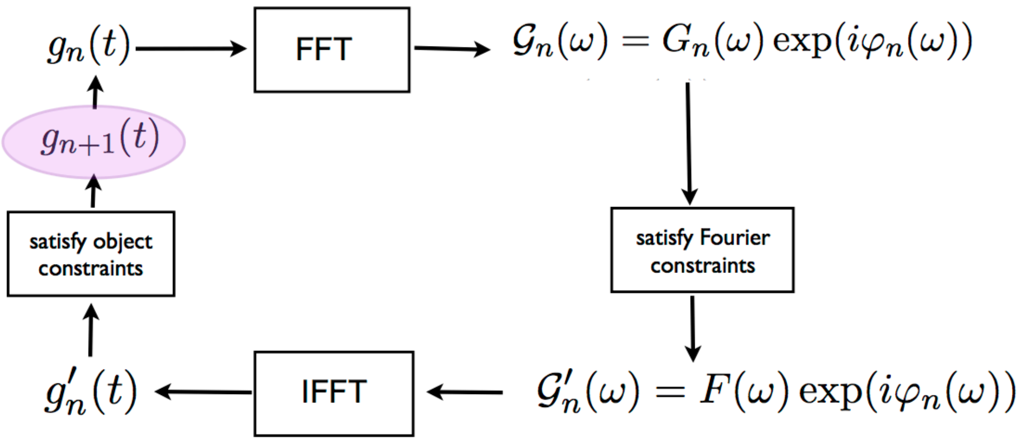
case 2
narrow peak at center
huge number of zeros



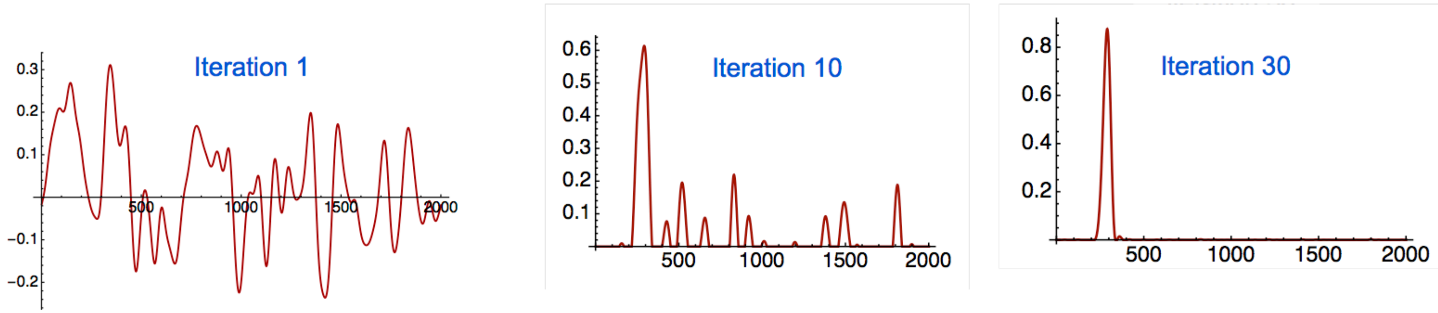


Method 2: Iterative phase retrieval

Gerchberg-Saxton algorithm



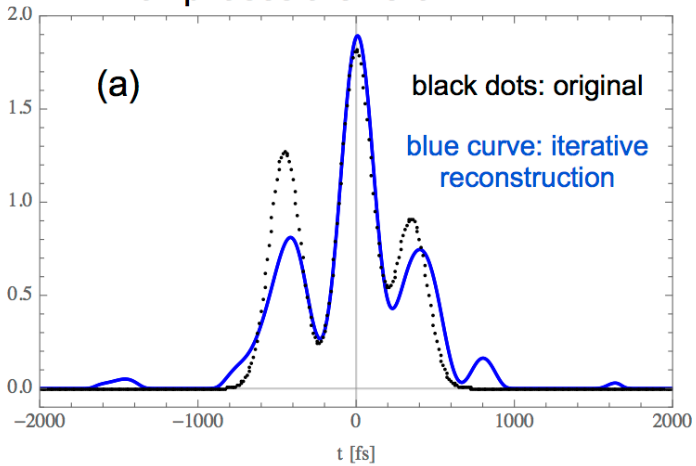
Example: single Gaussian. Start with known F(ω), choose random phase (Bernhard Schmidt)



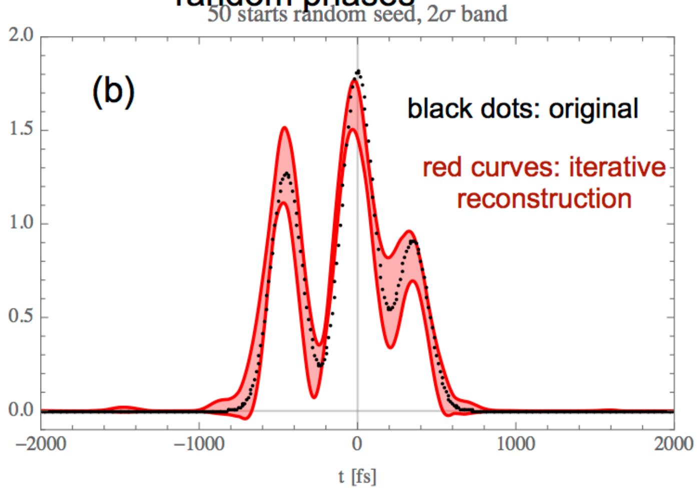
Previous Example 1:
3 Gaussians of equal width, equidistant

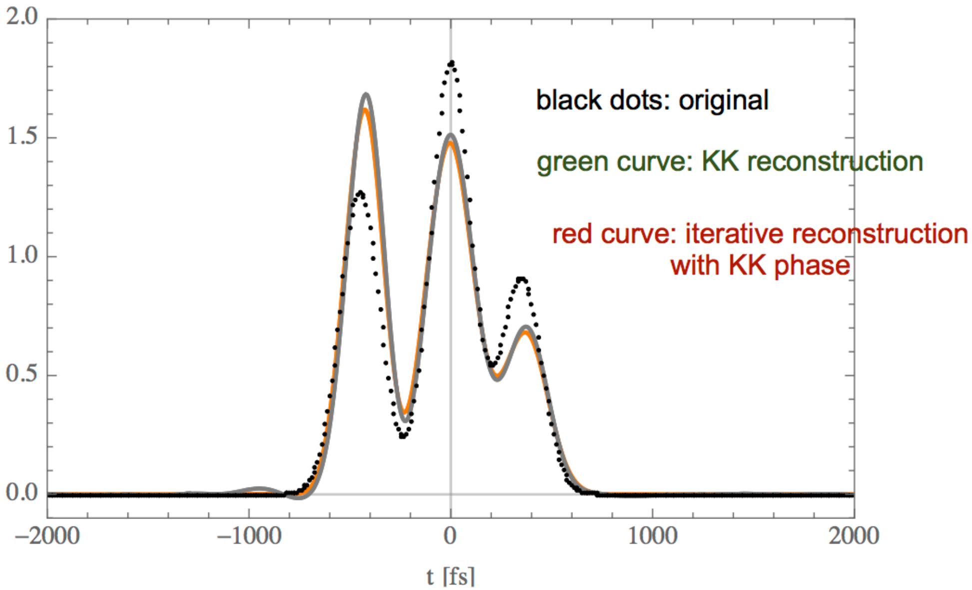
Start with known F(ω), use different initial phases (computed by Bernhard Schmidt)

all phases are zero



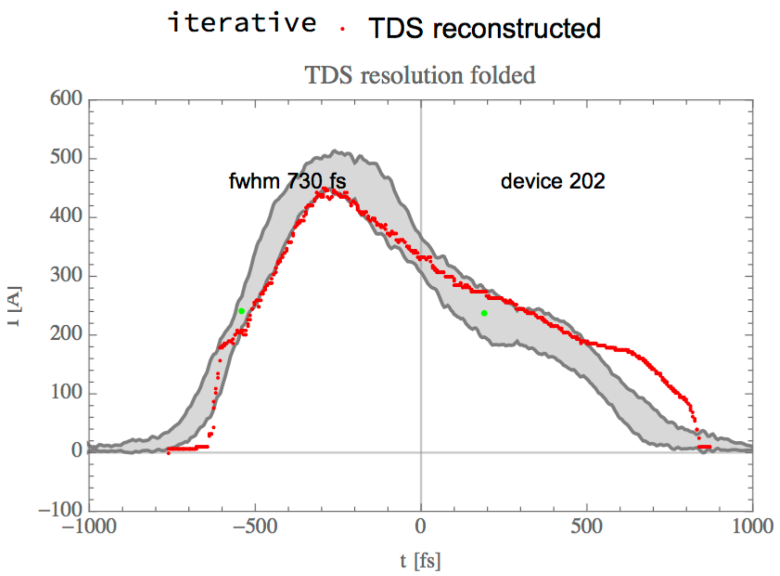
random phases

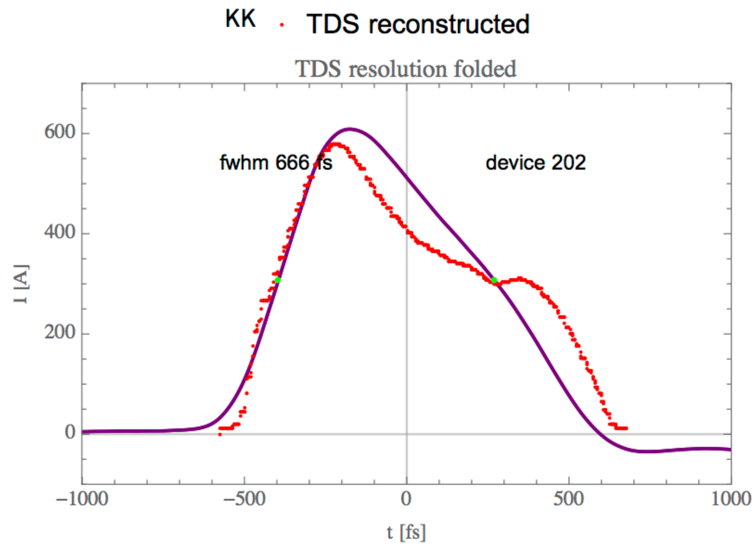


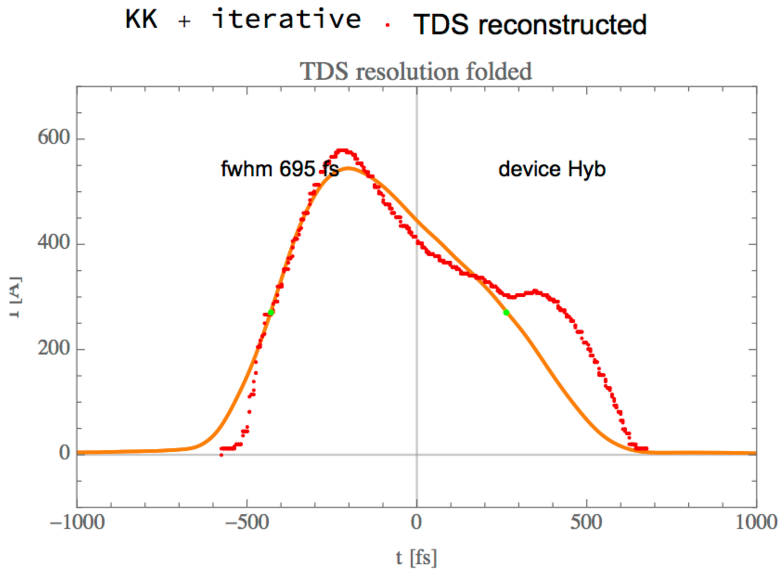


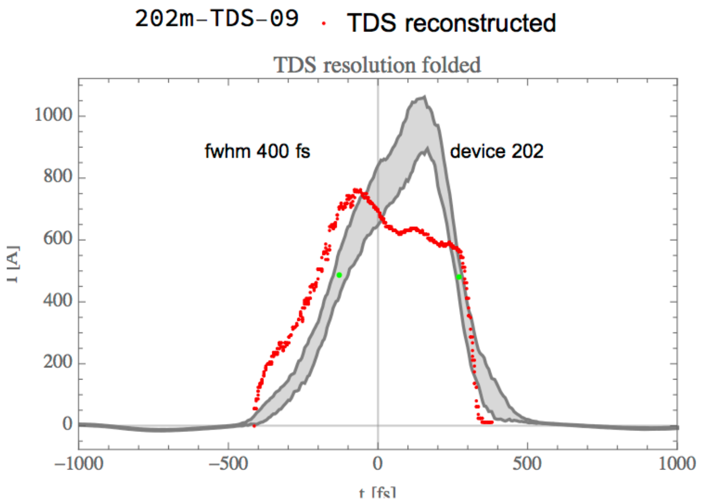
initial phase equal to KK phase

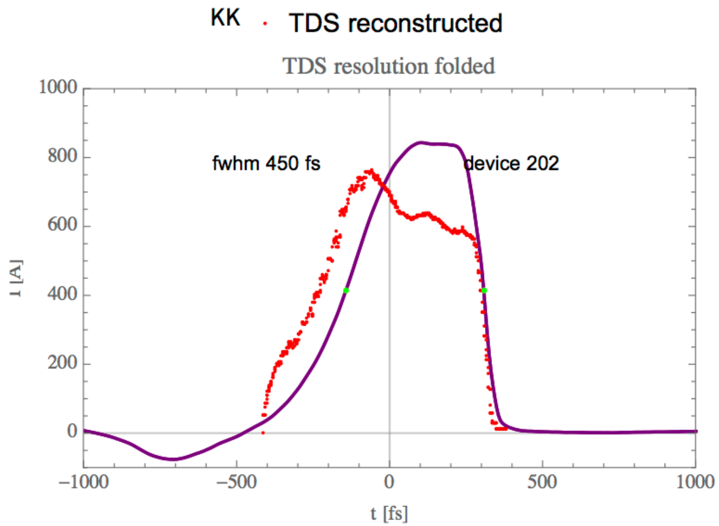
some experimental results (B. Schmidt et al.)

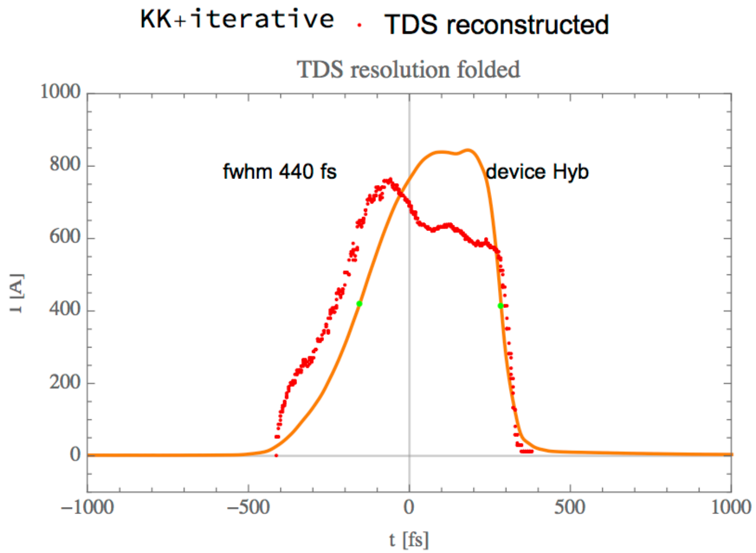







202m-TDS-09
TDS reconstructed
TDS resolution folded
fwhm 400 fs
device 202
I [A]
t [fs]


KK
TDS reconstructed
TDS resolution folded
fwhm 450 fs
device 202
I [A]
t [fs]


KK+iterative
TDS reconstructed
TDS resolution folded
fwhm 440 fs
device Hyb
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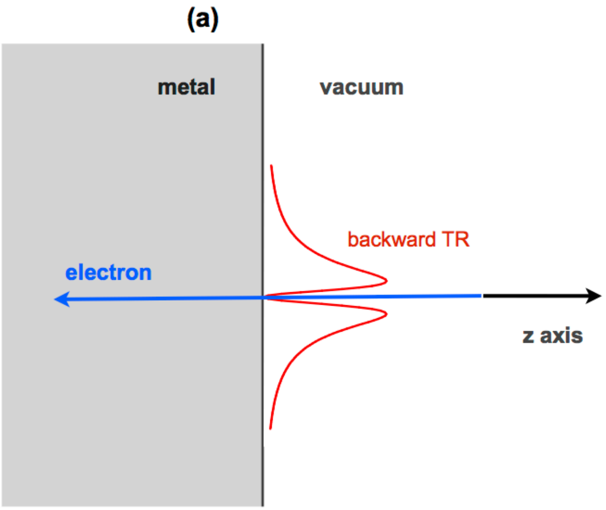
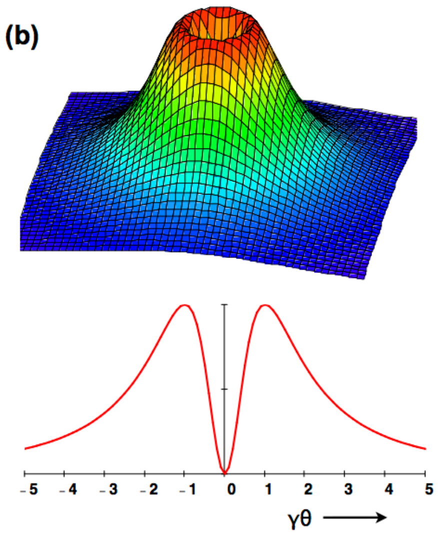
Backward transition radiation





(1)
$$\left[\frac{d^2U}{d\omega d\Omega}\right]_{\mathrm{GF}} = \frac{e^2}{4\pi^3\varepsilon_0 c}\cdot\frac{\beta^2\sin^2\theta}{(1-\beta^2\cos^2\theta)^2}$$

Ginzburg-Frank formula
far-field radiation from an infinite plane

(2)
$$\left[\frac{d^2U}{d\omega d\Omega}\right]_{\mathrm{far}} = \left[\frac{d^2U}{d\omega d\Omega}\right]_{\mathrm{GF}}\cdot[1-T(\theta,\omega)]^2$$

far-field radiation from a disc of radius a

$$T(\theta,\omega) = \frac{\omega a}{c\,\beta\gamma}J_0\left(\frac{\omega a\sin\theta}{c}\right)K_1\left(\frac{\omega a}{c\beta\gamma}\right)+\frac{\omega a}{c\beta^2\gamma^2\sin\theta}J_1\left(\frac{\omega a\sin\theta}{c}\right)K_0\left(\frac{\omega a}{c\beta\gamma}\right)$$

(3)
$$\left[\frac{d^2U}{d\omega d\Omega}\right]_{\mathrm{near}} = \frac{e^2\omega^4}{4\pi^3\varepsilon_0 c^5\beta^4\gamma^2}\left|\int_0^a J_1\left(\frac{\omega\rho\sin\theta}{c}\right)K_1\left(\frac{\omega\,\rho}{c\,\beta\gamma}\right)\exp\left(\frac{i\omega\,\rho^2}{2cR}\right)\rho\,d\rho\right|^2$$

near-field radiation
from a disc of radius a

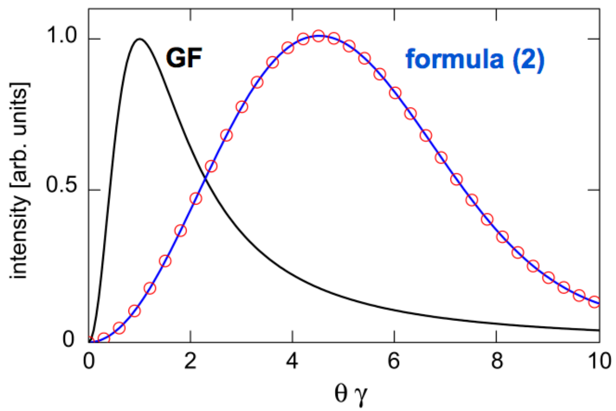
(2) far-field radiation from a finite disc of radius a

Ginzburg-Frank formula is not applicable in most practical cases

$$\left[\frac{d^2U}{d\omega d\Omega}\right]_{\text{far}} = \left[\frac{d^2U}{d\omega d\Omega}\right]_{\text{GF}} \cdot [1 - T(\theta,\omega)]^2$$

$$T(\theta,\omega) = \frac{\omega a}{c\,\beta\gamma} J_0\left(\frac{\omega a \sin\theta}{c}\right) K_1\left(\frac{\omega a}{c\beta\gamma}\right) + \frac{\omega a}{c\beta^2\gamma^2 \sin\theta} J_1\left(\frac{\omega a \sin\theta}{c}\right) K_0\left(\frac{\omega a}{c\beta\gamma}\right)$$

$$r_{\text{eff}} = \gamma\lambda$$ effective source size

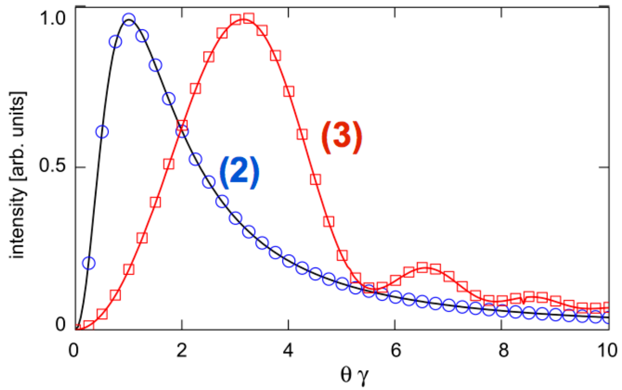


a < r_{eff} use formula (2)

angular distribution is wider for a small TR source

(3) near-field radiation from a finite disc of radius a

$$\left[\frac{d^2U}{d\omega d\Omega}\right]_{\text{near}} = \frac{e^2\omega^4}{4\pi^3\varepsilon_0 c^5\beta^4\gamma^2}\left|\int_0^a J_1\left(\frac{\omega\rho\sin\theta}{c}\right)K_1\left(\frac{\omega\,\rho}{c\,\beta\gamma}\right)\exp\left(\frac{i\omega\,\rho^2}{2cR}\right)\rho\,d\rho\right|^2$$



(2) far-field regime $D > \gamma^2\lambda$

(3) near-field regime $D < \gamma^2\lambda$

angular distribution is wider in the near-field regime

Impact of bunch radius

cylindrical beam with Gaussian profile

$$\rho_{\text{trans}}(x,y) = \frac{1}{\sqrt{2\pi}\,\sigma}\exp\left(-\frac{x^2}{2\,\sigma^2}\right)\frac{1}{\sqrt{2\pi}\,\sigma}\exp\left(-\frac{y^2}{2\,\sigma^2}\right).\qquad \tilde{F}_{\text{trans}}(k,\theta) = \exp\left(-\frac{k^2\sigma^2\sin^2\theta}{2}\right).$$

FLASH at 202 m

Lorentz factor $\gamma = 1000$, normalized emittance $\varepsilon_n = 2\,\mu\text{m}$, beta function $\beta_x = \beta_y = 7\,\text{m}$, $\sigma = 120\,\mu\text{m}$.

weighted average of squared transverse form factor

$$\langle|\tilde{F}_{\text{trans}}(k)|^2\rangle = \frac{\int_0^{\theta_{\text{ap}}} U(\theta,k)\,\exp\left(-k^2\sigma^2\sin^2\theta\right)\,\sin\theta\,d\theta}{\int_0^{\theta_{\text{ap}}} U(\theta,k)\,\sin\theta\,d\theta}$$