Methoden moderner Röntgenphysik: Streuung und Abbildung

Lecture 8	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2021		
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Location	online		
Date	Tuesdays	12:30 - 14:00	(starting 6.4.)
	Thursdays	8:30 - 10:00	(until 8.7.)

Methoden moderner Röntgenphysik: Online Info

Tuesday Zoom-Meeting
https://desy.zoom.us/j/92674682486
Meeting ID: 926 7468 2486
Passcode: 144456

Thursday Zoom-Meeting
https://desy.zoom.us/j/99738625981
Meeting ID: 997 3862 5981
Passcode: 841881

Tutorial Zoom-Meeting
https://desy.zoom.us/j/95288979489
Meeting ID: 952 8897 9489
Passcode: 832350

Literature

Basic concepts:

Moderne Röntgenbeugung
Röntgendiffraktometrie für Materialwissenschaftler, Physiker und Chemiker
Authors
(view affiliations)
Lothar Spieß
Robert Schwarzer
Herfried Behnken
Gerd Teichert
https://link.springer.com/book/10.1007/978-3-663-10831-3

Elements of Modern X-Ray Physics
J. A. Nielsen and D. McMorrow, J. Wiley&Sons (2001)

X-Ray Diffraction
B.E. Warren, DOVER Publications Inc., New York

Principles of Optics
M. Born and E. Wolf, Cambridge University Press, 7th ed.

Soft X-rays and Extreme Ultraviolet Radiation
D. Attwood, Cambridge University Press (2000)
http://www.coe.berkeley.edu/AST/sxreuv/

Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen
K. Wille, Teubner Studienbücher 1996

Lecture Notes

https://photon-science.desy.de/research/research_teams/coherent_x_ray_scattering/teaching/index_eng.html

Methoden moderner Röntgenphysik: Streuung und Abbildung

Small Angle Scattering, and Soft Matter
Introduction, Form Factor, Structure Factor, Applications, ...

Anomalous Diffraction
Introduction into Anomalous Scattering, ...

Introduction into Coherence
Concept, First Order Coherence, Spatial Coherence, Second Order Coherence, ...

Coherent Scattering
Imaging and Correlation Spectroscopy, ...

The Concept of Coherence: Classical Light

First Order Coherence

Coherence and Emission Spectrum

Spatial Coherence

Second Order Coherence

Chaotic Light

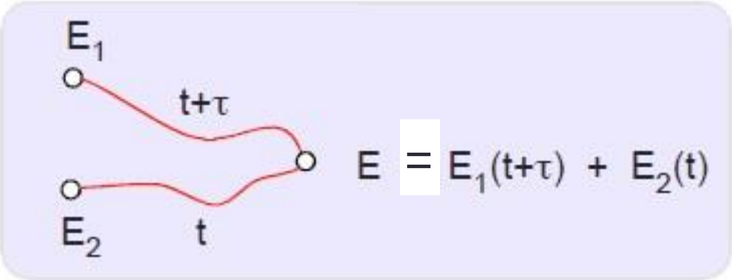
Basic concepts:

The quantum theory of light
Rodney Loudon, Oxford University Press (1990)

Quantum optics
Marlan O. Scully, M. Suhal Zubairy,
Cambridge University Press (1997)

The Concept of Coherence

Consider harmonic fields E_1, E_2 at positions r_1, r_2 at time t=0:



$$< I_n > \equiv < E_n(t)E_n^*(t) >, \qquad n \in \{1,2\}$$

$$< I > = < EE^* > = < I_1 > + < I_2 > + 2\,\mathrm{Re}\,[< E_1(t+\tau)E_2^*(t) >] \qquad \text{with } < f > \equiv \lim_{T\to\infty} < f >_T$$

$$< f >_T \equiv \left(\frac{1}{T}\right) \int_{-\frac{T}{2}}^{\frac{T}{2}} f(t)dt$$

Here lim T→∞ means that T is finite but sufficiently large such that $<f>_T$ does not depend on T

Normalized pair correlation function: $\gamma_{12}(\tau) \equiv \dfrac{<E_1(t+\tau)E_2^*(t)>}{(<I_1><I_2>)^{\frac{1}{2}}}$

$$\Rightarrow < I > = < I_1 > + < I_2 > + 2\,(< I_1 >< I_2 >)^{\frac{1}{2}}\ \mathrm{Re}[\gamma 12(\tau)]$$

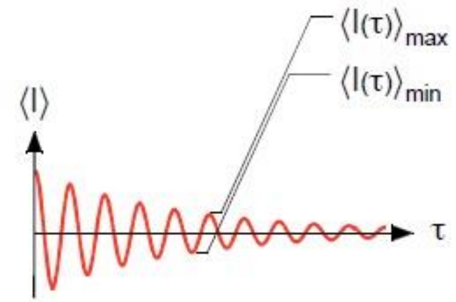
$$\gamma_{12}(\tau) = |\gamma_{12}(\tau)| \cos\big(\phi_{12}(\tau)\big) \Rightarrow I = \langle I_1 \rangle + \langle I_2 \rangle + 2(\langle I_1 \rangle \langle I_2 \rangle)^{\frac{1}{2}} \; |\gamma_{12}(\tau)| \cos(\phi_{12}(\tau))$$

Assume: $\phi_{12}(\tau)$ changes much faster than $|\gamma_{12}(\tau)|$ (quasi-coherent light)

$$\Rightarrow \langle I \rangle_{max/min} = \langle I_1 \rangle + \langle I_2 \rangle \pm 2(\langle I_1 \rangle \langle I_2 \rangle)^{\frac{1}{2}} \; |\gamma_{12}(\tau)|$$

Interference visibility κ :

$$\kappa \equiv \left| \frac{\langle I \rangle_{max} - \langle I \rangle_{min}}{\langle I \rangle_{max} + \langle I \rangle_{min}} \right| = 2 \frac{(\langle I_1 \rangle \langle I_2 \rangle)^{\frac{1}{2}}}{\langle I_1 \rangle + \langle I_2 \rangle} \; |\gamma_{12}(\tau)|$$



$$\langle I_1 \rangle = \langle I_2 \rangle \Rightarrow \kappa = |\gamma_{12}(\tau)|$$

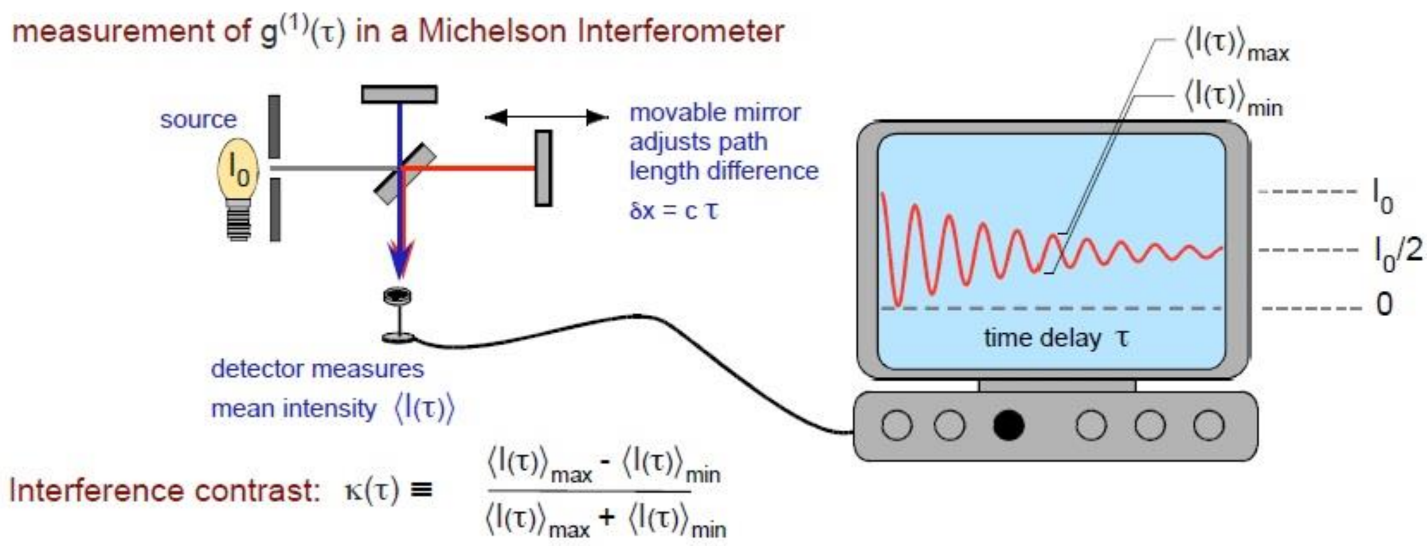
Definition:	$\|\gamma_{12}(\tau)\| = 1$	for all τ	$\Rightarrow$	complete coherence
	$0 < \|\gamma_{12}(\tau)\| < 1$	for some τ	$\Rightarrow$	partial coherence
	$\|\gamma_{12}(\tau)\| = 0$	for all τ	$\Rightarrow$	no coherence

Normalized autocorrelation function:

$$g^{(1)}(\tau) \equiv \frac{\langle E(t+\tau)E^*(t)\rangle}{\langle I\rangle}$$

with $g^{(1)}(0) = 1$ and $g^{(1)}(-\tau) = g^{(1)*}(\tau)$

Measurement of $g^{(1)}(\tau)$ in a Michelson Interferometer

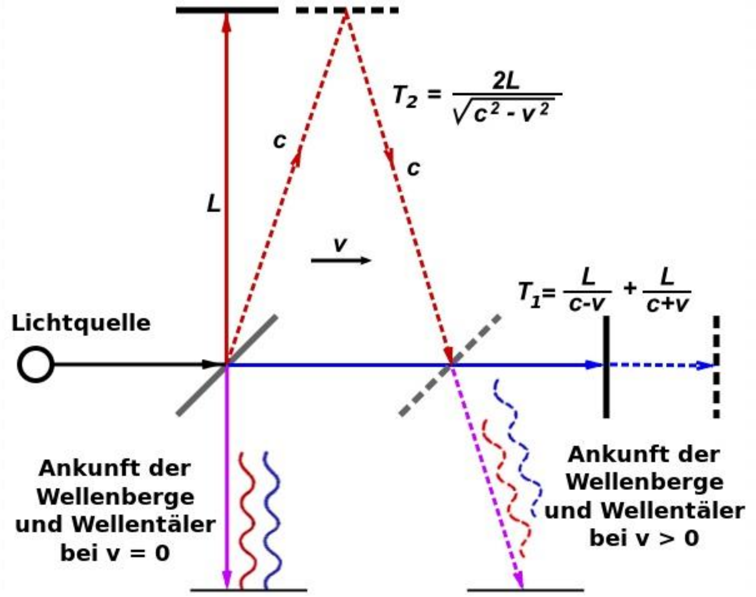


Maximal coherence: Interference contrast maximal for all τ 

Partial coherence: Interference contrast decreases for large τ 

The Michelson-Morley Experiment

by Albert Abraham Michelson: 1881 in Potsdam



Normalized autocorrelation function: $g^{(1)}(\tau) \equiv \dfrac{<E(t+\tau)E^*(t)>}{<I>}$

$$\text{with } g^{(1)}(0) = 1 \ \text{ and } \ g^{(1)}(-\tau) = g^{(1)*}(\tau)$$

<u>Example</u>: successive wave trains of duration τ_0 and length $c\tau_0$

$$E(t) = E_0 e^{i\omega t + i\phi(t)} \qquad \text{with } \phi(t) \text{ (see figure)}$$

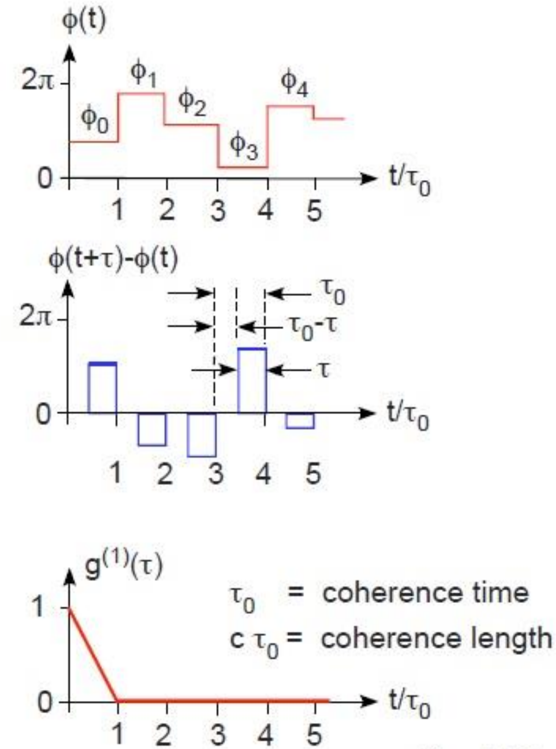
$$\Rightarrow g^{(1)}(\tau) = e^{i\omega\tau} < e^{i(\phi(t+\tau)-\phi(t))} >$$

$0 \leq \tau \leq \tau_0$:

$$< e^{i(\phi(t+\tau)-\phi(t))} > = \frac{1}{N\tau_0} \sum_{n=0}^{N+1} \int_{n\tau_0}^{(n+1)\tau_0} dt\, e^{i(\phi(t+\tau)-\phi(t))}$$

$$= \frac{1}{N\tau_0} \sum_{n=0}^{N+1} \left\{ (\tau_0 - \tau) + \tau\, e^{i(\phi_{n+1} - \phi_n)} \right\}$$

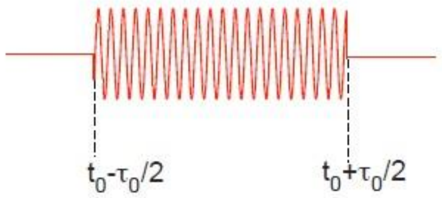
$$\Rightarrow g^{(1)}(\tau) = e^{i\omega t} \frac{(\tau_0 - \tau)}{\tau_0} \quad \begin{array}{ll} \text{x } 0 & \text{if } \tau_0 < \tau \\ \text{x } 1 & \text{if } 0 \leq \tau \leq \tau_0 \end{array}$$



<u>Note</u>: τ_0: coherence time; $\xi_l = \dfrac{\lambda}{2} \dfrac{\lambda}{\Delta\lambda} = c\tau_0$: longitudinal coherence length

Coherence and Emission Spectrum

Consider single wave train of duration τ_0, phase ϕ_0, frequency ω_0:

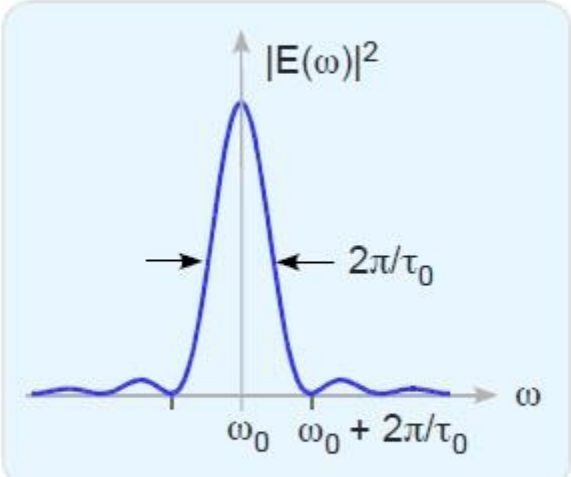


$$E(t) = e^{[-i\omega_0 t - i\phi_0]} \times 1 \qquad (\text{if } \frac{\tau_0}{2} \le \tau \le \frac{\tau_0}{2})$$

$$\times 0 \qquad \text{otherwise}$$

$$E(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt\; E(t)\; e^{i\omega t} = \sqrt{\frac{2}{\pi}} \frac{\sin\left(\frac{(\omega-\omega_0)\tau_0}{2}\right)}{(\omega-\omega_0)} \bullet e^{-i\phi_0}$$

N wave trains with the same frequency ω_0 but arbitrary phases ϕ_n:



$$|E(\omega)|^2 = \sum_{n=1}^{N} |E_n(\omega)|^2 = \frac{2}{\pi} \sum_{n=1}^{N} \frac{\sin^2\left(\frac{(\omega-\omega_0)\tau_n}{2}\right)}{(\omega-\omega_0)^2}$$

Emission bandwidth $\Delta\nu \cong \frac{1}{\tau}$ with $\tau \equiv \frac{1}{N}\sum_{n=1}^{N} \tau_n$

Example: Collision Broadened Light Source

Molecules of a gas radiate light $E(t) = E_0 e^{-i(\omega_0 t - \phi(t))}$ at frequency ω_0. Collisions yield random phase jumps, i.e., phase $\phi(t) \in [0, 2\pi]$ fluctuates.

Probability for a free flight of duration $t \in [\tau, \tau + d\tau]$: $P(t) = \frac{1}{\tau_0} \exp(\tau/\tau_0)$

kinetic gas theory (τ_0 means duration of free flight)

Coherence function: $g^{(1)}(\tau) = e^{i\omega_0\tau} < e^{i(\phi(t+\tau) - \phi(t))} >$

$e^{i(\phi(t+\tau) - \phi(t))}$ = 1 for free flights with duration > τ

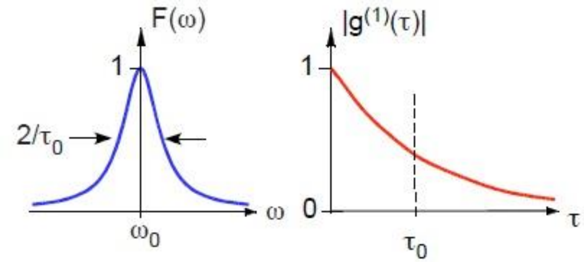
= $e^{i\chi}$ with $\chi \in [0, 2\pi]$ random for free flights with duration < τ

i.e., only flights of duration t > τ yield contribution to $< e^{i(\phi(t+\tau) - \phi(t))} >$:

$\Rightarrow$ $g^{(1)}(\tau) = e^{i\omega\tau} \,{}_{\tau}\!\int^{\infty} P(s)ds = e^{i\omega\tau} \exp(-\tau/\tau_0)$

$\Rightarrow$ $|g^{(1)}(\tau)| = \exp(\tau/\tau 0)$

$\Rightarrow$ $F(\omega) = \frac{1}{1+(\omega-\omega_0)^2 \tau_0^2}$ **Wiener-Khinchin Theorem**



Wiener Khinchin Theorem

$$E(\omega) \equiv \mathcal{F}[E(t)] \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt \; E(t) \; e^{i\omega t}$$

$$F(\omega) \equiv \frac{|E(\omega)|^2}{\int_{-\infty}^{\infty} dt |E(\omega)|^2}$$

normalized spectral density

$$\Rightarrow F(\omega) = \frac{1}{\sqrt{2\pi}} \mathcal{F}\left[g^{(1)}\right],$$

$\mathcal{F} \equiv$ Fourier-Transform

Wiener Khinchin Theorem

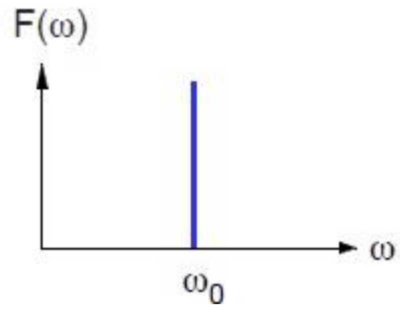
The spectral power density $F(\omega)$ is the Fourier transform of the normalized autocorrelation function $g^{(1)}(\tau)$

Example: Monochromatic Light

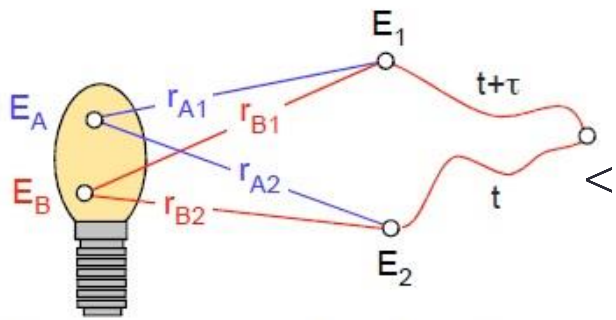
$$E(t) = e^{-i(\omega_0 t - \phi)}$$

$$g^{(1)}(\tau) = e^{i\omega_0 \tau}$$

$$\left|g^{(1)}(\tau)\right| = 1$$



Spatial Coherence



Light Source: mutually incoherent point sources $g^{(1)}(\tau) = \exp(i\omega\tau - \tau/\tau_0)$

$$E_1 = E_{A1} + E_{B1} \qquad E_{An} = E_A e^{\frac{i r_{An}\omega}{c}}$$

$$E_2 = E_{A2} + E_{B2} \qquad E_{Bn} = E_B e^{\frac{i r_{Bn}\omega}{c}}$$

$$\langle E_1(t+\tau)E_2^*(t)\rangle = \langle E_{A1}(t+\tau)E_{A2}^*(t)\rangle + \langle E_{B1}(t+\tau)E_{B2}^*(t)\rangle + \langle E_{A1}(t+\tau)E_{B2}^*(t)\rangle + \langle E_{B1}(t+\tau)E_{A2}^*(t)\rangle$$

$$\langle I_n\rangle = \langle E_n(t)E_n^*(t)\rangle = \langle E_{An}(t)E_{An}^*(t)\rangle + \langle E_{Bn}(t)E_{Bn}^*(t)\rangle + \langle E_{An}(t)E_{Bn}^*(t)\rangle + \langle E_{Bn}(t)E_{An}^*(t)\rangle$$

$$\Rightarrow \langle I_1\rangle = \langle I_2\rangle$$

$$\langle E_{A1}(t+\tau)E_{A2}^*(t)\rangle = \langle E_A(t+\tau)E_A^*(t)\rangle\, e^{\left[\frac{i(r_{A1}-r_{A2})\omega}{c}\right]} = \langle E_A(t+\tau_A)E_A^*(t)\rangle \text{ with } \tau_A \equiv \tau + \frac{(r_{A1}-r_{A2})}{c}$$

$$\langle E_{B1}(t+\tau)E_{B2}^*(t)\rangle = \langle E_B(t+\tau)E_B^*(t)\rangle\, e^{\left[\frac{i(r_{B1}-r_{B2})\omega}{c}\right]} = \langle E_B(t+\tau_B)E_B^*(t)\rangle \text{ with } \tau_B \equiv \tau + \frac{(r_{B1}-r_{B2})}{c}$$

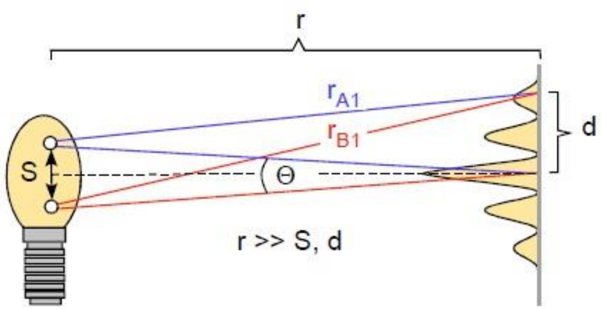
$$\Rightarrow \langle E_1(t+\tau)E_2^*(t)\rangle = \langle E_A(t+\tau_A)E_A^*(t)\rangle + \langle E_B(t+\tau_B)E_B^*(t)\rangle$$

$$\gamma_{12}(\tau) \equiv \frac{\langle E_1(t+\tau)E_2^*(t)\rangle}{(\langle I_1\rangle\langle I_2\rangle)^{\frac{1}{2}}} = \frac{1}{2}\left[g^{(1)}(\tau_A) + g^{(1)}(\tau_B)\right] = \frac{1}{2}\left[e^{i\omega\tau_A - \frac{\tau_A}{\tau_0}} + e^{i\omega\tau_B - \frac{\tau_B}{\tau_0}}\right]$$

$$4|\gamma_{12}(\tau)|^2 \equiv \left|g^{(1)}(\tau_A)\right|^2 + \left|g^{(1)}(\tau_B)\right|^2 + 2\left|g^{(1)}(\tau_A)\right|\left|g^{(1)}(\tau_B)\right|\cos(\omega(\tau_A - \tau_B))$$ **interference term**

$$4|\gamma_{12(\tau)}|^2 \equiv |g^{(1)}(\tau_A)|^2 + |g^{(1)}(\tau_B)|^2 + 2|g^{(1)}(\tau_A)|\,|g^{(1)}(\tau_B)|\,\cos(\omega(\tau_A - \tau_B))$$

Interference term depends on $\tau_A - \tau_B = \frac{r_{A1}-r_{A2}}{c} - \frac{r_{B1}-r_{B2}}{c}$



Light Source: mutually incoherent point sources $g^{(1)}(\tau) = \exp(i\omega\tau - \tau/\tau_0)$

symmetric: $r_{A2} - r_{B2} = 0 \Rightarrow \tau_A - \tau_B = \frac{r_{A1} - r_{B1}}{c}$

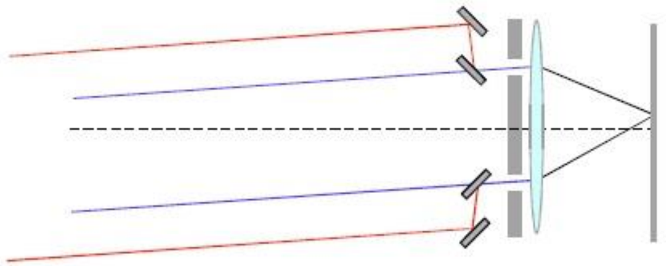
$$r_{A1} \cong r + \frac{\left(\frac{d-S}{2}\right)^2}{2r},\; r_{B1} \cong r + \frac{\left(\frac{d+S}{2}\right)^2}{2r}$$

$$\Rightarrow \tau_A - \tau_B \cong -\frac{Sd}{2rc}$$

First minimum of $|\gamma_{12}(\tau)|^2$:

$$\omega(\tau_A - \tau_B) = \pi; \quad S \cong r\theta \qquad \Rightarrow \; d \cong \frac{\lambda}{\theta}$$

transverse coherence length



Michelson stellar interferometer: adjustable slits, extension of slit separation by mirrors

Measurement of angular diameter of stars, angular separation of double stars, etc.

Second Order Coherence

Normalized autocorrelation function:

$$g^{(2)}(\tau) \equiv \frac{< I(t+\tau)I(t) >}{< I(t) >^2}$$

degree of second order coherence

Correlation of intensities

(1) $g^{(2)}(-\tau) = g^{(2)}(\tau)$

(2) $g^{(2)}(0) \geq 1$

(3) $g^{(2)}(\tau) \leq g^{(2)}(0)$

(4) $g^{(2)}(\tau \to \infty) = 1$ if correlations vanish

Proof (2):

$$\left(\frac{1}{N}\sum_{n=1}^{N} I_n\right)^2 = \frac{1}{N^2}\left(\sum_n I_n^2 + \sum_{n\neq m} I_n I_m\right) \leq \frac{1}{N^2}\left(\sum_n I_n^2 + \sum_{n\neq m} \frac{I_n^2 + I_m^2}{2}\right)$$

(inequality of arithmetic and geometric means)

$$= \frac{1}{N^2}\sum_{n,m} \frac{I_n^2 + I_m^2}{2} = \frac{1}{N}\sum_{n,m} I_n^2$$

$$\Rightarrow g^{(2)}(0) = \frac{< I(t)^2 >}{< I(t) >^2} = \frac{1}{N}\sum_{n,m} I_n^2 \Big/ \left(\frac{1}{N}\sum_{n=1}^{N} I_n\right)^2 \geq 1$$

Proof (3):

$$(< I(t+\tau)I(t) >)^2 = \left(\frac{1}{N}\sum_{n=1}^{N} I(t_n+\tau)I(t_n)\right)^2 \leq \left(\frac{1}{N}\sum_{n=1}^{N} I(t_n+\tau)^2\right)\left(\frac{1}{N}\sum_{n=1}^{N} I(t_n)^2\right) = (< I(t)^2 >)^2$$

(Cauchy-Schwarz inequality)

Proof (4):

$$\tau \to \infty \;\Rightarrow\; < I(t+\tau)I^*(t) > = < I(t+\tau) >< I(t) > \; = < I(t) >^2$$

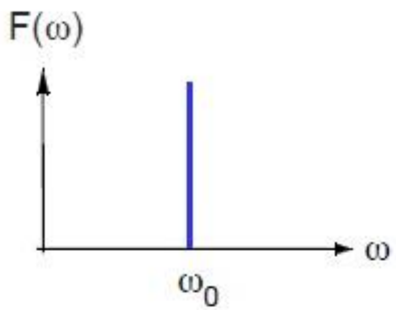
Example: **monochromatic light**

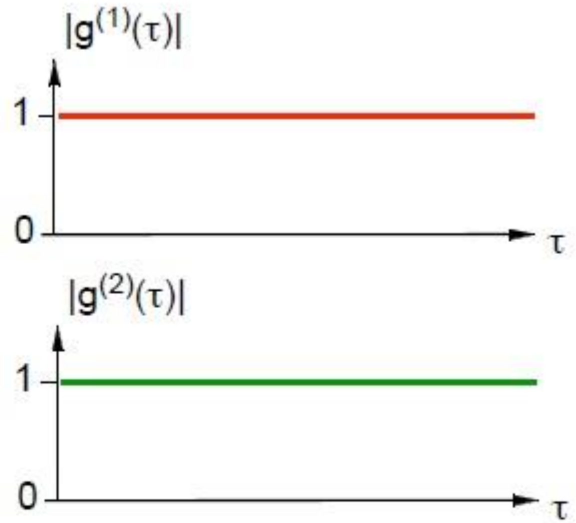
$$E(t) = E_0\, e^{i(\omega_0 t + \phi)}$$

$$I(t) = E_0 E_0^*$$

$$|g^{(1)}(\tau)| = 1$$

$$g^{(2)}(\tau) \equiv \frac{< I(t+\tau)I^*(t) >}{< I(t) >^2} = 1$$





Chaotic Light

$$E(t) = E_0 \sum_{n=1}^{N} e^{i\phi_n(t)}, \qquad \phi_n(t) = \text{random phase, uniform at any time t}$$

$$< e^{i(\phi_n(t+\tau)-\phi_n(t))} > = 0 \qquad \text{if } n \neq m,$$

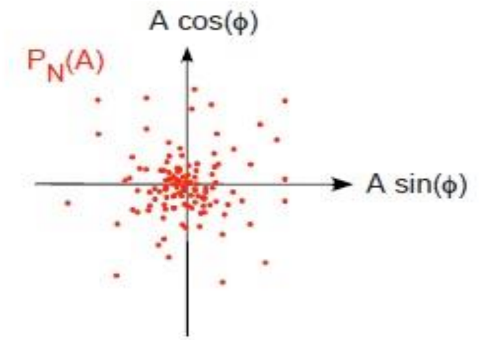
$$g^{(1)}(\tau) = \sum_{n=1}^{N} < e^{i(\phi_n(t+\tau)-\phi_n(t))} >$$

Theory of stochastic processes:

Probability for $\sum_n^N e^{i\phi_n}$ to fall within unit areas at the point (A,Φ) in the complex plane:

$$P_N(A) = \frac{1}{N}\pi e^{-\frac{A^2}{N}}$$

Probability for measuring an intensity $\in [I, I + dI]$: $P(I)dI = \frac{1}{\langle I \rangle} e^{-I/\langle I \rangle} dI$



moments: $< I^n > \equiv \int_0^\infty dI\, P(I)\, I^n = n! < I >^n$

$$\Delta I \equiv (< I^2 > - < I >^2)^{\frac{1}{2}} = < I >$$

Note: for chaotic light: $g^{(2)}(\tau) = 1 + |g^{(1)}(\tau)|^2$ **Siegert relation**

$E(t) = \sum_{n=1}^{N} E_n(t)$, with $E_n(t), E_m(t)$ uncorrelated for $n \neq m$:

$$< E(t+\tau)E(t)E^*(t)E(t+\tau)^* > = \sum_{n=1}^{N} < E_n(t+\tau)E_n(t)E_n^*(t)E_n^*(t+\;) >$$

$$+ \sum_{n \neq m}^{N} < E_n(t+\tau)E_n(t)E_m^*(t)E_m^*(t+\;) >$$

$$+ \sum_{n \neq m}^{N} < E_n(t+\tau)E_n^*(t+\tau)E_m^*(t)E_m(t) >$$

$$= N < E_n(t+\tau)E_n(t)E_n^*(t)E_n^*(t+\;) >$$

Only fields for each atom contribute

$$+ N(N-1) < E_n(t+\tau)E_n^*(t) >< E_m(t)E_m^*(t+\;) >$$
$$+ N(N-1) < E_n(t+\tau)E_n^*(t+\tau) >< E_m^*(t)E_m(t) >$$

N >>1

$$\cong N^2 |< E_n(t+\tau)E_n^*(t) >|^2 + N^2 < E_m^*(t)E_m(t) >^2 = N^2 < E_m^*(t)E_m(t) >^2 \left(\left|g^{(1)}(\tau)\right|^2 + 1\right)$$

$$= < I > \left(\left|g^{(1)}(\tau)\right|^2 + 1\right)$$

An example of chaotic light: collisional broadened source revisited

$$E(t) = E_0 \sum_{n=1}^{N} e^{i\phi_n(t)}, \qquad \phi_n(t) = -\omega_n t + \phi_n,\ \phi_n = \text{random phase} \Longrightarrow$$

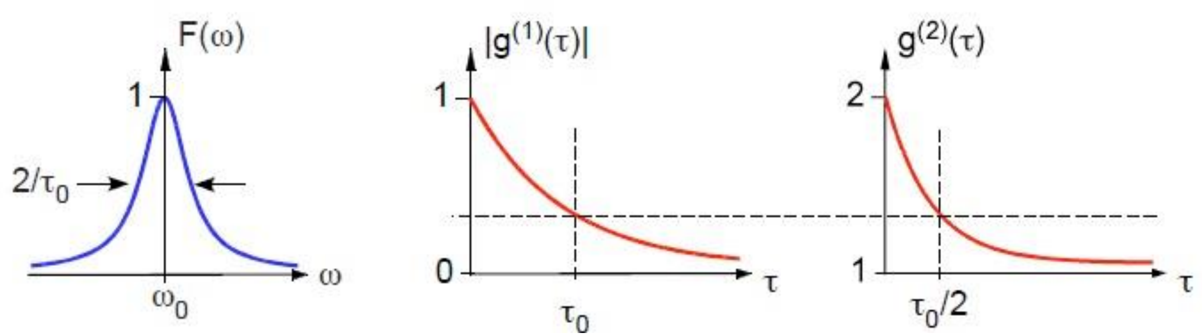
$$g^{(1)}(\tau) = \sum_{n=1}^{N} < e^{i(\phi_n(t+\tau)-\phi_n(t))} > = \sum_{n=1}^{N} < e^{i\omega_n \tau} > = \int_{-\infty}^{+\infty} d\omega\ e^{i\omega\tau}\, P(\omega)$$

Wiener-Khinchin

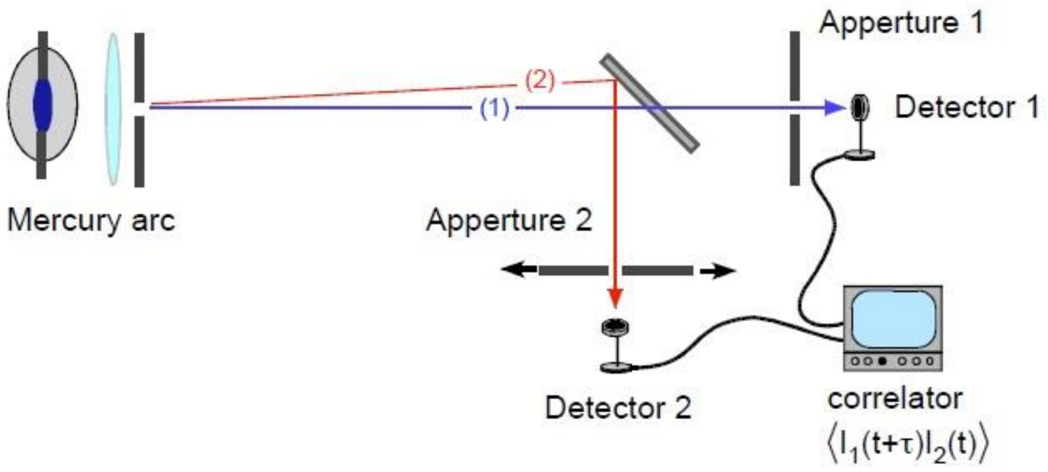
Example: assume Lorentzian spectrum (collision broadened light source)

$$P(\omega) = \frac{\tau_0}{\pi} \frac{1}{[1+(\omega_0-\omega)^2\tau_0^2]} \Rightarrow g^{(1)}(\tau) = e^{-i\omega_0\tau - \frac{|\tau|}{\tau_0}}$$

$$g^{(2)}(\tau) = 1 + e^{\frac{-2|\tau|}{\tau_0}}$$



Measurement of $g^{(2)}(\tau)$: Hanbury Brown & Twiss (1956)



Angular size of SIRIUS: 3×10^{-8} radians

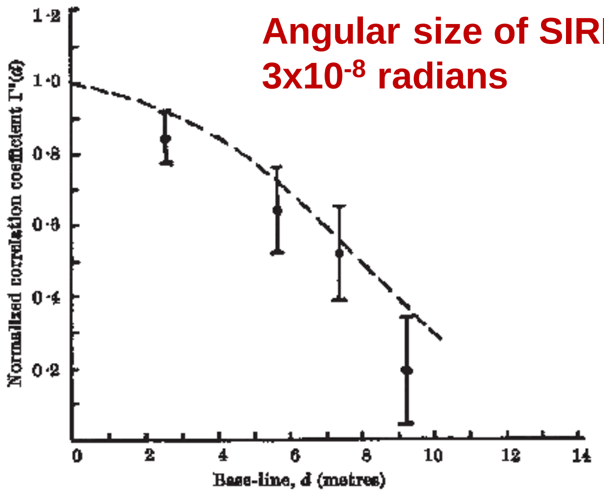


Fig. 2. Comparison between the values of the normalized correlation coefficient Γ²(d) observed from Sirius and the theoretical values for a star of angular diameter 0·0063″. The errors shown are the probable errors of the observations

Variation of aperture 2 allows a measurement of the transverse coherence length

⇒ Determination of the opening angle of the source