§7 ...

Das Fluktuations-Dissipations-Theorem

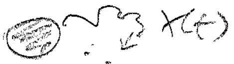
Fundamentale Beziehung
Flukt. einer Observablen eines Systems im thermodyn. GGW und der Antwort dieses Systems auf ext. Feld

Statistische Physik des Gleichgewichts

- $\langle E \rangle$, $\langle N \rangle$, ...
- Temperatur $T = \left(\frac{\partial U}{\partial S}\right)_V$
- Fluktuationen als Funktion von T
- Noise ... thermal noise

§1.1 Motivation

Beispiel 1: Diffusion (Einstein 1905)

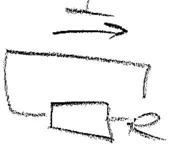


$$\langle x(t)^2 \rangle = 2Dt$$

$$D = k_B T \cdot \frac{1}{\gamma}$$

$\frac{1}{\gamma} = \frac{1}{6\pi\eta a}$ = hydrodyn. Mobilität

Beispiel 2: Elektrothermisches Rauschen
electrothermal noise
(Johnson, Nyquist, 1928)



$\langle I \rangle = 0$

Fluktuationsspektrum

$$S_I(\omega) = 2k_B T \cdot \frac{1}{R\pi} \quad (\hbar\omega \ll k_B T)$$

§2 Das FDT für klassische Systeme

(Callen, Welton 1951)

Mikrozustand microstate

$X = (p_1, \ldots, p_N, q_1, \ldots, q_N)$

Hamiltonian

$H_0(X)$

Observable A; $\langle A(t) \rangle = \int dx\, A(x)\, \rho(x,t)$

FDT $\quad \underbrace{S_A(\omega)}_{\text{Fluktuations-spektrum}} = 2 \cdot \frac{k_B T}{\omega} \underbrace{\operatorname{Im} \chi_A(\omega)}_{\text{Dissipative Antwort auf ext. Feld}}$

Dissipative response to external field

Two concepts needed:

- Boltzmann-Verteilung $\rho_0 \sim \exp(-\beta H_0)$

+

- Zeitpropagator $P(x_1, t_1 | x_0, t_0)$
  time propagator

§2a Fluktuationsspektrum $S_A(\omega)$

Autokorrelationsfunktion

$$C_A(\tau) = \langle A(t)\, A(t+\tau) \rangle - \langle A \rangle^2$$

[unabhängig von t,
gerade Funktion $C_A(\tau) = C_A(-\tau)$]
even function

$$= \int dx_0 \; A(x_0)\, A(x_1) \cdot \rho_0(x_0) \cdot P(x_1, t+\tau \mid x_0, t)$$
$$- \langle A \rangle^2$$

<u>Def.</u> (power spectrum)

$$S_A(\omega) = \tilde{C}_A(\omega) = \int d\tau \; C_A(\tau) \exp{+i\omega\tau}$$

Fourier transform (non-unitary, angular freq.)

[Wiener-Kinchin-Theorem: integral exists]

[• kann direkt gemessen werden, z.B. Dichtefluktuationen in Streuexperimenten]

Formally

$$\langle \tilde{A}(\omega)\, \tilde{A}^*(\omega') \rangle = S_A(\omega)\, \delta(\omega - \omega')$$

§26 Lineare ~~Antwortfunktion~~ χ_A.
linear response function

Hamiltonian
$$H(x,t) = H_0(x) - A(x)\, f(t)$$

Lineare ~~Antwort~~
$$\langle A(t)\rangle = \langle A\rangle_0 + \int_0^\infty d\tau\, \chi_A(\tau)\, f(t-\tau) + O(f^2)$$
$\Rightarrow$ definiert $\chi_A(\tau)$

Kausalität impliziert $\chi_A(\tau) = 0$ für $\tau < 0$

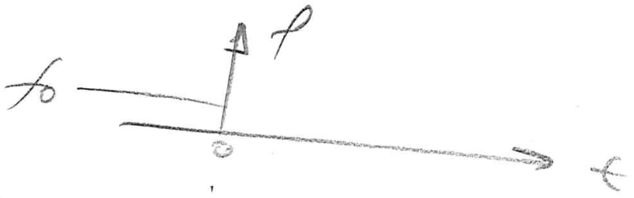
Fourier transformation
$$\tilde{\chi}_A(\omega) = \int_0^\infty d\tau\, \chi_A(\tau) \exp i\omega\tau.$$

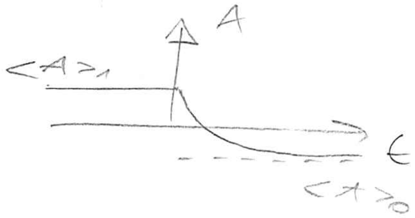
Oszillierendes Feld $f(t) = f_0 \cos\omega t$.
$$\langle A(t)\rangle = \langle A\rangle_0 + \mathrm{Re}\, \tilde{\chi}_A(\omega) f_0 \cos\omega t - \mathrm{Im}\, \tilde{\chi}_A(\omega) f_0 \sin\omega t$$

Vom Feld verrichtete Leistung
$$R = -f(t) \frac{d}{dt} A(t)$$
$$\langle R\rangle = \frac{1}{2}\omega f_0^2\, \mathrm{Im}\, \tilde{\chi}_A(\omega)$$

§2c Herleitung
Derivation

Sei $f(t) = f_0 \, \Theta(-t)$





Hamiltonian $H_1 = H_0 - A f_0$: H_0

Zustandsdichte
probability density $\rho_1(x)$: $\rho(x,t) \xrightarrow{t \to \infty} \rho_0(x)$

$$Z_1 = \int dx \, \exp - \beta H_1(x) \, , \quad \beta = \frac{1}{k_B T}$$

$$\rho_1(x) = \frac{1}{Z_1} \exp - \beta H_1(x)$$

$$\approx \rho_0(x) \left[1 + \beta f_0 \left(A(x) - \langle A \rangle_0 \right) \right] \quad (*)$$

$\to$ ÜA

Für $t > 0$:

$$\langle A(t) \rangle = \int dx \, A(x) \, \rho(x,t)$$

$$= \int dx \, A(x) \int dx_0 \, P_0(x,t | x_0, 0) \, \rho_1(x_0)$$

$$\overset{(*)}{=} \langle A \rangle_0 + \beta f_0 \, C_A(t)$$

$\to$ ÜA 6.6. (use *)

$$\overset{!}{=} \langle A \rangle_0 + \int_{-\infty}^{\infty} d\tau \, \chi_A(\tau) f_0 \Theta(\tau - t)$$

$$= \int dx \int dx_0 \; A(x) \; P(x,t \mid x_0, 0) \cdot \rho_0(x_0) \cdot \left[1 + \beta f_0 \left(A(x_0) - \langle A \rangle_0 \right) \right]$$

$$= \langle A \rangle_0 + \underbrace{\beta f_0 \cdot \langle A(t) \cdot A(0) \rangle_0 - \beta f_0 \langle A(t) \rangle_0 \langle A \rangle_0}_{\beta f_0 \, C_A(t)}$$

Ableitung nach t.

$$\chi_A(t) = \begin{cases} \beta \frac{d}{dt} C_A(t) & \text{für } t \geq 0 \\ 0 & t < 0 \end{cases}$$

Gerade/ungerade Funktionen

$$F(t) \begin{cases} F'(t) = \frac{1}{2}[F(t) + F(-t)] \longrightarrow \tilde{F}'(\omega) = \mathrm{Re}\,\tilde{F}(\omega) \\ F''(t) = \frac{1}{2}[F(t) - F(-t)] \longrightarrow \tilde{F}''(\omega) = i\,\mathrm{Im}\,\tilde{F}(\omega) \end{cases}$$

$C_A(t)$ = even
$\frac{d}{dt} C_A(t)$ = odd.

$$\chi_A''(t) = \frac{1}{2} \beta \frac{d}{dt} C_A(t)$$

$$i\,\mathrm{Im}\,\tilde{\chi}_A(\omega) = \frac{1}{2}\beta\,(+i\omega)\,S_A(\omega)$$

$\Rightarrow$
FDT.

⚠ Sign depends on convention for Fourier transform.

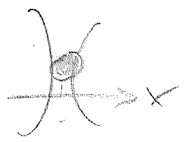
- Klassische Mechanik $\Rightarrow$ Quantenmechanik
  $\frac{1}{\beta} = kT$ $\Rightarrow \hbar\omega \coth \frac{\beta\hbar\omega}{2}$

inkl. Nullpunktsenergie, kann nicht übertragen werden
zero-point energie

6

Beispiel: Optische Falle
Optical trap

(Arthur Ashkin
Nobel prize 2018)



$L \sim 1\,\mu m$

$k x - \gamma \dot{x} = \gamma \xi(t)$

$\langle \xi(t) \rangle = 0.$

Rauschstärke

$$\int_{-\infty}^{\infty} d\tau \, \langle \xi(t)\, \xi(t-\tau) \rangle = 2D.$$

FDT

$$S_x(\omega) = \frac{2k_BT}{\omega}\, \mathrm{Im}\, \tilde{\chi}_x(\omega) = \frac{2k_BT/\gamma}{(k/\gamma)^2 + \omega^2}$$

- Bestimmung von k
  Eichung k.

- $\omega = 0$: $S_x(\omega) = \dfrac{2D\gamma^2}{|k + \gamma i \omega|^2}$

$$\Rightarrow D = \frac{k_BT}{\gamma}$$

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$\boxed{\text{Generalized example}}$

(*) $\sum_{k=0}^{n} a_k x^{(k)} = \xi(t)$.

lin. dif. op. Gaussian (white) noise.

$$\xrightarrow{\text{FT}} \underbrace{\sum_{k=0}^{n} a_k (i\omega)^k}_{\tilde{\chi}_A(\omega)^{-1}} \tilde{x}(\omega) = \tilde{\xi}(\omega)$$

product $\tilde{x}(\omega) = \tilde{\chi}_A(\omega) \cdot \tilde{\xi}(\omega)$.

$\Downarrow$ IFT

convolution $x(t) = \int_0^\infty d\tau \; \tilde{\chi}_A(\cancel{t-}\tau) \cdot \xi(t-\tau)$

$$S_x(\omega)\,\delta(\omega-\omega') = \langle \tilde{x}(\omega)\tilde{x}^*(\omega')\rangle$$
$$= |\tilde{\chi}_A(\omega)|^2 \cdot \langle \tilde{\xi}(\omega)\tilde{\xi}(\omega')\rangle$$
$$= |\tilde{\chi}_A(\omega)|^2 \cdot 2D \cdot \delta(\omega-\omega').$$

$$\Rightarrow S_x(\omega) = |\tilde{\chi}_A(\omega)|^2 \, 2D.$$

$$= \frac{2k_BT}{\omega} \operatorname{Im} \tilde{\chi}_A(\omega)$$

$$\Rightarrow 2D = 2k_BT \cdot \frac{\frac{1}{\omega} \operatorname{Im} \tilde{\chi}_A(\omega)}{|\tilde{\chi}_A(\omega)|^2}$$

Special case ($a_{2k+1} = 0$ except $a_1 = \gamma$)

$$\tilde{\chi}_A = \frac{1}{R(\omega) - i\omega\gamma} \Rightarrow \operatorname{Im} \tilde{\chi}_A = \frac{\omega\gamma}{R(\omega)^2 + \omega^2\gamma^2}$$

$$\Rightarrow D_{\cancel{x}} = \frac{k_BT}{\cancel{\gamma}}\gamma$$

$\Rightarrow$ white noise.

If we divide Eq (*) by γ, $D = \frac{k_BT}{\gamma}$ diffusion coef.)

Compute power-spectral density from finite time ~~series~~

tlist = np.arange(0, tmax, dt)
xlist.

xfft = fft(xlist). • depends on dt, tmax.

$$\boxed{psd = \frac{1}{tmax} |xfft|^2 \cdot dt^2}$$