準備

- トレースの循環性

$$ \begin{aligned} \text{Tr}[AB] &= A_{ij}B_{ji} \ &= B_{ji} A_{i j} \ &= \text{Tr}[BA] \end{aligned} $$

$$ \begin{aligned} \text{Tr} [AB] &= \int d\psi \bra{\psi} AB \ket{\psi} \ &= \int d\psi \bra{\psi} A \left(\int d\psi' \ket{\psi'}\bra{\psi'} \right) B \ket{\psi} \ &= \int d\psi \int d\psi' \bra{\psi} A \ket{\psi'}\bra{\psi'} B \ket{\psi} \ &= \int d\psi' \int d\psi \bra{\psi'} B \ket{\psi} \bra{\psi} A \ket{\psi'} \ &= \int d\psi' \bra{\psi'} B \left(\int d\psi \ket{\psi}\bra{\psi} \right) A \ket{\psi'} \ &= \int d\psi' \bra{\psi'} BA \ket{\psi'} \ &= \text{Tr} [BA] \end{aligned} $$

- 分布関数πの位置

$$ \begin{aligned} \langle A B \rangle_{eq} &= \sum_{\psi} \bra{\psi} A B \pi \ket{\psi} \ &= \text{Tr}\left[A B \pi \right] \ &= \text{Tr}\left[\pi A B \right] \ \ \ \ \ (\because \text{トレースの循環性}) \ &= \text{Tr}\left[B \pi A \right] \ \ \ \ \ (\because \text{トレースの循環性}) \ &\neq \text{Tr}\left[\pi B A \right] \ \ \ \ \ (ie. \neq \langle B A \rangle_{eq}) \ \end{aligned} $$

- Hが時間に陽に依存しない場合の、時間発展演算子$U_{(t)}$

$$ \begin{aligned} &U_{(t)} = e^{-\frac{i}{h}Ht} \ &U^{\dagger}{(t)} = U^{-1}{(t)} = e^{\frac{i}{h}Ht} \ \end{aligned} $$

$$ \begin{aligned} A_{(t)} &= U^{\dagger}{(t)} A U{(t)} \ \dot{A}{(t)} &= |frac{d}{dt} |left(U^{|dagger}{(t)} A U_{(t)} \right) \ &= U^{\dagger}{(t)} |frac{i}{|hbar} H A U{(t)} - U^{\dagger}{(t)} A |frac{i}{|hbar} H U{(t)} \ &= U^{\dagger}{(t)} |frac{i}{|hbar} [H, A] U{(t)} \ &= U^{\dagger}{(t)} |dot{A} U{(t)} \end{aligned} $$

- Hが時間に陽に依存する場合の、時間発展演算子$U_{(t)}$

$$ \begin{aligned} i \hbar \frac{\partial}{\partial t} \ket{\psi_{(t)}} &= H_{(t)} \ket{\psi_{(t)}} \ \therefore i \hbar \frac{\partial}{\partial t} U_{(t)} &= H_{(t)} U_{(t)} \ \therefore U_{(t + \Delta t)} &= \left(I - \frac{i}{\hbar} H_{(t)} \Delta t \right) U_{(t)} \end{aligned} $$

逐次積分

$$ \begin{aligned} U_{(\Delta t)} &= \left(I - \frac{i}{\hbar}H_{(0)} \Delta t \right) U_{(0)} = \left(I - \frac{i}{\hbar} H_{(0)} \Delta t \right) \ U_{(2\Delta t)} &= \left(I - \frac{i}{\hbar}H_{(\Delta t)} \Delta t \right) U_{(\Delta t)} = \left(I - \frac{i}{\hbar} H_{(\Delta t)} \Delta t \right) \left(I - \frac{i}{\hbar} H_{(0)} \Delta t \right) \ \cdots \ U_{(n\Delta t)} &= \prod^{n}{i} |left(I - |frac{i}{|hbar} H{(i \Delta t)} \Delta t \right) \ \therefore U_{(\tau)} &= \lim_{n \to \infty} \prod^{n}{i} |left(I - |frac{i}{|hbar} H{(\frac{i\tau}{n})} \frac{\tau}{n} \right) = I - \frac{i}{\hbar} \int^{\tau}0 dt H{(t)} + \left(\frac{i}{\hbar} \right)^2 \int^{\tau}{|tau'} dt |int^{|tau'}0 dt' H{(dt)} H{(dt')} + \cdots \ &\coloneqq \exp_{\leftarrow} \left(-\frac{i}{\hbar} \int^{\tau}_0 H dt \right) \ \ \ \ (\text{時間順序指数}) \end{aligned} $$

- 平衡状態における平均の時間非依存性

古典系

$$ \begin{aligned} \langle A_{(t)} \rangle_{eq} &\coloneqq \langle e^{L^{\dagger}0 t} A |rangle{eq} \ &= \int d\Gamma (e^{L^{\dagger}0 t} A) |pi | &= |int d|Gamma A e^{L_0 t} |pi | &= |int d|Gamma A |pi{(-t)} \ &= \int

d\Gamma A \pi \ &= \langle A \rangle_{eq} \end{aligned} $$

量子系

$$ \begin{aligned} \langle P^{-1} A P \rangle_{eq} &= \text{Tr} [P^{-1} A P] \ &= \text{Tr} [A P P^{-1}] \ &= \text{Tr}[A] \ &= \langle A \rangle_{eq} \end{aligned} $$

$$ \langle A_{(t)} \rangle_{eq} = \langle U^{\dagger}t A U_t \rangle{eq} = \langle A \rangle_{eq} \ \ \ \ \ (\because U_t\text{がユニタリ}) $$

$$ \begin{aligned} \langle A_{(t)} B_{(\tau)} \rangle_{eq} &= \langle U^{\dagger}t A U_t U^{\dagger}\tau B U_\tau \rangle_{eq} \ &= \langle A U_t U^{\dagger}\tau B{(\tau - t)} U_\tau U^\dagger_t \rangle_{eq} \ &= \langle A U^{\dagger}{(\tau - t)} B{(\tau - t)} U_{(\tau - t)} \rangle_{eq} \ &= \langle A B_{(\tau - t)} \rangle_{eq} \end{aligned} $$

- 微分が入った時間相関関数 $\cdots (公式1)$

$$ \begin{aligned} \left\langle \dot{B}{(\tau)} A{(t)} \right\rangle_{eq} &= \left\langle \left(\frac{d}{d\tau} B_{(\tau)} \right) A_{(t)} \right\rangle_{eq} \ &= \frac{d}{d\tau} \left\langle B_{(\tau)} A_{(t)} \right\rangle_{eq} \ &= \frac{d}{d\tau} \left\langle B A_{(t - \tau)} \right\rangle_{eq} \ &= - \frac{d}{dt} \left\langle B A_{(t - \tau)} \right\rangle_{eq} \ &= - \left\langle B \dot{A}{(t - \tau)} \right\rangle{eq} \ \end{aligned} $$

2.2 古典粒子系に対する揺動散逸定理 (続き)

応答関数を計算するときは、系が平衡状態$(H = H_{tot})$のときを考えればいよい。

$$ \begin{aligned} \alpha + \text{O}{(\epsilon)} \coloneqq \phi{\dot{x}x(t; H_{tot} - \epsilon x F_{(t)})} \ \alpha = \left. \phi_{\dot{x}x(t; H_{tot} - \epsilon x F_{(t)})} \right|{\epsilon = 0} = \phi{\dot{x}x(t; H_{tot})} \end{aligned} $$

$$ \begin{aligned} \langle \dot{x}{(\tau)} \rangle &\simeq \epsilon \int^{\tau}{-\infty} dt F_{(t)} \phi_{\dot{x}x(\tau - t; H_{tot} - \epsilon x F_{(t)})} \ &= \epsilon \int^{\tau}{-\infty} dt F{(t)} \left(\alpha + \text{O}{(\epsilon)} \right) \ &\simeq \epsilon \int^{\tau}{-\infty} dt F_{(t)} \alpha \ &= \epsilon \int^{\tau}{-\infty} dt F{(t)} \phi_{\dot{x}x(\tau - t; H_{tot})} \end{aligned} $$

応答関数 $\phi_{\dot{x}x}$

$$ \begin{aligned} \dot{x}_{(t)} &= e^{L^{\dagger}_0 t} \dot{x} \ &= e^{L^{\dagger}_0 t} L^{\dagger}_0 x \ &= \frac{d}{dt} e^{L^{\dagger}0 t} x \ &= \frac{d}{dt} x{(t)} \end{aligned} $$

$$ \begin{aligned} \phi_{\dot{x}x(\tau - t)} &\coloneqq \beta \langle \dot{x}{(\tau - t)} \dot{x} \rangle{eq} \ &= \beta \langle \dot{x}{(\tau)} \dot{x}{(t)} \rangle_{eq} \ &= \beta \langle \dot{x}{(\tau)} \frac{d}{dt} x{(t)} \rangle_{eq} \ &= \beta \frac{d}{dt} \langle \dot{x}{(\tau)} x{(t)} \rangle_{eq} \end{aligned} $$

長時間後に一定になった速度 $\cdots (2.11)$

$$ \begin{aligned} \frac{\langle \dot{x}{(\tau)} \rangle}{F_0} &= \int^{\tau}{-\infty} dt \phi_{\dot{x}x(\tau - t)} \ &= \int^{\infty}0 dt \phi{\dot{x}x(t)} \ \ \ \ \ (t \Rightarrow \tau - t) \ &= \beta \int^{\infty}0 dt \langle \dot{x}{(t)} \dot{x} \rangle_{eq} \ \therefore \frac{\langle \dot{x}{(\tau)} \rangle{eq}}{F_0} &= \frac{\langle \dot{x} \rangle_{eq}}{F_0} = \beta \int^{\infty}0 dt \langle \dot{x}{(t)} \dot{x} \rangle_{eq} \end{aligned} $$

ランジュバン方程式でのμ

$$ m \ddot{x} = F - \gamma \dot{x} + \xi $$

$$ \begin{aligned} m \langle \ddot{x} \rangle &= F - \gamma \langle \dot{x} \rangle + \langle \xi \rangle \ \therefore F &= \gamma \langle \dot{x} \rangle \ \ \ \ \ (\because \text{速度一定}) \ \therefore \frac{\langle \dot{x} \rangle}{F} &= \mu = \frac{1}{2k_B T} \int^{\infty}{-\infty} ds \langle \dot{x}{(s)} \dot{x} \rangle \ \ \ \ \ (\text{ref. } (1.12)) \end{aligned} $$

パルス入力に対する応答 $\cdots (2.12)$

$$ F_{(t)} = F_0 \delta_{(t - t')} $$

$$ \begin{aligned} \langle \dot{x}{(\tau)} \rangle &= \epsilon \int^{\tau}{-\infty} dt F_{(t)} \phi_{x\dot{x}(\tau - t)} \ &= \epsilon \int^{\tau}{-\infty} dt F_0 \delta{(t - t')} \phi_{x\dot{x}(\tau - t)} \ &= \epsilon F_{(0)} \phi_{x\dot{x}(\tau - t')} \ \ \ \ \ (\tau \ge t') \end{aligned} $$

フーリエ表示の揺動散逸定理 $\cdots (2.15)$

$$ \chi_{\dot{x}x(\omega)} = \chi'{(\omega)} + i \chi''{(\omega)} $$

$$ \begin{aligned} \chi'{(\omega)} &= \text{Re} \left[\int^{\infty}{0} dt \beta \langle \dot{x}{(t)} \dot{x} \rangle{eq} e^{i\omega t} \right] \ &= \beta \int^{\infty}{0} dt C{(t)} \text{Re} [e^{i\omega t}] \ &= \beta \int^{\infty}0 dt C{(t)} \cos{(\omega t)} \ &= \frac{\beta}{2} \int^{\infty}{0} dt C{(t)} \left(e^{i \omega t} + e^{-i \omega t} \right) \ &= \frac{\beta}{2} \left(\int^{\infty}{0} dt C{(t)} e^{i \omega t} - \int^{\infty}0 (-dt) C{(-t)} e^{-i \omega t} \right) \ &= \frac{\beta}{2} \left(\int^{\infty}{0} dt C{(t)} e^{i \omega t} + \int^0_{-\infty} dt C_{(t)} e^{i \omega t} \right) \ &= \frac{\beta}{2} C_{(\omega)} \end{aligned} $$

2.2 線形応答理論

§ 2.2.1 力学応答の線形応答

$$ H_{tot(t)} = H - BF_{(t)} $$

タイプ 1

$$ A \propto B $$

タイプ 2

$$ A \propto \dot{B} $$

§ 2.2.1.1 一般論

時間発展演算子 $\cdots (2.18)$

- 平衡状態の時間発展演算子を分離

$$ \begin{aligned} i \hbar \frac{\partial}{\partial t} U_{(t)} &= [H - FB] U_{(t)} \ \bar{U}{(t)} &\coloneqq e^{\frac{i}{\hbar}Ht} U{(t)} \ \end{aligned} $$

$$ \begin{align*} \frac{\partial}{\partial t} \bar{U}{(t)} &= \frac{i}{\hbar} H \bar{U}{(t)} - \frac{i}{\hbar} e^{\frac{i}{\hbar}Ht}[H - F_{(t)}B]U_{(t)} \ &= \frac{i}{\hbar} e^{\frac{i}{\hbar}Ht} F_{(t)}B U_{(t)} \ &= \frac{i}{\hbar} F_{(t)} \left(e^{\frac{i}{\hbar}Ht} B e^{-\frac{i}{\hbar}Ht} \right) e^{\frac{i}{\hbar} Ht} U_{(t)} \ &= F_{(t)}B_{(t)} \bar{U}_{(t)} \ \end{align*} $$

[note] Fについて一次の近似を考えるので、B の時間発展を考える時は、Fを考慮せず平衡状態のハミルトニアンで時間発展すると考えて良い。

- 逐次積分

$$ \begin{aligned} \bar{U}{(t + \Delta t)} &= \left(I + \frac{i}{\hbar} F{(t)}B_{(t)} \Delta t \right) \bar{U}{(t)} \ \therefore U{(t + \Delta t)} &= e^{- \frac{i}{\hbar}H(t+\Delta t)} \left(I + \frac{i}{\hbar} F_{(t)}B_{(t)} \Delta t \right) e^{\frac{i}{\hbar}Ht} U_{(t)} \ \therefore U_{(t)} &= e^{- \frac{i}{\hbar} H t} \prod^{n}{i} \left(e^{- \frac{i}{\hbar} H \Delta t} \left(I + \frac{i}{\hbar} F{(i\Delta t)}B_{(i \Delta t)} \Delta t \right) \right) e^{\frac{i}{\hbar}Ht_0} \ &\to e^{- \frac{i}{\hbar} Ht} \exp_{\leftarrow} \left(\frac{i}{\hbar} \int^t_{t_0} dt' F_{(t')} B_{(t')} \right) e^{\frac{i}{\hbar}Ht_0} \ \ \ \ \ (\Delta t \to 0) \end{aligned} $$

- 一次近似

$$ \begin{aligned} U_{(t)} &= e^{- \frac{i}{\hbar} H t} \prod^{n}{i} \left(e^{- \frac{i}{\hbar} H \Delta t} \left(I + \frac{i}{\hbar} F{(i\Delta t)}B_{(i \Delta t)} \Delta t \right) \right) e^{\frac{i}{\hbar}Ht_0} \ &= e^{- \frac{i}{\hbar} H t} \left(e^{- \frac{i}{\hbar} H \Delta t} \right)^n \left[1 + \sum^{n}{i} \left(\frac{i}{\hbar} F{(i\Delta t)}B_{(i \Delta t)} \Delta t \right) \right] e^{\frac{i}{\hbar}Ht_0} + \text{O}(F^2) \ &\to e^{- \frac{i}{\hbar} H t} \left(1 + \frac{i}{\hbar} \int^t_{t_0} dt' F_{(t')} B_{(t')} \right) e^{\frac{i}{\hbar} Ht_0} + \text{O}(F^2) \end{aligned} $$

演算子の期待値の時間発展 $\cdots (2.19)$

- 演算子の時間発展

$$ \begin{aligned} A_{(\tau)} &= U^{\dagger}{(\tau)} A U{(\tau)} \ &= e^{- \frac{i}{\hbar} H t_0} \left(1 - \frac{i}{\hbar} \int^\tau_{t_0} dt' F_{(t')} B_{(t')} \right) e^{\frac{i}{\hbar} H \tau} A e^{- \frac{i}{\hbar} H \tau} \left(1 + \frac{i}{\hbar} \int^\tau_{t_0} dt' F_{(t')} B_{(t')} \right) e^{\frac{i}{\hbar} Ht_0} + \text{O}(F^2) \ &= e^{\frac{i}{\hbar} H (\tau - t_0)} A e^{-\frac{i}{\hbar} H (\tau - t_0)} + e^{-\frac{i}{\hbar}Ht_0} \left[e^{\frac{i}{\hbar} H \tau} A e^{- \frac{i}{\hbar} H \tau}, \frac{i}{\hbar} \int^\tau_{t_0} dt' F_{(t')}B_{(t')} \right] e^{\frac{i}{\hbar}Ht_0} + \text{O}(F^2) \ &= e^{\frac{i}{\hbar} H (\tau - t_0)} A e^{-\frac{i}{\hbar} H (\tau - t_0)} + \frac{i}{\hbar} \int^\tau_{t_0} dt' F_{(t')} [A_{(\tau - t_0)}, B_{(t' - t_0)}] + \text{O}(F^2) \ \end{aligned} $$

[note] Fの一次近似を考えているので、積分の中では非平衡の時間発展と平衡の時間発展を区別する必要がない。

- 期待値の時間発展

$$ \begin{aligned} \langle A_{(\tau)} \rangle_{eq} - \langle A \rangle_{eq} &= \langle e^{\frac{i}{\hbar} H (\tau - t_0)} A e^{-\frac{i}{\hbar} H (\tau - t_0)} \rangle_{eq} + \frac{i}{\hbar} \int^\tau_{t_0} dt' F_{(t')} \langle [A_{(\tau - t_0)}, B_{(t' - t_0)}] \rangle_{eq} - \langle A \rangle_{eq} + \text{O}(F^2) \ &= \langle A \rangle_{eq} + \frac{i}{\hbar} \int^\tau_{t_0} dt' F_{(t')} \langle [A_{(\tau - t')}, B] \rangle_{eq} - \langle A \rangle_{eq} + \text{O}(F^2) \ &= \frac{i}{\hbar} \int^\tau_{t_0} dt' F_{(t')} \langle [A_{(\tau - t')}, B] \rangle_{eq} + \text{O}(F^2) \ \end{aligned} $$

十分に時間が経った時の期待値の変化量 $\cdots (2.20)$

$$ \begin{aligned} \langle \Delta A_{(\tau)} \rangle_{eq} &\coloneqq \lim_{t_0 \to - \infty} \langle A_{(\tau)} \rangle_{eq} - \langle A \rangle_{eq} \ &= \frac{i}{\hbar} \int^{\tau}{- \infty} dt F{(t)} \langle [A_{(\tau - t)}, B] \rangle_{eq} \ &= \frac{i}{\hbar} \int^{\infty}{0} dt F{(\tau - t)} \langle [A_{(t)}, B] \rangle_{eq} \ \ \ \ \ (t \to \tau - t) \ &= \int^{\infty}{0} dt \phi{AB(t)} F_{(\tau - t)} \end{aligned} $$

量子系の応答関数 $\cdots (2.21)$

$$ \phi_{AB(t)} \coloneqq \frac{i}{\hbar} \langle [A_{(t)}, B] \rangle_{eq} $$

- パルス応答

$$ \begin{aligned} \langle \Delta A_{(\tau)} \rangle_{eq} = F_0 \phi_{AB(\tau)} \ \ \ \ \ (\text{when. }F = F_0 \delta_{(t)}) \ \end{aligned} $$

- 書き換え

$$ \begin{aligned} \phi_{AB(t)} &= \frac{i}{\hbar}\langle [A_{(t)}, B] \rangle_{eq} \ &= \frac{i}{\hbar} \text{Tr} \left[\pi [A_{(t)}, B] \right] \ &= \frac{i}{\hbar} \left(\text{Tr} \left[\pi A_{(t)} B \right] - \text{Tr} \left[\pi B A_{(t)} \right] \right) \ &= - \frac{1}{i\hbar} \left(- \text{Tr} \left[A_{(t)} B \pi \right] + \text{Tr} \left[A_{(t)} \pi B \right] \right) \ &= \frac{1}{i\hbar} \text{Tr} \left[A_{(t)} [\pi, B] \right] \end{aligned} $$

カノニカル相関 $\cdots (2.22) \sim (2.27)$

- カノニカル相関

$$ \begin{aligned} \langle X; Y \rangle &\coloneqq \frac{1}{\beta} \int^{\beta}_0 du \text{Tr} \left[e^{uH} X e^{-u H} Y \pi \right] \ &= \frac{1}{\beta} \int^{\beta}_0 du \left(\text{Tr} \left[e^{uH} X e^{-u H} Y \pi \right] \right)^{\dagger} \ &= \frac{1}{\beta} \int^{\beta}_0 du \text{Tr} \left[\pi Y e^{-u H} X e^{uH} \right] \ &= \frac{1}{\beta} \int^{\beta}_0 du \text{Tr} \left[e^{uH} \pi Y e^{-u H} X \right] \ &= \frac{1}{\beta} \int^{\beta}_0 du \text{Tr} \left[\pi e^{uH} Y e^{-u H} X \right] \ &= \langle Y; X \rangle \end{aligned} $$

$$ \langle X; Y \rangle = \frac{1}{\beta} \int^{\beta}0 du |langle X{(-i\hbar u)} Y \rangle_{eq} \to \langle X Y \rangle_{eq} \ \ \ \ \ (\hbar \to 0) $$

- 交換子の書き換え

$$ \begin{aligned} [\pi, B] &= \frac{1}{Z} [e^{-\beta H}, B] \ &= \frac{1}{Z} (e^{-\beta H} B - B e^{-\beta H}) \ &= \frac{1}{Z} (e^{-\beta H} B e^{\beta H} - B) e^{-\beta H} \ &= \frac{1}{Z} \left[e^{-u H} B e^{u H} \right]^{u = \beta}_{u = 0} e^{-\beta H} \ &= \frac{1}{Z} \int^{\beta}_0 du \frac{d}{du} (e^{-u H} B e^{u H}) e^{-\beta H} \ &= \frac{i\hbar}{Z} \int^{\beta}_0 du \frac{d}{d(i \hbar u)} (e^{\frac{i}{\hbar} H (i \hbar u)} B e^{- \frac{i}{\hbar} H (i \hbar u)}) e^{-\beta H} \ &= \frac{i\hbar}{Z} \int^{\beta}0 du |dot{B}{(i\hbar u)} e^{-\beta H} \ &= i\hbar \int^{\beta}0 du |dot{B}{(i\hbar u)} \pi \ \ [\pi, B] &= \frac{1}{Z} e^{-\beta H} (B - e^{\beta H} B e^{-\beta H}) \ &= \cdots \ &= i\hbar \pi \int^{\beta}0 du |dot{B}{(-i\hbar u)} \end{aligned} $$

- 応答関数の書き換え

$$ \begin{aligned} \phi_{AB(t)} &= \frac{1}{i\hbar} \text{Tr} \left[A_{(t)} [\pi, B] \right] \ &= \frac{1}{i\hbar} \text{Tr} \left[A_{(t)} i\hbar \int^{\beta}0 du |dot{B}{(i\hbar u)} \pi \right] \ \end{aligned} $$

$$ \begin{aligned} \phi_{AB(t)} &= \frac{1}{i\hbar} \text{Tr} \left[A_{(t)} [\pi, B] \right] \ &= \frac{1}{i\hbar} \text{Tr} \left[A_{(t)} i\hbar \int^{\beta}0 du |dot{B}{(i\hbar u)} \pi \right] \ &= \int^\beta_0 du \text{Tr} \left[A_{(t)} \dot{B}{(i|hbar u)} |pi |right] | &= |int^|beta_0 du |langle A{(t)} \dot{B}{(i|hbar u)} |rangle{eq} \ &= \int^\beta_0 du \langle A_{(t - i\hbar u)} \dot{B} \rangle_{eq} \ &= \beta \langle A_{(t)}; \dot{B} \rangle \ &= \beta \langle \dot{B}; A_{(t)} \rangle \end{aligned} $$

$$ \phi_{AB(t)} \to \beta \langle A_{(t)} \dot{B} \rangle_{eq} \ \ \ \ \ (\hbar \to 0) $$

複素アドミッタンス $\cdots (2.28)$

$$ \chi_{AB(\omega)} \coloneqq \int^{\infty}0 dt \phi{AB(t)} e^{i\omega t} = \chi' + i \chi'' $$

$$ \begin{aligned} \chi_{AB(-\omega)} &= \int^{\infty}0 dt \phi{AB(t)} e^{-i \omega t} \ &= \int^{\infty}0 dt \phi{AB(t)} \left(e^{i \omega t} \right)^{} \ &= \left(\int^{\infty}0 dt \phi{AB(t)} e^{i \omega t} \right)^{} \ &= \chi_{AB(\omega)}^{*} \end{aligned} $$

演算子の応答 $\cdots (2.29)$

$$ F_{(t)} = F_0 \cos{(\omega t)} $$

$$ \begin{aligned} \langle \Delta A_{(\tau)} \rangle_{eq} &= \int^{\infty}{0} dt \phi{AB(t)} F_{(\tau - t)} \ &= \int^{\infty}{0} dt \phi{AB(t)} F_0 \cos{\omega (\tau - t)} \ &= F_0 \int^{\infty}{0} dt \phi{AB(t)} \text{Re} [e^{i \omega (\tau - t)}] \ &= F_0 \text{Re} \left[\int^{\infty}{0} dt \phi{AB(t)} e^{i \omega (\tau - t)} \right] \ &= F_0 \text{Re} \left[\int^{\infty}{0} dt \phi{AB(t)} e^{- i \omega t} e^{i \omega \tau} \right] \ &= F_0 \text{Re} \left[\chi_{AB(\omega)}^{*} e^{i \omega \tau} \right] \ &= F_0 \text{Re} \left[\chi_{AB(\omega)} e^{-i \omega \tau} \right] \ \end{aligned} $$

§ 2.2.1.2 クラマース・クローニッヒ関係

リーマン・ルベーグの補題

$$ \lim_{\omega \to 0} \left| \int^{\infty}0 dt \phi{AB(t)} e^{i \omega t} \right| = 0 \ \ \ \ \ (\text{Im}[\omega] > 0) $$

- 証明

$$ \begin{aligned} I &\coloneqq \int^{\infty}0 dt \phi{AB(t)} e^{i\omega t} \ &= \int^{\infty}{- \frac{\pi}{\omega}} ds \phi{AB(s + \frac{\pi}{\omega})} e^{i \omega (s + \frac{\pi}{\omega})} \ \ \ \ \ (s = t - \frac{\pi}{\omega}) \ &= \int^{\infty}{- \frac{\pi}{\omega}} ds \phi{AB(s + \frac{\pi}{\omega})} e^{i \omega s} e^{i \pi} \ &= - \left(\int^{\infty}0 ds \phi{AB(s + \frac{\pi}{\omega})} e^{i \omega s} + \int^0_{- \frac{\pi}{\omega}} ds \phi_{AB(s + \frac{\pi}{\omega})} e^{i \omega s} \right) \ \therefore 2I &= \int^{\infty}0 dt \left(\phi{AB(t)} - \phi_{AB(t + \frac{\pi}{\omega})} \right) e^{i \omega t} - \int^{0}{- \frac{\pi}{\omega}} dt \phi{AB(t + \frac{\pi}{\omega})} e^{i \omega t} \ \therefore \left| 2I \right| &\le \left| \int^{\infty}0 dt \left(\phi{AB(t)} - \phi_{AB(t + \frac{\pi}{\omega})} \right) e^{i \omega t} \right| + \left| \int^{0}{- \frac{\pi}{\omega}} dt \phi{AB(t + \frac{\pi}{\omega})} e^{i \omega t} \right| \ &\le \int^{\infty}0 dt \left| \phi{AB(t)} - \phi_{AB(t + \frac{\pi}{\omega})} \right| \left| e^{i \omega t} \right| + \int^{0}{- \frac{\pi}{\omega}} dt \left| \phi{AB(t + \frac{\pi}{\omega})} \right| \left| e^{i \omega t} \right| \ &\lt \int^{\infty}0 dt \left| \phi{AB(t)} - \phi_{AB(t + \frac{\pi}{\omega})} \right| + \int^{0}{- \frac{\pi}{\omega}} dt \left| \phi{AB(t + \frac{\pi}{\omega})} \right| \ \ \ \ \ (\because \text{Im}[\omega] > 0) \ \end{aligned} $$

- 積分の収束性

$$ \begin{aligned} \int^{\infty}0 dt \left| \phi{AB(t)} - \phi_{AB(t + \frac{\pi}{\omega})} \right| &= \lim_{\tau \to \infty} \int^{\tau}0 dt \left| \phi{AB(t)} - \phi_{AB(t + \frac{\pi}{\omega})} \right| \ &\le \lim_{\tau \to \infty} \int^{\tau}0 dt \left(\left| \phi{AB(t)} \right| + \left| \phi_{AB(t + \frac{\pi}{\omega})} \right| \right) \ &= 2 \int^{\infty}0 dt \left| \phi{AB(t)} \right| \ \ \ \ \ (\Rightarrow \text{有界かつ}\tau\text{について単調増加}) \end{aligned} $$

- 絶対値の極限

$$ \begin{aligned} \therefore \lim_{\omega \to \infty} \left| I \right| &= \lim_{\Delta t \to 0} \frac{1}{2} \int^{\infty}0 dt |left| |phi{AB(t + \Delta t)} - \phi_{AB(t)} \right| \ &= \lim_{\Delta t \to 0} \frac{1}{2} \lim_{\Delta t' \to 0} \sum_{i} \left| \phi_{AB(t_i + \Delta t)} - \phi_{AB(t_i)} \right| \Delta t' \ &= \lim_{\Delta t \to 0} \frac{1}{2} \sum_{i} \left| \phi_{AB(t_{i+1})} - \phi_{AB(t_i)} \right| \Delta t \ \ \ \ \ (\Delta t' = \Delta t \text{の条件で極限をとる})\ &\le \lim_{\Delta t \to 0} \frac{1}{2} \sum_{i} (M_i - m_i) \Delta t \ &= \lim_{\Delta t \to 0} \frac{1}{2} \left(S_{(\Delta t)} - s_{(\Delta t)} \right) \ &= 0 \ \ \ \ \ (\because \phi_{AB(t)}\text{はリーマン可積分}) \end{aligned} $$

複素アドミッタンス

$$ \begin{aligned} \chi_{AB(\omega)} &= \int^{\infty}0 |phi{AB(t)} e^{i\omega t} \end{aligned} $$

- 公式

$$ \begin{aligned} \int^a_b dx \frac{\epsilon}{x^2 + \epsilon^2} f_{(x)} &= \frac{1}{2i} \int^a_b dx \left(\frac{1}{x - i\epsilon} - \frac{1}{x + i\epsilon} \right) f_{(x)} \ &= \frac{1}{2i} \int^{a - i\epsilon}{b - i|epsilon} dz |frac{f{(z + i\epsilon)}}{z} + \int^{b + i\epsilon} {a + i|epsilon} dz |frac{f{(z - i\epsilon)}}{z} \ &= \frac{1}{2i} \oint dz \frac{f_{(z)}}{z} + \text{O}{(|epsilon)} | &|to |left{ |begin{split} &|pi f{(0)} \ \ \ \ \ (\text{原点が積分経路に含まれる}) \ &0 \ \ \ \ \ (\text{原点が積分経路に含まれない}) \end{split} \right. \end{aligned} $$

$$ \therefore \lim_{\epsilon \to 0} \frac{\epsilon}{x^2 + \epsilon^2} = \pi \delta(x) $$

$$ \begin{aligned} \frac{1}{x - i\epsilon} &= \frac{x + i\epsilon}{(x - i\epsilon)(x + i\epsilon)} \ &= \frac{x}{x^2 + \epsilon^2} + i \frac{\epsilon}{x^2 + \epsilon^2} \ &\to \text{Pv} \frac{1}{x} + i \pi \delta_{(x)} \end{aligned} $$

複素平面に拡張された複素アドミッタンス

$$ \frac{1}{2\pi i} \int^{\infty}{- |infty} d|omega' |frac{|chi{AB(\omega')}}{\omega' - z} = \left{ \begin{aligned} &\chi_{AB(z)} \ \ \ \ \ (\text{Im}[z] > 0) \ &0 \ \ \ \ \ (\text{Im}[z] < 0) \ \end{aligned} \right. $$

$$ \frac{1}{2\pi i} \int^{\infty}{|infty} d|omega' |frac{|chi{AB(\omega')}}{\omega' - (\omega + i \epsilon)} $$

$$ \begin{aligned} \frac{1}{2\pi i} \int^{\infty}{-|infty} d|omega' |frac{|chi{AB(\omega')}}{\omega' - (\omega + i \epsilon)} &= \frac{1}{2\pi i} \int^{\infty}{|infty} d|omega' |frac{|chi{AB(\omega')}}{(\omega' - \omega) - i \epsilon} \ &\to \frac{1}{2 \pi i} \int^{\infty}{-|infty} d|omega' |left(|text{Pv} |frac{|chi{AB(\omega')}}{\omega' - \omega} + i \pi \chi_{AB(\omega')} \delta_{(\omega' - \omega)} \right) \ &= \frac{1}{2 \pi i} \text{Pv} \int^{\infty}{-|infty} d|omega' |frac{|chi{AB(\omega')}}{\omega' - \omega} + \frac{1}{2} \chi_{AB(\omega)} \ \end{aligned} $$

クラマース・クローニッヒ関係 $\cdots (2.30)$

$$ \begin{aligned} \chi'{AB(|omega)} + i|chi''{AB(\omega)} &= \frac{1}{2 \pi i} \text{Pv} \int^{\infty}{- |infty} d|omega' |frac{|chi'{AB(\omega')} + i \chi''{AB(|omega')}}{|omega' - |omega} + |frac{1}{2} |left(|chi'{AB(\omega)} + i \chi''{AB(|omega)} |right) | |therefore |chi'{AB(\omega)} + i\chi''{AB(|omega)} &= |frac{1}{|pi} |text{Pv} |int^{|infty}{-\infty} d\omega' \frac{-i \chi'{AB(|omega')} + |chi''{AB(\omega')}}{\omega' - \omega} \end{aligned} $$

$$ \begin{aligned} \chi'{AB(|omega)} &= |frac{1}{|pi} |text{Pv} |int^{|infty}{-\infty} d\omega' \frac{\chi''{AB(|omega')}}{|omega' - |omega} | |chi''{AB(\omega)} &= - \frac{1}{\pi} \text{Pv} \int^{\infty}{- |infty} d|omega' |frac{|chi'{AB(\omega')}}{\omega' - \omega} \ \end{aligned} $$

2.2.2 力学応答の揺動散逸定理 (P. 27)

§ 2.2.2.1 パワーロス (P. 27)

$$ H_{tot} = H - BF_{(t)} $$

タイプ 1

$$ \Delta A_{(t)} = B_{(t)} $$

タイプ 2

$$ \Delta A_{(t)} = \dot{B}_{(t)} $$

一周期あたりの仕事 W $\cdots(2.31)$

$$ \begin{aligned} W &= \int^{\frac{2\pi}{\omega}}{0} dt \frac{dF{(t)}}{dt} \text{Tr}\left(\frac{\partial H_{tot}}{\partial F} \rho_{(t)} \right) \ &= - \int^{\frac{2\pi}{\omega}}{0} dt \frac{dF{(t)}}{dt} \langle B_{(t)} \rangle_{eq} \ \ \ \ \ \left(\because \frac{\partial H_{tot}} {\partial F} = -B \right) \ \end{aligned} $$

単位時間あたりの仕事P $\cdots(2.32)$

- タイプ 1 $(\Delta A_{(t)} = B_{(t)})$

$$ \begin{aligned} P^{(1)} &= - \frac{\omega}{2 \pi} \int^{\frac{2\pi}{\omega}}{0} dt \frac{dF{(t)}}{dt} \langle B_{(t)} \rangle_{eq} \ &= - \frac{\omega}{2 \pi} \int^{\frac{2\pi}{\omega}}{0} dt \frac{dF{(t)}}{dt} \langle \Delta A_{(t)} \rangle_{eq} \ \ \ \ \ \left(\because \Delta A_{(t)} = B_{(t)} \right) \ &= - \frac{\omega}{2 \pi} \int^{\frac{2\pi}{\omega}}{0} dt (-\omega) F_0 \sin{(\omega t)} F_0 \text{Re} \left[\chi{AB(\omega)} e^{-i\omega t} \right] \ &= \frac{\omega^2 F_0^2}{2 \pi} \text{Re} \left[\chi_{AB(\omega)} \int^{\frac{2\pi}{\omega}}{0} dt \sin{(\omega t)} e^{-i\omega t} \right] \ &= \frac{\omega^2 F_0^2}{2 \pi} \text{Re} \left[\chi{AB(\omega)} \int^{\frac{2\pi}{\omega}}{0} dt (-i) \sin^2{(\omega t)} \right] \ &= \frac{\omega F_0^2}{2} \chi''{AB(\omega)} \end{aligned} $$

- タイプ 2 $(\Delta A_{(t)} = \dot{B}_{(t)})$

$$ \begin{aligned} P^{(2)} &= - \frac{\omega}{2 \pi} \int^{\frac{2\pi}{\omega}}{0} dt \frac{dF{(t)}}{dt} \langle B_{(t)} \rangle_{eq} \ &= - \frac{\omega}{2 \pi} \left[F_{(t)} \langle B_{(t)} \rangle_{eq} \right]^{\frac{2\pi}{\omega}}{0} + \frac{\omega}{2 \pi} \int^{\frac{2\pi}{\omega}}{0} dt F_{(t)} \frac{d}{dt} \langle B_{(t)} \rangle_{eq} \ &= \frac{\omega}{2 \pi} \int^{\frac{2\pi}{\omega}}{0} dt F{(t)} \langle \dot{B}{(t)} \rangle{eq} \ \ \ \ \ \left(\because \text{定常状態の周期性} \right) \ &= \frac{\omega}{2 \pi} \int^{\frac{2\pi}{\omega}}{0} dt F{(t)} \langle \Delta A_{(t)} \rangle_{eq} \ \ \ \ \ \left(\because \Delta A_{(t)} = \dot{B}{(t)} \right) \ &= \frac{\omega}{2 \pi} \int^{\frac{2\pi}{\omega}}{0} dt F_0 \cos{(\omega t)} F_0 \text{Re} \left[\chi_{AB(\omega)} e^{-i\omega t} \right] \ &= \frac{\omega}{2 \pi} F_{0}^{2} \text{Re} \left[\chi_{AB(\omega)} \int^{\frac{2\pi}{\omega}}{0} dt \cos{(\omega t)} e^{-i\omega t} \right] \ &= \frac{\omega}{2 \pi} F{0}^{2} \text{Re} \left[\chi_{AB(\omega)} \int^{\frac{2\pi}{\omega}}{0} dt \cos^2{(\omega t)} \right] \ &= \frac{F_0^2}{2} \chi'{AB(\omega)} \end{aligned} $$

等温過程応答係数χ^{T}_{AB} $\cdots(2.34)$

$$ \begin{aligned} \chi^{T}{AB} &= \left. \frac{\partial}{\partial F_0} \frac{\text{Tr}\left[e^{-\beta (H - F_0 B)} A \right]}{\text{Tr}\left[e^{-\beta(H - F_0B)} \right]} \right/{F_0 \to 0} \ &= \left. \frac{1}{Z} \left{ \frac{\partial}{\partial F_0} \text{Tr}\left[e^{-\beta (H - F_0 B)} A \right] - \langle A \rangle_{eq} \frac{\partial}{\partial F_0} \text{Tr}\left[e^{-\beta(H - F_0B)} \right] \right} \right|{F_0 \to 0} \ &= \frac{1}{Z} \left{ \text{Tr} \left[\int^1_0 dy e^{-\beta H(1-y)} (\beta B) e^{-\beta H y}A \right] - \langle A \rangle{eq} \text{Tr} \left[\int^1_0 dy e^{-\beta H(1-y)} (\beta B) e^{-\beta H y} \right] \right} \ &= \frac{1}{Z} \text{Tr} \left[\int^1_0 dy e^{-\beta H(1-y)} (\beta B) e^{-\beta H y} (A - \langle A \rangle_{eq}) \right] \ &= \frac{1}{Z} \text{Tr} \left[\int^{\beta}0 du e^{(u H-\beta H)} B e^{-u H} (A - \langle A \rangle{eq}) \right] \ \ \ \ \ (u \coloneqq \beta y) \ &= \int^{\beta}0 du \frac{1}{Z} \text{Tr} \left[e^{-\beta H} e^{u H} B e^{-u H} (A - \langle A \rangle{eq}) \right] \ &= \int^{\beta}0 du \langle e^{u H} B e^{-u H} (A - \langle A \rangle{eq}) \rangle_{eq} \ &= \int^{\beta}0 du \langle B{(-i\hbar u)} (A - \langle A \rangle_{eq}) \rangle_{eq} \ \ \ \ \ \left(\because e^{u H}\text{を時間発展演算子とみなした} \right) \ &= \int^{\beta}0 du \langle B (A{(i \hbar u)} - \langle A \rangle_{eq}) \rangle_{eq} \ \ \ \ \ \left(\because \text{平衡状態の平均は時間に依存しない} \right) \ &= \int^{\beta}0 du \left(\langle B A{(i \hbar u)} \rangle_{eq} - \langle B \rangle_{eq} \langle A \rangle_{eq} \right) \ &= \int^{\beta}0 du \langle \Delta B \Delta A{(i \hbar u)} \rangle_{eq} \ \ \ \ \ \left(\text{ref.} \ \ \text{Cov}(xy) = \text{E}[xy] - \text{E}[x]\text{E}[y] \right) \ \end{aligned} $$

熱力学的応答関数と力学的応答関数の差 $\cdots(2.35)$

- 力学的応答関数の$\omega \to 0$極限を求める

$$ \begin{aligned} \lim_{\omega \to 0} \chi_{AB(\omega)} &= \lim_{\omega \to 0} \int^{\infty}0 dt \phi{AB(t)} e^{-i \omega t} \ &= \lim_{\tau \to \infty} \int^{\tau}0 dt \phi{AB(t)} \ &= \lim_{\tau \to \infty} \int^{\tau}0 dt \int^{\beta}0 du \langle \dot{B}{(-i \hbar u)} A{(t)} \rangle_{eq} \ \ \ \ \ (\because \text{(2.25)}) \ &= - \lim_{\tau \to \infty} \int^{\tau}0 dt \int^{\beta}0 du \frac{d}{dt} \langle B A{(t + i \hbar u)} \rangle{eq} \ \ \ \ \ (\because (公式1)) \ &= - \int^{\beta}0 du \lim{\tau \to \infty} \left[\langle B A_{(t + i \hbar u)} \rangle_{eq} \right]^{\tau}0 \ &= \int^{\beta}0 du \left(\langle B A{(i \hbar u)} \rangle{eq} - \lim_{\tau \to \infty} \langle B A_{(\tau + i \hbar u)} \rangle_{eq} \right) \end{aligned} $$

- 差を計算する

$$ \begin{aligned} \chi^{T}{AB} - \chi{AB} &= \int^{\beta}0 du \langle \Delta B \Delta A{(i \hbar u)} \rangle - \int^{\beta}0 du \left(\langle B A{(i \hbar u)} \rangle_{eq} - \lim_{\tau \to \infty} \langle B A_{(\tau + i \hbar u)} \rangle_{eq} \right) \ &= \int^{\beta}0 du \left(\langle B A{(i \hbar u)} \rangle_{eq} - \langle B \rangle_{eq} \langle A \rangle_{eq} \right) - \int^{\beta}0 du \left(\langle B A{(i \hbar u)} \rangle_{eq} - \lim_{\tau \to \infty} \langle B A_{(\tau + i \hbar u)} \rangle_{eq} \right) \ &= \int^{\beta}0 du \left(\lim{\tau \to \infty} \langle B A_{(\tau + i \hbar u)} \rangle_{eq} - \langle B \rangle_{eq} \langle A \rangle_{eq} \right) \ &= \lim_{\tau \to \infty} \int^{\beta}0 du \left(\langle B A{(\tau + i \hbar u)} \rangle_{eq} - \langle B \rangle_{eq} \langle A \rangle_{eq} \right) \ &= \lim_{\tau \to \infty} \int^{\beta}0 du \langle \Delta B \Delta A{(\tau + i \hbar u)} \rangle_{eq} \end{aligned} $$

§ 2.2.2.2 揺動散逸定理 (P. 29)

時間反転

$$ \begin{aligned} \langle [A_{(t)}, B] \rangle_{eq} &= \text{Tr} \left[\pi [A_{(t)}, B] \right] \ &= \text{Tr} \left[\left(T \pi [A_{(t)}, B] T^{\dagger} \right)^{\dagger} \right] \ &= \text{Tr} \left[[B^{\dagger}, A^{\dagger}{(-t)}] \pi^{\dagger} \right] \ &= - \text{Tr} \left[[A{(-t)}, B] \pi \right] \ &= - \langle [A_{(-t)}, B] \rangle_{eq} \ \end{aligned} $$

- タイプ 1 $(A = B)$

$$ \begin{aligned} \langle [A_{(t)}, B] \rangle_{eq} &= \langle [B_{(t)}, B] \rangle_{eq} \ &= \langle [B, B_{(-t)}] \rangle_{eq} \ &= - \langle [B_{(-t)}, B] \rangle_{eq} \ &= - \langle [A_{(-t)}, B] \rangle_{eq} \ \end{aligned} $$

- タイプ 2 $(A = \dot{B})$

$$ \begin{aligned} \langle [A_{(t)}, B] \rangle_{eq} &= \langle [\dot{B}{(t)}, B] \rangle{eq} \ &= \frac{d}{dt} \langle [B_{(t)}, B] \rangle_{eq} \ &= \frac{d}{dt} \langle [B, B_{(-t)}] \rangle_{eq} \ &= - \frac{d}{dt} \langle [B_{(-t)}, B] \rangle_{eq} \ &= \langle [\dot{B}{(-t)}, B] \rangle{eq} \ &= \langle [A_{(-t)}, B] \rangle_{eq} \ \end{aligned} $$

応答関数ϕ_{AB}

- タイプ 1

$$ \begin{aligned} \phi_{AB(\omega)} &= \int^{\infty}{\infty} dt \frac{i}{\hbar} \langle [A{(t)}, B] \rangle_{eq} e^{i\omega t} \ &= \int^{\infty}0 dt \frac{i}{\hbar} \langle [A{(t)}, B] \rangle_{eq} (e^{i \omega t} - e^{-i \omega t}) \ &= 2i \int^{\infty}0 dt \frac{i}{\hbar} \langle [A{(t)}, B] \rangle_{eq} \text{Im}[e^{i \omega t}] \ &= 2i \text{Im} \left[\int^{\infty}0 dt \frac{i}{\hbar} \langle [A{(t)}, B] \rangle_{eq} e^{i \omega t} \right] \ &= 2i \text{Im} [\chi_{AB(\omega)}] \ &= 2 \chi'_{AB(\omega)} \end{aligned} $$

- タイプ 2

$$ \begin{aligned} \phi_{AB(\omega)} &= \int^{\infty}{\infty} dt \frac{i}{\hbar} \langle [A{(t)}, B] \rangle_{eq} e^{i\omega t} \ &= \int^{\infty}0 dt \frac{i}{\hbar} \langle [A{(t)}, B] \rangle_{eq} (e^{i \omega t} + e^{-i \omega t}) \ &= 2 \int^{\infty}0 dt \frac{i}{\hbar} \langle [A{(t)}, B] \rangle_{eq} \text{Re}[e^{i \omega t}] \ &= 2 \text{Re} \left[\int^{\infty}0 dt \frac{i}{\hbar} \langle [A{(t)}, B] \rangle_{eq} e^{i \omega t} \right] \ &= 2 \text{Re} [\chi_{AB(\omega)}] \ &= 2 \chi''_{AB(\omega)} \end{aligned} $$

KMS 条件

- 一般論

$$ \begin{aligned} \langle AB_{(t + i\hbar\beta)} \rangle_{eq} &= \text{Tr}[\pi A e^{-\beta H} B_{(t)} e^{\beta H}] \ &= \frac{1}{Z} \text{Tr} [e^{-\beta H} A e^{-\beta H} B_{(t)} e^{\beta H}] \ &= \frac{1}{Z} \text{Tr} [A e^{-\beta H} B_{(t)} e^{\beta H} e^{-\beta H}] \ &= \frac{1}{Z} \text{Tr} [A e^{-\beta H} B_{(t)}] \ &= \frac{1}{Z} \text{Tr} [e^{-\beta H} B_{(t)} A] \ &= \langle B_{(t)} A \rangle_{eq} \end{aligned} $$

- 特に、

$$ \langle \Delta B \Delta A_{(t + i\hbar\beta)} \rangle_{eq} = \langle \Delta A_{(t)} \Delta B \rangle_{eq} $$

- KMS 条件 (積分形)

$$ \begin{aligned} \int_{C} dz \langle \Delta B \Delta A_{(z)} \rangle_{eq} e^{i \omega z} &= 0 \ \therefore \int^{\infty}{-\infty} dt \langle \Delta B \Delta A{(t)} \rangle_{eq} e^{i \omega t} &= \int^{\infty}{-\infty} dt \langle \Delta B \Delta A{(t + i \hbar \beta)} \rangle_{eq} e^{i \omega (t + i \hbar \beta)} \ &= e^{- \hbar \beta \omega}\int^{\infty}{-\infty} dt \langle \Delta B \Delta A{(t + i \hbar \beta)} \rangle_{eq} e^{i \omega t} \ &= e^{- \hbar \beta \omega} \int^{\infty}{-\infty} dt \langle \Delta A{(t)} \Delta B \rangle_{eq} e^{i \omega t} \ \end{aligned} $$

応答関数ϕ_{AB}

- 準備

$$ \begin{aligned} [A_{(t)}, B] &= [\Delta A_{(t)} + \langle A \rangle_{eq}, \Delta B + \langle B \rangle_{eq}] \ &= [\Delta A_{(t)}, \Delta B] \end{aligned} $$

- ϕ_{AB}を変形 $(\langle \Delta A_{(t)} \Delta B \rangle_{eq}\text{の形})$

$$ \begin{aligned} \phi_{AB} &= \frac{i}{\hbar} \int^{\infty}{-\infty} dt \langle [A{(t)}, B] \rangle_{eq} e^{i \omega t} \ &= \frac{i}{\hbar} \int^{\infty}{- \infty} dt \langle [\Delta A{(t)}, \Delta B] \rangle_{eq} e^{i \omega t} \ &= \frac{i}{\hbar} \int^{\infty}{- \infty} dt \left(\langle \Delta A{(t)}\Delta B \rangle_{eq} - \langle \Delta B \Delta A_{(t)} \rangle_{eq} \right) e^{i \omega t} \ &= \frac{i}{\hbar} \int^{\infty}{- \infty} dt \left(\langle \Delta A{(t)}\Delta B \rangle_{eq} - e^{-\hbar\beta\omega} \langle \Delta A_{(t)} \Delta B \rangle_{eq} \right) e^{i \omega t} \ &= \frac{i}{\hbar} (1 - e^{-\hbar\beta\omega}) \int^{\infty}{- \infty} dt \langle \Delta A{(t)}\Delta B \rangle_{eq} e^{i \omega t} \ \end{aligned} $$

- ϕ_{AB}を変形 $(\langle \Delta B \Delta A_{(t)} \rangle_{eq}\text{の形})$

$$ \begin{aligned} \phi_{AB} &= \frac{i}{\hbar} (1 - e^{-\hbar\beta\omega}) \int^{\infty}{- \infty} dt \langle \Delta A{(t)}\Delta B \rangle_{eq} e^{i \omega t} \ &= (\frac{i}{\hbar} 1 - e^{-\hbar\beta\omega}) \int^{\infty}{- \infty} dt e^{\hbar\beta\omega} \langle \Delta B \Delta A{(t)} \rangle_{eq} e^{i \omega t} \ &= \frac{i}{\hbar} (e^{\hbar\beta\omega} - 1) \int^{\infty}{- \infty} dt \langle \Delta B \Delta A{(t)} \rangle_{eq} e^{i \omega t} \ \end{aligned} $$

- ϕ_{AB}を変換 $(C_{AB}\text{の形})$ $\cdots (2.44)$

$$ \begin{aligned} C_{AB} &= \int^{\infty}{-\infty} dt \frac{1}{2} \left[\langle \Delta A{(t)} \Delta B \rangle_{eq} + \langle \Delta B \Delta A_{(t)} \rangle_{eq} \right] e^{i\omega t} \ &= \frac{1}{2} \left[\int^{\infty}{-\infty} dt \langle \Delta A{(t)} \Delta B \rangle_{eq} e^{i\omega t} + \int^{\infty}{-\infty} dt \langle \Delta B \Delta A{(t)} \rangle_{eq} e^{i\omega t} \right] \ &= \frac{1}{2} \left[\frac{1}{\frac{i}{\hbar} (1 - e^{-\hbar\beta\omega})} \phi_{AB} + \frac{1}{\frac{i}{\hbar} (e^{\hbar\beta\omega} - 1)} \phi_{AB} \right] \ &= \frac{\hbar}{2i} \frac{e^{\frac12 \hbar\beta\omega} + e^{-\frac12 \hbar\beta\omega}}{e^{\frac12 \hbar\beta\omega} - e^{-\frac12 \hbar\beta\omega}} \phi_{AB} \ &= \frac{\frac{\hbar\omega}{2}}{i\omega} \coth{\left(\frac{\hbar\beta\omega}{2} \right)} \phi_{AB} \ \therefore \phi_{AB} &= \frac{i\omega}{\left(\frac{\hbar\omega}{2} \right) \coth{\left(\frac{\beta\hbar\omega}{2} \right)}} C_{AB} \end{aligned} $$

散逸とゆらぎの関係

- タイプ１の χ''_{AB} $\cdots (2.45)$

$$ \begin{aligned} \chi''{AB} &= \frac{1}{2i} \phi{AB} \ &= \frac{1}{\hbar \coth{\left(\frac{\beta\hbar\omega}{2} \right)}} C_{AB} \end{aligned} $$

- タイプ２の χ'_{AB} $\cdots (2.46)$

$$ \begin{aligned} C_{A\dot{B}} &= \int^{\infty}{-\infty} dt \frac12 \left[\langle \Delta A{(t)} \Delta \dot{B} \rangle_{eq} + \langle \Delta \dot{B} \Delta A_{(t)} \rangle_{eq} \right] e^{i\omega t} \ &= - \int^{\infty}{- \infty} dt \frac12 \left(\frac{d}{dt} \left[\langle \Delta A{(t)} \Delta B \rangle_{eq} + \langle \Delta B \Delta A_{(t)} \rangle_{eq} \right] \right) e^{i\omega t} \ \ \ \ \ (\because (\text{公式1})) \ &= \int^{\infty}{-\infty} dt \frac12 \left[\langle \Delta A{(t)} \Delta B \rangle_{eq} + \langle \Delta B \Delta A_{(t)} \rangle_{eq} \right]

\frac{d}{dt} e^{i\omega t} \ \ \ \ \ (\because \text{混合性}) \ &= i \omega \int^{\infty}{-\infty} dt \frac12 \left[\langle \Delta A{(t)} \Delta B \rangle_{eq} + \langle \Delta B \Delta A_{(t)} \rangle_{eq} \right] e^{i\omega t} \ &= i \omega C_{AB} \ \end{aligned} $$

$$ \begin{aligned} \chi'{AB} &= \frac12 \phi{AB} \ &= \frac{i\omega}{\hbar\omega \coth{\left(\frac{\beta\hbar\omega}{2} \right)}} C_{AB} \ &= \frac{1}{\hbar\omega \coth{\left(\frac{\beta\hbar\omega}{2} \right)}} C_{A\dot{B}} \ \end{aligned} $$

タイプ 2: $\omega \to 0$の極限

$$ \begin{aligned} \chi'{AB} &= \frac{1}{\hbar\omega \coth{\left(\frac{\beta\hbar\omega}{2} \right)}} C{A\dot{B}} \ &\to \frac{\frac{\beta}{2} \frac{\beta\hbar\omega}{2}}{\frac{\beta\hbar\omega}{2}} \int^{\infty}{-\infty} dt C{A\dot{B}(to)} \ \ \ \ \ \left(\because \frac{1}{\coth{(x)}} = \tanh{(x)} = x + \text{O}(x^3) \right) \ &= \frac{\beta}{2} \int^{\infty}{-\infty} dt C{A\dot{B}(t)} \end{aligned} $$

2.2.3 分布応答の線形応答と揺動散逸定理 (P. 31)

$$ H_{tot} = H_s + \sum_{k} H_k + H_{ks} $$

分布関数 ρ_0

- $e^{-u (G+X)}$ を計算する $\cdots (2.53)$

$$ \begin{aligned} \sigma_u &\coloneqq e^{-u (G + X)} \ \bar{\sigma}_u &\coloneqq e^{uG}\sigma_u \end{aligned} $$

$$ \begin{aligned} \frac{\partial}{\partial u} \bar{\sigma}u &= e^{uG} G \sigma_u - e^{uG} (G + X) \sigma_u \ &= - e^{uG} X \sigma_u \ &= - e^{uG} X e^{-uG} \bar{\sigma}u \ &= - X{(-i\hbar u)} \bar{\sigma}u \ \therefore \bar{\sigma}\beta &= e^{-\int^{\beta}0 du X{(-i \hbar u)}} \ \therefore \sigma\beta &= e^{-uG} e^{-\int^{\beta}0 du X{(-i \hbar u)}} \ \end{aligned} $$

$$ \begin{aligned} \sigma_\beta &= e^{-\beta G} e^{-\int^{\beta}0 du X{(-i \hbar u)}} \ &= e^{-\beta G} \left(1 - \int^{\beta}0 du X{(-i \hbar u)} \right) + \text{O}{(X^2)} \ \sigma\beta &= e^{-\int^{\beta}0 du X{(i \hbar u)}} e^{-uG} \ \ \ \ \ (\because \sigma_\beta \text{はエルミート}) \ &= \left(1 - \int^{\beta}0 du X{(i \hbar u)} \right) e^{-\beta G} + \text{O}{(X^2)} \ \therefore \sigma\beta &\simeq e^{-\beta G} - \int^{\beta}0 du \frac12 \left[e^{-\beta G} X{(-i \hbar u)} + X_{(i \hbar u)} e^{-\beta G} \right] \end{aligned} $$

- $\text{Tr} [e^{-u (G + X)}]$を計算する

$$ \begin{aligned} \text{Tr} \left[e^{-u (G+X)} \right] &\simeq \text{Tr}\left[e^{-\beta G} - \int^{\beta}0 du \frac12 \left[e^{-\beta G} X{(-i \hbar u)} + X_{(i \hbar u)} e^{-\beta G} \right] \right] \ &= \text{Tr}\left[e^{-\beta G} \right] - \int^{\beta}0 du \frac12 \left(\text{Tr}\left[e^{-\beta G} X{(-i \hbar u)} \right] + \text{Tr}\left[X_{(i \hbar u)} e^{-\beta G} \right] \right) \ &= Z - \int^{\beta}0 du \frac{1}{2} (Z \langle X{(-i \hbar u)} \rangle_{eq} + Z \langle X_{(i \hbar u)} \rangle_{eq}) \ &= Z \left(1 - \int^{\beta}0 du \frac{1}{2} (\langle X{(-i \hbar u)} \rangle_{eq} + \langle X_{(i \hbar u)} \rangle_{eq}) \right) \end{aligned} $$

- 分配関数ρ_0を計算する $\cdots (2.54)$

$$ \frac{1}{1-x} = 1 + x + \text{O}_{(x^2)} $$

$$ \begin{aligned} \rho_0 &= \frac{e^{-\beta (G + X)}}{\text{Tr} e^{-\beta (G + X)}} \\ &\simeq \left(e^{-\beta G} - \int^{\beta}_0 du \frac12 \left[e^{-\beta G} X_{(-i \hbar u)} + X_{(i \hbar u)} e^{-\beta G} \right] \right) \frac{1}{Z} \left(1 + \int^{\beta}_0 du \frac{1}{2} (\langle X_{(-i \hbar u)} \rangle_{eq} + \langle X_{(i \hbar u)} \rangle_{eq}) \right) \\ &= \left(\pi - \int^{\beta}_0 du \frac12 \left[\pi X_{(-i \hbar u)} + X_{(i \hbar u)} \pi \right] \right) \left(1 + \int^{\beta}_0 du \frac{1}{2} (\langle X_{(-i \hbar u)} \rangle_{eq} + \langle X_{(i \hbar u)} \rangle_{eq}) \right) \\ &\simeq \pi - \int^{\beta}_0 du \frac12 \left[\pi X_{(-i \hbar u)} + X_{(i \hbar u)} \pi \right] + \int^{\beta}_0 du \frac{1}{2} (\pi \langle X_{(-i \hbar u)} \rangle_{eq} + \langle X_{(i \hbar u)} \rangle_{eq} \pi) \\ &= \pi - \int^{\beta}_0 du \frac12 \left[\pi \Delta X_{(-i \hbar u)} + \Delta X_{(i \hbar u)} \pi \right] \end{aligned} $$

演算子の時間発展 $\cdots (2.55)$

$$ \begin{aligned} \langle A_{(\tau)} \rangle_{eq} &= \text{Tr}[\rho_0 U^{\dagger} A U] \\ &= \text{Tr}[A U \rho_0 U^{\dagger}] \\ &= \text{Tr}[AU\pi U^{\dagger}] - \int^{\beta}_0 du \frac12 \left(\text{Tr}[AU\pi\Delta X_{(-i \hbar u)}U^{\dagger}] + \text{Tr}[AU\Delta X_{(i \hbar u)} \pi U^{\dagger}] \right) \\ &= \text{Tr}[\pi A] - \int^{\beta}_0 du \frac12 \left(\text{Tr}[\pi\Delta X_{(-i \hbar u - \tau)} A] + \text{Tr}[\pi A\Delta X_{(i \hbar u - \tau)}] \right) \\ &= \langle A \rangle_{eq} - \int^{\beta}_0 du \frac12 \left[\langle \Delta X_{(-i \hbar u - \tau)} A \rangle_{eq} + \langle A\Delta X_{(i \hbar u - \tau)} \rangle_{eq} \right] \\ &= \langle A \rangle_{eq} + \int^{\beta}_0 du \int^0_{-\tau} dt \frac12 \left[\langle \Delta \dot{X}_{(-i \hbar u + t)} \rangle_{eq} + \langle A \Delta \dot{X}_{(i \hbar u + t)} \rangle_{eq} \right] - \int^{\beta}_0 du \frac12 \left(\langle \Delta X_{(-i \hbar u)} A \rangle_{eq} + \langle A\Delta X_{(i \hbar u)} \rangle_{eq} \right) \end{aligned} $$