Title: PSI 2019/2020 - Quantum Theory (Dupuis) - Lecture 12

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TODAY: Perturbation theory

use to determine → Ground state energy

→ $\langle 0|T[\hat{x}(\tau_1)\cdots\hat{x}(\tau_n)|0\rangle$

1. Express quantities with propagator
2. Separate Lagrangian = "free" + "interacting"
3. Interacting propagator can be written in terms of free propagator + source term
4. Evaluation of free propagator + source term. ← Tutorial (Exact)
5. Functional derivatives on free propagator + source = perturbative expansion of interactive propagator

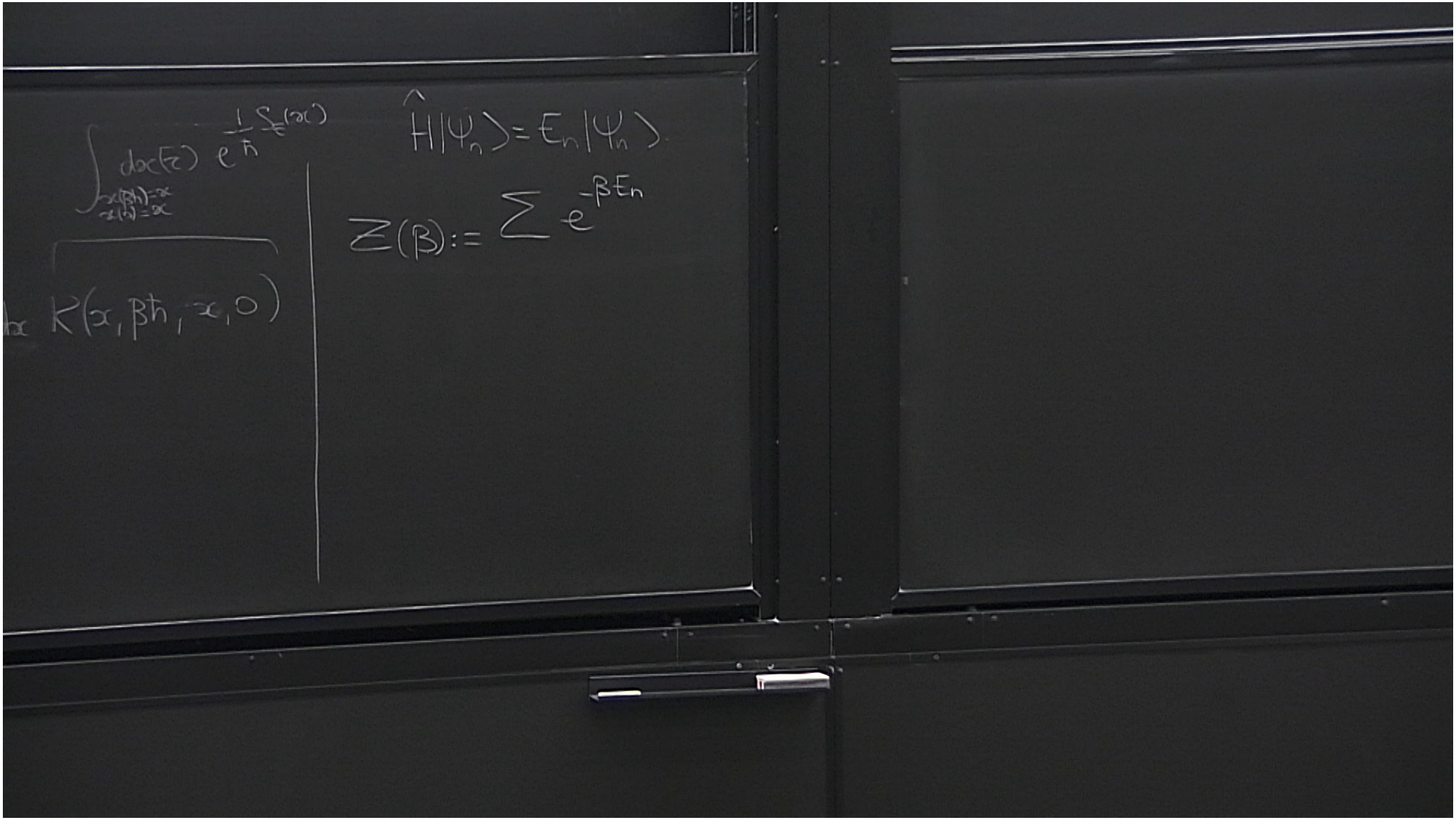
Ground state energy for the anharmonic oscillator

① Partition function

$$Z(\beta) := \mathrm{Tr}\, e^{-\beta H} = \mathrm{tr}\, U(\beta\hbar, 0) = \int dx'\, dx''\, \delta(x''-x') \underbrace{\langle x'' | U(\beta\hbar,0) | x' \rangle}_{K} = \int dx\, K(x, \beta\hbar, x, 0)$$

$$\overset{\text{PI}}{=} \int_{x(0)=x(\beta\hbar)} [dx]\, e^{-S_E(x)/\hbar}$$

$$= \int_{x(0)=x(\beta\hbar)=x} dx(\tau)\, e^{-\frac{1}{\hbar} S_E(x)} \Big| Z$$


$\int dx(\tau)\, e^{\frac{1}{\hbar} S_E(x)}$
$x(\beta\hbar) = x$
$x(0) = x$
$K(x, \beta\hbar, x, 0)$
$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$
$Z(\beta) := \sum e^{-\beta E_n}$

To extract E_0

$$\rightarrow K(0,\beta;0,0) = \langle x'=0 | e^{-\beta H} \sum_n |\psi_n\rangle\langle\psi_n| x'=0\rangle$$

$x''=0$ $x=0$

$$= \sum e^{-\beta E_n} \psi_n(0)\,\psi_n^*(0)$$

$$\beta \rightarrow \infty \qquad K(0,\beta;0,0) \simeq e^{-\beta E_0} \psi_0(0)\,\psi_0^* + \cdots$$

① To extract E_0

$$\rightarrow K(0,\beta;0,0) = \langle x''=0 | e^{-\beta H} \sum_n |\psi_n\rangle\langle\psi_n| x'=0\rangle$$

($x''=0$, $x=0$)

$$= \sum e^{-\beta E_n} \psi_n(0)\, \psi_n^*(0)$$

$$\beta \to \infty \qquad K(0,\beta;0,0) \simeq e^{-\beta E_0} \psi_0(0)\, \psi_0^* + \dots \qquad E_0 = -\lim_{\beta\to\infty} \frac{1}{\beta} \log\left(K(0,\beta;0,0)\right)$$

② Anharmonic oscillator

$$K(0,\beta;0,0) = \int dx(\tau)\, \exp -\frac{1}{\hbar} \int d\tau \left(\underbrace{\frac{1}{2} m\dot{x}^2 + \frac{m\omega^2 x^2}{2}}_{\text{HO} = \text{"free"}} + \underbrace{\lambda x^4}_{\text{interacting}} \right)$$

③ $K^0[J] = \int dx[\tau] \exp \frac{-1}{\hbar} \int d\tau \left(\underbrace{L^{(0)}}_{\frac{1}{2}m\dot{x}^2 + \frac{m}{2}\omega^2 x^2} - J(\tau)x(\tau) \right)$

$K(0,\beta,0,0) \overset{?}{\Longleftrightarrow} K^0[J]$

$$K[J] = \int dx[\tau]\, e^{-\frac{1}{\hbar}\int \left(L^{(0)} + \lambda x^4 - Jx\right) d\tau}$$

$$= \int dx[\tau] \sum_n \frac{1}{n!} \int \left(\frac{-\lambda}{\hbar}\right)^n x^4(\tau_1)\cdots x^4(\tau_n)\, e^{-\frac{1}{\hbar}\int (L^{(0)} - Jx) d\tau}\, d\tau_1 \cdots d\tau_n$$

② Anharmonic oscillator

$$K(0,\beta,0,0) = \int_{11} dx(\tau)\ \exp\left(-\frac{1}{\hbar}\int d\tau \underbrace{\left(\frac{1}{2}m\dot{x}^2 + \frac{m\omega^2 x^2}{2}\right)}_{\text{HO = "free"}} + \underbrace{\lambda x^4}_{\text{interacting}}\right)$$

③ $$K^0[J] = \int dx[\tau]\ \exp\left(-\frac{1}{\hbar}\int d\tau \left(\underbrace{L^{(0)}}_{\frac{1}{2}m\dot{x}^2 + \frac{m}{2}\omega^2 x^2} - J(\tau)x(\tau)\right)\right)$$

$$K(0,\beta,0,0) \overset{?}{\Longleftrightarrow} K^0[J]$$

$$K[J] = \int dx[\tau]\, e^{-\frac{1}{\hbar}\int \left(L^{(0)} + \lambda x^4 - Jx\right) d\tau}$$

$$= \int dx[\tau] \sum_n \frac{1}{n!} \int \left(-\frac{\lambda}{\hbar}\right)^n x^4(\tau_1)\cdots x^4(\tau_n)\, e^{-\frac{1}{\hbar}\int (L^{(0)} - Jx)\, d\tau}\, d\tau_1 \cdots d\tau_n$$

$$K(0,\beta,0,0) \overset{?}{\longleftrightarrow} K^\circ[J]$$

$$K[J] = \int dx[\tau]\, e^{-\frac{1}{\hbar}\int (L^{(0)} + \lambda x^4 - Jx)\,d\tau}$$

$$= \int dx[\tau] \sum_n \frac{1}{n!} \int \left(\frac{-\lambda}{\hbar}\right)^n x^4(\tau_1)\cdots x^4(\tau_n)\, e^{-\frac{1}{\hbar}\int (L^{(0)} - Jx)\,d\tau}\, d\tau_1 \cdots d\tau_n$$

$$= \sum_n \frac{1}{n!} \int \left(\frac{-\lambda}{\hbar}\right)^n \frac{\hbar^4 \delta^4}{\delta J^4(\tau_1)} \cdots \frac{\hbar^4 \delta^4}{\delta J^4(\tau_n)} K^\circ[J]\, d\tau_1 \cdots d\tau_n$$

$$\equiv \exp\left(-\int d\tau\, \hbar^3 \lambda \frac{\delta^4}{\delta J(\tau)^4}\right) K^\circ(J)$$

$$K(0,\beta,0,0) = \exp\left(-\int d\tau\, \lambda \frac{\delta^4}{\delta J(\tau)^4}\right) K^\circ[J]\Big|_{J=0} = K^\circ[J]\Big|_{J=0} - \lambda \left(\int d\tau \frac{\delta^4}{\delta J(\tau)^4}\right) K^\circ[J]\Big|_{J=0} + O(\lambda^2)$$

$\hbar = 1$

perturbat° expansion

$$K(0,\beta,0,0) \overset{?}{\Longleftrightarrow} K^\circ[J]$$

$$K[J] = \int dx[\tau]\, e^{-\frac{1}{\hbar}\int (L^{(0)} + \lambda x^4 - Jx)\,d\tau}$$

$$= \int_{\substack{x(0)=0 \\ x(\beta\hbar)=0}} dx[\tau] \sum_n \frac{1}{n!} \int \left(\frac{-\lambda}{\hbar}\right)^n x^4(\tau_1)\cdots x^4(\tau_n)\, e^{-\frac{1}{\hbar}\int (L^{(0)} - Jx)\,d\tau}\, d\tau_1 \cdots d\tau_n$$

$$= \sum_n \frac{1}{n!} \int \left(\frac{-\lambda}{\hbar}\right)^n \frac{\hbar^4 \delta^4}{\delta J^4(\tau_1)} \cdots \frac{\hbar^4 \delta^4}{\delta J^4(\tau_n)} K^\circ[J]\, d\tau_1 \cdots d\tau_n$$

$$\equiv \exp\left(-\int d\tau\, \hbar^3 \lambda \frac{\delta^4}{\delta J(\tau)^4}\right) K^\circ(J)$$

$$(\hbar = 1) \qquad K(0,\beta,0,0) = \exp\left(-\int d\tau\, \lambda \frac{\delta^4}{\delta J(\tau)^4}\right) K^\circ[J]\Big|_{J=0} = K^\circ[J]\Big|_{J=0} - \lambda \left(\int d\tau \frac{\delta^4}{\delta J(\tau)^4}\right) K^\circ[J]\Big|_{J=0} + O(\lambda^2)$$

perturbative expansion

$x(0) = x(\beta\hbar)$

④ $K^\circ[J] = \underbrace{e^{-\frac{1}{\hbar} S_E^J[x_c]}}_{} \times \underbrace{\int \mathcal{D}\, du[\tau]\; e^{-\frac{1}{2}\iint d\tau_1 d\tau_2\, u(\tau_1)\, A(\tau_1,\tau_2)\, u(\tau_2)}}_{\text{same term as for HO, } J=0}$

$$\frac{K^\circ[J]}{K^\circ} = e^{-\frac{1}{\hbar} S_E^J[x_c] + \frac{1}{\hbar} S_E^\circ[x_c^\circ]}$$

$$K^\circ = \left(\frac{m\omega}{2\pi\hbar\, \mathrm{sh}(\omega T)}\right)^{\frac{1}{2}} e^{-\frac{1}{\hbar} S_E^\circ[x_c^\circ]} \Bigg] \Rightarrow K^\circ[J] = \underbrace{\left(\frac{m\omega}{2\pi\, \mathrm{sh}(\omega T)}\right)^{\frac{1}{2}}}_{C} e^{-S_E^J[x_c]}.$$

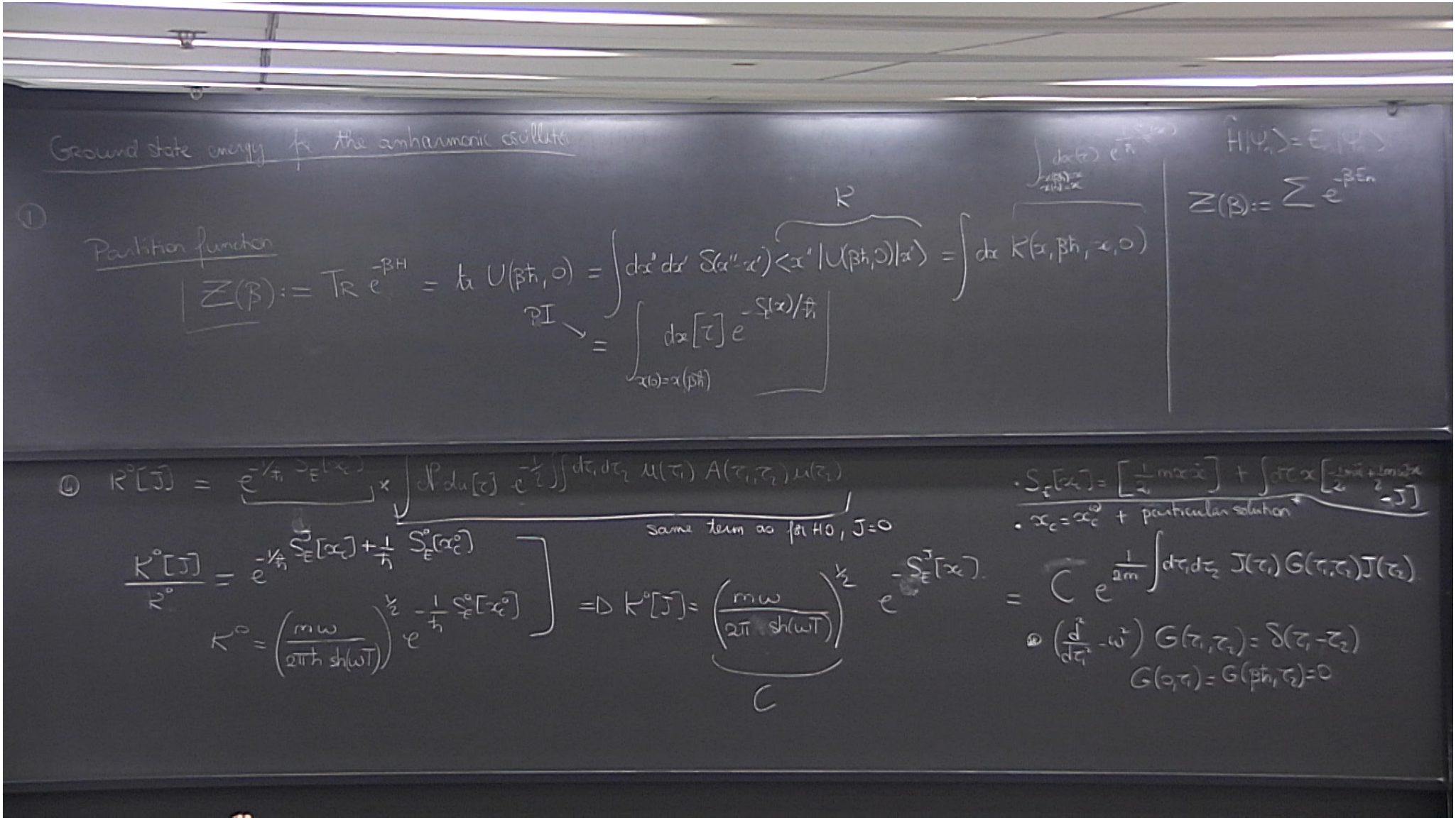
$$Z(\beta) := \mathrm{Tr}\, e^{-\beta \hat{H}} = \int dx\, \langle x | e^{-\beta \hat{H}} | x \rangle = \int_{x(0)=x(\beta\hbar)} \mathcal{D}x\, e^{-S_E(x)/\hbar}$$

① $K^J[J] = \underbrace{e^{-\frac{1}{\hbar} S_E^J[x_c]}}_{S_E} \times \underbrace{\int \mathcal{D}\mu[\tau]\, e^{-\frac{1}{2}\iint d\tau_1 d\tau_2\, \mu(\tau_1) A(\tau_1,\tau_2) \mu(\tau_2)}}_{\text{same term as for HO, } J=0}$

$$\frac{K^J[J]}{K^0} = e^{-\frac{1}{\hbar} S_E^J[x_c] + \frac{1}{\hbar} S_E^0[x_c^0]}$$

$$K^0 = \left(\frac{m\omega}{2\pi\hbar\, \mathrm{sh}(\omega T)}\right)^{\frac{1}{2}} e^{-\frac{1}{\hbar} S_E^0[x_c^0]}$$

$$\Rightarrow K^J[J] = \underbrace{\left(\frac{m\omega}{2\pi\hbar\, \mathrm{sh}(\omega T)}\right)^{\frac{1}{2}}}_{C} e^{-S_E^J[x_c]} = C\, e^{\frac{1}{2m}\int d\tau_1 d\tau_2\, J(\tau_1) G(\tau_1,\tau_2) J(\tau_2)}$$


Ground state energy for the anharmonic oscillator
Partition function
$Z(\beta) := \mathrm{Tr}\, e^{-\beta H} = \mathrm{tr}\, U(\beta\hbar, 0) = \int dx' dx'' \delta(x'' - x') \langle x' | U(\beta\hbar, 0) | x' \rangle = \int dx\, K(x, \beta\hbar, x, 0)$
PI
$= \int_{x(0)=x(\beta\hbar)} dx[\tau]\, e^{-S_E(x)/\hbar}$
K
$\int_{x(0)=x(\beta\hbar)=x} dx(\tau)\, e^{-S_E(x)/\hbar}$
$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$
$Z(\beta) := \sum e^{-\beta E_n}$
$K^\circ[J] = e^{-\frac{1}{\hbar} S_E^\circ[x_c]} \times \int dP\, du[\tau]\, e^{-\frac{1}{2}\int d\tau_1 d\tau_2\, u(\tau_1) A(\tau_1,\tau_2) u(\tau_2)}$
same term as for HO, J=0
$\frac{K^\circ[J]}{K^\circ} = e^{-\frac{1}{\hbar} S_E^J[x_c] + \frac{1}{\hbar} S_E^\circ[x_c^J]}$
$K^\circ = \left(\frac{m\omega}{2\pi\hbar\, \mathrm{sh}(\omega T)}\right)^{\frac{1}{2}} e^{-\frac{1}{\hbar} S_E^\circ[x_c^\circ]}$
$\Rightarrow K^\circ[J] = \underbrace{\left(\frac{m\omega}{2\pi\, \mathrm{sh}(\omega T)}\right)^{\frac{1}{2}}}_{C} e^{-S_E^J[x_c]}$
$\cdot S_E[x_c] = \left[\frac{1}{2} m x_c \dot{x}_c\right] + \int d\tau\, x \left[\frac{-\dots}{2} - J\right]$
$\cdot x_c = x_c^\omega + \text{particular solution}$
$= C\, e^{\frac{1}{2m}\int d\tau_1 d\tau_2\, J(\tau_1) G(\tau_1,\tau_2) J(\tau_2)}$
$\left(\frac{d^2}{d\tau^2} - \omega^2\right) G(\tau_1,\tau_2) = \delta(\tau_1 - \tau_2)$
$G(0,\tau_1) = G(\beta\hbar,\tau_2) = 0$

$$S_E[x_c] = \underbrace{\left[\frac{1}{2} m \dot{x} x\right]}_{=0} + \int d\tau \; x \left[\underbrace{-\frac{1}{2} m \ddot{x} + \frac{1}{2} m \omega^2 x}_{} - J\right]$$

$y \begin{cases} x'=0 \\ x''=0 \end{cases}$

$A(\tau_1,\tau_2)\,\mu(\tau_2)$

term as for $\hbar\to 0$, $J=0$

$$= \underbrace{\left(\frac{m\omega}{2\pi\,\sinh(\omega T)}\right)^{1/2}}_{C} e^{-S_E^J[x_c]}$$

- $S_E[x] = \left[\frac{1}{2}m x\dot{x}\right] + \int d\tau\, x\left[-\frac{1}{2}m\ddot{x} + \frac{1}{2}m\omega^2 x - J\right]$
- $x_c = x_c^{(0)}$ + particular solution *

$$= C\, e^{\frac{1}{2m}\int d\tau_1 d\tau_2\, J(\tau_1)\,G(\tau_1,\tau_2)\,J(\tau_2)}$$

* $\left(\frac{d^2}{d\tau_1^2} - \omega^2\right) G(\tau_1,\tau_2) = \delta(\tau_1-\tau_2)$

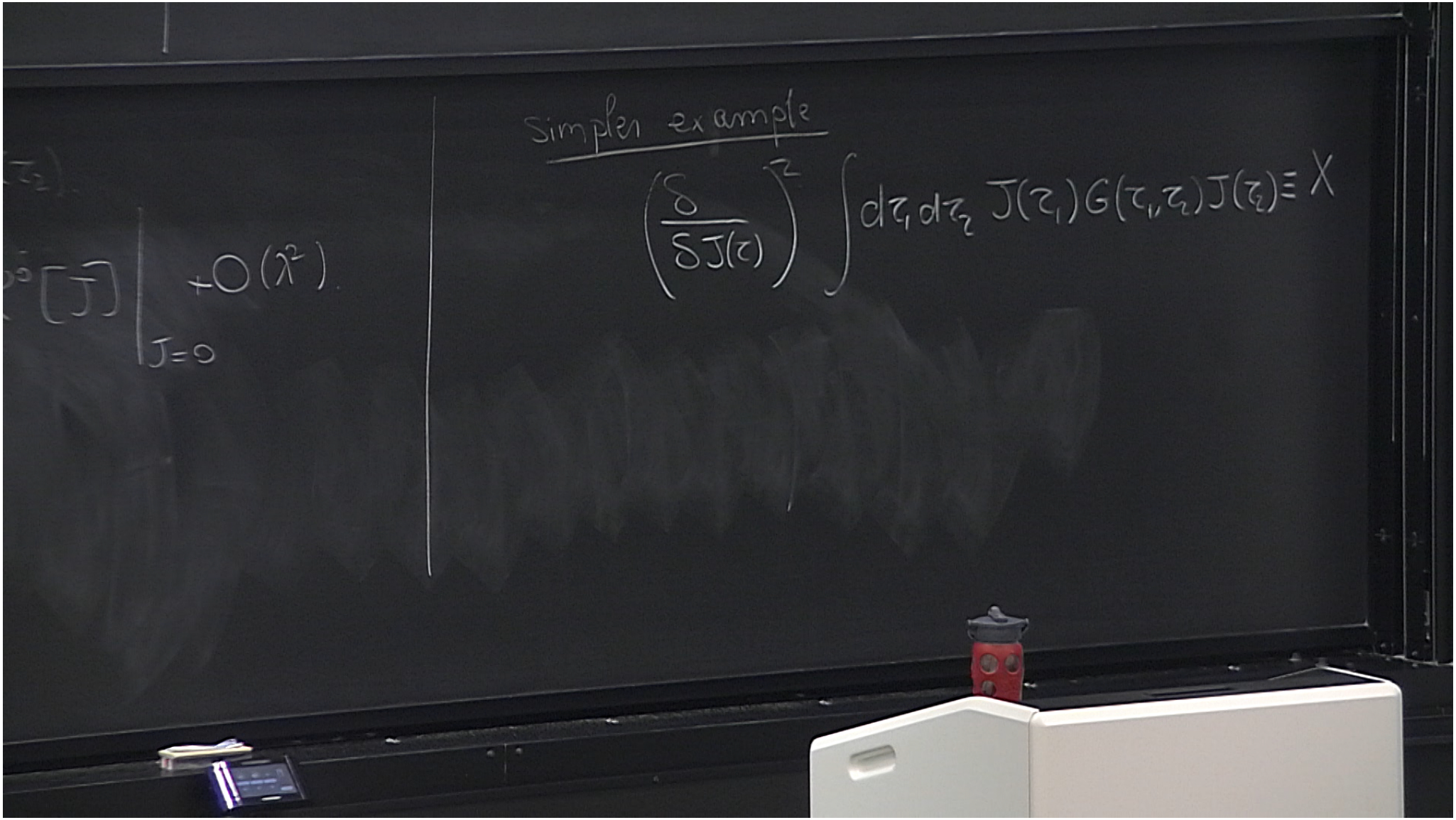
$G(0,\tau_1) = G(\beta\hbar,\tau_2) = 0$

$$C\, e^{-\frac{1}{2}\int d\tau\, x_c(\tau)J(\tau)}$$

C $\quad C\, e^{-\frac{1}{2}\int d\tau}$

$$S_E[x_c] = \underbrace{\left[\frac{1}{2} m \dot{x} x\right]}_{=0} + \int d\tau\, x \underbrace{\left[-\frac{1}{2} m \ddot{x} + \frac{1}{2} m \omega^2 x - J\right]}_{\text{eq of motion}} = -\frac{1}{2} \int d\tau\, x_c(\tau) J(\tau).$$

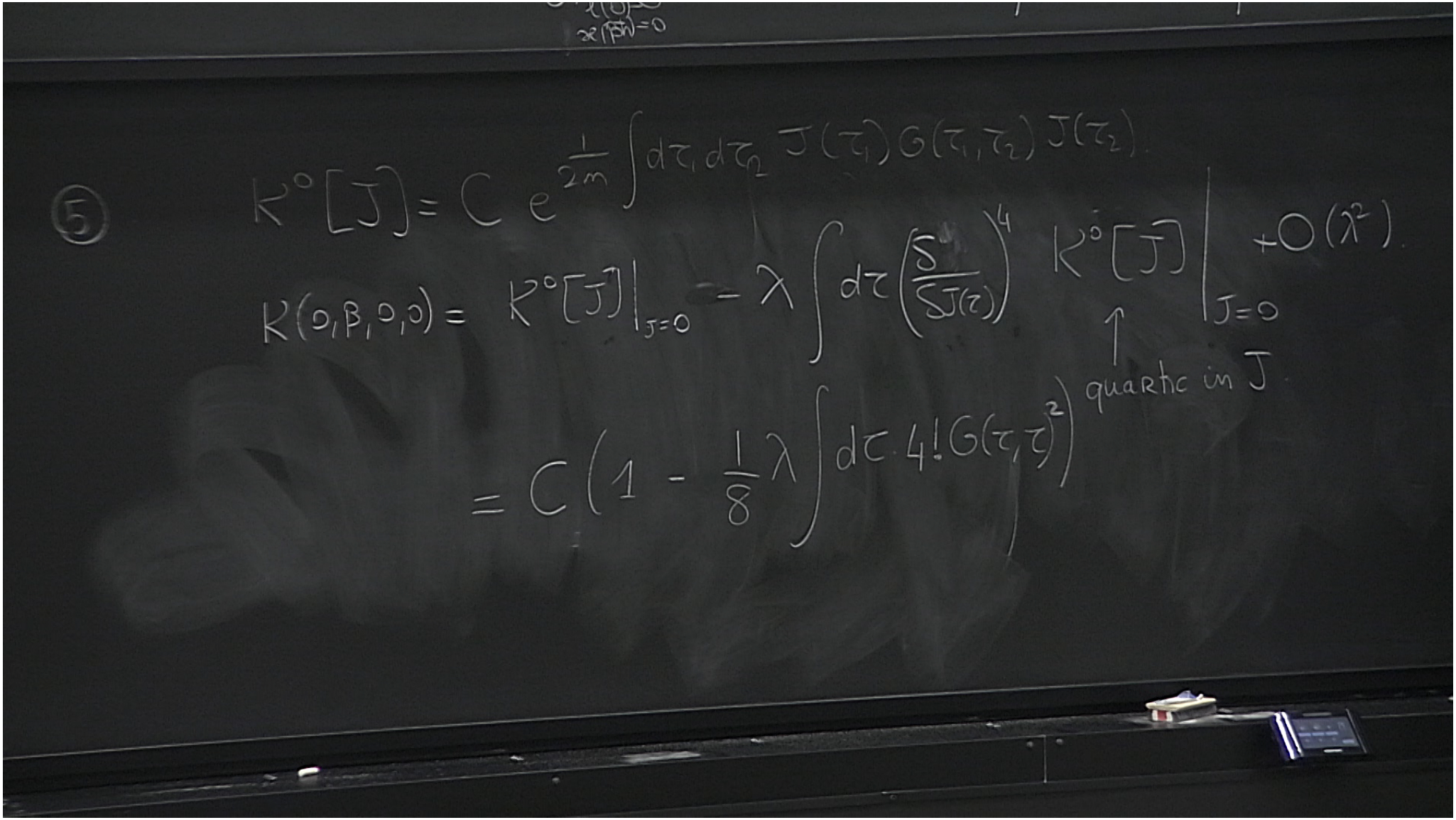
$$\text{if } \begin{cases} x'=0 \\ x''=0 \end{cases}$$


Simpler example
$\left(\frac{\delta}{\delta J(\tau)}\right)^2 \int d\tau_1 d\tau_2 \, J(\tau_1) G(\tau_1,\tau_2) J(\tau_2) \equiv X$
$+O(\lambda^2)$
$J=0$

$$C e^{\frac{1}{2}\int d\tau\, d\tau'}$$

$$X = \frac{\delta}{\delta J(\tau)} \left[\int d\tau_1 d\tau_2 \left(\delta(\tau - \tau_1)\, G(\tau_1, \tau_2)\, J(\tau_2) + J(\tau_1)\, G(\tau_1, \tau_2)\, \delta(\tau - \tau_2) \right) \right.$$

$$\left. = \frac{\delta}{\delta J(\tau)} \left[\int d\tau_2\, G(\tau, \tau_2)\, J(\tau_2) + \int d\tau_1\, J(\tau_1)\, G(\tau_1, \tau) \right] \right] = 2\, G(\tau, \tau)$$


⑤
$K^0[J] = C\, e^{\frac{1}{2m}\int d\tau_1 d\tau_2\, J(\tau_1) G(\tau_1,\tau_2) J(\tau_2)}$
$K(0,\beta,0,0) = K^0[J]\big|_{J=0} - \lambda \int d\tau \left(\frac{\delta}{\delta J(\tau)}\right)^4 K^0[J]\Big|_{J=0} + O(\lambda^2)$
quartic in J
$= C\left(1 - \frac{1}{8}\lambda \int d\tau\, 4!\, G(\tau,\tau)^2\right)$

$$K(0,\beta,0,0) = \int_{x(0)=0}^{x(\beta\hbar)=0} \mathcal{D}x(\tau)\, \exp\frac{-1}{\hbar}\int d\tau \left(\underbrace{\frac{1}{2}m\dot{x}^2 + \frac{m\omega^2}{2}x^2}_{\text{HO} = \text{"free"}} + \underbrace{\lambda x^4}_{\text{interacting}}\right)$$

simplest

⑤ $$K^0[J] = C\, e^{\frac{1}{2m}\int d\tau_1 d\tau_2\, J(\tau_1) G(\tau_1,\tau_2) J(\tau_2)}$$

$$K(0,\beta,0,0) = K^0[J]\Big|_{J=0} - \lambda \int d\tau \left(\frac{\delta}{\delta J(\tau)}\right)^4 K^0[J]\Big|_{J=0} + O(\lambda^2)$$

↑ quartic in J

$$= C\left(1 - \frac{1}{8}\lambda \int d\tau\, 4!\, G(\tau,\tau)^2\right)$$

with $G(\tau,\tau) = \frac{-1}{2m\omega}$ ($\lim_{\tau_1\to-\infty} G(\tau_1,\tau_2) = 0$, $\lim_{\tau_2\to\infty} G(\tau_1,\tau_2) = 0$)

$$K(0,\beta,0,0) = C(\beta)\left(1 - \frac{\beta\lambda}{32m^2\omega^2} + O(\lambda^2)\right) = C\, e^{-\beta\lambda/32m^2\omega^2} + O(\lambda^2)$$

$$\hookrightarrow E_0 = -\lim_{\beta\to\infty} \frac{1}{\beta} K(0,\beta,0,0) \rightarrow E_0 = \frac{\hbar\omega}{2} + \frac{\hbar^2\lambda}{32m^2\omega^3} + O(\lambda^2)$$

re-introducing $\hbar$ (check units!)

Correlation functions / generating functional

- $G^{(n)}(t_1 \dots t_n) = \langle 0 | T[\hat{x}(t_1) \dots \hat{x}(t_n)] | 0 \rangle$ ← correlation function
- $Z[J] = \langle 0 | T\, e^{\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\, J(t)\hat{x}(t)} | 0 \rangle$ ← generating functional

Time-ordered product $A(t), B(t)$ Heisenberg operators $\quad T[A(t_1)B(t_2)] = A(t_1)B(t_2)\,\Theta(t_1 - t_2) + B(t_2)A(t_1)\,\Theta(t_2 - t_1)$

↑ Heaviside function $\Theta(t) = \begin{cases} 0 & t < 0 \\ 1 & t \geq 0 \end{cases}$