

# Fit functions for correlations on Lattice

## Basics

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Complete basis in the Fock space

$$I = \sum_{H'} \int \frac{d^3 \vec{p}'}{(2\pi)^3} |H'_{\vec{p}'}\rangle \langle H'_{\vec{p}'}|$$

Time and space transition, note here we did Wick rotation  $it_M = t_E$ , all the time below are in the Euclidean space

$$\begin{aligned}\hat{O}_H(\vec{x}, t_{\text{sep}}) &= e^{-i\vec{p}\cdot\vec{x}} \hat{O}_H(\vec{0}, t_{\text{sep}}) e^{i\vec{p}\cdot\vec{x}} \\ \hat{O}_H(\vec{0}, t_{\text{sep}}) &= e^{\hat{H}t} \hat{O}_H(\vec{0}, 0) e^{-\hat{H}t}\end{aligned}$$

## Two-point correlation function

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### Correlation on Lattice

$$C_{2\text{pt}} = \int d^3 \vec{x} e^{-i\vec{p}\cdot\vec{x}} \langle \Omega | \hat{O}_H(\vec{x}, t_{\text{sep}}) \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle$$

Inserting complete basis, we have

$$\begin{aligned}C_{2\text{pt}} &= \int d^3 \vec{x} e^{-i\vec{p}\cdot\vec{x}} \sum_{H'} \int \frac{d^3 \vec{p}'}{(2\pi)^3} \langle \Omega | \hat{O}_H(\vec{0}, t_{\text{sep}}) | H'_{\vec{p}'} \rangle e^{i\vec{p}'\cdot\vec{x}} \langle H'_{\vec{p}'} | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle \\ &= \sum_{H'} \int d^3 \vec{p}' \langle \Omega | \hat{O}_H(\vec{0}, t_{\text{sep}}) | H'_{\vec{p}'} \rangle \delta(\vec{p} - \vec{p}') \langle H'_{\vec{p}'} | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle \\ &= \sum_{H'} \langle \Omega | \hat{O}_H(\vec{0}, 0) | H'_{\vec{p}} \rangle e^{-H' t_{\text{sep}}} \langle H'_{\vec{p}} | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle\end{aligned}$$

The operator  $\hat{O}$  will project the state with specific quantum numbers, but it is still a superposition of the eigenstates of Hamiltonian, because there are many excited states with the same quantum numbers, so we got

$$C_{2\text{pt}} = \sum_{E_n} e^{-E_n t_{\text{sep}}} \langle \Omega | \hat{O}_H(\vec{0}, 0) | E_n \rangle \langle E_n | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle$$

### Correlation in software

We would like to construct 2pt operator in Chroma / QLUA / GPT etc., we take the  $\pi^+$  as an example

$$\hat{O}_{\pi^+}(\vec{x}, t) = \bar{u}(\vec{x}, t) \gamma^5 d(\vec{x}, t)$$

so the operator is

$$\begin{aligned}\hat{O}_{\pi^+}(\vec{x}, t) \hat{O}_{\pi^+}^\dagger(\vec{0}, 0) &= \bar{u}(\vec{x}, t) \gamma^5 d(\vec{x}, t) \bar{d}(\vec{0}, 0) \gamma^5 u(\vec{0}, 0) \\ &= \text{tr} \left[ u(\vec{0}, 0) \bar{u}(\vec{x}, t) \gamma^5 d(\vec{x}, t) \bar{d}(\vec{0}, 0) \gamma^5 \right] = \text{tr} \left[ S_u(\vec{0}, 0; \vec{x}, t) \gamma^5 S_d(\vec{x}, t; \vec{0}, 0) \gamma^5 \right]\end{aligned}$$

note the hermiticity relation

$$S_u(\vec{0}, 0; \vec{x}, t) = \gamma^5 S_u^\dagger(\vec{x}, t; \vec{0}, 0) \gamma^5$$

### Fit function

We define overlap factors as

$$\begin{aligned}z_n &= \langle \Omega | \hat{O}_H(\vec{0}, 0) | E_n \rangle \\ z_n^\dagger &= \langle E_n | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle\end{aligned}$$

Then we got the fit function for 2pt correlation

$$C_{2\text{pt}} = \sum_n z_n z_n^\dagger \cdot e^{-E_n t_{\text{sep}}} \approx z_0^2 e^{-E_0 t_{\text{sep}}} (1 + c_1 e^{-\Delta E t_{\text{sep}}})$$

## Three-point correlation function

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### Correlation on Lattice

$$C_{3\text{pt}} = \int d^3 \vec{x} e^{-i\vec{p} \cdot \vec{x}} \int d^3 \vec{y} \langle \Omega | \hat{O}_H(\vec{x}, t_{\text{sep}}) \hat{O}_C(\vec{y}, t) \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle$$

in which  $\hat{O}_C$  is the inserted current.

Inserting complete basis, we have

$$\begin{aligned}C_{3\text{pt}} &= \int d^3 \vec{x} e^{-i\vec{p} \cdot \vec{x}} \int d^3 \vec{y} \sum_{H'} \int \frac{d^3 \vec{p}'}{(2\pi)^3} \sum_{H''} \int \frac{d^3 \vec{p}''}{(2\pi)^3} \\ &\times \langle \Omega | \hat{O}_H(\vec{0}, t_{\text{sep}}) | H_{\vec{p}'}^\dagger \rangle e^{i\vec{p}' \cdot \vec{x}} e^{-i\vec{p}' \cdot \vec{y}} \langle H_{\vec{p}'}^\dagger | \hat{O}_C(\vec{0}, t) | H_{\vec{p}''}^\dagger \rangle e^{i\vec{p}'' \cdot \vec{y}} \langle H_{\vec{p}''}^\dagger | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle \\ &= \sum_{H'} \int d^3 \vec{p}' \sum_{H''} \int d^3 \vec{p}'' \\ &\times \langle \Omega | \hat{O}_H(\vec{0}, t_{\text{sep}}) | H_{\vec{p}'}^\dagger \rangle \delta(\vec{p} - \vec{p}') \langle H_{\vec{p}'}^\dagger | \hat{O}_C(\vec{0}, t) | H_{\vec{p}''}^\dagger \rangle \delta(\vec{p}' - \vec{p}'') \langle H_{\vec{p}''}^\dagger | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle \\ &= \sum_{H', H''} \langle \Omega | \hat{O}_H(\vec{0}, t_{\text{sep}}) | H_{\vec{p}'}^\dagger \rangle \langle H_{\vec{p}'}^\dagger | \hat{O}_C(\vec{0}, t) | H_{\vec{p}''}^\dagger \rangle \langle H_{\vec{p}''}^\dagger | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle \\ &= \sum_{H', H''} \langle \Omega | \hat{O}_H(\vec{0}, 0) | H_{\vec{p}'}^\dagger \rangle e^{-H' t_{\text{sep}}} e^{H' t} \langle H_{\vec{p}'}^\dagger | \hat{O}_C(\vec{0}, 0) | H_{\vec{p}''}^\dagger \rangle e^{-H'' t} \langle H_{\vec{p}''}^\dagger | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle\end{aligned}$$

The operator  $\hat{O}$  will project the state with specific quantum numbers, but it is still a superposition of the eigenstates of Hamiltonian, because there are many excited states with the same quantum numbers, so we got

$$C_{3\text{pt}} = \sum_{n, m} \langle \Omega | \hat{O}_H(\vec{0}, 0) | E_n \rangle e^{-E_n(t_{\text{sep}} - t)} \langle E_n | \hat{O}_C(\vec{0}, 0) | E_m \rangle e^{-E_m t} \langle E_m | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle$$

### Fit function

We define overlap factors as

$$z_n = \langle \Omega | \hat{O}_H(\vec{0}, 0) | E_n \rangle$$
$$z_n^\dagger = \langle E_n | \hat{O}_H^\dagger(\vec{0}, 0) | \Omega \rangle$$

define matrix elements as

$$O_{nm} = \langle E_n | \hat{O}_C(\vec{0}, 0) | E_m \rangle$$

Then we got the fit function for 3pt correlation

$$C_{3\text{pt}} = \sum_{n,m} z_n O_{nm} z_m^\dagger \cdot e^{-E_n(t_{\text{sep}}-t)} e^{-E_m t}$$
$$\approx z_0^2 O_{00} \cdot e^{-E_0 t_{\text{sep}}} + z_0 O_{01} z_1^\dagger \cdot e^{-E_0 t_{\text{sep}}} e^{-\Delta E t} + z_1 O_{10} z_0^\dagger \cdot e^{-E_1 t_{\text{sep}}} e^{\Delta E t} + z_1^2 O_{11} \cdot e^{-E_1 t_{\text{sep}}}$$

## Ratio

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### Definition

$$R(t_{\text{sep}}, t) = \frac{C_{3\text{pt}}(t_{\text{sep}}, t)}{C_{2\text{pt}}(t_{\text{sep}})}$$

### Fit function

With the fit function of 2pt and 3pt above, we have

$$R(t_{\text{sep}}, t) = \frac{\sum_{n,m} z_n O_{nm} z_m^\dagger \cdot e^{-E_n(t_{\text{sep}}-t)} e^{-E_m t}}{\sum_n z_n z_n^\dagger \cdot e^{-E_n t_{\text{sep}}}}$$

If we just keep 2 states, then we have approximation

$$\sum_n z_n z_n^\dagger \cdot e^{-E_n t_{\text{sep}}} \approx z_0^2 e^{-E_0 t_{\text{sep}}} (1 + c_1 e^{-\Delta E t_{\text{sep}}})$$
$$R(t_{\text{sep}}, t) \approx \frac{O_{00} + a_1 (e^{-\Delta E t} + e^{-\Delta E(t_{\text{sep}}-t)}) + a_2 e^{-\Delta E t_{\text{sep}}}}{1 + c_1 e^{-\Delta E t_{\text{sep}}}}$$

$$\text{in which } c_1 = \frac{z_1^2}{z_0^2}, a_1 = \frac{z_0 O_{01} z_1^\dagger}{z_0^2} = \frac{z_1 O_{10} z_0^\dagger}{z_0^2} \text{ and } a_2 = \frac{z_1^2 O_{11}}{z_0^2}.$$

## Feynman-Hellmann correlation

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### Definition

$$FH(t_{\text{sep}}, \tau_{\text{cut}}, dt) = \left( \sum_{t=\tau_{\text{cut}}}^{t=t_{\text{sep}}+dt-\tau_{\text{cut}}} R(t_{\text{sep}} + dt, t) - \sum_{t=\tau_{\text{cut}}}^{t=t_{\text{sep}}-\tau_{\text{cut}}} R(t_{\text{sep}}, t) \right) / dt$$

### **Fit function**

Firstly, let's derive the fit function of the summation as

$$S(t_{\text{sep}}, \tau_{\text{cut}}) = \sum_{t=\tau_{\text{cut}}}^{t=t_{\text{sep}}-\tau_{\text{cut}}} C_{3\text{pt}}(t_{\text{sep}}, t) = \sum_{t=\tau_{\text{cut}}}^{t=t_{\text{sep}}-\tau_{\text{cut}}} \sum_{n,m} z_n O_{nm} z_m^\dagger \cdot e^{-E_n(t_{\text{sep}}-t)} e^{-E_m t}$$

For  $n = m$  part, we got

$$\sum_{t=\tau_{\text{cut}}}^{t=t_{\text{sep}}-\tau_{\text{cut}}} z_n O_{nn} z_n^\dagger \cdot e^{-E_n(t_{\text{sep}}-t)} e^{-E_n t} = (t_{\text{sep}} - 2\tau_{\text{cut}} + 1) \cdot z_n O_{nn} z_n^\dagger \cdot e^{-E_n t_{\text{sep}}}$$

For  $n \neq m$  part, we got

$$\begin{aligned} \sum_{t=\tau_{\text{cut}}}^{t=t_{\text{sep}}-\tau_{\text{cut}}} z_n O_{nm} z_m^\dagger \cdot e^{-E_n(t_{\text{sep}}-t)} e^{-E_m t} &= \sum_{t=\tau_{\text{cut}}}^{t=t_{\text{sep}}-\tau_{\text{cut}}} z_n O_{nm} z_m^\dagger e^{-E_n t_{\text{sep}}} \cdot e^{\Delta_{nm} t} \\ &= z_n O_{nm} z_m^\dagger e^{-E_n t_{\text{sep}}} \cdot e^{\Delta_{nm} \tau_{\text{cut}}} \frac{1 - e^{\Delta_{nm}(t_{\text{sep}} - 2\tau_{\text{cut}} + 1)}}{1 - e^{\Delta_{nm}}} \end{aligned}$$

So, when realize it in the code, the suggestion is defining a function for the summation  $S(t_{\text{sep}}, \tau_{\text{cut}})$ , then calculate the FH correlation as

$$FH(t_{\text{sep}}, \tau_{\text{cut}}, dt) = \frac{S(t_{\text{sep}} + dt, \tau_{\text{cut}}) - S(t_{\text{sep}}, \tau_{\text{cut}})}{dt}$$