Fit functions for correlations on Lattice

Basics

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

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

Two-point correlation function

<u>Correlation on Lattice</u>

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

Inserting complete basis, we have

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

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

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

<u>Correlation in software</u>

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

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

so the operator is

$$\hat{O}_{\pi^+}(\vec{x},t)\,\hat{O}^\dagger_{\pi^+}(\vec{0},0) = \overline{u}(\vec{x},t)\gamma^5 d(\vec{x},t)\overline{d}(\vec{0},0)\gamma^5 u(\vec{0},0)$$
$$= tr\Big[u(\vec{0},0)\overline{u}(\vec{x},t)\gamma^5 d(\vec{x},t)\overline{d}(\vec{0},0)\gamma^5\Big] = tr\Big[S_u(\vec{0},0;\vec{x},t)\,\gamma^5\,S_d(\vec{x},t;\vec{0},0)\,\gamma^5\Big]$$

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

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

Then we got the fit function for 2pt correlation

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

Three-point correlation function

Correlation on Lattice

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

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

Inserting complete basis, we have

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

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

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

Fit function

We define overlap factors as

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

define matrix elements as

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

Then we got the fit function for 3pt correlation

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

Ratio

Definition

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

Fit function

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

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

If we just keep 2 states, then we have approximation

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

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

Feynman-Hellmann correlation

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

$$\sum_{t=\tau_{\text{cut}}}^{t=t_{\text{sep}}-\tau_{\text{cut}}} z_n O_{nm} z_m^\dagger \cdot e^{-E_n(t_{\text{sep}}-t)} e^{-E_m t} = \sum_{t=\tau_{\text{cut}}}^{t=t_{\text{sep}}-\tau_{\text{cut}}} z_n O_{nm} z_m^\dagger e^{-E_n t_{\text{sep}}} \cdot e^{\Delta_{nm} t}$$

$$= z_n O_{nm} z_m^\dagger e^{-E_n t_{\text{sep}}} \cdot e^{\Delta_{nm}\tau_{\text{cut}}} \frac{1 - e^{\Delta_{nm}(t_{\text{sep}} - 2\tau_{\text{cut}} + 1)}}{1 - e^{\Delta_{nm}}}$$

here $\Delta_{nm} = E_n - E_m$.

If we preserve the first two energy states,

$$\frac{S(t_{\text{sep}}, \tau_{\text{cut}})}{C_{2\text{pt}}(t_{\text{sep}})} = \frac{(t_{\text{sep}} - 2\tau_{\text{cut}} + 1) \cdot z_0^2 O_{00} \cdot e^{-E_0 t_{\text{sep}}} \left(1 + b_1 e^{-\Delta E t_{\text{sep}}}\right) + b_2 e^{-E_0 t_{\text{sep}}} + b_3 e^{-E_1 t_{\text{sep}}}}{z_0^2 e^{-E_0 t_{\text{sep}}} \left(1 + c_1 e^{-\Delta E t_{\text{sep}}}\right)}$$

$$= \frac{(t_{\text{sep}} - 2\tau_{\text{cut}} + 1) \cdot O_{00} \cdot \left(1 + b_1 e^{-\Delta E t_{\text{sep}}}\right)}{1 + c_1 e^{-\Delta E t_{\text{sep}}}} + \frac{b_2 e^{-E_0 t_{\text{sep}}} + b_3 e^{-E_1 t_{\text{sep}}}}{e^{-E_0 t_{\text{sep}}} + c_1 e^{-E_1 t_{\text{sep}}}}$$

$$= (t_{\text{sep}} - 2\tau_{\text{cut}} + 1) \cdot O_{00} \cdot \left(\frac{b_1}{c_1} + \frac{1 - b_1/c_1}{1 + c_1 e^{-\Delta E t_{\text{sep}}}} \right) + b_2 + \frac{(b_3 - c_1 b_2) e^{-E_1 t_{\text{sep}}}}{e^{-E_0 t_{\text{sep}}} + c_1 e^{-E_1 t_{\text{sep}}}}$$

we can redefine $b_1 \equiv b_1 / c_1$ and $b_3 \equiv b_3 - c_1 b_2$, then

$$\frac{S(t_{\text{sep}}, \tau_{\text{cut}})}{C_{2\text{pt}}(t_{\text{sep}})} = (t_{\text{sep}} - 2\tau_{\text{cut}} + 1) \cdot O_{00} \cdot \left(b_1 + \frac{1 - b_1}{1 + c_1 e^{-\Delta E t_{\text{sep}}}} \right) + b_2 + \frac{b_3 e^{-\Delta E t_{\text{sep}}}}{1 + c_1 e^{-\Delta E t_{\text{sep}}}}$$

$$= (t_{\text{sep}} - 2\tau_{\text{cut}} + 1) \cdot O_{00} \cdot \left(b_1 + \frac{1 - b_1}{1 + c_1 e^{-\Delta E t_{\text{sep}}}} \right) + \frac{b_2 + b_3 e^{-\Delta E t_{\text{sep}}}}{1 + c_1 e^{-\Delta E t_{\text{sep}}}}$$

If we ignore e.s. to set $\Delta E = \infty$, then it becomes

$$\frac{S(t_{\text{sep}}, \tau_{\text{cut}})}{C_{2\text{pt}}(t_{\text{sep}})} = (t_{\text{sep}} - 2\tau_{\text{cut}} + 1) \cdot O_{00} + b_2$$

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

$$FH(t_{\mathrm{sep}}, \tau_{\mathrm{cut}}, dt) = \left[\frac{S(t_{\mathrm{sep}} + dt, \tau_{\mathrm{cut}})}{C_{\mathrm{2pt}}(t_{\mathrm{sep}} + dt)} - \frac{S(t_{\mathrm{sep}}, \tau_{\mathrm{cut}})}{C_{\mathrm{2pt}}(t_{\mathrm{sep}})} \right] / dt$$